UFMG

UNIVERSIDADE FEDERAL DE MINAS GERAIS
Pós-Graduação em Ecologia, Conservação e Manejo da Vida Silvestre
Instituto de Ciências Biológicas – UFMG Campus Pampulha
Avenida Antônio Carlos, 6627, Pampulha, Cep 31270-901, Belo Horizonte - MG
Telefone: (31) 3409 2569
E-mail: ecmvs@icb.ufmg.br – web site: www.ufmg.br/pos/ecologia

ECMVS

Tese defendida em 30 de maio de 2019 e aprovada pela banca examinadora constituída pelos membros:

Tatiana Cornelissen

Doutor(a) Tatiana Garabini Cornelissen

Mário Almeida Neto

Doutor(a) Mário Almeida Neto

Doutor(a) Paulo Enrique Cardoso Peixoto

Aristóteles Góes Neto

Doutor(a) Aristóteles Góes Neto

Doutor(a) Marco Aurélio Ribeiro de Mello
(Presidente da Banca)

As topologias de redes de interações ecológicas e suas origens

Rafael Barros Pereira Pinheiro

Belo Horizonte

Minas Gerais - Brasil

2019

Rafael Barros Pereira Pinheiro

As topologias de redes de interações ecológicas e suas origens

Tese apresentada ao Programa de Pós-Graduação em Ecologia, Conservação e Manejo da Vida Silvestre da Universidade Federal de Minas Gerais como requisito para a obtenção do título de Doutor.

Orientador: Prof. Marco Aurélio Ribeiro de Mello

Belo Horizonte

Minas Gerais - Brasil

2019

Scientists are responsible for **truth**, **knowledge**, **wisdom**, and **understanding**.

Truth is what is - it is the underlying reality of all existence.

Knowledge is what we think we know about truth. Knowledge, however, is always an imperfect assessment, and is always subject to revision and improvement. The realization that there are discrepancies and weaknesses in knowledge is **wisdom**.

Wisdom leads to a process, called the philosophy of science, through which knowledge is modified to better fit the truth. Philosophy means the love of wisdom, and doctors of philosophy are supposed, before all else, to be experts in wisdom.

Understanding, as defined in Job (28:28), is the effort to avoid evil. We may think of understanding as what we use in order to adequately apply our wisdom and our knowledge in guiding our **actions**.

Stephen D. Fretwell (1975)

“Viver é melhor que sonhar ...”

Belchior (1976)

AGRADECIMENTOS

Ao meu orientador, Marco Mello, pelo apoio, confiança e muitos ensinamentos.

Ao meu orientador na universidade de Freiburg: Carsten Dormann.

Ao meu colaborador: Gabriel.

Aos muitos cientistas que contribuíram com ideias, sugestões e revisões durante a realização desse trabalho e na escrita e publicação dos capítulos.

À UFMG, minha segunda casa nos últimos 11 anos, e a todos os professores, colegas, funcionários e amigos com quem convivi durante esse tempo.

À Débora pelo suporte, companheirismo e amor. Ao seu lado as dificuldades se tornaram suportáveis e as vitórias ainda mais especiais.

À minha família, pelo apoio em todo o tempo.

Aos amigos, pois eu sei que tenho os melhores.

SUMÁRIO

LISTA DE FIGURAS

INTRODUÇÃO GERAL

CAPÍTULO 1: A NEW MODEL EXPLAINING THE ORIGIN OF DIFFERENT TOPOLOGIES IN INTERACTION NETWORKS

CAPÍTULO 2: A NOVEL PERSPECTIVE ON NESTEDNESS AND A THEORY-ORIENTED PROCEDURE FOR THE USE OF NULL MODELS

LISTA DE TABELAS

CAPÍTULO 2: A NOVEL PERSPECTIVE ON NESTEDNESS AND A THEORY-ORIENTED PROCEDURE FOR THE USE OF NULL MODELS

LISTA DE APÊNDICES

MATERIAIS SUPLEMENTARES DO CAPÍTULO 1

MATERIAIS SUPLEMENTARES DO CAPÍTULO 2

Dedico esse trabalho à Brumadinho, minha cidade, meu lar, meu cantinho nesse mundo; e ao seu povo, meus conterrâneos. Mesmo quando estive longe, meu coração e mente jamais saíram das margens do Paraopeba.

RESUMO

A ciência de redes é uma ferramenta útil para analisar interações ecológicas e já produziu importantes descobertas, como a existência de topologias prevalentes, especialmente o aninhamento e a modularidade. Alguns estudos atribuem a prevalência desses padrões a um processo de seleção baseado na estabilidade das redes. Assim, tais topologias seriam mais comumente observadas na natureza por gerarem redes estáveis. Outros autores, porém, argumentam que essas topologias podem emergir diretamente dos processos que guiam as interações entre espécies. No primeiro capítulo desta tese, desenvolvemos um modelo que simula a evolução de espécies consumidoras usando espécies recursos, seguindo regras simples baseadas na hipótese integradora da especialização. Sem aplicar seleção por estabilidade, nosso modelo reproduziu todas as topologias comumente observadas em redes de interações. Simulações contendo recursos homogêneos formaram redes aninhadas e altamente generalizadas, enquanto simulações com alta heterogeneidade de recursos formaram principalmente redes de topologia combinada: formada por módulos internamente aninhados. No segundo capítulo, através de argumentos lógicos, mostramos que o aninhamento resulta de diferenças nas somas marginais de matrizes sem preferências. Processos que geram desigualdades nas frequências de interação das espécies, sem produzir preferências, resultam em aninhamento. Diferenças na abundância, aptidão e detectabilidade entre espécies, portanto, são potenciais causas dessa topologia. Adicionalmente, essa nova perspectiva nos permitiu relacionar modelos nulos com hipóteses explícitas sobre o aninhamento: o modelo equiprovável contém matrizes de topologia aleatória enquanto o modelo proporcional contém matrizes de topologia aninhada. A partir das evidências obtidas nos dois capítulos, concluímos que processos que guiam as interações entre espécies são capazes de produzir as principais topologias observadas em redes empíricas. A modularidade emerge como o resultado de *trade-offs* adaptativos enfrentados pelas espécies em sistemas diversos, enquanto o aninhamento resulta de processos que geram desigualdades nas frequências de interação das espécies. Por fim, a interação entre esses processos pode gerar redes de topologia combinada.

PALAVRAS-CHAVES: Aninhamento; análise de modelos nulos; interações ecológicas; modularidade; redes consumidor-recurso; redes de interações, topologia combinada; topologia de redes; *trade-offs* adaptativos.

ABSTRACT

Network science is a powerful tool to study ecological interactions and produced several discoveries, as the existence of prevalent topologies, mainly nestedness and modularity. Some studies argue that these topologies result from selection against unstable networks, whereas others propose that they likely emerge from processes driving the interactions between pairs of species. In the first chapter of this thesis, we developed a model that simulates the evolution of consumer species using resource species, following rules based on the integrative hypothesis of specialization. Without applying selection on stability, our model produced all the topologies commonly observed in species interaction networks. Simulations with homogeneous resources resulted in highly generalized nested networks, while simulation with high resource heterogeneity resulted mainly in networks with compound topologies: modular with internally nested modules. In the second chapter, through logical arguments, we show that nestedness results from marginal sum inequalities in matrices without row-column preferences. Processes that increase inequalities in the interaction frequencies of species, without introducing preferences, promote nestedness. Unequal abundances, fitness and detectability, thus, may cause nestedness. Additionally, the new perspective allowed us to related null models with explicitly hypotheses on nestedness: the equiprobable model is made by random topology matrices, while the proportional model is made by nested matrices. From the evidences obtained in both chapters, we conclude that the processes driving species interactions are able to produce the main topologies observed in real-world species interaction networks. Modularity emerges from the adaptive trade-off faced by species in diverse systems, while nestedness results from processes that promote inequalities in the interaction frequencies of species. For last, the interaction between those processes may produce networks with compound topologies.

KEYWORDS: Adaptive trade-offs; consumer-resource networks; compound topology; interaction networks; modularity; nestedness; network topology; null model analysis; species interaction

INTRODUÇÃO GERAL

A teia da vida

Nós vivemos em um planeta de exuberante diversidade. Desde a origem da vida, há cerca de 4 bilhões de anos[1], o processo evolutivo gerou uma profusão de seres vivos com diferentes formas, tamanhos e hábitos (Fig. 1). Hoje, seres tão variados quanto baleias azuis pesando 150 toneladas, arqueias microscópicas capazes de sobreviver em água fervente, samambaias, formigas cortadeiras, protozoários que parasitam hemácias, ipês-amarelos, cangurus e cogumelos compartilham conosco, uma espécie de primata bípede, a superfície da Terra. Acredita-se que aqui existam 8,7 milhões de espécies eucariotas[2], além de uma enorme e pouco conhecida diversidade de bactérias e vírus. Essa estonteante riqueza é um dos alvos mais antigos da curiosidade humana: há milênios estudamos, catalogamos e classificamos os seres vivos. E, apesar disso, 85% das espécies ainda são desconhecidas para a ciência[2].

Fig. 1. Uma das características mais marcantes da Terra é a diversidade da vida. Atualmente nosso planeta abriga 8,7 milhões de espécies eucariotas com diferentes formas, tamanhos e hábitos. Fotos disponíveis no Unsplash: https://unsplash.com/.

Não há, porém, um único local onde toda essa riqueza possa ser contemplada. Cada espécie se distribui de forma restrita no globo terrestre. Por isso, essa enorme biodiversidade se reflete em uma enorme diversidade de comunidades e ecossistemas[3]. Por séculos, cientistas buscam entender por que diferentes locais e ambientes abrigam diferentes conjuntos de espécies. Em 1799, o naturalista alemão Alexander Von Humboldt viajou da Europa à América do Sul, onde se maravilhou com a fauna e a flora tropicais: tão distintas das de sua terra natal e tão diversas[4]. Na famosa figura *Naturgemälde* (em português, pintura da natureza), Humboldt ilustra a variação nas fitofisionomias de plantas entre diferentes altitudes no vulcão Chimborazo, Equador (Fig. 2). Para Humboldt, a distribuição dessas espécies não era aleatória, mas seguia padrões guiados pelas condições ambientais. Além disso, Humboldt via comunidades como unidades coesas, dentro das quais diferentes espécies cumpriam diferentes papeis. Essa perspectiva moldou a concepção moderna de natureza[4]. Meio século depois, a questão da distribuição dos seres vivos se tornaria o tópico seminal da nascente disciplina nomeada de *ecologia*[3].

Fig. 2. Naturgemälde de Alexander Von Humboldt. Uma ilustração do vulcão Chimborazo no Equador e das espécies vegetais que crescem em diferentes altitudes em sua encosta. Originalmente publicada no livro *Ideen zu einer Geographie der Pflanzen*, 1807; disponível para download em: http://geographical.co.uk/places/mapping/item/1542-the-invention-of-nature.

É fácil constatar que, em um ambiente natural as espécies não vivem em isolamento, mas podem interagir, afetar e depender umas das outras. No nosso planeta, somente alguns organismos, como as plantas, algas e as bactérias quimiossintetizantes, assimilam a matéria e a energia de fontes inorgânicas. Os demais seres vivos, precisam consumir matéria derivada de outros organismos, formando assim teias alimentares. A maior parte desse fluxo de matéria e energia ocorre através da interação direta entre espécies, por exemplo, através do consumo de folhas e frutos de plantas por animais, e da predação de animais por outros animais. Além disso, essa mesma necessidade de recursos gera a competição entre os organismos.

Charles Darwin, em *A origem das espécies* (1859)[5], descreve uma colina emaranhada, repleta de plantas, pássaros, insetos e vermes interagindo de maneiras complexas. Por causa desse emaranhamento, é difícil prever a forma como as espécies podem se afetar mutuamente. Em um dos mais influentes experimentos ecológicos[6], o ecólogo americano Robert Paine removeu estrelas-do-mar predadoras (*Pisaster*) em áreas de um costão rochoso e observou a diversidade de suas presas cair. Ao consumir preferencialmente a espécie de presa mais abundante, as estrelas-do-mar evitavam a monopolização do espaço no costão por uma espécie dominante, facilitando a coexistência. O experimento de Paine demonstrou que em um sistema de interações entre espécies, os impactos de uma interação específica podem se espalhar em cascata através das demais interações, gerando efeitos indiretos.

Além disso, se as espécies são capazes de afetar umas às outras, é provável que essas interações colaborem, juntamente com as condições ambientais, em determinar suas distribuições. O ecólogo Jared Diamond estudou a distribuição de aves em ilhas de Papua Nova Guiné e, em 1975, propôs suas famosas e polêmicas regras de montagem da comunidade[7]. Para Diamond, a composição regional de espécies, ou seja, do arquipélago, era resultado de processos evolutivos mais lentos que respondem tanto a fatores ambientais quanto históricos. A composição de cada ilha, porém, resultava das interações competitivas entre as espécies. Assim, as espécies se dispersavam livremente entre as ilhas e enquanto algumas combinações de espécies, por causa da competição, não perduravam em cada ilha, outras se mostravam estáveis e eram mais facilmente observadas.

Alguns anos depois, os ecólogos Edward Connor e Daniel Simberloff demonstraram que muitos dos padrões que Diamond explicava através das regras de montagem eram inconsistentes ou podiam surgir ao acaso[8]. Dentre outras abordagens, esses autores fizeram simulações nas quais as espécies de aves eram distribuídas aleatoriamente entre as ilhas: modelos nulos. A partir desses dois estudos, se seguiu uma intensa discussão na literatura ecológica, com uma sequência de artigos apresentando argumentos e contra-argumentos, ao ponto de tal controvérsia ficar popularmente conhecida como “a guerra dos modelos nulos” [9]. Apesar da polêmica, o estudo de Diamond é considerado um marco para a ecologia moderna e um dos seus muitos efeitos foi trazer para o centro do debate ecológico o papel das interações entre espécies na montagem das comunidades biológicas.

Desde então, se consolidou o entendimento de que interações entre espécies são fenômenos de grande importância em uma comunidade, que influenciam e são influenciados por processos ecológicos e evolutivos[10]. Isso fomentou o interesse em estudar diretamente os sistemas de interações entre espécies, e não somente seus efeitos na composição das comunidades. Mas, se estudar as espécies, suas distribuições e as comunidades formadas já são tarefas árduas, entender como dezenas ou centenas de espécies interagem umas com as outras dentro de cada comunidade envolve uma ordem superior de complexidade. Nesse contexto, a ciência de redes, uma área interdisciplinar desenvolvida sobretudo na física, se mostrou uma ferramenta especialmente útil[11–13].

Redes são abstrações de sistemas na forma de elementos (nós) e conexões entre esses elementos (ligações). Em uma rede de interações ecológicas, geralmente os nós representam as espécies e as ligações representam as interações entre elas. Essa não é uma forma de abstração estranha à tradição ecológica: a analogia de *teia da vida*, provavelmente criada pelo pastor luterano John Bruckner no século XVIII[14], tem sido frequentemente usada desde então. Além disso, com base na ideia de que espécies desempenham diferentes papéis ecológicos em um sistema trófico, cujo principal defensor foi o ecólogo inglês Charles Elton no princípio do século XX[15], tais sistemas são classicamente representados em termos de cadeias ou teias alimentares. E talvez seja por essa semelhança que análises de rede desenvolvidas nas últimas décadas foram rapidamente incorporadas ao *kit* de ferramentas da ecologia e aplicadas ao estudo da *teia da vida*.

As análises de redes ecológicas possibilitaram uma mudança de perspectiva no estudo de interações entre espécies: das interações específicas entre pares de espécies, para o sistema de interações como um todo. Nessa nova perspectiva, conceitos ecológicos clássicos foram operacionalizados de forma mais objetiva, antigas questões ecológicas ganharam nova roupagem e novas perguntas surgiram[12]. Redes ecológicas são hoje usadas como uma lente para observar a unidade da natureza, como contemplada por Humboldt e Elton, e como uma ferramenta para desvendar a complexidade subjacente, ilustrada por tantas analogias, dos *ramos* na *colina de Darwin* aos *fios* na *teia da vida*.

Analisando redes de interações ecológicas

O *pensamento de redes* já faz parte do estudo de interações tróficas há várias décadas, através das teias alimentares, mas só foi aplicado a outros tipos de interações entre espécies mais recentemente[16]. Isso se deveu principalmente a dois fatores: em primeiro lugar, porque outras interações, como os mutualismos e parasitismos, foram por um longo tempo negligenciadas ou consideradas pouco importantes para as comunidades biológicas[17], resultando numa escassez de dados. O estudo do ecólogo espanhol Pedro Jordano (1987)[18], analisando estatisticamente sistemas de polinização e de dispersão de sementes, foi um dos primeiros a desafiar essa percepção e iniciar o estudo das redes mutualistas. Semelhantemente, estudos pioneiros de sistemas parasito-hospedeiro, como o do zoólogo canadense Robert Poulin em 1992[19], revelaram uma diversidade e complexidade desconhecidas, atraindo o interesse dos ecólogos. E em segundo lugar, porque as ferramentas disponíveis até então, não eram apropriadas para grande parte dos sistemas de interações ecológicas. Com o desenvolvimento das análises de redes bipartidas, porém, essa limitação foi superada.

Redes bipartidas são compostas por duas classes de nós e suas ligações só ocorrem entre nós de classes diferentes. Essa é uma abstração ideal para vários sistemas de interações ecológicas, como as diversas formas de interações entre animais e plantas e as relações entre parasitos e hospedeiros. Em uma rede de polinização, por exemplo, há dois tipos de nós: polinizadores e plantas, e uma vez que um polinizador não pode polinizar outro polinizador, nem uma planta ser polinizada por outra planta, interações somente ocorrem entre pares polinizador-planta. Redes de interações são representadas principalmente através de dois objetos matemáticos: grafos e matrizes (Fig. 3).

Dois artigos considerados fundacionais para a estudo de redes ecológicas bipartidas foram publicados em 2003[20,21], ambos pelos ecólogos espanhóis Pedro Jordano e Jordi Bascompte, e pelo ecólogo dinamarquês Jens Olesen (além do ecólogo espanhol Carlos Melián em somente um deles). Um dos artigos[20] mostra que algumas propriedades comuns em teias tróficas aparentam ser também universais em redes de interações entre animais e plantas. Já o foco do outro estudo[21] é a topologia de redes de mutualismos: polinização e dispersão de sementes, e sua principal conclusão foi que tais redes não apresentam arquiteturas aleatórias, mas são fortemente aninhadas. Isso é: espécies que interagem com menos parceiros interagem com um subconjunto dos parceiros das espécies que interagem com mais parceiros.

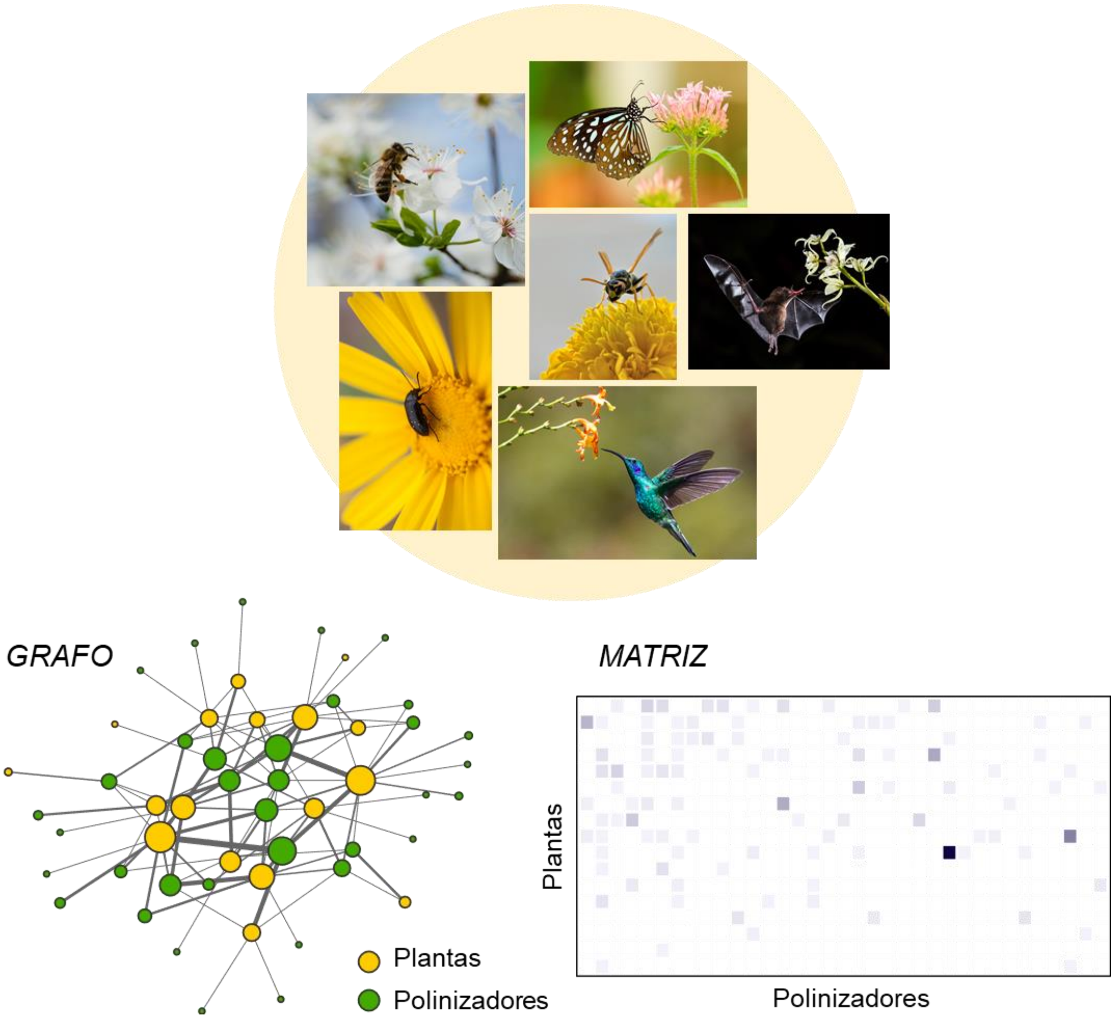


Fig. 3. Redes de interações entre espécies são tradicionalmente representadas através de dois objetos matemáticos: grafos e matrizes. Aqui ilustramos um sistema hipotético de interações entre espécies de plantas e seus polinizadores. Na ilustração via grafo, os círculos representam as espécies, separadas por cores entre polinizadores (verdes) e plantas (amarelos), enquanto as linhas representam as interações. A espessura da linha é ponderada pelo número de vezes que aquela interação foi observada. Já na matriz, espécies são representadas por linhas (plantas) e colunas (polinizadores), enquanto o valor de cada célula indica o número de vezes que a interação entre

linha e coluna foi observada. Para facilitar a visualização, a frequência de cada interação é indicada pela intensidade da cor nas células da matriz, ao invés de valores numéricos. Fotos meramente ilustrativas, disponíveis no Unsplash: https://unsplash.com/.

Desde a publicação destes artigos em 2003, uma extensa literatura em redes de interações ecológicas foi produzida. Ecólogos estudaram sistemas de interações entre parasitos e hospedeiros[22], polinizadores e plantas[23], dispersores de sementes e plantas[24], herbívoros e plantas[25], mutualismos defensivos entre plantas e formigas[26], mutualismos entre peixes e anêmonas[27], dentre outros. Outros padrões recorrentes foram descobertos em redes ecológicas, como a modularidade[23], e seus efeitos na estabilidade e robustez das redes foram estudados[28]. Por fim, nesse período, avanços metodológicos significativos foram obtidos, como o desenvolvimento de métodos para a estudo de redes ponderadas[29,30], e o surgimento das redes multicamadas[31], ideais para a análise de sistemas contemplando mais de um tipo de interação[32].

As topologias de redes de interações ecológicas

Uma das descobertas feitas no estudo de redes de interações entre espécies é a prevalência de duas topologias principais nesses sistemas: o aninhamento e a modularidade. As topologias são padrões que descrevem o sistema de interações como um todo, ou seja, o formato ou arquitetura geral da rede. O aninhamento foi observado em diversos tipos de interações ecológicas[33] e se caracteriza por espécies com menos parceiros interagirem com subconjuntos dos parceiros das espécies que têm mais parceiros. Assim, o aninhamento em uma matriz bipartida é a combinação de duas propriedades: desigualdades nos totais marginais, já que há espécies que interagem com mais parceiros e espécies que interagem com menos parceiros, e sobreposição nas interações, pois diferentes espécies interagem preferencialmente com os mesmos parceiros[34]. Em redes ponderadas, além da identidade dos parceiros, deve-se considerar a força ou frequência dessas interações[30] (Fig. 4a).

Outro padrão comum em redes de interações é a modularidade[23,35]. Em uma rede modular cada espécie interage preferencialmente dentro de um subgrupo de espécies altamente conectadas, ou conectadas por interações mais intensas e frequentes (em redes ponderadas) (Fig. 4b). Assim, a sobreposição de interações é grande entre espécies de um mesmo módulo, mas pequena entre espécies de módulos diferentes. Esses módulos são muitas vezes formados por espécies filogeneticamente próximas[22] ou funcionalmente semelhantes [24].

Apesar de aninhamento e modularidade serem topologias logicamente diferentes [36] e negativamente correlacionadas em redes empiricas[28,37], muitas redes apresentam uma combinação desses dois padrões[23]. Uma possível solução para esse paradoxo é que tais redes apresentem uma topologia composta[25,38]: modular, com módulos internamente aninhados (Fig. 4c). Essa topologia foi originalmente proposta pelo ecólogo Thomas Lewinsohn e colaboradores em 2006[25], mas permaneceu pouco testada por vários anos. A partir de 2013, porém, com o desenvolvimento de novos métodos para sua detecção[38,39], topologias compostas foram encontradas em sistemas de diversos tipos de interações[32,35,39,40].

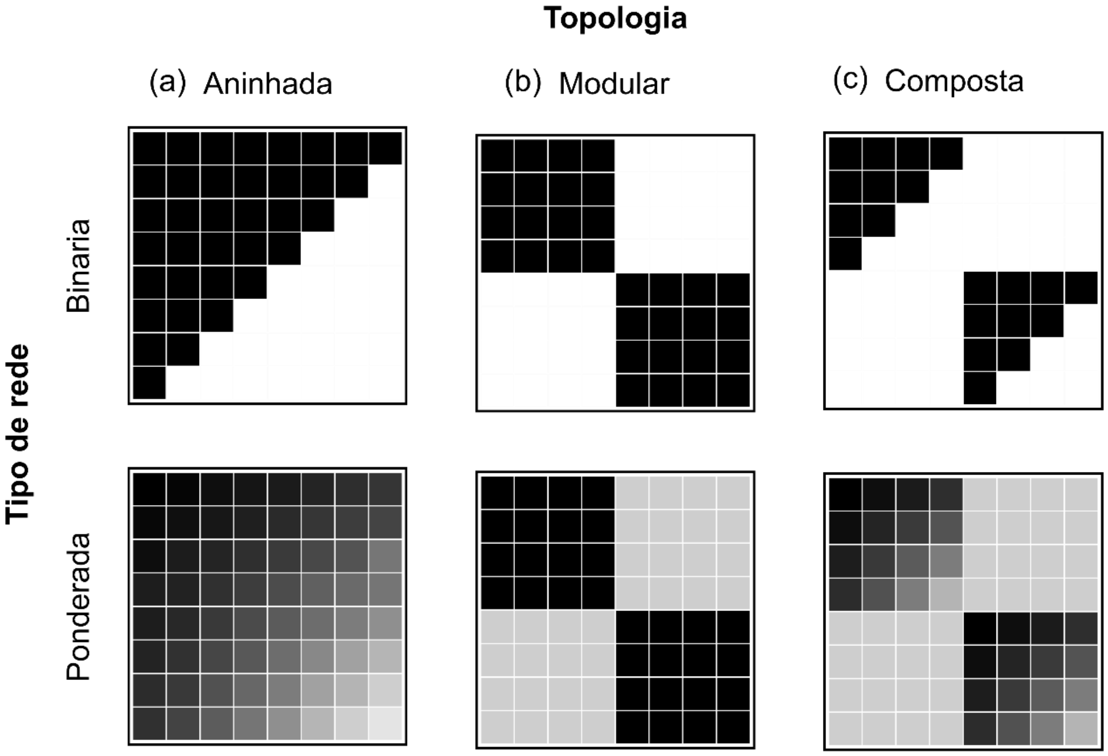


Fig. 4. Arquétipos das principais topologias encontradas em redes de interações ecológicas entre espécies. Nas redes ponderadas, o padrão pode ser formado pelas diferenças em intensidades ou frequências de interações e não somente pela ocorrência ou não ocorrência das mesmas. Por exemplo, em uma rede ponderada modular, não é necessário que a conectância dentro do módulo seja maior do que fora do módulo, somente que tais interações sejam realizadas mais frequentemente. No trabalho original de Lewinsohn e colaboradores, em 2006, foi proposta ainda uma quarta topologia: a topologia em gradiente, na qual há preferências de interações que variam

de maneira gradual entre as espécies, sem a formação de módulos. Esse padrão, porém, ainda não foi observado em redes de interações.

Como detectar topologias?

Testar estatisticamente redes de interações para as diferentes topologias é uma tarefa desafiadora. Para esses testes, as redes são geralmente representadas através de matrizes e a primeira etapa é a aplicação de uma métrica quantificando o grau de aninhamento ou modularidade presentes na matriz. Atualmente existe uma grande variedade de métricas para ambos os padrões disponíveis na literatura, tanto para matrizes binarias quanto ponderadas[30,41,42]. A escolha entre essas métricas é uma etapa importante e deve levar em consideração, não somente a eficiência dos índices, mas também aspectos conceituais: índices podem medir diferentes definições da mesma topologia. Os índices de aninhamento, por exemplo, podem ser divididos entre aqueles que somente mensuram a sobreposição de interações na matriz e os que consideram a desigualdade de somas marginais. Essa divisão reflete diferentes definições para o aninhamento presentes na literatura[43].

A segunda etapa dos testes envolve a comparação entre redes reais (i.e., observadas na natureza) e modelos nulos (i.e., redes artificiais geradas através de aleatorizações). Uma vez que as células de uma matriz de interações não são estatisticamente independentes entre si, não é possível realizar inferência paramétrica. Assim, para testes de significância, os valores das métricas de topologias observados em matrizes reais precisam ser comparados com valores obtidos em matrizes aleatorizadas[44].

Essa segunda etapa na detecção de topologias em redes de interações é considerada a mais controversa pela maioria dos pesquisadores por causa da escolha do algoritmo nulo. Existe na literatura uma variedade de algoritmos para a construção de modelos nulos, os quais assumem diferentes pressupostos e conservam diferentes propriedades das matrizes originais. Há, por exemplo, modelos nulos em que somente as dimensões e a soma total da matriz original são conservadas, enquanto outros conservam também as somas marginais[44]. Não há, porém, uma ligação explicita entre esses modelos e as topologias a serem testadas, sendo normalmente escolhidos por pesquisadores com base no seu conservadorismo para a detecção das diferentes topologias. Assim, essa escolha é vista como uma troca entre as chances de erros estatísticos do tipo I e do tipo II[45]. Essa não é uma abordagem ideal e gera controvérsias[46]. Idealmente, os diferentes algoritmos nulos deveriam estar ligados a hipóteses claras sobre as topologias das redes examinadas, permitindo assim a comparação entre os valores observados e os esperados em cada uma dessas hipóteses.

Métricas e modelos nulos específicos para a detecção de topologias compostas só foram desenvolvidos mais recentemente[38,39]. Uma rede de topologia composta é uma rede modular cujos módulos são internamente aninhados e, portanto, o primeiro passo é testar a modularidade da matriz. Uma vez que a matriz seja detectada como modular, é preciso testar o aninhamento interno de seus módulos. Em 2013, o físico mexicano César Flores e colaboradores[39] propuseram métricas através das quais é possível medir separadamente o aninhamento entre espécies que pertencem ao mesmo módulo e o aninhamento entre espécies em módulos diferentes. Segundo esses autores, em uma rede de topologia composta podemos esperar que o primeiro tipo de aninhamento seja muito maior do que o segundo.

Em um estudo feito pelo nosso grupo de pesquisa (Laboratório de Síntese Ecológica, USP), cujo *pre-print* foi disponibilizado em 2017[38], argumentamos que, pela própria definição de modularidade, a sobreposição de interações é necessariamente maior dentro dos módulos e consequentemente o aninhamento. Assim, mesmo em uma rede modular sem topologia composta, o aninhamento seria maior entre espécies que pertencem ao mesmo módulo. Para solucionar esse problema, nós propusemos um modelo nulo que conserva a estrutura modular nas matrizes aleatórias (*modelo nulo restrito*), desfazendo assim somente o aninhamento interno das diferentes regiões da matriz. A comparação do aninhamento de espécies do mesmo módulo entre a matriz observada e o modelo nulo deve então ser utilizada para a detecção de topologias compostas.

A origem das topologias

Os motivos pelos quais diferentes redes podem apresentar diferentes topologias permanecem um mistério. Estudos sugeriram que o aninhamento resulta, por exemplo, das desigualdades de abundâncias entre as espécies[47], de neutralidade pura[48] ou de restrições morfológicas[49]. Já a modularidade pode ser causada por conservadorismo filogenético[22], complementariedade funcional[50] ou fenologia [51], dentre outros fatores. Além disso, o grau de intimidade das interações ecológicas, ou seja, o encaixe necessário entre as espécies para a ocorrência das interações, parece afetar a topologia das redes[52-53]. A maior parte desses estudos, porém, se encontra dentro de uma abordagem puramente fenomenológica e pouco informativa sobre os mecanismos subjacentes a partir dos quais as topologias emergem.

Alguns pesquisadores acreditam que a prevalência dessas topologias em redes de interações ecológicas se deva a um processo de seleção contra rede instáveis. Assim, padrões que aumentam a estabilidade e a persistência no tempo de redes, seriam mais frequentemente observados na natureza[28,54]. Outros estudos argumentam que as topologias provavelmente surgem a partir dos processos que guiam as interações entre espécies[55,56]. A prevalência dessas topologias, portanto, não seria o resultado de seleção por estabilidade, mas um produto secundário da forma como as redes são formadas. Nós, porém, ainda conhecemos muito pouco sobre as regras que governam as interações entre espécies e menos ainda sobre a capacidade dessas regras de montar redes com diferentes topologias.

Uma abordagem promissora para essa questão é o desenvolvimento de modelos que simulam processos ecológicos e evolutivos. Nos últimos anos houve uma mudança significativa de foco na literatura de redes: de abordagens puramente fenomenológicas para a produção de modelos mecanísticos[40,55–58]. Tais modelos foram capazes de recuperar diversos padrões conhecidos em redes ecológicas reais, mostrando que estes podem emergir através de processos ecológicos e evolutivos agindo nas espécies, sem a necessidade de seleção por estabilidade ao nível da rede. Quanto à questão das diferentes topologias, se destacam o modelo proposto por Beckett e Williams (2013)[59] capaz de gerar redes de topologias compostas e o modelo de Leung e Weitz (2016)[40] que produz redes aninhadas, modulares ou com topologias compostas, dependendo dos pressupostos assumidos. Ambos os modelos foram baseados em interações entre parasitos e hospedeiros.

Um próximo passo lógico nessa abordagem seria o desenvolvimento de modelos baseados em processos ecológicos e evolutivos capazes de reproduzir, a partir de um mecanismo único, as diferentes topologias em diferentes circunstâncias. Adicionalmente, um avanço necessário é o desenvolvimento de modelos quantitativos, uma vez que a maioria dos modelos, até então, só é capaz de produzir redes binárias.

A hipótese integradora da especialização

Uma hipótese ecológica que potencialmente pode nos ajudar a entender melhor o processo de emergência das topologias de redes é a hipótese integradora da especialização (abreviada como IHS, do inglês). Essa hipótese foi proposta por nosso grupo de pesquisa, na minha dissertação de mestrado, e em um artigo científico em 2016[60]. O objetivo inicial desse estudo era explicar as diferentes relações descritas na literatura entre a performance e a especificidade de parasitos. Apesar de inicialmente focada em sistemas de interações entre parasitos e hospedeiros, os argumentos da IHS podem ser aplicados ao contexto mais geral de interações entre espécies consumidoras e espécies recursos.

Uma previsão intuitiva é a de que consumidores especialistas sejam mais eficientes em explorar cada espécie hospedeira do que consumidores generalistas. Essa previsão ficou conhecida como hipótese do *trade-off*, uma vez que os consumidores estariam submetidos a um *trade-off* adaptativo em suas performances em diferentes recursos[61]. Nesse cenário, a capacidade de um parasito de explorar eficientemente uma determinada espécie hospedeira, só se desenvolve ao custo de sua eficiência na exploração das demais espécies hospedeiras. Estes *trade-offs* poderiam resultar em restrições na capacidade dos consumidores de usar diferentes recursos (*constraints*). Já os consumidores generalistas, que não se restringissem a utilização de um ou poucos recursos, teriam seus desempenhos reduzidos. Apesar de alguns estudos reportarem evidências para essa hipótese[62], muitos outros encontraram resultados contrários[63,64], criando uma controvérsia na literatura.

A IHS prediz que a importância de *trade-offs* adaptativos num sistema de consumidores e recursos depende sobretudo da heterogeneidade dos recursos. Quando os recursos são similares uns aos outros, eles exigem dos consumidores características semelhantes para exploração[64]. Já quando os recursos são muito diferentes uns dos outros, diferentes características são necessárias para utilizar cada um deles, e por isso os consumidores enfrentam *trade-offs* adaptativos. Comunidades com alta diversidade de recursos podem também ser compostas por agrupamentos de espécies hospedeiras similares, enquanto os agrupamentos são muito diferentes uns dos outros. Nesse caso, a IHS prediz que fortes *trade-offs* adaptativos devem existir na performance dos consumidores em recursos de diferentes agrupamentos, mas não dentro dos agrupamentos[60].

Além de explicar a relação entre o desempenho e a especialização de consumidores, as predições da IHS podem ser estendidas para a topologia de redes de interações[35,38]. Em redes contendo recursos muito homogêneos, por exemplo por causa de uma alta proximidade taxonômica ou filogenética entre eles, o aninhamento deveria prevalecer. Já em redes diversas com agrupamentos de recursos, devemos esperar uma alta modularidade por causa dos fortes *trade-offs* no desempenho de consumidores em diferentes agrupamentos de recursos. Porém, dentro de cada agrupamento, o aninhamento poderia ainda emergir, gerando uma topologia composta. O ponto é que os módulos representam um limiar nas escalas de uma rede composta, com diferentes processos predominando dentro e fora deles, e por isso resultando em diferentes padrões.

Note que as explicações derivadas da IHS para a emergência das diferentes topologias em redes de interações não presumem qualquer forma de seleção por estabilidade ao nível das redes. Pelo contrário, as previsões apresentadas assumem que os *trade-offs* adaptativos, produzidos pela heterogeneidade dos recursos, determinam o padrão de formação de interações entre consumidores e recursos. Esses efeitos então seriam capazes de escalonar do nível das espécies e interações para o nível da rede, moldando sua topologia. Isso faz da IHS uma hipótese promissora para o desenvolvimento de um modelo mecanístico, focado na emergência das diferentes topologias em redes de interações entre espécies.

Referências

1. Dodd, M. S. et al. Evidence for early life in Earth's oldest hydrothermal vent precipitates. Nature 543, 60–64 (2017).
2. Mora, C., Tittensor, D. P., Adl, S., Simpson, A. G. B. & Worm, B. How many species are there on earth and in the ocean? PLoS Biol. 9, e1001127 (2011).
3. Begon, M., Townsend, C. R. & Harper, J. L. Ecologia: de indivíduos a ecossistemas. (Artmed, 2007).
4. Wulf, A. The invention of nature: Alexander von Humboldt's new world. (2015).
5. Charles Darwin. A origem das espécies. (1859).
6. Paine, R. T. Food web complexity and species diversity. *Am. Nat.* **100**, 65–75 (1966).
7. Diamond, J. M. Assembly of species comunnities. in *Ecology and Evolution of communities* (eds. Cody, M. & Diamond, J. M.) 342–444 (Harvard University Press, 1975).
8. Connor, E. F. & Simberloff, D. The assembly of species communities: chance or competition? *Ecology* **60**, 1132 (1979).
9. Fox, J. W. Why ecologists should refight the 'null model wars' (UPDATED). *Dinamic Ecology* (2011). Available at: https://dynamicecology.wordpress.com/2011/06/01/why-ecologists-should-refight-the-null-model-wars/. (Accessed: 5th April 2019)
10. Toju, H. *et al.* Species-rich networks and eco-evolutionary synthesis at the metacommunity level. *Nat. Ecol. Evol.* **1**, 0024 (2017).
11. Proulx, S., Promislow, D. & Phillips, P. Network thinking in ecology and evolution.

Trends Ecol. Evol. **20**, 345–353 (2005).

12. Delmas, E. *et al.* Analysing ecological networks of species interactions. *Biol. Rev.* 112540 (2018). doi:10.1111/brv.12433

13. Dormann, C. F., Fründ, J. & Schaefer, H. M. Identifying causes of patterns in ecological networks: opportunities and limitations. *Annu. Rev. Ecol. Evol. Syst.* **48**, 559–584 (2017).

14. Worster, D. Nature's economy: the roots of ecology. (Sierra Club, 1977).

15. Elton, C. Animal ecology. (Sidgwick and Jackson, 1927).

16. Ings, T. C. *et al.* Ecological networks - Beyond food webs. *J. Anim. Ecol.* **78**, 253–269 (2009).

17. Bronstein, J. L. Our current understanding of mutualism. *Q. Rev. Biol.* **69**, 31–51 (1994).

18. Jordano, P. Patterns of mutualistic interactions in pollination and seed dispersal: connectance, dependence asymmetries, and coevolution. *Am. Nat.* **129**, 657–677 (1987).

19. Poulin, R. Determinants of host-specificity in parasites of freshwater fishes. *Int. J. Parasitol.* **22**, 753–758 (1992).

20. Jordano, P., Bascompte, J. & Olesen, J. M. Invariant properties in coevolutionary networks of plant-animal interactions. *Ecol. Lett.* **6**, 69–81 (2003).

21. Bascompte, J., Jordano, P., Melian, C. J. & Olesen, J. M. The nested assembly of plant-animal mutualistic networks. *Proc. Natl. Acad. Sci.* **100**, 9383–9387 (2003).

22. Krasnov, B. R. *et al.* Phylogenetic signal in module composition and species connectivity in compartmentalized host-parasite networks. *Am. Nat.* **179**, 501–511 (2012).

23. Olesen, J. M., Bascompte, J., Dupont, Y. L. & Jordano, P. The modularity of pollination networks. *Proc. Natl. Acad. Sci.* **104**, 19891–19896 (2007).

24. Mello, M. A. R. *et al.* The modularity of seed dispersal: differences in structure and robustness between bat– and bird–fruit networks. *Oecologia* **167**, 131–140 (2011).

25. Lewinsohn, T. M., Inácio Prado, P., Jordano, P., Bascompte, J. & M. Olesen, J. Structure in plant-animal interaction assemblages. *Oikos* **113**, 174–184 (2006).

26. Dáttilo, W., Guimarães, P. R. & Izzo, T. J. Spatial structure of ant-plant mutualistic networks. *Oikos* **122**, 1643–1648 (2013).

27. Ollerton, J., McCollin, D., Fautin, D. G. & Allen, G. R. Finding NEMO: nestedness engendered by mutualistic organization in anemonefish and their hosts. *Proc. Biol. Sci.* **274**, 591–598 (2007).

28. Thebault, E. & Fontaine, C. Stability of ecological communities and the architecture of mutualistic and trophic networks. *Science (80-.).* **329**, 853–856 (2010).

29. Dormann, C. F. & Strauss, R. A method for detecting modules in quantitative bipartite networks. *Methods Ecol. Evol.* **5**, 90–98 (2014).

30. Almeida-Neto, M. & Ulrich, W. A straightforward computational approach for measuring nestedness using quantitative matrices. *Environ. Model. Softw.* **26**, 173–178 (2011).

31. Pilosof, S., Porter, M. A., Pascual, M. & Kéfi, S. The multilayer nature of ecological networks. *Nat. Ecol. Evol.* **1**, 0101 (2017).

32. Genrich, C. M., Mello, M. A. R., Silveira, F. A. O., Bronstein, J. L. & Paglia, A. P. Duality of interaction outcomes in a plant-frugivore multilayer network. *Oikos* **126**, 361–368 (2017).

33. Bascompte, J. & Jordano, P. Plant-animal mutualistic networks: the architecture of biodiversity. *Annu. Rev. Ecol. Evol. Syst.* **38**, 567–593 (2007).

34. Almeida-Neto, M., Guimarães, P., Guimarães, P. R., Loyola, R. D. & Ulrich, W. A consistent metric for nestedness analysis in ecological systems: reconciling concept and measurement. *Oikos* **117**, 1227–1239 (2008).

35. Mello, M. A. R. *et al.* Insights on the assembly rules of a continent-wide multilayer network. *bioRxiv* (2018). doi:10.1101/452565

36. Ulrich, W. *et al.* A comprehensive framework for the study of species co-occurrences, nestedness and turnover. *Oikos* 1607–1616 (2017). doi:10.1111/oik.04166

37. Trøjelsgaard, K. & Olesen, J. M. Macroecology of pollination networks. *Glob. Ecol. Biogeogr.* **22**, 149–162 (2013).

38. Felix, G. M., Pinheiro, R. B. P., Poulin, R., Krasnov, B. R. & Mello, M. A. R. The compound topology of a continent-wide interaction network explained by an integrative hypothesis of specialization. *bioRxiv* (2017). doi:10.1101/236687

39. Flores, C. O., Valverde, S. & Weitz, J. S. Multi-scale structure and geographic drivers of cross-infection within marine bacteria and phages. *ISME J.* **7**, 520–532 (2013).

40. Leung, C. Y. (Joey) & Weitz, J. S. Conflicting attachment and the growth of bipartite networks. *Phys. Rev. E* **93**, 032303 (2016).

41. Ulrich, W., Almeida-Neto, M. & Gotelli, N. J. A consumer's guide to nestedness analysis. *Oikos* **118**, 3–17 (2009).

42. Beckett, S. J. Improved community detection in weighted bipartite networks. *R. Soc. Open Sci.* **3**, 140536 (2016).

43. Ulrich, W. & Almeida-Neto, M. On the meanings of nestedness: back to the basics. *Ecography (Cop.).* **35**, 865–871 (2012).

44. Ulrich, W. & Gotelli, N. J. Null model analysis of species nestedness patterns. *Ecology* **88**, 1824–1831 (2007).

45. Strona, G., Ulrich, W. & Gotelli, N. J. Bi-dimensional null model analysis of presence-absence binary matrices. *Ecology* **99**, 103–115 (2018).

46. Dormann, C. F. What's wrong with null models? *Theoretical Ecology* (2017). Available at: https://theoreticalecology.wordpress.com/2017/06/06/whats-wrong-with-null-models/. (Accessed: 25th April 2019)

47. Vázquez, D. P. *et al.* Species abundance and asymmetric interaction strength in ecological networks. *Oikos* **116**, 1120–1127 (2007).

48. Krishna, A., Guimarães Jr, P. R., Jordano, P. & Bascompte, J. A neutral-niche theory of nestedness in mutualistic networks. *Oikos* **117**, 1609–1618 (2008).

49. Stang, M., Klinkhamer, P. G. L. & van der Meijden, E. Asymmetric specialization and extinction risk in plant–flower visitor webs: a matter of morphology or abundance? *Oecologia* **151**, 442–453 (2007).

50. Montoya, D., Yallop, M. L. & Memmott, J. Functional group diversity increases with modularity in complex food webs. *Nat. Commun.* **6**, 7379 (2015).

51. Schleuning, M. *et al.* Ecological, historical and evolutionary determinants of modularity in weighted seed-dispersal networks. *Ecol. Lett.* **17**, 454–463 (2014).

52. Pires, M. M. & Guimaraes, P. R. Interaction intimacy organizes networks of antagonistic interactions in different ways. *J. R. Soc. Interface* **10**, 20120649–20120649 (2012).

53. Hembry, D. H. *et al.* Does biological intimacy shape ecological network structure? A test using a brood pollination mutualism on continental and oceanic islands. *J. Anim. Ecol.* **87**, 1160–1171 (2018).

54. Borrelli, J. J. Selection against instability: stable subgraphs are most frequent in empirical food webs. *Oikos* **124**, 1583–1588 (2015).

55. Valverde, S. *et al.* The architecture of mutualistic networks as an evolutionary spandrel. *Nat. Ecol. Evol.* **2**, 94–99 (2018).

56. Maynard, D. S., Serván, C. A. & Allesina, S. Network spandrels reflect ecological assembly. *Ecol. Lett.* **21**, 324–334 (2018).

57. Zhang, F., Hui, C. & Terblanche, J. S. An interaction switch predicts the nested architecture of mutualistic networks. *Ecol. Lett.* **14**, 797–803 (2011).

58. Sebastián-González, E., Pires, M. M., Donatti, C. I., Guimarães, P. R. & Dirzo, R. Species traits and interaction rules shape a species-rich seed-dispersal interaction network. *Ecol. Evol.* **7**, 4496–4506 (2017).

59. Beckett, S. J. & Williams, H. T. P. Coevolutionary diversification creates nested-modular structure in phage-bacteria interaction networks. *Interface Focus* **3**, 20130033–20130033 (2013).

60. Pinheiro, R. B. P. *et al.* Trade-offs and resource breadth processes as drivers of performance and specificity in a host–parasite system: a new integrative hypothesis. *Int. J. Parasitol.* **46**, 115–121 (2016).

61. Futuyma, D. J. & Moreno, G. The evolution of ecological specialization. *Annu. Rev. Ecol. Syst.* **19**, 207–233 (1988).

62. Poulin, R. Large-scale patterns of host use by parasites of freshwater fishes. *Ecol. Lett.* **1**, 118–128 (1998).

63. Hellgren, O., Pérez-Tris, J. & Bensch, S. A jack-of-all-trades and still a master of some: prevalence and host range in avian malaria and related blood parasites. *Ecology* **90**, 2840–2849 (2009).

64. Krasnov, B. R., Poulin, R., Shenbrot, G. I., Mouillot, D. & Khokhlova, I. S. Ectoparasitic

“Jacks-of-all-trades”: relationship between abundance and host specificity in fleas (siphonaptera) parasitic on small mammals. *Am. Nat.* **164**, 506–516 (2004).

CONTEXTUALIZAÇÃO DOS CAPÍTULOS

Problema estudado

A presente tese é composta por dois capítulos, ambos focados na origem das diferentes topologias em redes de interações interespecíficas. Esses dois estudos são unidos por uma pergunta central: quais processos ecológicos e evolutivos, atuando no nível das interações par a par entre espécies produzem as topologias observadas em redes na natureza?

No primeiro capítulo, desenvolvemos um modelo que simula a evolução de espécies de consumidores usando espécies de recursos, com regras simples baseadas na hipótese integradora da especialização (IHS)[1]. Esse modelo foi capaz de produzir redes consumidor-recurso ponderadas, com todas as topologias comumente observadas em redes de interações: aninhada, modular e composta[2]. Nosso modelo se baseia em processos de seleção e deriva no nível das espécies de consumidores, e não inclui qualquer forma de seleção por estabilidade ao nível da rede. Assim, os resultados encontrados são evidência de que as topologias observadas no mundo real podem de fato emergir através de processos ecológicos e evolutivos que afetam as interações entre os pares de espécies[3].

O nosso modelo matemático serve como uma prova de conceito da IHS[4], pois demonstra que a emergência de diferentes topologias em redes consumir-recurso depende da heterogeneidade dos recursos. Simulações contendo recursos homogêneos formaram redes aninhadas e altamente generalizadas, enquanto simulações com alta heterogeneidade de recursos formaram principalmente redes com topologia composta (i.e., modulares, mas com módulos internamente aninhados).

Os resultados do primeiro capítulo indicam que a modularidade tende a emergir como efeito de *trade-offs* adaptativos enfrentados pelos consumidores ao usar recursos muito dissimilares. Por outro lado, tais resultados geraram um questionamento sobre a emergência do aninhamento nas nossas simulações: por que redes sem *trade-offs* tendem a ser aninhadas? O que é necessário para que tal padrão ocorra em uma matriz de interações? Com base nesses questionamentos e em *insights* obtidos a partir do modelo IHS, fizemos o estudo que resultou no segundo capítulo desta tese.

No segundo capítulo, através de argumentos lógicos, demonstramos que o aninhamento resulta de desigualdades nos totais marginais em matrizes de interações sem preferências.

Portanto, processos que geram desigualdades nas frequências gerais de interação das espécies, sem produzir preferências, resultam em aninhamento. Diferenças na abundância, aptidão e detectabilidade entre espécies são, por isso, potenciais causas dessa topologia. Adicionalmente, essa nova perspectiva nos permitiu produzir avanços metodológicos na análise topológica de redes de interações.

Publicação dos capítulos

Os dois capítulos que compõem essa tese foram escritos em inglês no formato de artigos científicos. Ambos os estudos foram liderados por mim, Rafael Pinheiro; e coautorados por meu colaborador, Gabriel Felix; por meu coorientador durante o período *sandwich* na Universidade de Freiburg na Alemanha, Carsten Dormann; e pelo meu orientador principal, Marco Mello.

O primeiro capítulo, *A new model explaining the origin of different topologies in interaction networks*, foi publicado como artigo[5] (https://doi.org/10.1002/ecy.2796) no periódico *Ecology*, da *Ecological Society of America*, e se encontra formatado de acordo com as regras do mesmo. Uma versão anterior do manuscrito foi depositada como *preprint* no repositório bioRxiv (https://doi.org/10.1101/362871). Materiais suplementares foram incluídos na seção final da presente tese e códigos de programação comentados (em linguagem R) estão disponíveis no GitHub (http://dx.doi.org/10.5281/zenodo.1486121).

O segundo capítulo, *A novel perspective on nestedness and a theory-oriented procedure for the use of null models*, se encontra em um formato geral de artigo científico, mas ainda não foi submetido a nenhum periódico. Nesse capítulo, adotamos um vocabulário mais geral, evitando jargões específicos da literatura ecológica, uma vez que a argumentação apresentada é apropriada também para outros tipos de matrizes e redes. Materiais suplementares foram incluídos na seção final da presente tese e códigos de programação comentados (em linguagem R) para reprodução integral das análises do estudo estão disponíveis no GitHub (http://dx.doi.org/10.5281/zenodo.2653181).

Série de estudos

Os dois estudos que compõem esta tese são originais e foram realizados com vistas à obtenção do título de doutorado. Esses trabalhos não representam esforços científicos isolados, mas fazem parte de uma linha de pesquisa que abrange dezenas de estudos, realizados principalmente nos últimos 20 anos, pelo nosso grupo de pesquisa no Laboratório de Síntese Ecológica da USP (junto com os nossos colaboradores) e por outros grupos ao redor do mundo.

Além de trabalhos anteriores focados principalmente em teias tróficas, podemos dizer que o estudo das topologias de redes de interações entre espécies se iniciou com o trabalho liderado por Jordi Bascompte em 2003[6] focado no aninhamento. Em 2007, outro estudo de grande relevância foi realizado por Jens Olensen[7] e colaboradores, desta vez focado na modularidade. Nessa mesma época, um estudo liderado por Thomas Lewinsohn, em 2006[2], incluiu as diferentes topologias em um arcabouço teórico. Esse estudo criou a base conceitual sobre a qual construímos a hipótese integradora da especialização (IHS).

Posteriormente, em um estudo liderado por Elisângela Bezerra em 2009[8], do qual Marco Mello, orientador desta tese, é autor correspondente, foram obtidas evidências que corroboram indiretamente a topologia composta proposta por Lewinsohn e colaboradores em 2006. Em outras palavras, redes de interações formadas apenas por um táxon parecem ser módulos do que seriam redes completas com vários táxons envolvidos. E esses módulos teriam uma estrutura mais aninhada do que as redes às quais pertencem. Evidências indiretas adicionais de topologias compostas foram obtidos em estudos subsequentes, um liderado por Marco Mello em 2011[9] e outro por Raissa Sarmento em 2014[10].

Envolvi-me com esta linha de pesquisa a partir do meu mestrado. O primeiro trabalho que liderei, diretamente relacionado a esta tese, é o artigo resultante do meu projeto de mestrado, publicado em 2016 no *International Journal for Parasitology*[1]. Nesse trabalho propusemos, de forma gráfica e discursiva, a IHS a partir da qual foi desenvolvido o modelo matemático descrito no capítulo 1. Portanto, considero o meu projeto de doutorado como um aprofundamento do projeto que desenvolvi no mestrado.

A partir da proposta da IHS, foram conduzidos estudos visando fazer testes empíricos de previsões derivadas da hipótese. O estudo de Genrich e colaboradores (2017)[11], do qual Marco Mello é autor correspondente, detectou uma topologia composta em um sistema formado por dois tipos diferentes de interações, em uma rede multicamada de interações de dispersão e destruição de sementes entre plantas e mamíferos. Semelhantemente, o estudo de Mello e colaboradores (2018), do qual eu sou coautor[12], detectou uma topologia composta em uma rede multicamadas de interações entre morcegos e plantas, incluindo frugivoria e nectarivoria. Esse estudo foi além dos testes de topologia e demonstrou que diferentes processos predominavam em diferentes níveis hierárquicos da rede: os módulos e camadas eram filogeneticamente definidos, enquanto as interações entre espécies dependiam de coocorrência geográfica.

Por fim, e extremamente relevante para os métodos utilizados nessa tese, há o estudo conduzido por Gabriel Félix, enquanto esse era aluno de mestrado orientado por Marco Mello, e colaboradores[13], do qual eu também sou coautor. Nesse estudo, além de testar previsões da IHS usando como modelo um sistema parasito-hospedeiro, desenvolvemos o método para a detecção de topologias compostas que foi utilizado no primeiro capítulo da tese. É importante destacar que esse método, é um aprimoramento do método apresentado por César Flores e colaboradores em 2013[14].

Há, obviamente, vários outros artigos que são referências fundamentais para essa tese, os quais não foram realizados pelo nosso grupo de pesquisa e dos quais eu não participei. Estes foram devidamente citados nas referências de cada capítulo.

Referências

1. Pinheiro, R. B. P. *et al.* Trade-offs and resource breadth processes as drivers of performance and specificity in a host–parasite system: a new integrative hypothesis. *Int. J. Parasitol.* **46**, 115–121 (2016).
2. Lewinsohn, T. M., Inácio Prado, P., Jordano, P., Bascompte, J. & M. Olesen, J. Structure in plant-animal interaction assemblages. *Oikos* **113**, 174–184 (2006).
3. Maynard, D. S., Serván, C. A. & Allesina, S. Network spandrels reflect ecological assembly. *Ecol. Lett.* **21**, 324–334 (2018).
4. Servedio, M. R. *et al.* Not Just a Theory—The Utility of Mathematical Models in Evolutionary Biology. *PLoS Biol.* **12**, e1002017 (2014).
5. Pinheiro, R. B. P., Félix, G. M. F., Dormann, C. F. & Mello, M. A. R. A new model explaining the origin of different topologies in interaction networks. *Ecology.* Accepted articles (2019).
6. Bascompte, J., Jordano, P., Melian, C. J. & Olesen, J. M. The nested assembly of plant-animal mutualistic networks. *Proc. Natl. Acad. Sci.* **100**, 9383–9387 (2003).
7. Olesen, J. M., Bascompte, J., Dupont, Y. L. & Jordano, P. The modularity of pollination networks. Proc. Natl. Acad. Sci. U. S. A. **104**, 19891–19896 (2007).
8. Bezerra, E. L. S., Machado, I. C. & Mello, M. A. R. Pollination networks of oil-flowers: a tiny world within the smallest of all worlds. *J. Anim. Ecol.* **78**, 1096–1101 (2009).

9. Mello, M. A. R. *et al.* The modularity of seed dispersal: differences in structure and robustness between bat– and bird–fruit networks. *Oecologia* **167**, 131–140 (2011).

10. Sarmento, R., Alves-Costa, C. P., Ayub, A. & Mello, M. A. R. Partitioning of seed dispersal services between birds and bats in a fragment of the Brazilian Atlantic Forest. *Zool.* **31**, 245–255 (2014).

11. Genrich, C. M., Mello, M. A. R., Silveira, F. A. O., Bronstein, J. L. & Paglia, A. P. Duality of interaction outcomes in a plant-frugivore multilayer network. *Oikos* **126**, 361–368 (2017).

12. Mello, M. A. R. *et al.* Insights on the assembly rules of a continent-wide multilayer network. *bioRxiv* (2018). doi:10.1101/452565

13. Felix, G. M., Pinheiro, R. B. P., Poulin, R., Krasnov, B. R. & Mello, M. A. R. The compound topology of a continent-wide interaction network explained by an integrative hypothesis of specialization. *bioRxiv* (2017). doi:10.1101/236687

14. Flores, C. O., Valverde, S. & Weitz, J. S. Multi-scale structure and geographic drivers of cross-infection within marine bacteria and phages. *ISME J.* **7**, 520–532 (2013).

CAPÍTULO 1

A NEW MODEL EXPLAINING THE ORIGIN OF DIFFERENT TOPOLOGIES IN INTERACTION NETWORKS

A new model explaining the origin of different topologies in interaction networks

Rafael Barros Pereira Pinheiro [1], Gabriel Moreira Félix Ferreira [2], Carsten F. Dormann [3], Marco Aurelio Ribeiro Mello [1,4]

[1] Programa de Pós-Graduação em Ecologia, Conservação e Manejo da Vida Silvestre, Universidade Federal de Minas Gerais, Brasil. [2] Programa de Pós-Graduação em Ecologia, Universidade Estadual de Campinas, Brasil. [3] Departamento de Biometria e Análise de Sistema Ambientais, Universidade de Freibug, Alemanha. [4] Departamento de Ecologia, Universidade de São Paulo, Brasil.

ABSTRACT

Nestedness and modularity have been recurrently observed in species interaction networks. Some studies argue that those topologies result from selection against unstable networks, while others propose that they likely emerge from processes driving the interactions between pairs of species. Here we present a model that simulates the evolution of consumer species using resource species following simple rules derived from the integrative hypothesis of specialization (IHS). Without any selection on stability, our model reproduced all commonly observed network topologies. Our simulations demonstrate that resource heterogeneity drives network topology. On the one hand, systems containing only homogeneous resources form generalized nested networks, in which generalist consumers have higher performance on each resource than specialists. On the other hand, heterogeneous systems tend to have a compound topology: modular with internally nested modules, in which generalists that divide their interactions between modules have low performance. Our results demonstrate that all real-world topologies likely emerge through processes driving interactions between pairs of species. Additionally, our simulations suggest that networks containing similar species differ from heterogeneous networks and that modules may not present the topology of entire networks.

Keywords: assembly rules; compound topology; consumer-resource networks; interaction networks; modularity; nestedness; network topology; specialization; species interactions; trade-offs;

INTRODUCTION

Network science, focusing on entire systems rather than species, can be an outstanding tool for the study of species interactions (Delmas et al. 2018). This approach led to important discoveries, including the existence of widespread topologies, among which nestedness and modularity stand out (Fortuna et al. 2010). Some studies claim that the prevalence of such topologies results from a selection against unstable networks, and, thus, patterns that increase network stability are more often observed (Thebault and Fontaine 2010, Borrelli 2015). Other authors, although, argue that network patterns likely emerge from processes that drive interactions between pairs of species, and, thus, selection on network stability is not necessary to explain them (Valverde et al. 2018, Maynard et al. 2018). However, knowledge about node linkage rules is still incipient, and we know little about whether these rules can scale up and shape entire networks (Ings et al. 2009), a critical issue to advance the debate.

Nestedness has been observed in a variety of networks (Bascompte et al. 2003). In a perfectly nested network, the links made by species with fewer interaction partners are a subset of the links made by species with more interaction partners (Bascompte and Jordano 2007). Other studies reported modularity in similar networks (Olesen et al. 2007, Guimerà et al. 2010, Krasnov et al. 2012). A modular network is characterized by each species interacting preferentially within a cohesive subgroup of species. Modules are often composed of phylogenetically related species (Krasnov et al. 2012) or species with similar traits (Mello et al. 2011).

Despite nestedness and modularity being logically different topologies (Ulrich et al. 2017) and negatively correlated with one another in real-world networks (Thebault and Fontaine 2010, Pires and Guimaraes 2012, Trøjelsgaard and Olesen 2013), several networks show combinations of them (Olesen et al. 2007, Flores et al. 2013). A potential explanation is that networks may present a compound topology: modular, but with internally nested modules (Lewinsohn et al. 2006). Compound topologies have been detected in empirical (Flores et al. 2013, Felix et al. 2017, Genrich et al. 2017, Mello et al. 2018) and simulated (Beckett and Williams 2013, Leung and Weitz 2016) interaction networks.

Traditionally, interaction network patterns and their underlying causes have been studied through phenomenological approaches (reviewed by Ings et al. 2009). Recently, though, this focus shifted, boosting the development of models that mimic ecological and evolutionary processes (e.g., Zhang et al. 2011, Guimarães et al. 2017, Valverde et al. 2018, Maynard et al. 2018). Despite several patterns being recovered by those models, the question of why networks present different topologies was seldom addressed (but see Leung and Weitz 2016). Here, we use recent theoretical developments on consumer-resource interactions to build a model focused on topology emergence.

The abstraction of consumer species exploiting resource species can be applied to different kinds of species interactions, such as parasite-host, pollinator-plant, and predator-prey interactions (Holland and DeAngelis 2010). An intuitive expectation is that generalist consumers should be outperformed by specialist consumers in the consumption of each resource (Futuyma & Moreno 1988). In other words, the higher the diversity of resources consumed (i.e., generalism), the lower should be the fitness obtained by the consumer on each resource (i.e., performance). The underlying assumption of this expectation is the existence of adaptive trade-offs: different traits are necessary for a consumer to optimally consume different resources, and, thus, increased performance on one resource comes at the cost of decreased performance on the other resources (Joshi and Thompson 1995). The importance of adaptive trade-offs in consumer-resource interactions, however, remains unclear, as studies of different systems found different results (Poulin 1998, Krasnov et al. 2004, Muchhala 2007, García-Robledo and Horvitz 2012).

The integrative hypothesis of specialization (IHS), initially called the integrative hypothesis of parasite specialization (Pinheiro et al. 2016), predicts that the intensity of trade-offs on a consumer-resource network, mostly depends on the heterogeneity of resources. When resources are similar to one another, they require similar traits for efficient consumption from a consumer. However, if resources are too dissimilar, consumers likely face adaptive trade-offs. Diverse communities can also comprise clusters of similar resource species, each cluster being highly different from the other (Pinheiro et al. 2016). In this case, the IHS predicts that strong trade-offs may exist on the performance of consumers on resources from different clusters, but not within clusters.

Beyond the relationship between performance and generalism of consumers, the IHS predictions may be extended to network topology (Felix et al. 2017, Mello et al. 2018). In networks that contain narrow phylogenetic or functional subsets of species, nestedness should prevail. In diverse networks with clustered resources, on the other hand, modularity may emerge because of the trade-offs in the performance of consumers on dissimilar clusters. However, within each cluster, as trade-offs are absent, nestedness may still emerge and produce a compound topology. These explanations do not assume selection on network stability, but assume that resource dissimilarities drive the formation of links and shape network topology.

Here, we propose a new model for interaction networks based on the IHS. Our new model simulates the evolution of consumer species using resource species, under three assumptions: (i) each resource species has a set of traits that affect its consumption by each consumer species, and, thus, resource species can be more or less similar to one another from the consumers' perspective. (ii) Any characteristic that enhances a consumer's ability to use a given resource tends to improve the consumption of similar resources, but diminish the consumption of dissimilar resources. And, (iii) the capacity of a consumer to use each resource on a given moment is contingent on its cumulative previous adaptations and maladaptations.

Following these simple assumptions, and adjusting a set of five parameters, the IHS model was able to: (1) reproduce the diverse relationships between performance and generalism of consumers observed in natural systems; (2) reproduce the main topologies observed in interaction networks; (3) explain the general conditions that affect the emergence of those patterns; and (4) generate predictions that are consistent with ecological and evolutionary theories and coherent with real-world observations.

THE IHS MODEL

Core structure

Our model produces species-based networks. For increased text fluency, hereafter, we call consumer species "consumers" and resource species "resources". The core of our model consists of two evolving matrices: the match matrix, and the performance matrix. In addition, there are two static inputs: a matrix with pairwise dissimilarities between resources, and a vector of resource availabilities (Fig. 1).

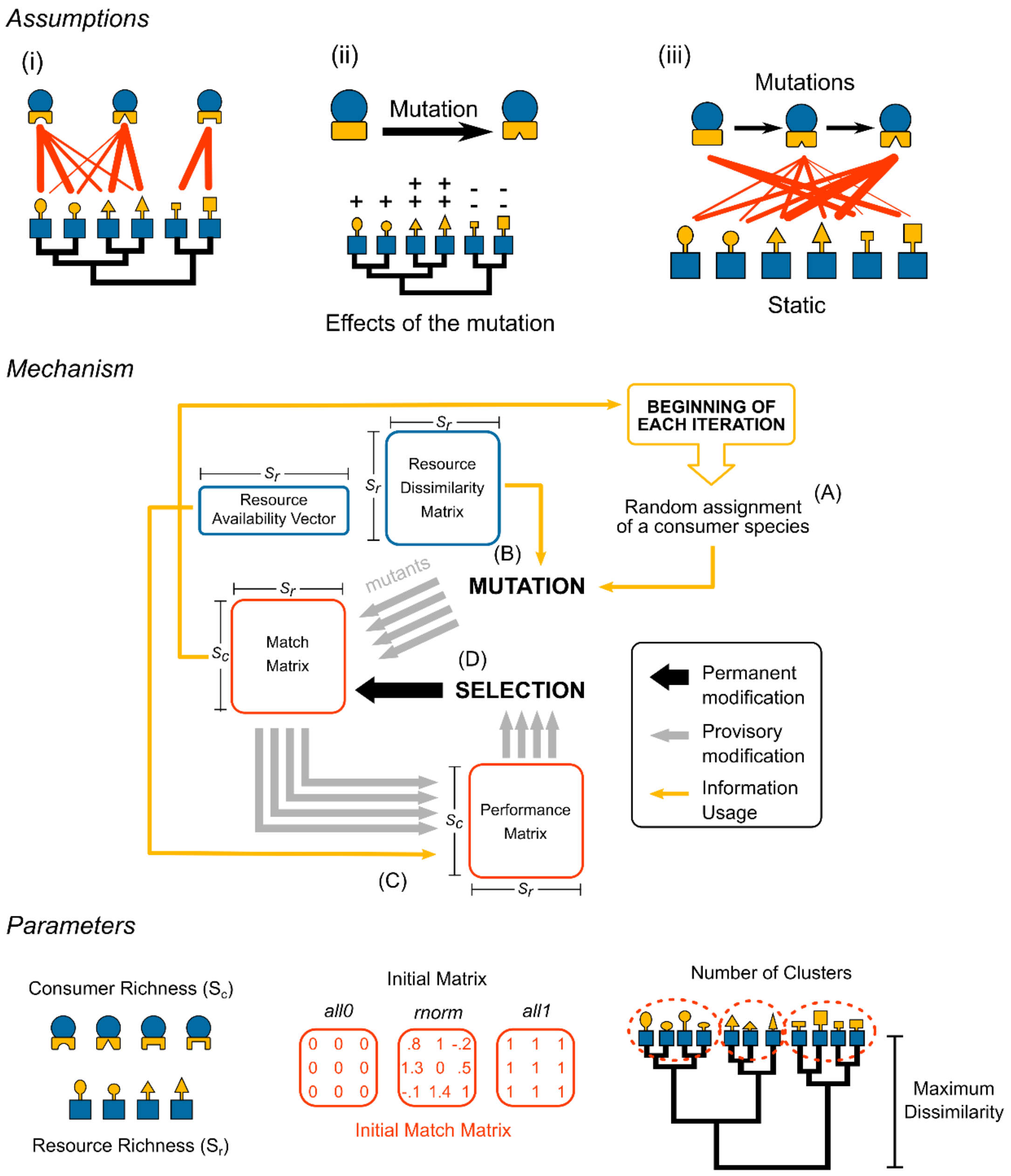


Fig. 1. The IHS model. *Assumptions*: Our model is based on three assumptions: (i) each resource species (squares) has a set of traits that affect its consumption by each consumer species (circles). Consumption efficiency is represented by the match between the yellow shapes of consumers and resources. (ii) A mutation that enhances consumer's ability to use a given resource tends to improve the consumption of similar resources, but diminish its consumption of dissimilar resources. The figure illustrates the effect a hypothetical mutation on the capacity of a consumer to use each resource: "+" means increased consumption and "-" means decreased consumption. And, (iii) the capacity of a consumer to use each resource is a result of its previous adaptations and maladaptations. In our model consumers evolve through gradual mutations, which may modify their interactions with resources. However, our model does not simulate resource

evolution (resource dissimilarity structure is kept static). *Mechanism:* An iteration starts with the assignment of a random consumer that will evolve (A). This consumer suffers alternative mutations, each generating a mutant with its own match with each resource. Each mutation is focused on a given resource (focal resource) but affects the consumer's matches with all resources. The consequence of each mutation for the consumer's match with a given resource depends on the dissimilarity between this resource and the focal resource, which is given by the resource dissimilarity matrix (B). Then the performance of each mutant is calculated taking into account resource availabilities (C). The mutant with the highest total performance is selected and replaces the original consumer in the match matrix to be used in the next iteration of the model (unless all mutations result in decreased total performance, in which case the original consumer is maintained) (D). For a detailed example of one iteration of the IHS model see Appendix S1. Elements in blue are static inputs: they do not change during the simulation, and elements in red are evolving matrices. S_r = resource richness; S_c = consumer richness. *Parameters:* We adjusted five parameters in our simulations: (1) the resource species richness, (2) the consumer species richness, (3) the method to generate the initial match matrix (initial matrix), (4) the maximum dissimilarity between resources, and (5) the number of clusters in the structure of dissimilarities between resources.

The match between a consumer and a resource summarizes how all characteristics of the consumer (e.g., morphology, physiology, and behavior) affect its ability to consume the resource. In our approach, match values are not bounded and may be even negative. When a consumer has a negative match with a resource, it is unable to consume it. The more negative the value, the greater the mismatch with the resource, and more adaptations would be necessary for consumption.

The dissimilarity between two resources is a measure of how different they are from one another from the consumer's perspective. Similar resources require from the consumer the same adaptations for efficient consumption (i.e., there are no trade-offs). For instance, two plant species whose fruits have similar shape, size, and consistency require the same type of beak from frugivorous birds. Thus, a bird with the appropriate beak may efficiently consume fruits from both plants. Resources are distant from one another when they require opposite adaptations of the consumers, and therefore, improving the consumption of one comes at the cost of lower efficiency in consuming another (i.e., there are trade-offs). For instance, two plant species whose fruits are more easily consumed by, respectively, small-beaked and large-beaked birds. In this case, a bird may be very efficient in consuming fruits from one plant species, but not both. The availability of each resource is the limit for the overall performance of its consumers.

The performance matrix represents the strength of interactions taking place in a consumer-resource system. Consumers that have negative match with a given resource, have zero performance on it. For consumers that have positive match with a given resource, the performances are the resource's availability divided between these consumers proportionally to their matches.

Mutation phase

At the beginning of each iteration, a consumer is randomly assigned to evolve. This consumer is submitted to alternative mutations, one focused on each resource (focal resource), therefore generating S_r (resource richness) mutants of the consumer.

Each mutation changes the match of the assigned consumer with the focal resource by summing a value randomly drawn from a normal distribution with mean 1 (standard deviation: 0.3). The mutation effect on the other resources is also drawn from normal distributions whose means are defined by their dissimilarity to the focal resource. The higher this dissimilarity, the lower the mean of the normal distribution (mean = 1 – dissimilarity). When the dissimilarity of a resource from the focal resource is more than 1, this mean is negative, and the mutation tends to decrease the match of the mutating consumer with the resource.

Selection phase

In the selection phase, the total performance of each mutant consumer is compared with the total performance of the original consumer (before mutations). If at least one mutant increased its total performance, the mutant with the largest total performance is selected, replacing the original consumer (i.e., evolutionary changes occurred). However, if all mutations result in decreased total performance, the original consumer is retained, and the simulation goes to the next iteration without evolutionary changes.

Our model has a strong optimization focus. First, because resource traits are summarized as dissimilarities, consumer mutations must be focused on the resources. That way, the model easily allows, beyond modification on the identity of resources consumed, increases and decreases in consumers generalism. The drawback of this approach is that mutations are not fully random: they always increase the match with at least one resource.

This is, however, unlikely to biases the model, as fully negative mutations should not be selected anyway. Second, in every iteration, the evolving consumer has available a wide range of mutations, which decreases the chance of it getting stuck in local minima and accelerates network evolution.

End of the simulation

The simulation ends after a pre-defined number of iterations and the final performance matrix is used as the simulated consumer-resource network (hereafter referred to as "simulated network"). It contains the information about the consumer and resource species in the network (nodes), the consumer-resource interactions (links), and the performance of consumers on each resource (weights). The simulated network is bipartite (two-mode). For a complete example of an iteration of the IHS model, see Appendix S1.

SIMULATIONS

Inputs and parameters of the simulations

List of parameters

In our simulations we adjusted five parameters: consumer richness, resource richness, method used to generate the initial match matrix (initial matrix), maximum dissimilarity between two resources (maximum dissimilarity), and number of resource clusters (number of clusters).

Initial match matrix

To start each simulation, we need to provide an initial match matrix. We built matrices with different consumer richness and resource richness. To fill the matrix we used three different methods: *all0*: all consumers score 0 in the match with all resources; *rnorm*: the match between each consumer and each resource is randomly drawn from a normal distribution with mean = 1 and standard deviation = 1; and *all1:* all consumers score 1 in the match with all resources.

Resource availability vector

The availability of each resource was defined by randomly drawing a value from a normal distribution with mean = 200 and standard deviation = 50.

Matrix of resource dissimilarities

The IHS predicts that network topology emerges as a function of the dissimilarity between resources and the degree of clustering of those dissimilarities. To test this prediction, we generated dissimilarity matrices with a range of values for the maximum dissimilarity between two resources and the number of clusters it contains. Those parameters define the heterogeneity of resources.

To produce the dissimilarities, we randomly assigned values for each resource in simulated dimensions and calculated the pairwise Euclidian distance, then we rescaled all distances based on the defined maximum. In simulations with clusters, each resource was first assigned to a cluster. Then, when defining values in the dimensions, a different range of possible values was used for each cluster, forcing dissimilarities within clusters to be lower than between clusters.

Running simulations

The IHS model was coded in R version 3.4.0 (R Core Team 2017). Commented codes and details of the model are available in GitHub (http://dx.doi.org/10.5281/zenodo.1486121).

Preliminary simulations

First, we performed 40 preliminary simulations with varied parameter values, to visualize the evolution of network topology during the procedure. In these tests we analyzed the network in intermediary steps of the simulations, to visually check: 1) if its evolution follows a unique trend in all simulations or if it depends upon the parameter values, 2) whether it tends to stabilization, and 3) if so, how many iterations are necessary to achieve it. Details and complete results of these simulations are presented in Appendix S2: Section S1.

Simulated networks

The next step was to generate a pool of simulated networks. The parameter values used were: consumer richness: 5, 10, 50, 100, and 200; resource richness: 50, 100, and 200; initial matrix: *all0*, *rnorm*, and *all1*; maximum dissimilarity: 1, 1.5, 2, 2.5, 3, 3.5, and 4; and number of clusters: 1, 2, and 4. We ran one simulation for each combination of those values, totalizing 945 setups. The number of iterations for each simulation was defined as consumer richness times 50 (see Appendix S2: Section S1 for justification).

As in each iteration of the model it is possible that no evolutionary changes occur, it is also possible that the entire simulation goes on without or with few modifications from the initial matrix (Appendix S2: Section S2). In these cases, the simulated networks did not reflect the mechanism of the model, but rather mirrored the initial matrices. Therefore, we removed from our pool the simulations in which evolutionary changes occurred in less than 80% of iterations. After this filtering, 672 simulated networks were retained for analysis.

ANALYSIS OF SIMULATED NETWORKS

Here, we used several indices and performed several analyses to describe the topology and specialization of simulated networks. Then we fitted generalized linear and additive models to understand how these features were driven by model parameters. A complete report of all the analysis performed in this study is presented in Appendix S2.

Network specialization

First, for each simulated network, we calculated binary and weighted network specialization metrics: connectance and H_2’, respectively (Blüthgen et al. 2008). Connectance is the proportion of potential links that are actually observed in the network, while H_2’ measures the degree of mutual specialization between nodes in the network, accounting for the quantitative information.

Network topology

Modularity and nestedness

We measured modularity and determined module composition of each simulated network using the DIRTLPAwb+ algorithm for weighted bipartite networks (Beckett 2016), available at the *bipartite* package for R (Dormann et al. 2008).

To compute nestedness we used a new metric, which we named WNODA (weighted nestedness based on overlap and decreasing abundance). WNODA is a modification of WNODF index (weighted nestedness based on overlap and decreasing fill) (Almeida-Neto and Ulrich 2011). Contrary to WNODF, WNODA does not demand binary decreasing fill to account for weighted nestedness, but rather decreasing marginal totals. It is, thus, less affected by weak links, and can be used to compare completely filled matrices (in which case WNODF is always 0). Detailed information about WNODA and comparisons between metrics are presented in Appendix S3.

Considering the possibility of a compound topology in our simulated networks, we used the approach proposed by Flores *et al.* (2013) and adapted by Felix *et al.* (2017), in which we separately computed the nestedness between species belonging to the same module and the nestedness between species belonging to different modules. In a network with a compound topology we expect the WNODA between species of the same module (WNODA_{SM}) to be much higher than the WNODA between species of different modules (WNODA_{DM}). An R function (*nest.smdm*) to compute these components of nestedness is now available at the *bipartite* package for R.

Null model analysis

We used null model analysis to define which topology, modular, nested, or compound, described best each simulated network. First, we tested for nested and modular topologies using free null models: null models that do not conserve the modular structure of the matrix (Felix et al. 2017). We applied a modified version of the algorithm proposed by Vázquez *et al.* (2007), in which randomized matrices rigidly conserve the original connectance and the total sum of weights, and probabilistically conserve the marginal sums. The original algorithm was modified to better deal with continuous link weights instead of counts (details in Appendix S2: Section S9).

A network has a compound topology when it is significantly modular and presents a significant WNODA_{SM} (i.e., modular with internally nested modules). To test for the significance of WNODA_{SM} in each modular network we used a restricted null model: a null model that conserve the modular structure of the matrix in the randomization. As, by definition, nodes in the same modules overlap more than nodes in different modules, not conserving the modular structure on the randomized matrix would result in an inflated type I error ratio for WNODA_{SM} (Felix et al. 2017).

To avoid excessively low consumer richness in each module, we excluded the networks with 10 or fewer consumer species and kept 415 simulated networks for these and subsequent analysis. Each null model was composed by 500 randomized matrices, and metric values were compared through Z-tests. Null model analysis was performed in the

Sagarana High-Performance Computing cluster from the High-Performance Processing Center, Institute of Biological Sciences, Federal University of Minas Gerais, Brazil.

Relationship between performance and generalism of consumers

Performance vs generalism

For each consumer in the simulated networks we calculated the mean performance: its average performance on all resources it consumes. We also calculated two generalism indices: (1) basic resource generalism, the richness of resources consumed, and (2) structural resource generalism, the diversity of resources consumed measured with the Shannon index (Poisot et al. 2012). Then, we calculated Spearman correlations between the mean performance and the generalism indices for each simulated network.

Performance vs between-module generalism

To measure the between-module generalism of consumers in each modular simulated network we calculated its participation coefficient (P) (Guimerà and Nunes Amaral 2005). The P measures how much the consumer's links are divided between different modules. We also used a weighted version of P (Appendix S2: Section S11). Then, for each network, we calculated Spearman correlations between the mean performance and the between-module generalism of consumers (binary and weighted).

Statistical analysis

To test the effect of model parameter in each of the descriptors of simulated networks, we fitted generalized and additive linear models. After building each complete model, we performed analysis of variance to reduce it to a minimum model, and used the deviance explained by each variable as a measure of effect size (Dobson and Barnett 2008). See Appendix S2 for the setup, reduction, and results of each model.

RESULTS

The evolution of networks in the preliminary simulations followed no unique trend. For instance, connectance may increase, decrease or remain constant in the course of the iterations, depending on model parameter values. Network topology and specialization tend to stabilize, and the number of iterations used to generate our pool of simulated networks was enough, in most of the preliminary simulations, to reach a very stable state (Appendix S2: Section S1).

The IHS model was able to generate a diverse set of simulated networks for every metric calculated in this study: from highly generalized to highly specialized (connectance: 0.12 to 1; H_2': <0.01 to 0.79), and from highly modular to highly nested (modularity: <0.01 to 0.80; WNODA: 0.07 to 0.95). Also, correlation between performance and generalism varied from positive to negative (basic generalism: -1 to 0.87; structural generalism: -1 to 1). Of the 415 networks tested for topologies, 268 (65%) were modular, 198 (48%) were nested, and 51 (12%) were both modular and nested. Of the 268 modular networks, 142 (53%) presented a compound topology: modules that are internally nested.

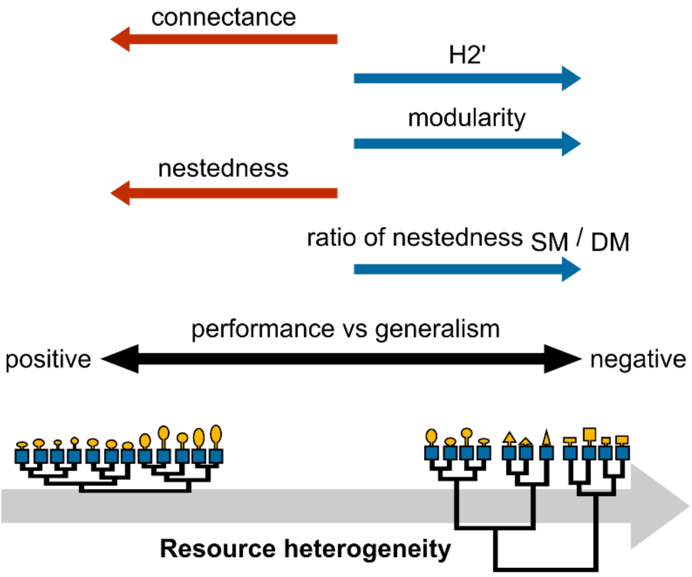


Fig. 2. Effects of resource heterogeneity in network specialization and topology. Parameters maximum dissimilarity and number of clusters that define resource heterogeneity have mostly driven simulation outputs. Specialization increases (lower connectance and higher H2'), nestedness decreases, and modularity increases with increased resource heterogeneity. The ratio between nestedness of species in the same module (nestedness $_{SM}$) and nestedness of species in different modules (nestedness $_{DM}$) is higher in simulated networks with more heterogeneous resources, boosting the emergence of compound topologies. For last, the relationship between performance and generalism of consumers shifts from highly positive to highly negative, depending on resource heterogeneity. Blue and red arrows: metric values, respectively, increase and decrease with increased maximum dissimilarity and number of clusters. Complete results in Appendix S2.

Out of the five parameters adjusted, maximum dissimilarity and number of clusters, which are related to resource heterogeneity, disproportionately drove simulated network specialization and topology (Fig. 2). The initial matrix had weak effects in most of the analysis showing that network evolution has overcome initial patterns. Consumer richness had a moderate effect in the detection of significative nestedness, likely resulting from an increased statistical power in the analysis (Appendix S2: Section S9). But, overall, consumer and resource richness did not strongly influence the simulation outputs. For the effect of each parameter in each model see Appendix S2.

Consequently, two main different patterns have emerged in our simulations. On the one hand, simulations with homogeneous resource mostly resulted in highly generalized, highly connected, nested, and non-modular networks (Fig. 3). In these simulations, there is a positive correlation between performance and generalism of consumers.

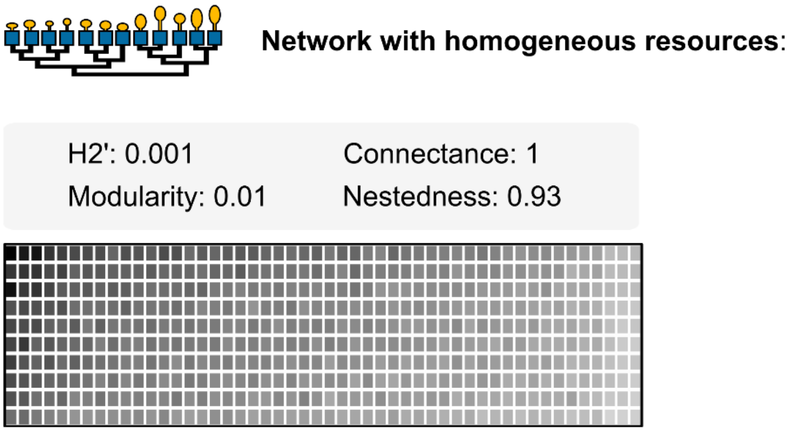


Fig. 3. Predictions of our model for networks with homogeneous resources. Here we illustrate the main pattern that emerged in simulations with highly homogeneous resources, using as example one of the simulated networks. The maximum dissimilarity between two resources in this simulation is 1, and, thus, consumers do not face trade-offs on its performances on different resources. The simulated network is generalized, non-modular, fully connected, and nested. Rows in the matrix are consumers, columns are resources, and the gray tones represent the weight of each interaction. Nestedness is evidenced by the general trend of decreasing weights from top-down to left-right corners.

On the other hand, simulations with heterogeneous resources mostly resulted in highly specialized, sparsely connected, non-nested, and modular networks with internally nested modules (compound topology) (Fig. 4). In most of the modular networks, the performance of consumers has a negative relationship with between-module generalism (P): 75% of the networks for the binary metric and 84% for the weighted metric.

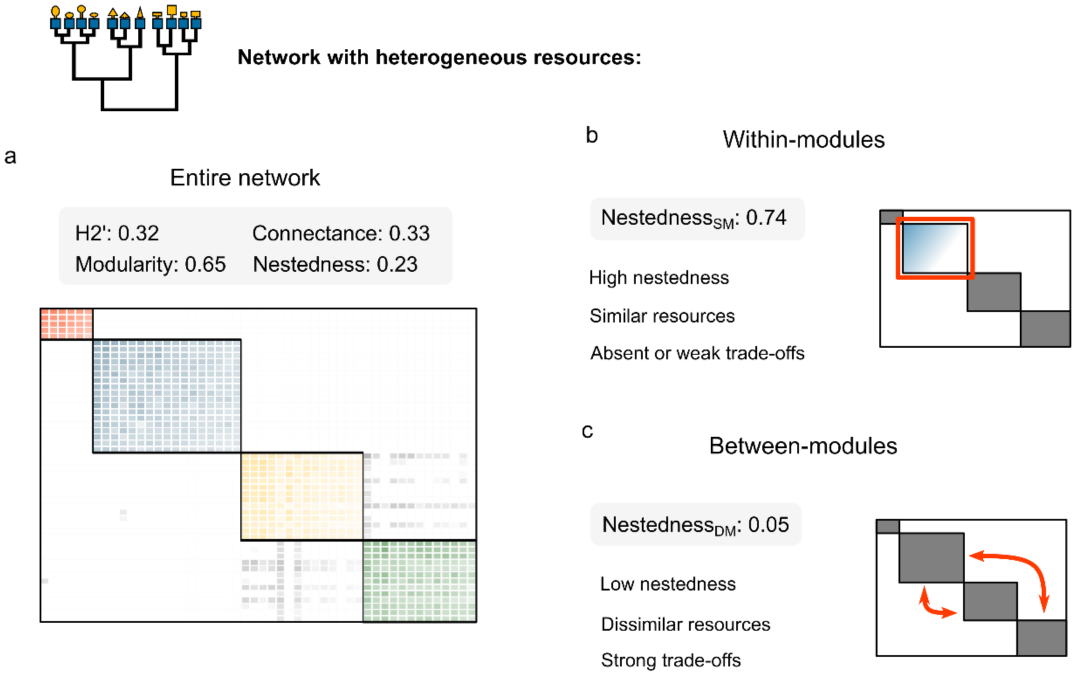


Fig. 4. Predictions of our model for networks with heterogeneous resources. Here we illustrate the main pattern that emerged in simulations with highly heterogeneous resources, using as example one of the simulated networks. The maximum dissimilarity between two resources in this simulation is 2.5 and the structure of dissimilarities is composed of 4 clusters. The simulated network is sparse, specialized, non-nested, and presents a compound topology: modular with internally nested modules (a). Within-modules (b) there is high nestedness, resources are homogeneous, and consumers are submitted to weak or absent trade-offs, resembling the patterns in Fig. 3. However, between-modules (c) nestedness is very low, resources are dissimilar, and multi-module generalists face strong trade-offs which results in decreased performances. Rows in (a) are consumers, columns are resources, colors represent modules, and the tones represent the weight of each interaction. Nestedness $_{SM}$: nestedness between species in the same module; nestedness $_{DM}$: nestedness between species in different modules.

DISCUSSION

Topology emergence

The IHS model produced a highly diverse set of simulated consumer-resource networks. In these simulations, specialization varied widely, and we detected the three main topologies observed in real-world interaction networks: nested, modular, and compound.

We also found positive and negative relationships between performance and generalism of consumers. Those patterns did not emerge through selection on network stability, but rather from rules on the evolution of consumers that use different sets of resources. As far as we know, our model is the first to implement a single mechanism able to generate all those patterns under different circumstances.

The IHS predicts that modularity in interaction networks mirrors discontinuities in dissimilarities between species (Pinheiro et al. 2016). Clusters are, thus, imposed on the model and drive link formation, which produces modules in the network. Our model does not address the origin of clustering on biological communities (but see Allen 2006, Scheffer and van Nes 2006). However, it is remarkable that even in simulations without clusters, modular networks emerged (see Appendix S4 for an example). This is an intriguing result, that strengthens the evidence of topology emerging from up-scaling of node linkage rules.

In our model, resource heterogeneity defines the intensity of trade-offs in the performances of each consumer on different resources. When trade-offs are strong, highly generalistic consumers are very inefficient on each resource or, cannot even exist, and the network is highly specialized, modular, and non-nested. However, when trade-offs are weak, a consumer can consume a wide range of resources, and the network is generalized and nested.

Limitations of the model

The main limitation of the IHS model is that it only simulates the evolution of consumer species. In nature, consumption is likely to be a selective force that also drives resource species evolution (Thompson 1994, Guimarães et al. 2017). We must admit that this simplification strongly reduces the realism of our model, especially when consumption has a strong effect on resource species fitness. We decided to follow this approach, however, because the inclusion of resource evolution would result in a much more complex and intricate model.

A related limitation is that our model does not include the effect of consumer abundances on performances. In obligate interactions (e.g., endoparasitism), the abundance of the consumer species is itself a measure of interaction weight, as a consumer only survives by interacting with resources. However, when consumer abundance is less dependent on the interaction, it may be important to consider the separate effect of consumer abundances in link formation.

In our model, we explicitly favored generalism and simplicity over realism: we aimed at producing a wide range of patterns through a simple mechanism. And, despite somewhat simplistic assumptions, it was indeed able to recover the most common topological patterns observed in interaction networks.

Compound topology

On the one hand, several simulated networks presented both significant nestedness and modularity. On the other hand, nestedness and modularity are driven in opposite directions by the same main parameters and are strongly negatively correlated (Spearman rho: -0.94, Appendix S2: Section S7), as usually found in empirical ecological networks (Thebault and Fontaine 2010, Pires and Guimaraes 2012, Trøjelsgaard and Olesen 2013). This scenario does not support the perspective of entire networks having a mixed nested and modular topology (Fortuna et al. 2010), but supports the perspective that, in modular networks, nestedness may predominate within modules (Lewinsohn et al. 2006, Felix et al. 2017). Indeed, in nested-modular simulated networks, nestedness between species of the same module was always much higher than nestedness between species of different modules.

Our study reinforces the prediction that highly diverse networks tend to present a compound topology (Lewinsohn et al. 2006, Flores et al. 2011, Felix et al. 2017). In these networks, consumers specialize in a group of homogeneous resource species instead of a single species and multi-module generalist have decreased efficiency, which corroborates that network modules may be the real unity of specialization and coevolution (Olesen et al. 2007).

Additionally, our results show that the taxonomic, phylogenetic, and functional diversity of species included in a network may have a strong influence on the patterns observed. Interaction networks containing only similar species show patterns that are not observed in heterogeneous networks (Bezerra et al. 2009), as well as a module does not present the topology of the entire network (Flores et al. 2013). Studies are often focused on modules of the network or in taxonomically defined assemblage subsets (Olesen et al. 2007, Jordano 2016), and only a few studies investigated diverse systems (Donatti et al. 2011). Thus, the literature is probably biased towards low-diversity patterns (as suggested by

Mello et al. 2011). This may explain the paradigm of mutualisms being nested (Bascompte and Jordano 2007) and the dominance of positive relationships between the performance and host range of parasites (Krasnov et al. 2004, Hellgren et al. 2009). We should expect that several of the published nested interaction networks are in fact modules of more diverse networks with compound topologies.

Other models of compound topologies

Beckett & Williams (2013) predicted a compound topology for phage-bacteria networks, using a relaxed lock-and-key model. Despite their model including a larger number of parameters and having a more complex and less general mechanism than ours, the assumptions of the IHS model are at least partially met by it. We believe that our model is not contradictory to the relaxed lock-and-key model, but rather more comprehensive.

Leung & Weitz (2016) proposed a bipartite network growth model that generates modular, nested, and compound networks. In their model, the network grows by duplication of nodes, and links, once formed, are kept constant. In our model the contrary is true, species richness is constant, and links submitted to evolution. Additionally, their model produces only binary networks. These differences make it difficult to compare both models. However, Leung & Weitz (2016) found that, when there are trade-offs, modularity emerges in networks, otherwise, hosts and parasites enter an arms race that results in nestedness. These results are highly consonant with our main predictions using the IHS model.

Conclusion

The proposed model based on the integrative hypothesis of specialization (IHS) reproduced the main network topologies and its predictions are coherent to real-world observations and consonant with current evolutionary and ecological theories. Our results show that the IHS model is useful to generate weighted, bipartite, consumer-resource networks and supports the IHS as a theoretical framework to study interaction specialization and network topology.

ACKNOWLEDGEMENTS

We thank our institutions and many colleagues, who helped us in different ways during this project. We thank J. Miguel Ortega, Tetsu Sakamoto, and Verônica de Melo Costa for help with the use of Sagarana HPC cluster. The Graduate School in Ecology of the Federal University of Minas Gerais (ECMVS), Brazil, provided us with a scholarship from the Brazilian Council for Scientific and Technological Development (CNPq) granted to RBPP. Infrastructure for this study was provided by ECMVS, the Department of Ecology of the University of São Paulo (USP), and the Department of Biometry and Environmental System Analysis of the University of Freiburg, Germany. The Graduate School in Ecology of the State University of Campinas (PPGE-UNICAMP), Brazil, provided GMFF with a scholarship from the Brazilian Coordination for the Improvement of Higher Education Personnel (CAPES). RBPP received a scholarship from the joint program between CAPES, CNPq, and Deutscher Akademischer Austauschdienst (DAAD) (88887.161398/2017-00). MARM was funded by the Research Dean of the University of São Paulo (PRP-USP: 18.1.660.41.7), CNPq (#302700/2016-1), Minas Gerais Research Foundation (FAPEMIG: PPM-00324-15), and Alexander von Humboldt Foundation (AvH: 3.4-8151/15037). We thank Pedro Jordano, Matthias Speich, Carine Emer, and anonymous reviewers for valuable suggestions for improving this manuscript. Tiago Quental and Paulo Guimarães Jr. helped us with discussion on the assembly rules of ecological networks.

DATA ACCESSIBILITY: In this study we used only simulated data that can be reproduced using codes provided on GitHub (http://dx.doi.org/10.5281/zenodo.1486121).

LITERATURE CITED

Allen, C. R. 2006. Discontinuities in ecological data. Proceedings of the National Academy of Sciences 103:6083–6084.

Almeida-Neto, M., and W. Ulrich. 2011. A straightforward computational approach for measuring nestedness using quantitative matrices. Environmental Modelling & Software 26:173–178.

Bascompte, J., and P. Jordano. 2007. Plant-Animal Mutualistic Networks: The Architecture of Biodiversity. Annual Review of Ecology, Evolution, and Systematics 38:567–593.

Bascompte, J., P. Jordano, C. J. Melian, and J. M. Olesen. 2003. The nested assembly of plant-animal mutualistic networks. Proceedings of the National Academy of Sciences 100:9383–9387.

Beckett, S. J. 2016. Improved community detection in weighted bipartite networks. Royal Society Open Science 3:140536.

Beckett, S. J., and H. T. P. Williams. 2013. Coevolutionary diversification creates nested-modular structure in phage-bacteria interaction networks. Interface Focus 3:20130033–20130033.

Bezerra, E. L. S., I. C. Machado, and M. A. R. Mello. 2009. Pollination networks of oil-flowers: a tiny world within the smallest of all worlds. Journal of Animal Ecology 78:1096–1101.

Blüthgen, N., J. Fründ, D. P. Vázquez, and F. Menzel. 2008. What do interaction network metrics tell us about specialization and biological traits. Ecology 89:3387–3399.

Borrelli, J. J. 2015. Selection against instability: stable subgraphs are most frequent in empirical food webs. Oikos 124:1583–1588.

Delmas, E., M. Besson, M.-H. Brice, L. A. Burkle, G. V. Dalla Riva, M.-J. Fortin, D. Gravel, P. R. Guimarães, D. H. Hembry, E. A. Newman, J. M. Olesen, M. M. Pires, J. D. Yeakel, and T. Poisot. 2018. Analysing ecological networks of species interactions. Biological Reviews:112540.

Dobson, A. J., and A. G. Barnett. 2008. An Introduction to Generalized Linear Models. Third. Taylor & Francis Group, Boca Raton, USA.

Donatti, C. I., P. R. Guimarães, M. Galetti, M. A. Pizo, F. M. D. Marquitti, and R. Dirzo. 2011. Analysis of a hyper-diverse seed dispersal network: modularity and underlying mechanisms. Ecology Letters 14:773–781.

Dormann, C. F., B. Gruber, and J. Fründ. 2008. Introducing the bipartite Package: Analysing Ecological Networks. R News 8:8–11.

Felix, G. M., R. B. P. Pinheiro, R. Poulin, B. R. Krasnov, and M. A. R. Mello. 2017. The compound topology of a continent-wide interaction network explained by an integrative hypothesis of specialization. bioRxiv.

Flores, C. O., J. R. Meyer, S. Valverde, L. Farr, and J. S. Weitz. 2011. Statistical structure of host-phage interactions. Proceedings of the National Academy of Sciences 108:E288–E297.

Flores, C. O., S. Valverde, and J. S. Weitz. 2013. Multi-scale structure and geographic drivers of cross-infection within marine bacteria and phages. The ISME Journal 7:520–532.

Fortuna, M. A., D. B. Stouffer, J. M. Olesen, P. Jordano, D. Mouillot, B. R. Krasnov, R. Poulin, and J. Bascompte. 2010. Nestedness versus modularity in ecological networks: two sides of the same coin? Journal of Animal Ecology 79:811–817.

Futuyma, D. J., and G. Moreno. 1988. The Evolution of Ecological Specialization. Annual Review of Ecology and Systematics 19:207–233.

García-Robledo, C., and C. C. Horvitz. 2012. Jack of all trades masters novel host plants: positive genetic correlations in specialist and generalist insect herbivores expanding their diets to novel hosts. Journal of Evolutionary Biology 25:38–53.

Genrich, C. M., M. A. R. Mello, F. A. O. Silveira, J. L. Bronstein, and A. P. Paglia. 2017. Duality of interaction outcomes in a plant-frugivore multilayer network. Oikos 126:361–368.

Guimarães, P. R., M. M. Pires, P. Jordano, J. Bascompte, and J. N. Thompson. 2017. Indirect effects drive coevolution in mutualistic networks. Nature.

Guimerà, R., and L. A. Nunes Amaral. 2005. Functional cartography of complex metabolic networks. Nature 433:895–900.

Guimerà, R., D. B. Stouffer, M. Sales-Pardo, E. A. Leicht, M. E. J. Newman, and L. A. N. Amaral. 2010. Origin of compartmentalization in food webs. Ecology 91:2941–2951.

Hellgren, O., J. Pérez-Tris, and S. Bensch. 2009. A jack-of-all-trades and still a master of some: prevalence and host range in avian malaria and related blood parasites. Ecology 90:2840–2849.

Holland, J. N., and D. L. DeAngelis. 2010. A consumer–resource approach to the density-dependent population dynamics of mutualism. Ecology 91:1286–1295.

Ings, T. C., J. M. Montoya, J. Bascompte, N. Bl??thgen, L. Brown, C. F. Dormann, F. Edwards, D. Figueroa, U. Jacob, J. I. Jones, R. B. Lauridsen, M. E. Ledger, H. M. Lewis, J. M. Olesen, F. J. F. Van Veen, P. H. Warren, and G. Woodward. 2009. Ecological networks - Beyond food webs. Journal of Animal Ecology 78:253–269.

Jordano, P. 2016. Sampling networks of ecological interactions. Functional Ecology 30:1883–1893.

Joshi, A., and J. N. Thompson. 1995. Trade-offs and the evolution of host specialization. Evolutionary Ecology 9:82–92.

Krasnov, B. R., M. A. Fortuna, D. Mouillot, I. S. Khokhlova, G. I. Shenbrot, and R. Poulin. 2012. Phylogenetic Signal in Module Composition and Species Connectivity in Compartmentalized Host-Parasite Networks. The American Naturalist 179:501–511.

Krasnov, B. R., R. Poulin, G. I. Shenbrot, D. Mouillot, and I. S. Khokhlova. 2004. Ectoparasitic “Jacks-of-All-Trades”: Relationship between Abundance and Host Specificity in Fleas (Siphonaptera) Parasitic on Small Mammals. The American Naturalist 164:506–516.

Leung, C. Y. (Joey), and J. S. Weitz. 2016. Conflicting attachment and the growth of bipartite networks. Physical Review E 93:032303.

Lewinsohn, T. M., P. Inácio Prado, P. Jordano, J. Bascompte, and J. M. Olesen. 2006. Structure in plant-animal interaction assemblages. Oikos 113:174–184.

Maynard, D. S., C. A. Serván, and S. Allesina. 2018. Network spandrels reflect ecological assembly. Ecology Letters 21:324–334.

Mello, M. A. R., G. M. Felix, R. B. P. Pinheiro, R. L. Muylaert, C. Geiselman, S. E. Santana, M. Tschapka, N. Lotfi, F. A. Rodrigues, and R. D. Stevens. 2018. Insights on the assembly rules of a continent-wide multilayer network. bioRxiv.

Mello, M. A. R., F. M. D. Marquitti, P. R. Guimarães, E. K. V. Kalko, P. Jordano, and M. A. M. de Aguiar. 2011. The modularity of seed dispersal: differences in structure and robustness between bat– and bird–fruit networks. Oecologia 167:131–140.

Muchhala, N. 2007. Adaptive Trade-Off in Floral Morphology Mediates Specialization for Flowers Pollinated by Bats and Hummingbirds. The American Naturalist 169:494–504.

Olesen, J. M., J. Bascompte, Y. L. Dupont, and P. Jordano. 2007. The modularity of pollination networks. Proceedings of the National Academy of Sciences 104:19891–19896.

Pinheiro, R. B. P., G. M. F. Félix, A. V. Chaves, G. A. Lacorte, F. R. Santos, É. M. Braga, and M. A. R. Mello. 2016. Trade-offs and resource breadth processes as drivers of performance and specificity in a host–parasite system: a new integrative hypothesis. International Journal for Parasitology 46:115–121.

Pires, M. M., and P. R. Guimaraes. 2012. Interaction intimacy organizes networks of antagonistic interactions in different ways. Journal of The Royal Society Interface 10:20120649–20120649.

Poisot, T., E. Canard, N. Mouquet, and M. E. Hochberg. 2012. A comparative study of ecological specialization estimators. Methods in Ecology and Evolution 3:537–544.

Poulin, R. 1998. Large-scale patterns of host use by parasites of freshwater fishes. Ecology Letters 1:118–128.

R Core Team. 2017. R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. URL https://www.R-project.org/.

Scheffer, M., and E. H. van Nes. 2006. Self-organized similarity, the evolutionary emergence of groups of similar species. Proceedings of the National Academy of Sciences 103:6230–6235.

Thebault, E., and C. Fontaine. 2010. Stability of Ecological Communities and the Architecture of Mutualistic and Trophic Networks. Science 329:853–856.

Thompson, J. N. 1994. The coevolutionary process. University of Chicago Press, Chicago, USA.

Trøjelsgaard, K., and J. M. Olesen. 2013. Macroecology of pollination networks. Global Ecology and Biogeography 22:149–162.

Ulrich, W., W. Kryszewski, P. Sewerniak, R. Puchałka, G. Strona, and N. J. Gotelli. 2017. A comprehensive framework for the study of species co-occurrences, nestedness and turnover. Oikos:1607–1616.

Valverde, S., J. Piñero, B. Corominas-Murtra, J. Montoya, L. Joppa, and R. Solé. 2018. The architecture of mutualistic networks as an evolutionary spandrel. Nature Ecology & Evolution 2:94–99.

Vázquez, D. P., C. J. Melián, N. M. Williams, N. Blüthgen, B. R. Krasnov, and R. Poulin. 2007. Species abundance and asymmetric interaction strength in ecological networks. Oikos 116:1120–1127.

Zhang, F., C. Hui, and J. S. Terblanche. 2011. An interaction switch predicts the nested architecture of mutualistic networks. Ecology Letters 14:797–803.

CAPÍTULO 2

A NOVEL PERSPECTIVE ON NESTEDNESS AND A THEORY-ORIENTED PROCEDURE FOR THE USE OF NULL MODELS

A novel perspective on nestedness and a theory-oriented procedure for the use of null models

Rafael Barros Pereira Pinheiro [1], Carsten F. Dormann [2], Gabriel Moreira Félix Ferreira [3], Marco Aurelio Ribeiro Mello [1,4]

[1] Programa de Pós-Graduação em Ecologia, Conservação e Manejo da Vida Silvestre, Universidade Federal de Minas Gerais, Brasil. [2] Departamento de Biometria e Análise de Sistema Ambientais, Universidade de Freibug, Alemanha. [3] Programa de Pós-Graduação em Ecologia, Universidade Estadual de Campinas, Brasil. [4] Departamento de Ecologia, Universidade de São Paulo, Brasil.

ABSTRACT

Nestedness is a long-known pattern in metacommunity matrices, later discovered in species interactions, and currently recognized as a common topology of different types of networks. Statistically testing for nestedness in a matrix is challenging because, beyond calculating a metric, it is necessary to compare observed values with null models. There are several available algorithms to produce null models and the choice between them likely affects test outcomes. However, as algorithms are mostly not linked to hypotheses about nestedness, there are no theory-oriented rules to follow. Here, we propose a different look at the meaning of nestedness to address this problem. Nestedness is a combination of marginal sum inequality and high overlap. First, we show that, the higher the overlap in a matrix, the more predictable are cell values by marginal sums. From this, we argue that two different null model algorithms can be used to test two different hypotheses. The equiprobable algorithm produces matrices with random topologies and is a lower bound of expectations for nestedness significance. The proportional algorithm, on the contrary, produces nested matrices, and tests whether a network significantly deviates from a nested topology. Beyond reconciling contradictions in null model analysis, this novel perspective delimits the range of possible explanations for nestedness. The only way a process can increase nestedness in a matrix is by increasing marginal sum inequalities, but without concomitantly introducing preferences. For instance, in a species interaction network, any explanation of nestedness should address the question of why some species systematically interacts more frequently than others. Unequal abundances and fitness differences are, thus, reasonable explanations for nestedness, while processes that introduces preferences on the matrix, are not. Finally, we evaluate the ability of several nestedness indices to separate random and nested topologies, and illustrate the proposed procedures using a pollination network.

KEYWORDS: network science; nestedness; network topology; metacommunity; species interactions; null-model analysis; community ecology;

INTRODUCTION

The concept of nestedness has its origins in the study of insular biotas. Nestedness was first defined as the biogeographical pattern that faunas of poorer islands within an archipelago constitute a subset of the faunas of richer islands [1]. Such patterns have been earlier recognized by biogeographers [2]. But it was only after the influential work of Diamond [3] that the structure of metacommunities, using species *vs* site matrices, turned into a major focus of ecological studies, boosting the search for nestedness. In the following decades nestedness of species occurrences have been found in islands [1,4], along gradients [5], in mountain ranges [6], and in several other habitats [7]. The later observation of nestedness in species interaction networks [8–10] exposed it as a very common pattern in ecological systems.

Nestedness of species occurrences is traditionally explained as the result of ordered selective colonization [1,2] or extinction [6] in local communities. Such order could arise, for instance, as the combined results of differential colonization abilities (or extinction vulnerability) by species and differential probabilities of colonization (or extinction) on islands depending on island size and isolation [11]. Similarly, nestedness in species interactions is often related to ordered probabilities of species to interact [12], resulting, for instance, from unequal abundances [13]. Currently, nestedness is recognized as a common network topology [14] and has been detected several systems beyond ecology, for instance social [15] and economic [16] networks.

To measure nestedness, networks are usually represented as adjacency matrices, where rows and columns represent the nodes (e.g., pollinators and plants in a pollination network) and cells represent the links between them (e.g., pollination). There are currently several nestedness metrics available [17]. Additionally, nestedness tests require the use of null models to quantify random expectations [17], which introduces an additional source of complexity to the methods. And although the choice of null model algorithms strongly affects the outcome [18], there are no theory-oriented rules to follow. Null models that only conserve matrix dimensions and total sum are considered less rigorous, but more sensitive, than null models that conserve matrix marginal sums. And, as algorithms are not linked to explicit hypotheses, this choice is often regarded simply as a trade-off between type I and type II statistical errors [18,19].

A more recent advancement was the development of nestedness metrics for weighted matrices [20–22]. In real systems, interactions between nodes are not all equivalent, but vary in frequency or intensity. For instance, links in a pollination network might be weighted by the frequency of pollination events observed for each plant-pollinator combination [23]. Weighted matrices are more informative and reveal patterns that are often hidden in their binary counterparts [24,25].

In this study we propose a novel perspective on nestedness in binary and weighted matrices. We believe that both the way in which nestedness is compared with null models and the interpretation of these findings can be improved, and some contradictions reconciled by taking a different look at what nestedness actually quantifies. In several steps, we first define nestedness in a matrix as a combination of marginal sum inequalities and overlap. Secondly, we show that overlap measures the predictive power of marginal sums on cell values. From this, thirdly, we argue that two commonly used null model algorithms are not alternative, but complementary, as they test different hypotheses. The equiprobable null model is appropriate for testing the significance of nestedness, while the proportional null model is useful to test whether the matrix topology is fully defined by nestedness (i.e., has a nested topology). Forth, we compare the efficiency of several nestedness metrics within our new perspective, using both binary and weighted matrices. Lastly, we illustrate our novel perspective using a pollination network.

METHODS

A novel perspective on nestedness

While we focus our examples and discussion on bipartite species interaction networks, the arguments presented here are not related to the nature of the studied interactions, and therefore apply similarly to other ecological (e.g., species vs. sites matrices) and non-ecological (e.g. social) systems. Also, for increased generality, we use general terms for the study of matrices and networks [26]. In an adjacency matrix, (1) rows and columns, (2) cells, (3) cell values, and (4) marginal sums, represent, respectively, network (1) nodes, (2) links, (3) link weights, and (4) node strengths, for weighted networks, or node degrees, for binary networks.

Orders of information on a network

Network information can be partitioned into three levels of complexity [27]. First-order information comprises the most general features of the adjacency matrix: its dimensions (number of rows and columns) and the sum of all cell values (hereafter, total sum). In a weighted species interaction network, it is the richness of species in each side of the interaction and the total number of interactions observed. Second-order information represent the specific properties of each row and column: the marginal sums. In a weighted species interaction network, it is the number of interactions made by each species. Finally, third-order information is the actual cell values. In a weighted species interaction network, it is the number of interactions between each pair of species.

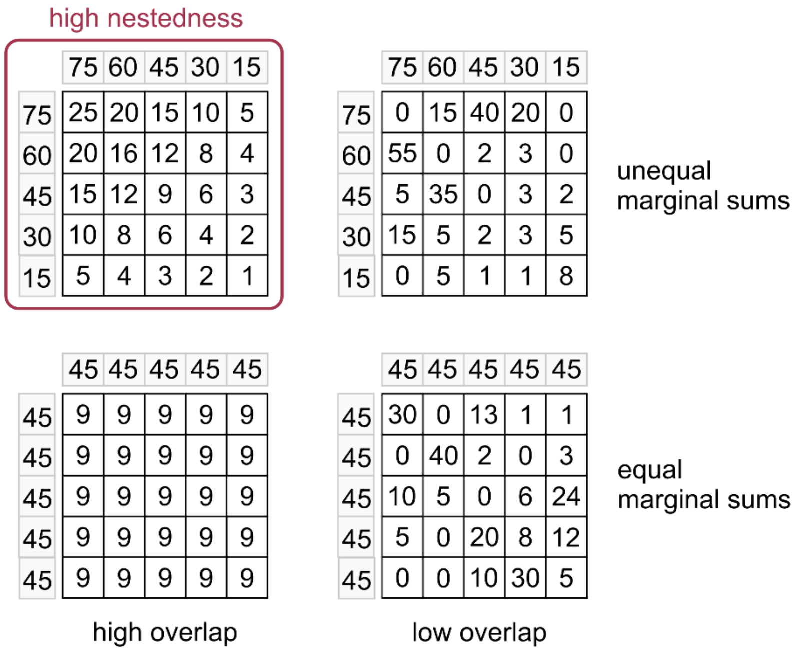
Definition of nestedness

The concept of *nestedness* was first proposed as a pattern of species occurrence, latter generalized to binary networks, and only recently applied to weighted networks. Thus, it is not trivial to provide a general definition of nestedness for all kinds of matrices. Below, we provide a verbal general definition, and additionally, a visual description, which is easier to understand and operationalize.

Binary nestedness is the tendency of rows / columns with lower marginal sums to have links (1s) with a subset of partners from those of rows / columns with higher marginal sums. For the weighted nestedness, beyond the identity of partners, we may account for cell values. Thus, weighted nestedness is the tendency of rows / columns with lower marginal sums to present weaker links (lower cell values) with the same set or a subset of partners from those of the rows / columns with higher marginal sums. To visualize nestedness we must organize matrix rows and columns by decreasing marginal sums. In a binary matrix, nestedness is visualized as a tendency of 1s to be located in the top-left, while 0s are in the bottom-right corner of the matrix. In a weighted matrix, nestedness is a tendency of decreasing link weights from the top-left to the bottom-right corner (Fig. 1).

Overlap is the tendency of rows / columns to interact with a similar set of partners. The core of any nestedness metric is assessing the overlap between rows / columns with different marginal sums, more specifically, testing whether rows / columns with lower marginal sums interact with the same partners as rows / columns with higher marginal sums. Weighted metrics of overlap account for, not only the identity of partners, but whether row / columns distribute weights among these partners in similar proportions. Several nestedness indices are indeed, purely measures of overlap (e.g., temperature [28] and spectral radius [22]). The opposite of overlap: a tendency of nodes to interact with different partners is often called *turnover*, *specialization*, or *preferences*. Here, we opt for *preferences*. But notice that this term is referred exclusively as the tendency opposed to matrix overlap (exactly as Blüthgen *et all.* [29] refer to *specialization*). Those may or may not be good proxies for the ecological concepts of specialization and preferences.

However, as pointed by previous studies [12,30], the original concept of nestedness also assumes a gradient in marginal sums. Such realization prompted the development of nestedness metrics demanding marginal sum inequalities (hereafter, "true nestedness" metrics), for instance, NODF (Nestedness based on Overlap and Decreasing Fill) [30]. Nestedness is, thus, a combination of these two features: high overlap and unequal marginal sums (Fig. 1).



	75	60	45	30	15
75	25	20	15	10	5
60	20	16	12	8	4
45	15	12	9	6	3
30	10	8	6	4	2
15	5	4	3	2	1

	75	60	45	30	15
75	0	15	40	20	0
60	55	0	2	3	0
45	5	35	0	3	2
30	15	5	2	3	5
15	0	5	1	1	8

	45	45	45	45	45
45	9	9	9	9	9
45	9	9	9	9	9
45	9	9	9	9	9
45	9	9	9	9	9
45	9	9	9	9	9

	45	45	45	45	45
45	30	0	13	1	1
45	0	40	2	0	3
45	10	5	0	6	24
45	5	0	20	8	12
45	0	0	10	30	5

Fig. 1. Nestedness is a combination of high overlap and marginal sums inequality. Weighted overlap is the tendency of rows / columns to establish links with the same partners and to distribute weights among these partners in similar proportions. In a matrix with unequal marginal sums (gray boxes), high overlap results in nestedness. Here, we focus on weighted matrices, as similar explanations for binary matrices were presented elsewhere [12,30].

A novel perspective on overlap

Here, we propose a new interpretation on the meaning of overlap and its implications for the understanding of nestedness. For this we use a hypothetical bipartite species interaction matrix as an example (see Fig. 2 legends for the same explanation in general notation for the study of matrices).

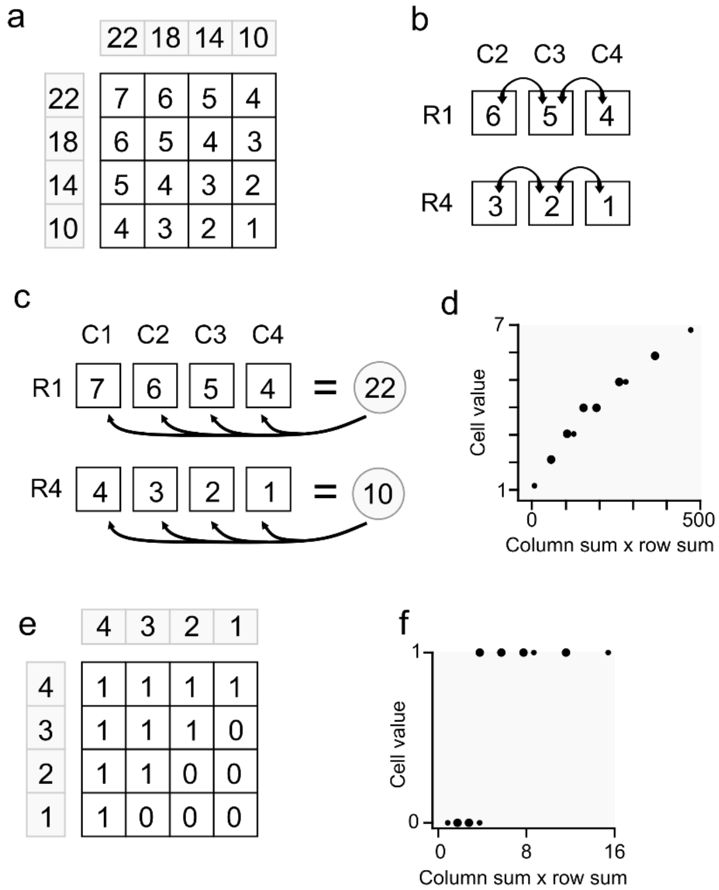


Fig. 2. In a nested weighted matrix organized by decreasing marginal sums (boxes in gray), cell values decrease from the top-left to the bottom-right corner (a). The high overlap on the matrix means that a cell value is partially predictable from its neighbor cells within a row (b). For instance, if R1 has a stronger link with C4 than R4, then, it will also have a stronger link with C3 and C2 than R4. As cell values within each row partially predicts one another and sum to the row sums, thus, row sums are themselves predictors of cell values in a nested matrix (c). If this same reasoning is applied to columns, we see that overlap in a matrix is also a measure of how much each cell value is predictable by its respective marginal sums. This property is illustrated in (d): cell values in our nested matrix increase monotonically with the outer product of their marginal sums. The same logic applies to binary matrices (e-f).

Imagine that the matrix in Fig. 2a represents the observed number of interactions between four pollinator species (rows: R1, R2, R3, and R4) and four plant species (columns: C1, C2, C3, and C4). A high overlap of interactions between plant species means that the number of interactions made by a given pollinator with any plant is a partial predictor of its interactions with the other plants. For instance, as the pollinator R1 interacts more frequently with the plant C4 than the pollinator R4, we would expect it to also interact more frequently than R4 with C3 and C2 (Fig. 2b).

The interactions of a pollinator with each plant (cell values within a row) sum to its total number of interactions (row sums). Thus, the total number of interactions of a pollinator is also a partial predictor of its interactions with each plant in a nested matrix (Fig. 2c). Applying the same logic to plants (columns), we conclude that the number of interactions between each pollinator-plant pair, in a nested matrix, can be well predicted by the total number of interactions of each pollinator and each plant species (marginal sums) (Fig. 2d). The same logics applies to binary nested matrices: the occurrence of interaction can be predicted by marginal sums (Fig. 2e-f).

This is the first key insight: the higher the overlap in a matrix, the higher the predictive power of marginal sums on cell values. However, when all marginal sums are equal, they provide no further information compared to a prediction based only on the first-order information. For instance, in a fully homogeneous matrix (matrix with high-overlap and equal marginal sums in Fig. 1) by knowing the marginal sums, we can perfectly predict all cell values. But we could achieve this same result just by guessing the mean cell value (total sum divided by the number of cells). Thus, the second key insight: for a given overlap, the higher the inequalities in marginal sums, the higher the differences between a prediction informed by the second-order information and a prediction only based on the first-order information.

Putting the two insights together, we find that nestedness is directly related to how much information about cell values we gain by knowing, beyond the first-order, also the second-order properties of a network. In a matrix with high nestedness, assuming that each cell value is proportional to the product of row and column sums is a much more accurate prediction than guessing that all cells present the mean weight. As nestedness decreases, this difference decreases too.

A theory-oriented procedure for the use of null models

Nestedness significance

The main challenge for testing nestedness is that cell values in a matrix are not independent from each other, and parametric inference is currently not possible. Even in a network formed by random interactions between similar nodes, we would expect to find some degree of overlap and marginal sum inequalities in the matrix, and thus, nestedness. Additionally, the first-order properties of a network delimit the universe of possibilities for second-order properties, and therefore, to its effect on cell values. In binary matrices, for instance, degree distribution and, hence, nestedness are highly conditioned by connectance [31].

Therefore, to test a matrix for significant nestedness, we must first state the expectations using a first null model. This first null model must derive from an equiprobable algorithm that only conserves first-order information: matrix dimensions and total sum [17] (hereafter called "equiprobable null model"). The equiprobable null model aims at simulating matrices void of nestedness, as the inequality of marginal sums and the overlap on them derive from randomness. The topology of equiprobable matrices can be consistently called a "random topology".

As the equiprobable model ignores the second-order information of the networks, its nestedness is due to the first-order properties and randomness, and, thus, a lower bound of expectations for significance tests.

The nested topology

After inferring that a given network presents significant nestedness compared to a random topology, the next logical question is whether it significantly deviates from a perfectly nested network. To proceed with this test, we must use a second null model that conserve the marginal sum inequalities and maximize overlap, accounting for the expected variance. The most appropriate algorithm for this task is one in which the probability of each cell to receive a unit of weight is proportional to marginal sums, hereafter, called proportional null model [32]. In matrices from a proportional null model, cell values are fully driven by the second-order information, and therefore, following our perspective, they have a truly nested topology.

Notice, though, that many of the currently available proportional null algorithms for weighted matrices, beyond conserving marginal sums and total sum, also conserves connectance, a binary matrix property (e.g., the *vaznull* model implemented in the R package *bipartite* [13,33]). This mixed use of binary and weighted information is undesirable for our approach, as it cannot be linked to any specific hypothesis about nestedness.

Proportional null models are traditionally used as a lower expectation to test nestedness significance. However, as overlap relates to the correlation between marginal sums and cell values, there is no point in testing whether a given matrix presents higher nestedness than randomized matrices in which cell probabilities are fully determined by marginal sums. This null model should be considered the upper bound of expectations for nestedness, rather than the lower bound. Otherwise, as earlier stated by Wright and Reeves [4], it hides the own pattern that we attempt to detect.

In this study, we differentiate between *nestedness* as a continuous tendency and a *nested topology* as a high-level classification of the entire matrix structure. A nested matrix not only present significant nestedness, but is statistically defined by it. So, two conditions are necessary for a matrix to be nested: first, nestedness must be significantly higher than the equiprobable null model; second, nestedness must not be significantly lower than the proportional null model (Fig. 3).

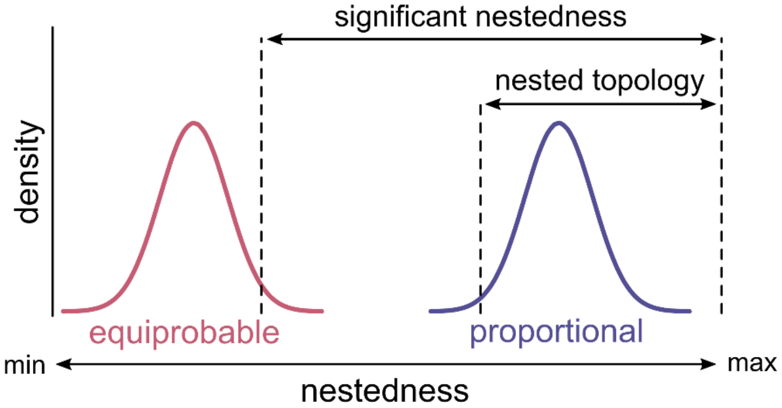


Fig. 3. A theory-oriented procedure for the use of null models in tests of nestedness. First, we defined nestedness as a combination of marginal sums inequality and high overlap. Second, we demonstrate that overlap can be measured as the predictive power of marginal sums in cell values. Through this novel perspective we are able to link two null models to two different explicit hypotheses about nestedness. The equiprobable null model conserves only the first-order properties of the matrix (dimensions and total sum) and have a random topology. The proportional null model conserves the second-order properties (marginal sums) and maximize the overlap (by

defining cell probabilities based on marginal sums), and thus shows a nested topology. Nestedness significance is checked by the comparison of the observed value with the equiprobable null model. For a network to have a truly nested topology, though, two conditions are necessary: first, nestedness must be significantly higher than in a random topology; second, nestedness must not be significantly lower than the proportional null model.

Nestedness metrics

In our perspective, the main function of a nestedness metric is to distinguish between matrices with randomly distributed cell values (non-significant nestedness, random topology), matrices in which cell values are partially predictable by marginal sums (significant nestedness, but non-nested topology), and matrices in which cell values are fully predictable by marginal sums (nested topology). The procedure proposed is appropriate for any nestedness metric that is efficient in this task.

There is, however, a possible drawback of using true nestedness metrics in null model analysis. Penalizing marginal sum equality on an index and then comparing values with null models that discard or conserve marginal sum distribution is circular. Metrics affected only by overlap are more appropriate for comparisons with null models, even if they are by themselves, that is without null models, less informative. This is a contradiction embedded in any nestedness test so far, for which we still have no solution. Here, we regard the ability to locate a matrix between the two null model bounds as the more important property.

Analysis

Binary and weighted matrices

In real-world systems, interactions almost always have a quantitative nature (e.g., frequencies or intensity). However, due to the way data are compiled [34], networks are often studied through binary matrices. When based on binary data, marginal sum distributions are highly contingent on connectance [31] and poor proxies for the weighted marginal sums, especially for matrices with high connectances (Fig. S1). Proportional null models when applied to binary matrices often cannot conserve the marginal sum distribution on the randomized matrix [7]. Such distortion is likely to cause underestimation of nestedness in the null model.

Comparisons between nestedness indices

Here, we analyzed the capacity of several nestedness indices in distinguishing between matrices with random (equiprobable null model) and nested (proportional null model) topologies. First, we produced probability matrices with dimensions: 5 x 5, 10 x 10, and 20 x 20, based on three different marginal probabilities: constant across rows / columns, linear decrease, and log-normal. These represent a gradient between an equiprobable null model and a proportional null model based on a steeper marginal sum distribution. Then, we sampled from these probabilities with different intensities: 50, 100, 200, 400, 800, 1600, 3200, and 6400 (Fig. S2). For each unique setup we produced 10,000 matrices. For each matrix we calculated a set of nestedness indices (Table 1), including both binary and quantitative metrics, and graphically inspected the capacity of separating results between the equiprobable (constant) and the proportional (linear decrease and lognormal) null models.

Table 1- Nestedness indices compared in this study. Type: overlap = indices that only account for overlap; true nestedness = indices that account for overlap and marginal sum inequalities.

Metric	Type	Reference
Binary		
Temperature	overlap	28
Manhattan distance	overlap	35
NODF	true nestedness	30
β_{NES}	true nestedness	36
Binary spectral radius	overlap	22
Weighted		
WNODF	true nestedness	20
WNODA	true nestedness	21
Spectral radius	overlap	22

As, binary matrices do not have quantitative information, we cannot fix the true total sum of weights on the null models, only connectance. For a more appropriate comparison of binary metrics, we generated binary matrices from the probabilities with fixed connectances of 0.3, 0.5, 0.7, 0.9, 0.92, 0.94, 0.96, and 0.98. Moreover, in analysis of binary matrices, we usually do not know the original weighted marginal sums, only its binary respective. To inspect the distortion caused by this approximation, for each matrix produced with fixed connectance, we produced a randomized matrix using a proportional algorithm based on binary information (null model 2 of Bascompte *et al.*[8]).

An issue with any randomizing algorithm based on probabilities is that it may produce matrices with empty rows or columns. In general, these are not likely to bias network analysis [32]. Here, for the weighted matrices we kept all matrices. However, reducing matrix dimension modifies its connectance. Thus, when producing each binary matrix, we discarded all the matrices with reduced dimensions.

Case study

To illustrate our novel perspective we used a weighted plant-pollinator network, originally described by Kaiser-Bunbury *et al.*[37] and available at the Web of Life database (www.web-of-life.es, network: M_PL_060_17). The network includes 52 nodes, being 17 plant species and 35 pollinator species, and has a connectance of 0.17. Weights are the number of floral visits observed between each pollinator and each plant species (total of 444 visits). This network was arbitrarily chosen from the database, without any preliminary analysis, following the only criterion of propitious dimensions for illustrational purposes (i.e., between 10 and 50 species in each side).

We produced an equiprobable and a proportional null model, with 10,000 matrices each, and calculated the WNODA for each matrix. Similarly, we analysed the binary structure of the network using the NODF. We then produced a proportional null model based on binary information, to inspect whether it would result in a distortion on NODF values compared to the proportional null model based on quantitative data.

Codes and R functions

Analysis were performed in R program version 3.4.0 (R Core Team 2017). Commented scripts to reproduce the study and R functions for applying the proposed procedures on alternative networks are available at GitHub (http://dx.doi.org/10.5281/zenodo.2653181).

RESULTS

Weighted nestedness metrics vary substantially in their capacities of distinguishing between random and nested matrices (Fig. 4, Appendix S1). WNODF, because of confounding weighted (overlap) and binary (decreasing fill) information [20], has a complex behavior and is not appropriate to highly or fully connected matrices. WNODA and spectral radius presented good separation and are the better discriminating at higher sampling intensity. Additionally, connectance increases faster with increased sampling, on matrices with more homogeneous marginal sum distributions.

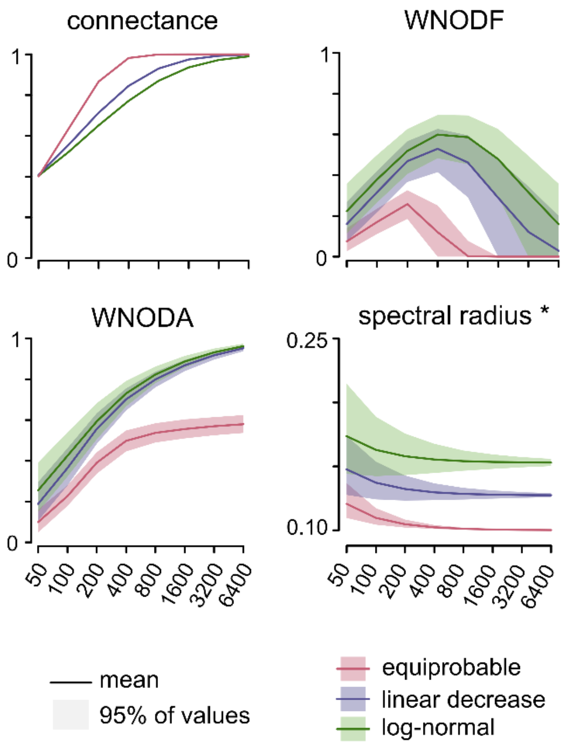


Fig. 4. Ability of weighted metrics to distinguish between nested matrices (cell values are determined by marginal sums: linear decrease and log-normal) and random matrices (cell values are randomly distributed: equiprobable), on different sampling intensities. In the presented perspective, the main function of a nestedness metric is to distinguish between those groups of matrices. Index values in y-axis and sampling (total weight of the matrix) on the x-axis. Spectral radius values were divided by sampling intensity for a better visualization. Only results from the 10 x 10 matrices are included in the figure, see Appendix S1 for other matrix dimensions and for binary indices.

As expected, matrices with a steeper marginal sum distribution (log-normal) are more easily distinguished from the equiprobable null model than matrices with more similar marginal sums (linear-decrease). The sampling required for the stabilization of the indices is higher in larger matrices (Appendix S1). WNODF, however, because of being contingent on connectance, is uninformative for the smallest matrices (5 x 5) even with intermediary sampling (Appendix S1).

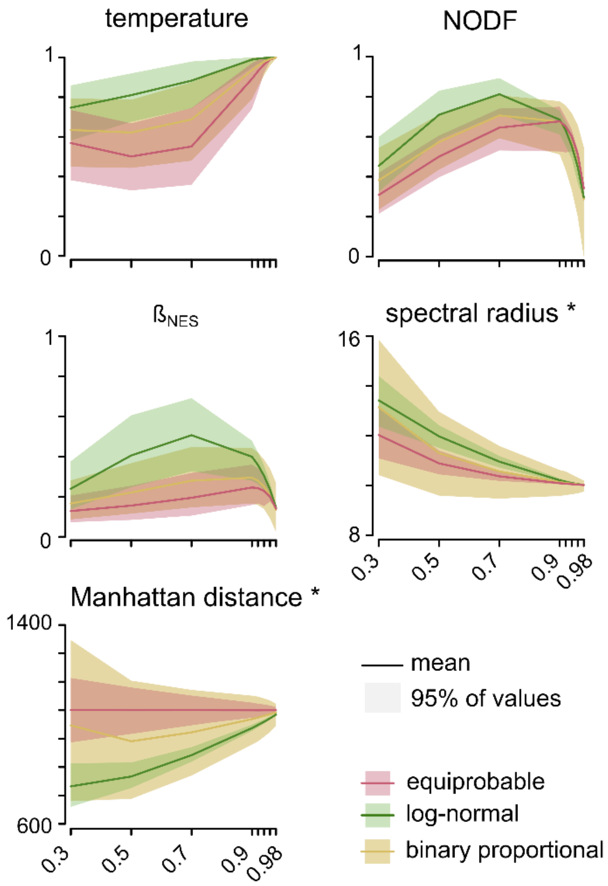


Fig. 5. Ability of binary metrics to distinguish between nested matrices (cell values are determined by marginal sums: log-normal) and random matrices (cell values are randomly distributed: equiprobable), on different connectances. As binary matrices do not provide information on weighted marginal sums, we produced a proportional null model based on the binary marginal sums of the matrices generated with the log-normal probabilities. Ideally, values for the binary proportional model (yellow) would match values for the matrices based on log-normal probabilities (green). They are, however, largely distorted: for temperature, NODF, and β_{NES} values are highly underestimated, while for spectral radius and Manhattan distance they present a much larger variability. Index values in y-axis and connectance on the x-axis. Binary spectral radius and Manhattan distance values were divided by the connectance, providing a better visualization. Only results from the 10 x 10 matrices are presented here, see Appendix S2 for other matrix dimensions and details.

Binary metrics varied in their capacity to distinguish between nested matrices formed by log-normal probabilities and random matrices with fixed connectance (Fig. 5, Appendix S2). Manhattan distance had an outstanding ability over the entire range of connectance. True nestedness indices (NODF and β_{NES}), by requiring inequalities in marginal sums, presented a complex behavior. Binary nestedness metrics were more efficient in larger matrices and in intermediary connectances (Appendix S2).

The use of binary information to estimate probabilities on the proportional null model resulted in large distortions. Nestedness values for the proportional null matrices based on the binary probabilities do not match the range of values for the matrices produced from quantitative information (Fig. 5). For most of the indices, those values are highly underestimated. However, for spectral radius and for Manhattan distance they presented a large variability, encompassing both groups.

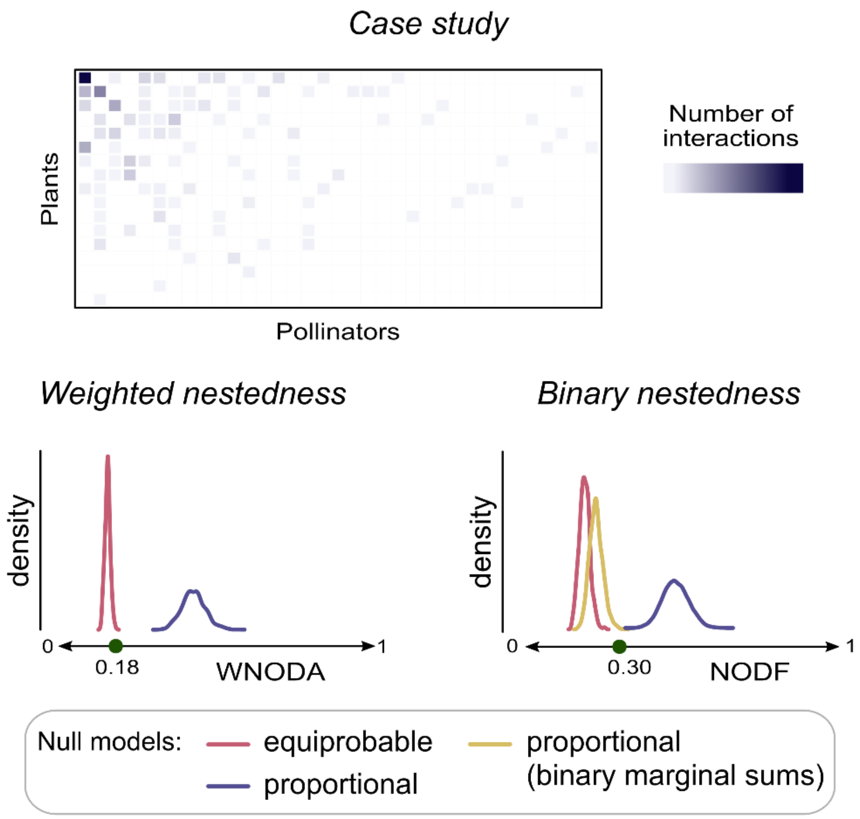


Fig. 6. *Case study* using a weighted empirical plant-pollinator network to illustrate the proposed procedures. *Weighted nestedness:* the observed weighted nestedness based on overlap and decreasing abundance (WNODA) is high compared to the equiprobable null model, meaning that there is significative nestedness in the network. Nestedness is, though, not similar to the values on the proportional model, meaning that network structure deviates from a nested topology. We can, thus, conclude that there are preferences in the pattern of observed interactions between plants and pollinators. *Binary nestedness:* we analyzed the binary topology of the network using the NODF index. When quantitative information was used to generate the proportional null model, conclusions were similar to the analysis with the weighted metric. However, when we

based the proportional null model on node degrees (marginal sums of the binary matrix), using the null model 2 of Bascompte *et al.*[8], it resulted in much lower values. In comparison, the observed nestedness seemed higher than the expected given the degree distribution. This is, thus, a result of the distortion caused by using binary information instead of quantitative. The empirical pollination network was obtained from the Web of Life database (www.web-of-life.es, network: M_PL_060_17, originally described by Kaiser-Bunbury *et al.*[37]).

The empirical plant-pollinator network showed significant nestedness (WNODA = 0.18, comparison against the equiprobable model: Z = 2.73, p = 0.006), but not a nested topology (comparison against the proportional model: Z = -6.73, p < 0.001) (Fig. 6: *Weighted nestedness*). The binary metric (NODF) leads to similar conclusions (NODF: 0.30; comparison against the equiprobable model: Z = 6.61, p < 0.001; comparison against the proportional model: Z = -4.87, p < 0.001). However, when the probabilities for the proportional null model are based in binary information, there is a large underestimation of nestedness in the randomized matrices (Fig. 6: *Binary nestedness*), and because of that, the observed nestedness is seemingly too high compared to the proportional model (Z = 3.35, p < 0.001).

DISCUSSION

Nestedness and null models

In the present study we demonstrate that nestedness in a matrix can only result from marginal sum inequalities. In difference to previous studies making similar claims [38,39], our conclusions do not arise from comparisons between empirical networks and null models, but rather from a deductive argument. We show that overlap, one of the two defining elements of nestedness, simply quantifies how well cell values are predictable by marginal sums. Preferences on the matrix, thus, reduce nestedness. In addition, for a matrix to present nestedness, it must have marginal sum inequalities, otherwise, marginal sums provide no increased information compared to matrix dimensions and total sum. I other word, nestedness is a measure of how better we can predict each cell value in a matrix if we account for marginal sums instead of just averaging.

This understanding delimits appropriate explanations for nestedness. The only way that a process can increase nestedness is by increasing marginal sum inequalities, without introducing preferences on the matrix. Thus, any explanation for nestedness in a species interaction network should address the question of “why some species interact more frequently than others?”. Unequal abundances is an obvious first guess [13], but not always true [40], and other factors may be involved, as differences in species fitness, activity, or detectability between species. Phylogenetic [41] and trait [42] specialization, on the other hand, lead to preferences and reduce the predictive power of second-order information on cell values.

Analogously, in an archipelago, differences in island isolation and area, may result in different chances of receiving or supporting species and promote nestedness of species occurrences. Local adaptation or competitive exclusion between pair of species, on the other hand, may result in preferences in the matrix, decreasing nestedness. Indeed, factors producing a hierarchy between sites and between species, and consequently marginal sum inequalities, have been traditionally pointed out as the causes of nestedness in metacommunity matrices [1,11].

The use of null models is regarded as the most controversial step on nestedness tests, as there are no strict rules on the choice of randomizing algorithms, but it may strongly affect inference [17]. The procedure proposed here overcomes this controversy by liking null models to explicit hypotheses to be tested. The equiprobable null model is used to test whether a given matrix present significantly higher nestedness than the expected in a random matrix, while the proportional null model tests whether nestedness statistically defines the entire matrix: a nested topology. We strongly disagree with the general understanding that null model choice is a decision between type I and type II statistical errors: there is no common hypothesis being tested, but rather different hypotheses. Those null models are, thus, not alternative, but complementary.

Ecological networks tend to have significative nestedness [7,8] and many explanations have been proposed to the ubiquity of nestedness, including its effect on network stability [43]. In our perspective, though, these results are not unexpected at all and no complex explanation is required. After all, unequal marginal sums promote nestedness and real-world networks are never formed by random connections between species with equal abundances, fitness and activities. However, for a network to be as nested as the proportional null model, it cannot include any preferences between nodes. This may be the case in homogeneous and small-scale systems, but much less probable in more diverse networks [10]. For instance, in a pollination network containing few plants with very similar flowers, we may expect no differential preferences of pollinators to plants. However, if the network comprises several plant families or plants with varied pollination syndromes, it is more likely that different pollinators preferentially interact with each plant or group of plants [11]. Nested topologies are, thus, expected in species interaction networks with low phylogenetic diversity [44], but not in highly diverse networks [45]. In diverse networks, topologies that includes preferences, as modularity, tends to predominate [46].

Methodological issues

Additionally, our study sheds light on the efficiency of nestedness indices. Indices that penalize marginal sum equalities aim at a better fit between the metric and the concept of nestedness [30] but were, in general, less able to separate nested from random matrices. As the null models are based on the removal or inclusion of second-order information, the accounting for marginal sums inequality on the raw value of the index includes some circularity on the analysis, which may explain these results.

The use of binary marginal sums to derive node probabilities in proportional null models have resulted in large distortions, both on our simulated matrices as in the case study, and, for most of the indices, resulted in underestimation of nestedness in the null model. This is a long known, but mostly overlooked, problem [4,7]. And it may be on the root of several studies finding much higher nestedness in empirical binary ecological networks and metacommunity matrices than in proportional null models [1,8], even when, as we discussed, this is not expected. Moreover, as the relationship between connectance and sampling depends on marginal sums, connectance is also not a direct proxy for the first-order information of the original weighted matrix. We echo previous authors in their call for a move beyond binary towards weighted matrices in ecological studies [24,25,47]. We agree that there might be reasons to study the binary instead of the weighted structure of a matrix [48], but even in these cases, null models based on weighted information are more appropriate. In other words, to study the binary structure of a weighted matrix is a better option than to study a binary matrix.

Topologies beyond nestedness

Random matrices are well defined by its first-order properties: dimensions and total weights. Nested matrices require and are explained by its second-order properties. Nevertheless, several matrices are shaped by preferences between row-column pairs, therefore are not random neither nested, and require more information for a better description of its topology. Preferences are often grouped, for instance, by phenology or phylogeny in a species interaction network, resulting in modularity. A nested matrix, in our definition, cannot be modular at the same time, because it presents no preferences. Thus, nestedness and modularity cannot be two sides of the same coin, as suggested by previous studies [49]. However, nestedness and modularity are also not the opposite extremes of a continuum, as in a modular matrices preferences are grouped and nestedness may still prevail within each group [10,50]. Thus, modular matrices may present more nestedness than random topologies, but less than nested matrices.

The relationship between nestedness and topologies that requires third-order information still demands clarification, and our novel perspective may help to address this challenge more efficiently. A consequence of the argument developed here is that, in order to test the significance of modularity or of any other topology beyond nestedness and randomness, we should use the proportional null model conserving the second-order information as the lower bound of expectations.

Conclusion

Here we show through a logic argument that nestedness quantifies the effect of unequal marginal sums on cell values of a matrix. This change of perspectives allowed us a clearer understanding on the meaning of nestedness and on the range of potential processes generating it. Moreover, by linking each algorithm to explicit hypotheses, it allows a more theory-oriented use of null model for testing topologies. We hope that these advances contribute to solve old contradictions and work towards a better understanding of the topology of metacommunities, species interactions, and other ecological and non-ecological networks.

ACKNOWLEDGEMENTS

We thank our institutions and colleagues, who helped us in different ways during this project. The Graduate School in Ecology of the Federal University of Minas Gerais (ECMVS), Brazil, provided RBPP with a scholarship from the Brazilian Council for Scientific and Technological Development (CNPq). Infrastructure for this study was provided by ECMVS, the Department of Ecology of the University of São Paulo (USP), and the Department of Biometry and Environmental System Analysis of the University of Freiburg, Germany. The Graduate School in Ecology of the State University of Campinas (PPGE-UNICAMP), Brazil, provided GMFF with a scholarship from the

Brazilian Coordination for the Improvement of Higher Education Personnel (CAPES). RBPP received a scholarship from the joint program between CAPES, CNPq, and Deutscher Akademischer Austauschdienst (DAAD) (88887.161398/2017-00). MARM was funded by the Minas Gerais Research Foundation (FAPEMIG: PPM-00324-15), the Alexander von Humboldt Foundation (AvH: 3.4-8151/15037), CNPq (#302700/2016-1), and the Research Dean of the University of São Paulo (PRP-USP: 18.1.660.41.7).

REFERENCES

1. Patterson, B. D. & Atmar, W. Nested subsets and the structure of insular mammalian faunas and archipelagos. *Biol. J. Linn. Soc.* **28**, 65–82 (1986).
2. Darlington, P. J. *Zoogeography: the geographical distribution of animals*. (John Wiley & Sons, 1957).
3. Diamond, J. M. Assembly of species comunnities. in *Ecology and Evolution of communities* (eds. Cody, M. & Diamond, J. M.) 342–444 (Harvard University Press, 1975).
4. Wright, D. H. & Reeves, J. H. On the meaning and measurement of nestedness of species assemblages. *Oecologia* **92**, 416–428 (1992).
5. Harrison, S., Ross, S. J. & Lawton, J. H. Beta diversity on geographic gradients in Britain. *J. Anim. Ecol.* **61**, 151 (1992).
6. Cutler, A. H. Nested faunas and extinction in fragmented habitats. *Conserv. Biol.* **5**, 496–504 (1991).
7. Wright, D. H., Patterson, B. D., Mikkelson, G. M., Cutler, A. & Atmar, W. A comparative analysis of nested subset patterns of species composition. *Oecologia* **113**, 1–20 (1997).
8. Bascompte, J., Jordano, P., Melian, C. J. & Olesen, J. M. The nested assembly of plant-animal mutualistic networks. *Proc. Natl. Acad. Sci.* **100**, 9383–9387 (2003).
9. Ollerton, J., McCollin, D., Fautin, D. G. & Allen, G. R. Finding NEMO: nestedness engendered by mutualistic organization in anemonefish and their hosts. *Proc. Biol. Sci.* **274**, 591–598 (2007).
10. Lewinsohn, T. M., Inácio Prado, P., Jordano, P., Bascompte, J. & M. Olesen, J. Structure in plant-animal interaction assemblages. *Oikos* **113**, 174–184 (2006).
11. Cutler, A. H. Nested biotas and biological conservation: metrics, mechanisms, and meaning of nestedness. *Landsc. Urban Plan.* **28**, 73–82 (1994).
12. Ulrich, W. & Almeida-Neto, M. On the meanings of nestedness: back to the basics. *Ecography (Cop.).* **35**, 865–871 (2012).
13. P. Vázquez, D. *et al.* Species abundance and asymmetric interaction strength in ecological networks. *Oikos* **116**, 1120–1127 (2007).
14. Delmas, E. *et al.* Analysing ecological networks of species interactions. *Biol. Rev.* 112540

(2018). doi:10.1111/brv.12433

15. Borge-Holthoefer, J., Baños, R. A., Gracia-Lázaro, C. & Moreno, Y. Emergence of consensus as a modular-to-nested transition in communication dynamics. *Sci. Rep.* **7**, 41673 (2017).

16. Bustos, S., Gomez, C., Hausmann, R. & Hidalgo, C. A. The dynamics of nestedness predicts the evolution of industrial ecosystems. *PLoS One* **7**, e49393 (2012).

17. Ulrich, W., Almeida-Neto, M. & Gotelli, N. J. A consumer's guide to nestedness analysis. *Oikos* **118**, 3–17 (2009).

18. Ulrich, W. & Gotelli, N. J. Null model analysis of species nestedness patterns. *Ecology* **88**, 1824–1831 (2007).

19. Strona, G., Ulrich, W. & Gotelli, N. J. Bi-dimensional null model analysis of presence-absence binary matrices. *Ecology* **99**, 103–115 (2018).

20. Almeida-Neto, M. & Ulrich, W. A straightforward computational approach for measuring nestedness using quantitative matrices. *Environ. Model. Softw.* **26**, 173–178 (2011).

21. Pinheiro, R. B. P., Félix, G. M. F., Dormann, C. F. & Marco, A. R. A new model explaining the origin of different topologies in interaction networks. *bioRxiv* 1–30 (2018). doi:10.1101/362871

22. Staniczenko, P. P. A., Kopp, J. C. & Allesina, S. The ghost of nestedness in ecological networks. *Nat. Commun.* **4**, 1391 (2013).

23. Watts, S., Dormann, C. F., Martín González, A. M. & Ollerton, J. The influence of floral traits on specialization and modularity of plant–pollinator networks in a biodiversity hotspot in the Peruvian Andes. *Ann. Bot.* **118**, 415–429 (2016).

24. Scotti, M., Podani, J. & Jordán, F. Weighting, scale dependence and indirect effects in ecological networks: A comparative study. *Ecol. Complex.* **4**, 148–159 (2007).

25. Banašek-Richter, C., Cattin, M.-F. & Bersier, L.-F. Sampling effects and the robustness of quantitative and qualitative food-web descriptors. *J. Theor. Biol.* **226**, 23–32 (2004).

26. Barabási, A. L. *Network Science*. (Cambridge University Press, 2016).

27. Dormann, C. F., Fründ, J. & Schaefer, H. M. Identifying causes of patterns in ecological networks: opportunities and limitations. *Annu. Rev. Ecol. Evol. Syst.* **48**, 559–584 (2017).

28. Rodriguez-Girones, M. A. & Santamaria, L. A new algorithm to calculate the nestedness temperature of presence-absence matrices. *J. Biogeogr.* **33**, 924–935 (2006).

29. Blüthgen, N., Menzel, F. & Blüthgen, N. Measuring specialization in species interaction networks. *BMC Ecol.* **6**, 9 (2006).

30. Almeida-Neto, M., Guimarães, P., Guimarães, P. R., Loyola, R. D. & Ulrich, W. A consistent metric for nestedness analysis in ecological systems: reconciling concept and measurement. *Oikos* **117**, 1227–1239 (2008).

31. Poisot, T. & Gravel, D. When is an ecological network complex? Connectance drives degree distribution and emerging network properties. *PeerJ* **2**, e251 (2014).

32. Gotelli, N. J. Null model analysis of species co-occurrence patterns. *Ecology* **81**, 2606–2621 (2000).

33. Dormann, C. F., Gruber, B. & Fründ, J. Introducing the bipartite package: analysing ecological networks. *R News* **8**, 8–11 (2008).

34. Dormann, C. F. & Blüthgen, N. Food webs versus interaction networks: principles, pitfalls, and perspectives. in *Adaptive Food Webs* 9–18 (Cambridge University Press, 2017). doi:10.1017/9781316871867.003

35. Corso, G. & Britton, N. F. Nestedness and τ-temperature in ecological networks. *Ecol. Complex.* **11**, 137–143 (2012).

36. Baselga, A. Partitioning the turnover and nestedness components of beta diversity. *Glob. Ecol. Biogeogr.* **19**, 134–143 (2010).

37. Kaiser-Bunbury, C. N., Muff, S., Memmott, J., Müller, C. B. & Caflisch, A. The robustness of pollination networks to the loss of species and interactions: a quantitative approach incorporating pollinator behaviour. *Ecol. Lett.* **13**, 442–452 (2010).

38. Jonhson, S., Domínguez-García, V. & Muñoz, M. A. Factors determining nestedness in complex networks. *PLoS One* **8**, e74025 (2013).

39. Borrás, C. P., Hernández, L. & Moreno, Y. Breaking the spell of nestedness. *arXiv* 1–17 (2017). doi:10.1101/216564

40. Vizentin-Bugoni, J., Maruyama, P. K. & Sazima, M. Processes entangling interactions in communities: forbidden links are more important than abundance in a hummingbird-plant network. *Proc. R. Soc. B Biol. Sci.* **281**, 20132397–20132397 (2014).

41. Pinheiro, R. B. P. *et al.* Trade-offs and resource breadth processes as drivers of performance and specificity in a host–parasite system: a new integrative hypothesis. *Int. J. Parasitol.* **46**, 115–121 (2016).

42. Minoarivelo, H. O. & Hui, C. Trait-mediated interaction leads to structural emergence in mutualistic networks. *Evol. Ecol.* **30**, 105–121 (2016).

43. Thebault, E. & Fontaine, C. Stability of ecological communities and the architecture of mutualistic and trophic networks. *Science (80-.).* **329**, 853–856 (2010).

44. Flores, C. O., Meyer, J. R., Valverde, S., Farr, L. & Weitz, J. S. Statistical structure of host-phage interactions. *Proc. Natl. Acad. Sci.* **108**, E288–E297 (2011).

45. Flores, C. O., Valverde, S. & Weitz, J. S. Multi-scale structure and geographic drivers of cross-infection within marine bacteria and phages. *ISME J.* **7**, 520–532 (2013).

46. Mello, M. A. R. *et al.* Insights on the assembly rules of a continent-wide multilayer network. *bioRxiv* (2018). doi:10.1101/452565

47. Ings, T. C. *et al.* Ecological networks - Beyond food webs. *J. Anim. Ecol.* **78**, 253–269 (2009).

48. Fründ, J., McCann, K. S. & Williams, N. M. Sampling bias is a challenge for quantifying specialization and network structure: lessons from a quantitative niche model. *Oikos* **125**, 502–513 (2016).

49. Fortuna, M. A. *et al.* Nestedness versus modularity in ecological networks: two sides of the same coin? *J. Anim. Ecol.* **79**, 811–817 (2010).

50. Felix, G. M., Pinheiro, R. B. P., Poulin, R., Krasnov, B. R. & Mello, M. A. R. The compound topology of a continent-wide interaction network explained by an integrative hypothesis of specialization. *bioRxiv* (2017). doi:10.1101/236687

CONCLUSÃO GERAL

A principal conclusão que tiramos a partir dos resultados apresentados na presente tese é que processos ecológicos e evolutivos atuando no nível das espécies e guiando as interações entre elas, são capazes de produzir as principais topologias encontradas em redes de interações ecológicas observadas no mundo real. Assim, não se fazem necessárias explicações mais complexas, como as que envolvem seleção por estabilidade no nível da rede, para entender a prevalência de tais topologias em sistemas naturais.

Esta conclusão destaca a importância de desvendarmos as regras que controlam as interações entre espécies. Isso nos permite avançar da descrição e detecção de padrões, para a compreensão dos seus mecanismos subjacentes. Essa é uma percepção que ganhou momento na ecologia na última década, propiciando o desenvolvimento de variados modelos de redes ecológicas que simulam mecanismos ecológicos e evolutivos, em contraste com as tradicionais abordagens puramente fenomenológicas.

O modelo da hipótese integradora da especialização (IHS) se mostrou muito eficiente, produzindo uma grande variedade de padrões a partir de um mecanismo simples baseado em três pressupostos, e do ajuste de cinco parâmetros. Nosso modelo tem uma configuração minimalista, simulando somente a evolução dos consumidores sem incluir explicitamente a evolução dos recursos ou a coevolução entre consumidores e recursos. É notável que, ainda assim, ele seja capaz de reproduzir topologias aninhadas, modulares e compostas, o que confirma o potencial da IHS para explicar padrões em redes de interações.

Os resultados dessa tese contradizem a noção de que o aninhamento e a modularidade são topologias equivalentes. Tanto as redes produzidas pelo modelo IHS, quanto a argumentação desenvolvida no segundo capítulo, inequivocamente apontam para os dois padrões como conflitantes e com causas distintas. Enquanto o aninhamento emerge em redes sem preferências, a partir de desigualdades nas frequências totais de interações das espécies; a modularidade demanda fortes preferências, as quais resultam de *trade-offs* adaptativos enfrentados pelas espécies no processo evolutivo. Em uma rede modular, porém, o aninhamento ainda pode prevalecer internamente aos módulos, formando uma topologia composta. Nesse caso, os padrões conflitantes e seus processos generativos não se anulam, mas predominam em diferentes níveis hierárquicos.

Por fim, a emergência de topologias compostas, os resultados do modelo IHS e a discussão teórica desenvolvida, predizem uma forte influência da diversidade taxonômica, filogenética e funcional das espécies incluídas em uma rede de interações ecológicas sobre os padrões topológicos observados. Redes contendo somente espécies similares não apresentam os padrões encontrados em redes mais diversas, assim como módulos não reproduzem a topologia de uma rede completa. Isso nos leva a refletir sobre boa parte das redes analisadas na literatura dos últimos 20 anos, que são fortemente enviesadas para um táxon (por exemplo, redes de dispersão de sementes formadas apenas por aves). No futuro, deveríamos estudar um maior número de redes empíricos multi-táxon, como feito em poucos trabalhos até o momento.

MATERIAIS SUPLEMENTARES DO CAPÍTULO 1

A NEW MODEL EXPLAINING THE ORIGIN OF DIFFERENT TOPOLOGIES IN INTERACTION NETWORKS

Appendix S1. An example of one iteration of the IHS model.

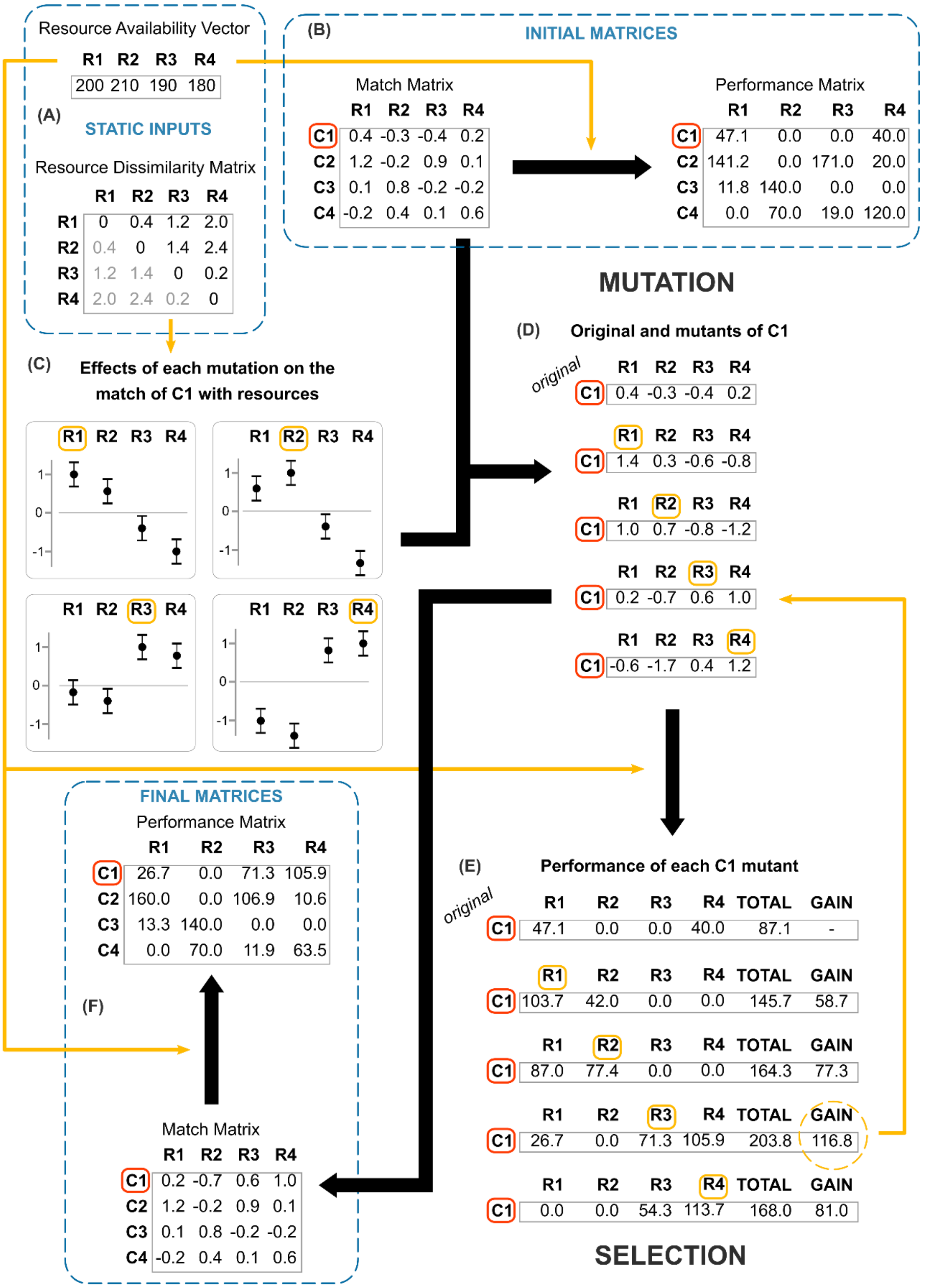
Appendix S2. Full report of statistical analysis.

Appendix S3. Weighted nestedness based on overlap and decreasing abundance (WNODA).

Appendix S4. Modularity emergence without resource dissimilarity discontinuities.

Appendix S1. An example of one iteration of the IHS model.

Rafael Barros Pereira Pinheiro, Gabriel Moreira Félix Ferreira, Carsten F. Dormann, Marco Aurelio Ribeiro Mello. A new model explaining the origin of different topologies in interaction networks.



Resource Availability Vector

R1	R2	R3	R4
200	210	190	180

Resource Dissimilarity Matrix

	R1	R2	R3	R4
R1	0	0.4	1.2	2.0
R2	0.4	0	1.4	2.4
R3	1.2	1.4	0	0.2
R4	2.0	2.4	0.2	0

Match Matrix

	R1	R2	R3	R4
C1	0.4	-0.3	-0.4	0.2
C2	1.2	-0.2	0.9	0.1
C3	0.1	0.8	-0.2	-0.2
C4	-0.2	0.4	0.1	0.6

Performance Matrix

	R1	R2	R3	R4
C1	47.1	0.0	0.0	40.0
C2	141.2	0.0	171.0	20.0
C3	11.8	140.0	0.0	0.0
C4	0.0	70.0	19.0	120.0

	R1	R2	R3	R4
C1	0.4	-0.3	-0.4	0.2

	R1	R2	R3	R4
C1	1.4	0.3	-0.6	-0.8

	R1	R2	R3	R4
C1	1.0	0.7	-0.8	-1.2

	R1	R2	R3	R4
C1	0.2	-0.7	0.6	1.0

	R1	R2	R3	R4
C1	-0.6	-1.7	0.4	1.2

	R1	R2	R3	R4	TOTAL	GAIN
C1	47.1	0.0	0.0	40.0	87.1	-

	R1	R2	R3	R4	TOTAL	GAIN
C1	103.7	42.0	0.0	0.0	145.7	58.7

	R1	R2	R3	R4	TOTAL	GAIN
C1	87.0	77.4	0.0	0.0	164.3	77.3

	R1	R2	R3	R4	TOTAL	GAIN
C1	26.7	0.0	71.3	105.9	203.8	116.8

	R1	R2	R3	R4	TOTAL	GAIN
C1	0.0	0.0	54.3	113.7	168.0	81.0

Performance Matrix

	R1	R2	R3	R4
C1	26.7	0.0	71.3	105.9
C2	160.0	0.0	106.9	10.6
C3	13.3	140.0	0.0	0.0
C4	0.0	70.0	11.9	63.5

Match Matrix

	R1	R2	R3	R4
C1	0.2	-0.7	0.6	1.0
C2	1.2	-0.2	0.9	0.1
C3	0.1	0.8	-0.2	-0.2
C4	-0.2	0.4	0.1	0.6

Figure S1. An example of one iteration of the IHS model. To start, each iteration requires the availability of each resource species (A), the pairwise dissimilarity between them (A), and the match matrix (B). We can also calculate the initial performance of each consumer in exploiting each resource. At the beginning of the iteration, a consumer is randomly assigned to evolve: C1. Then C1 is submitted to 4 different mutations each one focused on a resource (yellow squares).

In (C) we show the means (dots) and the standard deviations (arrows) of the normal distributions from which the effect of each mutation on the match between C1 and each resource is drawn. For simplicity here, we will take the mean value of each normal distributions. Then, the new matches of C1 mutants with each resource is exactly the original values, plus the effects of the respective mutation (D). After defining the matches of each mutant with resources, we calculate their performances. The total performance of the mutants and the original C1 (without mutations) is compared and the one with the higher value is selected (E), in this example: the mutant whose mutation was focused in R3. For last, the selected mutant replaces the original C1 (F). Then, if this is an intermediate iteration, the new match matrix goes for the next round. If this is the last iteration, the performance matrix is calculated and returned as the simulated network.

Appendix S2. Full report of statistical analysis

Rafael Barros Pereira Pinheiro, Gabriel Moreira Felix Ferreira, Carsten F. Dormann, Marco Aurelio Ribeiro Mello. A new model explaining the origin of different topologies in interaction networks.

Section S1. Preliminary simulations: evolution of network structure during simulations

Rationale of the analysis

To better understand the evolution of consumer-resource network structures during simulations of the IHS model, we ran preliminary simulations with varied parameter values and measured network metrics, not only on the final simulated networks but also in intermediary rounds of the model.

In this analysis, we aimed at answering three main questions: First, do the network structures follow a general trend during simulations regardless of the parameter values? If so, that would represent a flaw of the model, as the outputs would reflect more the number of iterations in each simulation than the parameters. For instance, if connectance always increases (or decreases) during the simulations, regardless of the parameter values, comparing the connectance of simulated networks would only reflect differences on the number of iterations and, maybe, on the speed of network structure evolution between them. Second, do the network structures tend to stabilize during the simulations? And, third, how many iterations are necessary to capture this tendency?

Here, we performed 40 simulations with varied parameter values (20 setups, 2 simulations with each setup). As summaries of network structure, we calculated connectance, nestedness, modularity, and H2’. For each simulation, the number of iterations was consumer richness times 100, and we measured network metrics 100 times during the simulation. We also evaluated the initial matrices, however, when the initial matrix is all0 or all1, it is not possible to calculate most of the network metrics on the initial matrix, as it is, respectively, completely empty or completely filled and homogeneous.

Results are presented in AppendixS2: Fig. S1-S2.

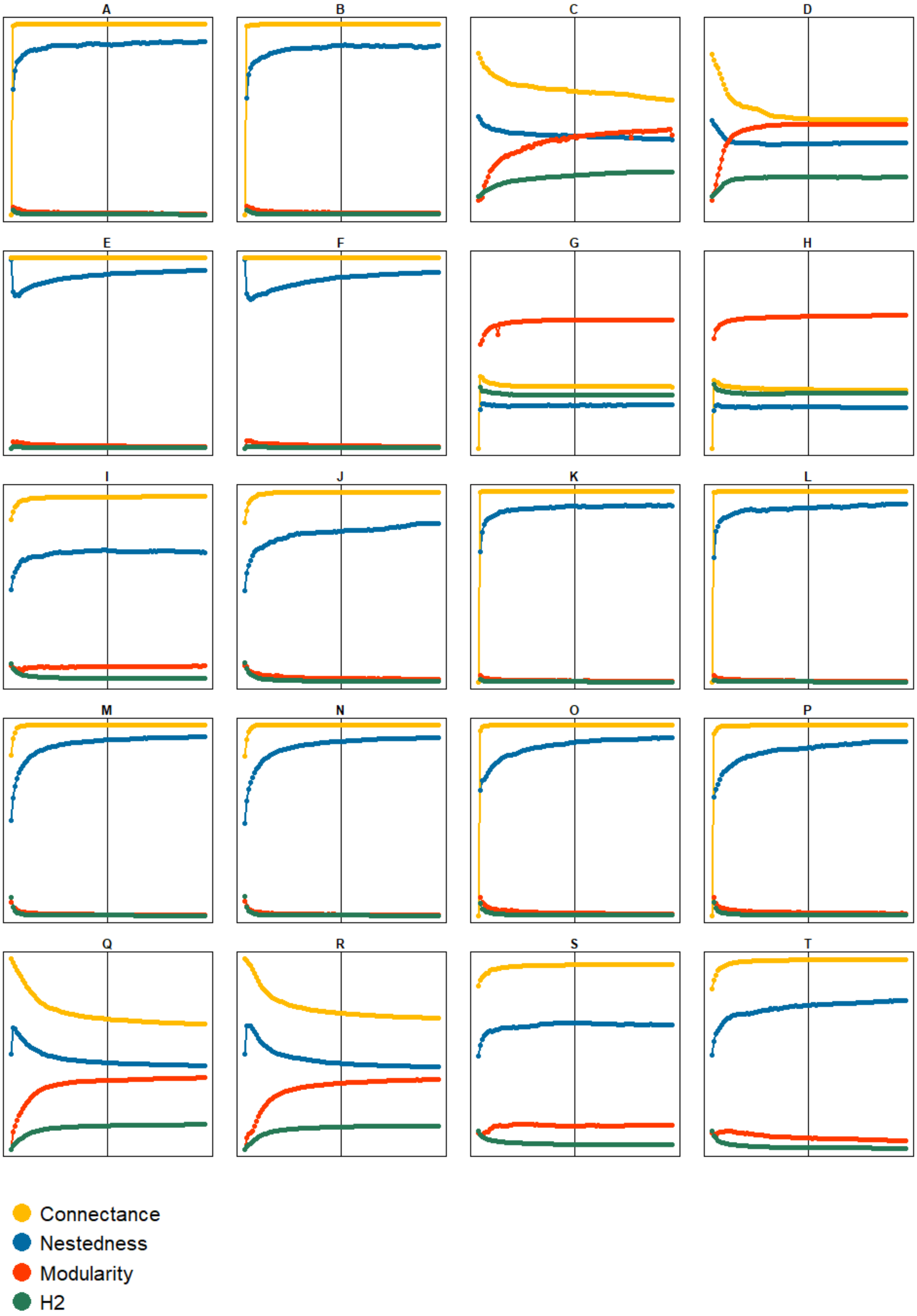


Figure S1. Evolution of network structures in the course of the simulations. Plots show that network structures follow no unique trend in all simulations, but depends on the parameter values. Also, there is an evident stabilization of the network during simulations. For most of the simulations, the topology is fully established with the number of iterations used to generate the simulated networks of our study (consumer richness times 50, vertical line on plots). The vertical axis goes from 0 to 1 and presents the metric values. The horizontal axis goes from 0 to the number of iterations performed in each simulation (consumer richness times 100). Network metrics were measured 100 times for each simulation. Parameter values for simulations in the figure: A-B: *maxdis*= 1, *initial_matrix*= all0, *nclust*= 1, *Sres*= 50, *Scon*= 50. C-D: *maxdis*= 3, *initial_matrix*= rnorm, *nclust*= 2, *Sres*= 100, *Scon*= 50. E-F: *maxdis*= 1.5, *initial_matrix*= all1, *nclust*= 1, *Sres*= 100, *Scon*= 10. G-H: *maxdis*= 2.5, *initial_matrix*= all0, *nclust*= 4, *Sres*= 100, *Scon*= 100. I-J: *maxdis*= 2, *initial_matrix*= rnorm, *nclust*= 1, *Sres*= 50, *Scon*= 50. K-L: *maxdis*= 0.5, *initial_matrix*= all0, *nclust*= 2, *Sres*= 50, *Scon*= 50. M-N: *maxdis*= 0.5, *initial_matrix*= rnorm, *nclust*= 1, *Sres*= 100, *Scon*= 50. O-P: *maxdis*= 1.5, *initial_matrix*= all0, *nclust*= 1, *Sres*= 50, *Scon*= 10. Q-R: *maxdis*= 2.5, *initial_matrix*= all1, *nclust*= 2, *Sres*= 100, *Scon*= 100. S-T: *maxdis*= 1.5, *initial_matrix*= rnorm, *nclust*= 4, *Sres*= 50, *Scon*= 50.

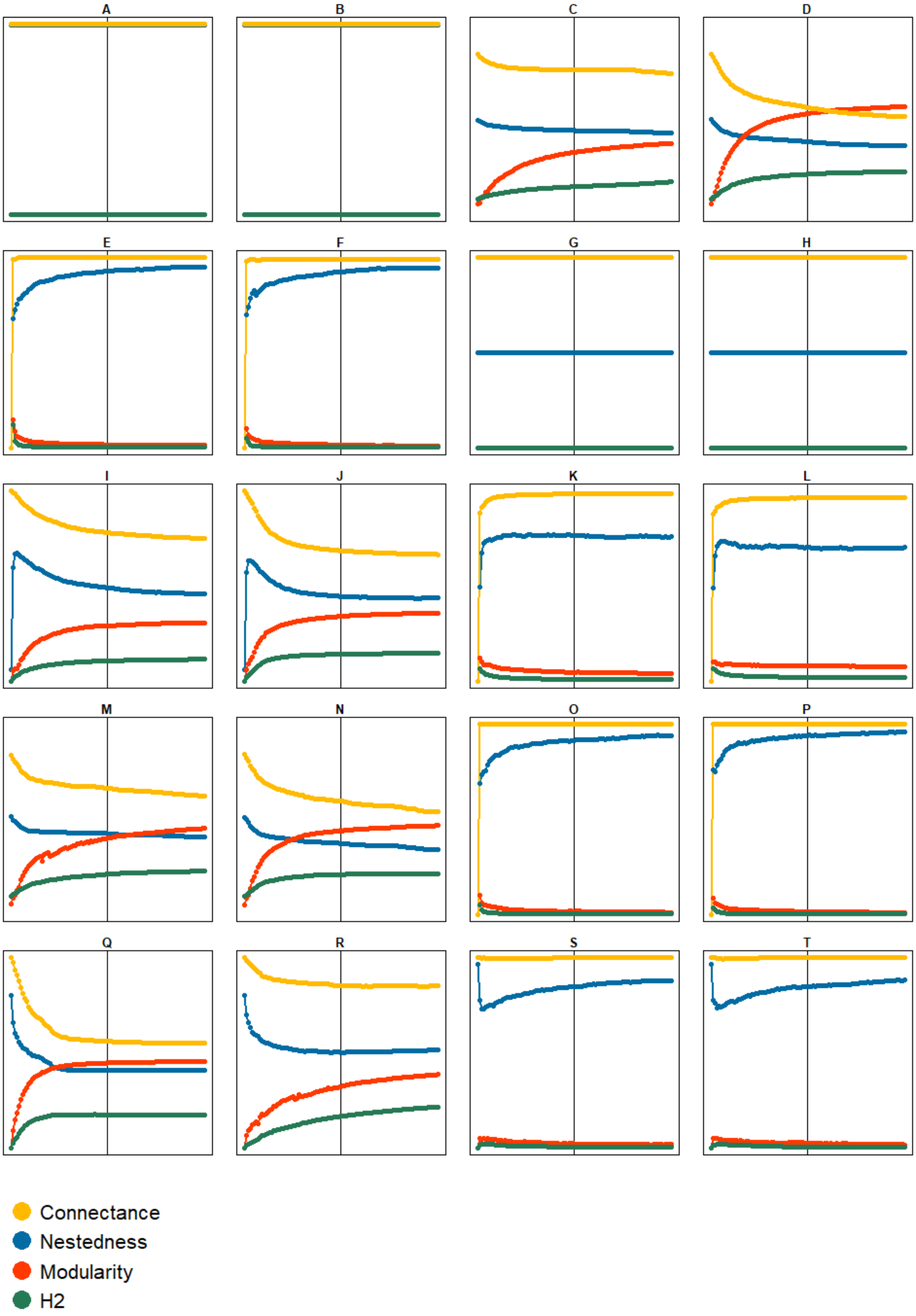


Figure S2. Evolution of network structures in the course of the simulations. Plots show that network structures follow no unique trend in all simulations, but depends on the parameter values. Also, there is an evident stabilization of the network during simulations. For most of the simulations, the topology is fully established with the number of iterations used to generate the simulated networks of our study (consumer richness times 50, vertical line on plots). The vertical axis goes from 0 to 1 and presents the metric values. The horizontal axis goes from 0 to the number of iterations performed in each simulation (consumer richness times 100). Network metrics were measured 100 times for each simulation. Parameter values for simulations in the figure: A-B: *maxdis*= 4, *initial_matrix*= all1, *nclust*= 1, *Sres*= 200, *Scon*= 10. C-D: *maxdis*= 2.5, *initial_matrix*= rnorm, *nclust*= 4, *Sres*= 200, *Scon*= 100. E-F: *maxdis*= 1, *initial_matrix*= all0, *nclust*= 2, *Sres*= 100, *Scon*= 5. G-H: *maxdis*= 3.5, *initial_matrix*= all1, *nclust*= 2, *Sres*= 50, *Scon*= 50. I-J: *maxdis*= 2.5, *initial_matrix*= all1, *nclust*= 2, *Sres*= 50, *Scon*= 200. K-L: *maxdis*= 2, *initial_matrix*= all0, *nclust*= 1, *Sres*= 50, *Scon*= 100. M-N: *maxdis*= 3, *initial_matrix*= rnorm, *nclust*= 2, *Sres*= 200, *Scon*= 50. O-P: *maxdis*= 1, *initial_matrix*= all0, *nclust*= 1, *Sres*= 50, *Scon*= 5. Q-R: *maxdis*= 3, *initial_matrix*= all1, *nclust*= 2, *Sres*= 100, *Scon*= 50. S-T: *maxdis*= 1.5, *initial_matrix*= all1, *nclust*= 4, *Sres*= 50, *Scon*= 10.

Summary of results and brief discussion

The results presented in Appendix S2: Fig. S1-S2 answer the questions that boosted this preliminary analysis. First, does the network topology follow a general trend during simulations regardless of the parameter values? No. The direction of change, increasing or decreasing, varied for all measured metrics among the tested simulations. For instance, connectance in Fig. S2Q is initially 1 and decreases to around 0.55. Although, in Fig. S2L, connectance follows an opposite tendency, going from 0 to 0.97. For last, in Fig. S2S connectance changes much less during the iterations.

Second, the consumer-resource networks tend to stabilize during the simulations? Yes. There is a clear tendency of stabilization in all the simulations. For some simulations, the values of network metrics are almost unchanged since the first iterations, while, for other, the values change gradually towards an asymptote. The time required to stabilization seems to depend on the difference between the initial network (defined by the initial matrix), and the stable state, given the others parameters.

And, third, how many iterations are required to capture this tendency? There is a great variation, but for most of the simulations, consumer richness times 50 are enough to result in a fully stabilized network structure, or at least for network metrics to show an asymptotic tendency.

Section S2. Proportion of iterations in which occurred evolutionary changes

Rationale of the analysis

For each simulation we calculated the proportion of iterations in which occurred evolutionary changes. For some simulations, the proportion was very low (or even 0), and, therefore, the final innate and realized matrices were highly similar (or identical) to the initial matrices.

Here, we used GLMs to test whether the parameter values affected the proportion of iterations in which occurred evolutionary changes. This analysis is not directly related to the hypothesis tested in our study, but it may provide us a better understanding on the behavior of the model.

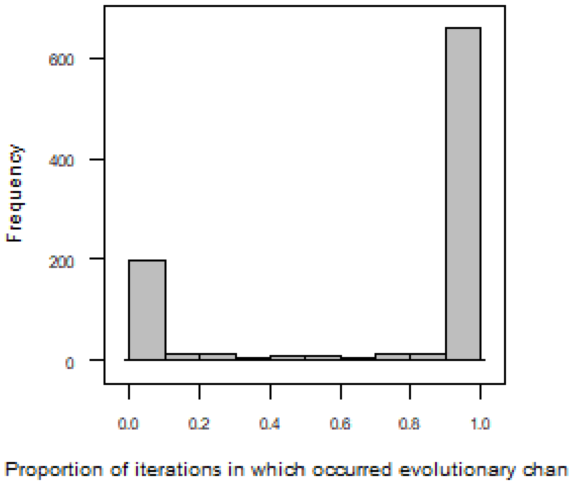


Figure S3. Histogram for the proportion of iterations in which occurred evolutionary changes. Absolute frequencies on vertical axis. There were several simulations in which did not occur evolutionary change at all. However, in most of the simulations, the proportion is higher than 90%.

Model

Method: Generalized Linear Model

Family: Quasibinomial

Link function: Logit

Response variable: Proportion of iterations in which occurred evolutionary changes

Explanatory variables on the full model: 1- Maximum dissimilarity (maxdis), 2- Initial matrix (initial_matrix), 3- Number of clusters (nclust), 4- Resource richness (Sres), 5- Consumer richness (Scon), 6- Interaction (variables 1 and 2), 7- Interaction (variables 1 and 3), 8- Interaction (variables 2 and 3), 9- Interaction (variables 1, 2, and 3)

N: 945

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			944	963.52		
maxdis	1	406.93	943	556.60	3954.22	0.0000
initial_matrix	2	332.23	941	224.36	1614.21	0.0000
nclust	2	135.85	939	88.51	660.05	0.0000
Sres	1	1.84	938	86.67	17.91	0.0000
Scon	1	3.20	937	83.46	31.11	0.0000
maxdis:initial_matrix	2	10.86	935	72.61	52.74	0.0000
maxdis:nclust	2	3.29	933	69.32	15.98	0.0000
initial_matrix:nclust	4	5.76	929	63.56	13.99	0.0000
maxdis:initial_matrix:nclust	4	1.19	925	62.37	2.89	0.0214

All explanatory variables were statistically significant. We maintained the full model.

Estimates on the minimum model

	Estimates
(Intercept)	11.4934
maxdis	-1.8449
initial_matrixall1	12.3411
initial_matrixrnorm	11.4521
nclust2	2.6454
nclust4	-3.1549
Sres	0.0046
Scon	0.0053
maxdis:initial_matrixall1	-5.7594
maxdis:initial_matrixrnorm	-5.2539
maxdis:nclust2	-1.2317
maxdis:nclust4	-0.0090
initial_matrixall1:nclust2	0.2227
initial_matrixrnorm:nclust2	-3.5935
initial_matrixall1:nclust4	4.9183
initial_matrixrnorm:nclust4	4.9543
maxdis:initial_matrixall1:nclust2	-0.4309
maxdis:initial_matrixrnorm:nclust2	1.0634
maxdis:initial_matrixall1:nclust4	-3.5226
maxdis:initial_matrixrnorm:nclust4	-3.4413

Plots

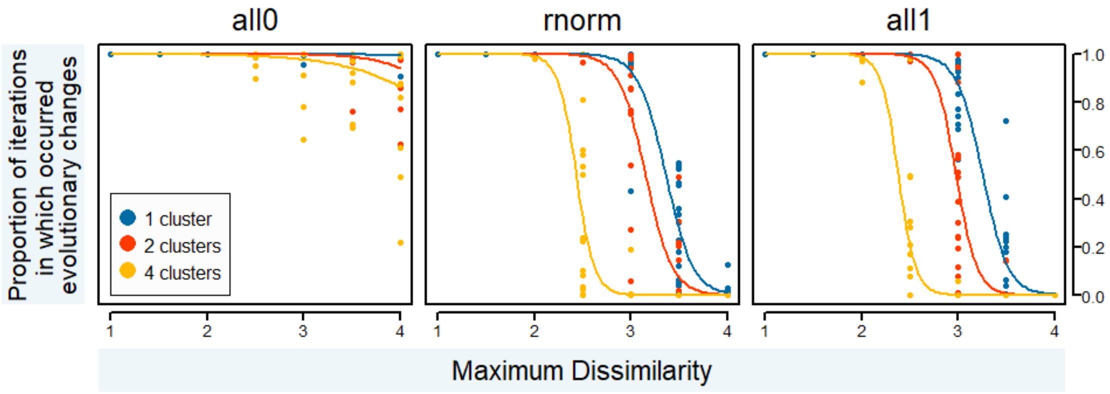


Figure S4. Proportion of iterations in which occurred evolutionary changes as a function of maximum dissimilarity (horizontal axis), number of clusters (colors), and initial matrix (plots). Average values of consumer and resource richness were used to draw the curves.

Summary of results and brief discussion

The proportion of iterations in which occurred evolutionary changes is negatively related to maximum dissimilarity and number of clusters. Also, it tends to be lower in simulations with initial matrix all1 and rnorm. Besides consumer and resource richness are statistically significant explanatory variables, they have very weak effects. For a consumer, when the adaptive trade-off on different resources is to strong, an increase in the performance on one resource leads to a large decrease in the performance on other resources. Thus, if a consumer starts the simulation already having performance on several resources, as in the initial matrixs all1 and rnorm, it might be advantageous to avoid these costs by not changing. This cannot occur in simulations with the initial matrix all0. Since the initial performance of consumers is 0, any mutation will result in benefit to the consumer and one of those mutations will inevitably be selected. However, it is possible that, after the first iterations, the system stabilizes, with each consumer’s niche already defined, and then a similar situation may occur.

Important observations

We removed the simulations in which evolutionary changes occurred in less than 80% of iterations from the pool of simulated networks. There remained 672 simulations.

Section S3. Connectance

Rationale of the analysis

Connectance is the number of non-zero cells in a matrix, divided by its total size (the number of rows times the number of columns). In an interaction matrix, connectance represents the proportion of possible interactions that are effectively made. We used GLMs to test whether model parameters affected the connectance of the simulated network.

Model

Method: Generalized Linear Model

Family: Quasibinomial

Link function: Logit

Response variable: Connectance

Explanatory variables on the full model: 1- Maximum dissimilarity (*maxdis*), 2- Initial matrix (*initial_matrix*), 3- Number of clusters (*nclust*), 4- Resource richness (*Sres*), 5- Consumer richness (*Scon*), 6- Interaction (variables 1 and 2), 7- Interaction (variables 1 and 3), 8- Interaction (variables 2 and 3), 9- Interaction (variables 1, 2, and 3)

N: 672

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			671	316.81		
maxdis	1	237.89	670	78.92	4289.24	0.0000
initial_matrix	2	2.46	668	76.46	22.15	0.0000
nclust	2	21.53	666	54.93	194.12	0.0000
Sres	1	1.32	665	53.61	23.84	0.0000
Scon	1	0.29	664	53.32	5.22	0.0227
maxdis:initial_matrix	2	9.48	662	43.84	85.43	0.0000
maxdis:nclust	2	0.14	660	43.70	1.28	0.2787
initial_matrix:nclust	4	2.41	656	41.29	10.85	0.0000
maxdis:initial_matrix:nclust	4	1.00	652	40.29	4.52	0.0013

All explanatory variables were statistically significant. We maintained the full model.

Estimates on the minimum model

	Estimates
(Intercept)	5.5476
maxdis	-1.7770
initial_matrixall1	4.6038
initial_matrixrnorm	4.3120
nclust2	-0.2681
nclust4	-1.3613
Sres	0.0024
Scon	-0.0008
maxdis:initial_matrixall1	-1.6473
maxdis:initial_matrixrnorm	-1.5639
maxdis:nclust2	0.0303
maxdis:nclust4	0.0335
initial_matrixall1:nclust2	0.0170
initial_matrixrnorm:nclust2	-1.2003
initial_matrixall1:nclust4	3.2436
initial_matrixrnorm:nclust4	0.6957
maxdis:initial_matrixall1:nclust2	-0.1937
maxdis:initial_matrixrnorm:nclust2	0.3773
maxdis:initial_matrixall1:nclust4	-2.2291
maxdis:initial_matrixrnorm:nclust4	-0.8049

Plots

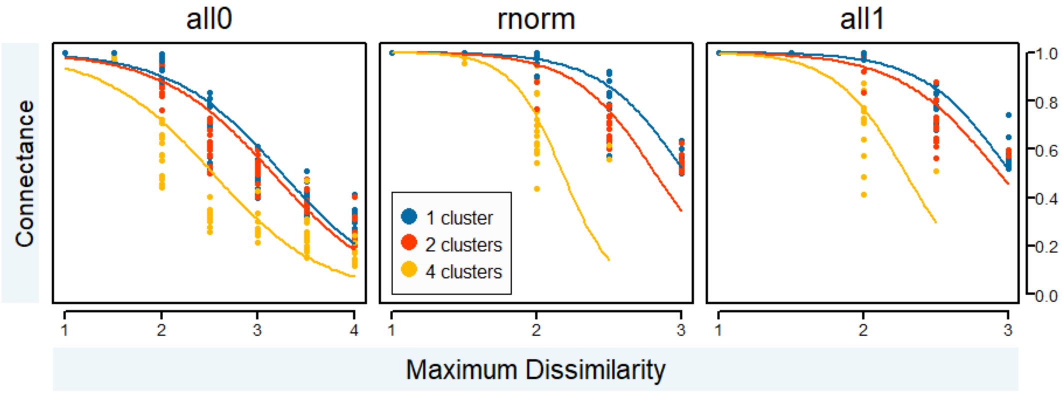


Figure S5. Connectance of simulated networks as a function of maximum dissimilarity (horizontal axis), number of clusters (colors), and initial matrix (plots). Average values of consumer and resource richness were used to draw the curves.

Summary of results:

As expected, maximum dissimilarity is the major factor that explains connectance in our simulated networks, followed by the number of clusters. Both variables are related to resource heterogeneity. Resource richness and consumer richness had statistically significant but very weak effects.

Section S4. H2’

Rationale of the analysis

H2’ is a network-level specialization index, appropriated to weighted matrices (Bluthgen 2006). The higher the value of H2’, the more specialized the network. In our simulations, the H2’ of the simulated networks varied from <0.001 to 0.79. We used GLMs to test whether and how parameter values affected the H2’ of the simulated networks.

Model

Method: Generalized Linear Model
Family: Quasibinomial
Link function: Logit
Response variable: H2’
Explanatory variables on the full model: 1- Maximum dissimilarity (*maxdis*), 2- Initial matrix (*initial_matrix*), 3- Number of clusters (*nclust*), 4- Resource richness (*Sres*), 5- Consumer richness (*Scon*), 6- Interaction (variables 1 and 2), 7- Interaction (variables 1 and 3), 8- Interaction (variables 2 and 3), 9- Interaction (variables 1, 2, and 3)
N: 672

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			671	185.55		
maxdis	1	125.26	670	60.29	2968.29	0.0000
initial_matrix	2	1.23	668	59.06	14.53	0.0000
nclust	2	9.63	666	49.43	114.12	0.0000
Sres	1	1.10	665	48.33	26.06	0.0000
Scon	1	9.04	664	39.29	214.28	0.0000
maxdis:initial_matrix	2	7.03	662	32.26	83.29	0.0000
maxdis:nclust	2	0.82	660	31.45	9.67	0.0001
initial_matrix:nclust	4	1.16	656	30.29	6.88	0.0000
maxdis:initial_matrix:nclust	4	0.67	652	29.62	3.96	0.0035

All explanatory variables were statistically significant. We maintained the full model.

Estimates on the minimum model

	Estimates
(Intercept)	-4.9128
maxdis	1.4451
initial_matrixall1	-4.4251
initial_matrixrnorm	-3.8790
nclust2	0.0685
nclust4	1.5573
Sres	-0.0024
Scon	-0.0057
maxdis:initial_matrixall1	1.6251
maxdis:initial_matrixrnorm	1.4185
maxdis:nclust2	-0.0043
maxdis:nclust4	-0.2235
initial_matrixall1:nclust2	0.8889
initial_matrixrnorm:nclust2	1.1742
initial_matrixall1:nclust4	-1.7120
initial_matrixrnorm:nclust4	-0.9103
maxdis:initial_matrixall1:nclust2	-0.2388
maxdis:initial_matrixrnorm:nclust2	-0.3535
maxdis:initial_matrixall1:nclust4	1.3664
maxdis:initial_matrixrnorm:nclust4	0.8247

Plots

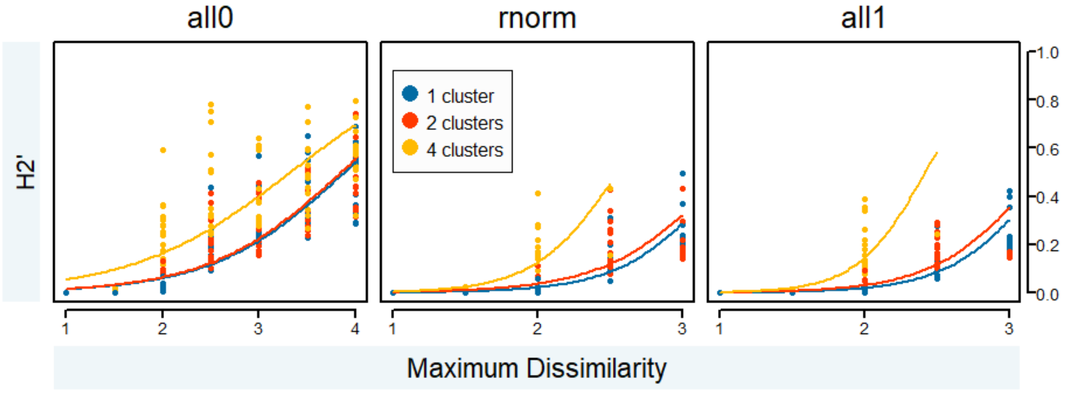


Figure S6. H2' (frequency-based specialization index) of simulated networks as a function of maximum dissimilarity (horizontal axis), number of clusters (colors), and initial matrix (plots). Average values of consumer and resource richness were used to draw the curves.

Summary of results:

Maximum dissimilarity is the major simulation parameter affecting H2' of the simulated networks. As expected, the greater the difference between resources, the greater the specialization of the network. The number of clusters, consumer richness and the interaction between maximum dissimilarity and initial matrix have weak but non-trivial explanatory powers on the model. The other variables have minor effects.

Section S5. Modularity

Rationale of the analysis

We used the DIRTLPAwb+ algorithm (Beckett 2016) to detect modules and to compute modularity in the simulated networks. Then we used GLMs to test which simulation parameters affected the modularity values.

Model

Method: Generalized Linear Model
Family: Quasibinomial
Link function: Logit
Response variable: Modularity
Explanatory variables on the full model: 1- Maximum dissimilarity (*maxdis*), 2- Initial matrix (*initial_matrix*), 3- Number of clusters (*nclust*), 4- Resource richness (*Sres*), 5- Consumer richness (*Scon*), 6- Interaction (variables 1 and 2), 7- Interaction (variables 1 and 3), 8- Interaction (variables 2 and 3), 9- Interaction (variables 1, 2, and 3)
N: 672

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			671	252.25		
maxdis	1	185.13	670	67.12	3656.33	0.0000
initial_matrix	2	1.17	668	65.95	11.60	0.0000
nclust	2	17.65	666	48.30	174.32	0.0000
Sres	1	1.00	665	47.30	19.72	0.0000
Scon	1	0.15	664	47.15	2.87	0.0907
maxdis:initial_matrix	2	9.58	662	37.57	94.58	0.0000
maxdis:nclust	2	0.30	660	37.27	2.97	0.0519
initial_matrix:nclust	4	1.58	656	35.69	7.82	0.0000
maxdis:initial_matrix:nclust	4	1.17	652	34.52	5.76	0.0001

We removed the variable Consumer richness (Scon). Then we tested the new model (Model 2) against the full model using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Full model	652	34.52				
Model 2	653	34.64	-1	-0.12	2.35	0.1259

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			671	252.25		
maxdis	1	185.13	670	67.12	3647.44	0.0000
initial_matrix	2	1.17	668	65.95	11.57	0.0000
nclust	2	17.65	666	48.30	173.89	0.0000
Sres	1	1.00	665	47.30	19.67	0.0000
maxdis:initial_matrix	2	9.64	663	37.65	95.01	0.0000
maxdis:nclust	2	0.30	661	37.36	2.92	0.0545
initial_matrix:nclust	4	1.57	657	35.78	7.74	0.0000
maxdis:initial_matrix:nclust	4	1.14	653	34.64	5.62	0.0002

Estimates on the minimum model

	Estimates
(Intercept)	-4.6302
maxdis	1.4652
initial_matrixall1	-3.1656
initial_matrixrnorm	-2.7115
nclust2	0.5613
nclust4	1.2109
Sres	-0.0019
maxdis:initial_matrixall1	1.1940
maxdis:initial_matrixrnorm	1.0226
maxdis:nclust2	-0.1589
maxdis:nclust4	-0.0531
initial_matrixall1:nclust2	-0.2171
initial_matrixrnorm:nclust2	0.2657
initial_matrixall1:nclust4	-2.5475
initial_matrixrnorm:nclust4	-1.2465
maxdis:initial_matrixall1:nclust2	0.2301
maxdis:initial_matrixrnorm:nclust2	-0.0395
maxdis:initial_matrixall1:nclust4	1.6976
maxdis:initial_matrixrnorm:nclust4	0.9380

Plots

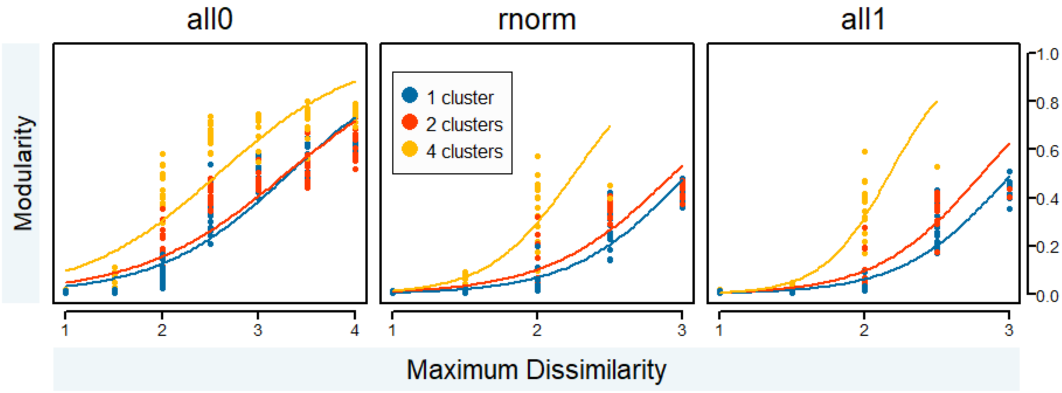


Figure S7. Modularity of simulated networks as a function of maximum dissimilarity (horizontal axis), number of clusters (colors), and initial matrix (plots). The average value of resource richness was used to draw the curves.

Summary of results

Modularity is strongly positively affected by maximum dissimilarity, and in a lesser extent, to the number of clusters. Consumer richness has no effect in modularity. The other variables, besides being statistically significant, have minor effects.

Section S6. Nestedness

Rationale of the analysis

We calculated the WNODA index (Appendix S3) for the simulated networks. To facilitate the analysis, we divided the WNODA by 100, resulting in values between 0 and 1. Then we used GLMs to test which model parameters affected the WNODA of the networks.

Model

Method: Generalized Linear Model

Family: Quasibinomial

Link function: Logit

Response variable: Nestedness (WNODA)

Explanatory variables on the full model: 1- Maximum dissimilarity (*maxdis*), 2- Initial matrix (*initial_matrix*), 3- Number of clusters (*nclust*), 4- Resource richness (*Sres*), 5- Consumer richness (*Scon*), 6- Interaction (variables 1 and 2), 7- Interaction (variables 1 and 3), 8-

Interaction (variables 2 and 3), 9- Interaction (variables 1, 2, and 3)

N: 672

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			671	232.71		
maxdis	1	195.37	670	37.34	6716.37	0.0000
initial_matrix	2	0.61	668	36.74	10.43	0.0000
nclust	2	12.98	666	23.76	223.06	0.0000
Sres	1	1.36	665	22.40	46.67	0.0000
Scon	1	0.85	664	21.55	29.26	0.0000
maxdis:initial_matrix	2	1.56	662	19.99	26.83	0.0000
maxdis:nclust	2	0.46	660	19.53	7.89	0.0004
initial_matrix:nclust	4	0.29	656	19.25	2.46	0.0443
maxdis:initial_matrix:nclust	4	0.45	652	18.80	3.86	0.0041

All explanatory variables were statistically significant. We maintained the full model.

Estimates on the minimum model

	Estimates
(Intercept)	3.5475
maxdis	-1.4116
initial_matrixall1	0.8737
initial_matrixrnorm	0.6438
nclust2	-0.1871
nclust4	-0.5618
Sres	0.0018
Scon	-0.0012
maxdis:initial_matrixall1	-0.3276
maxdis:initial_matrixrnorm	-0.2593
maxdis:nclust2	0.0566
maxdis:nclust4	-0.0987
initial_matrixall1:nclust2	0.0177
initial_matrixrnorm:nclust2	-0.0975
initial_matrixall1:nclust4	0.8356
initial_matrixrnorm:nclust4	0.5926
maxdis:initial_matrixall1:nclust2	-0.0655
maxdis:initial_matrixrnorm:nclust2	0.0255
maxdis:initial_matrixall1:nclust4	-0.6175
maxdis:initial_matrixrnorm:nclust4	-0.4173

Plots

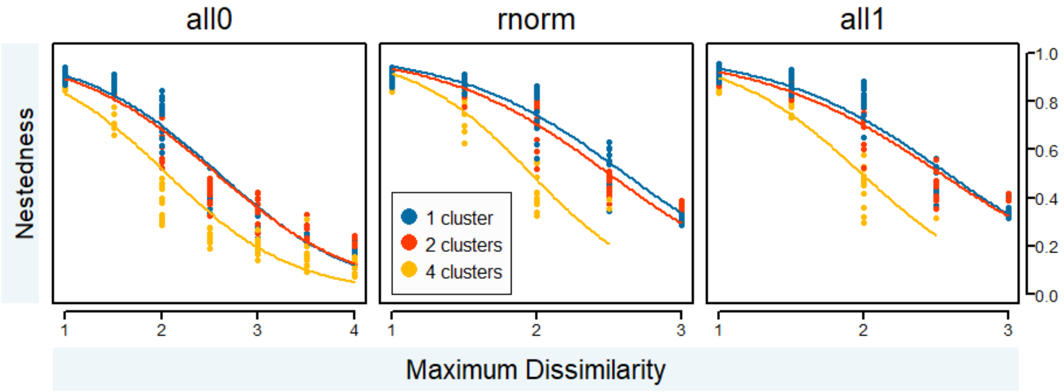


Figure S8. Nestedness (WNODA) of simulated networks as a function of maximum dissimilarity (horizontal axis), number of clusters (colors), and initial matrix (plots). Average values of consumer and resource richness were used to draw the curves.

Summary of results

Nestedness is strongly negatively affected by maximum dissimilarity, and in a lesser extent, to the number of clusters. The other variables, despite being statistically significant, have minor effects.

Section S7. Correlation between nestedness and modularity

Analysis

We tested the Spearman correlation between nestedness and modularity in the simulated networks.

```
##  Spearman's rank correlation rho
##
## data:  WNODA and modularity
## S = 98172000, p-value < 2.2e-16
## alternative hypothesis: true rho is not equal to 0
## sample estimates:
##      rho
## -0.94103
```

As expected, since they are higly driven in opposite directions by the same parameters, we found a very negative correlation.

Plot

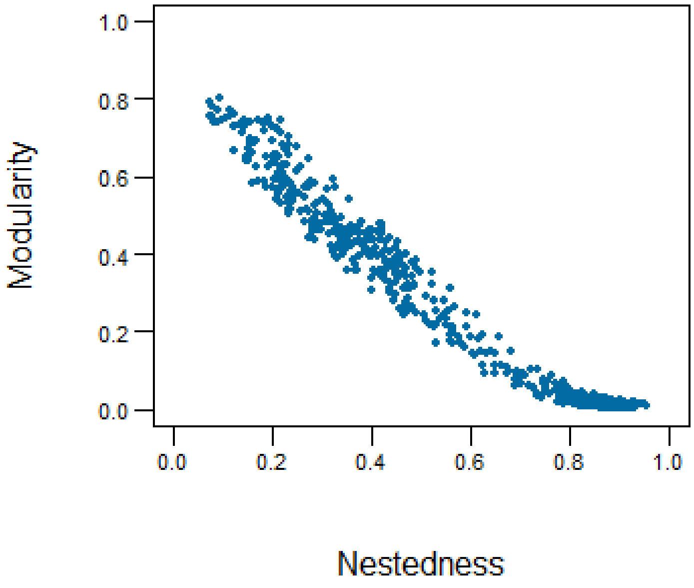


Figure S9. Relationship between modularity and nestedness in the simulated networks.

Section S8. Nestedness between nodes belonging to the same module and nestedness between nodes belonging to different modules

Rationale of the analysis

We calculated the nestedness between nodes belonging to the same module ($\mathrm{WNODA}_{\mathrm{SM}}$) and between nodes belonging to different modules ($\mathrm{WNODA}_{\mathrm{DM}}$) (Appendix S3) for each simulated network. To facilitate the analysis, we divided the values by 100, resulting in values between 0 and 1.

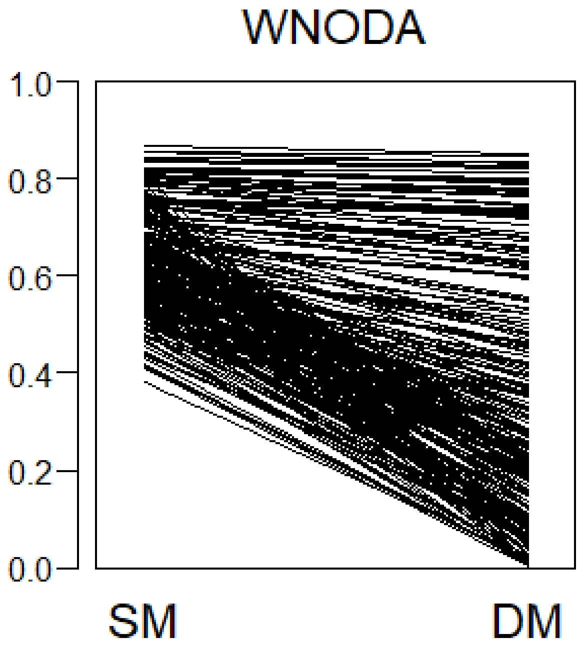


Figure S10. Nestedness (WNODA) between nodes belonging to the same module (SM) and nestedness between nodes belonging to different modules (DM) for each of the 268 modular networks. $WNODA_{DM}$ is usually much lower than $WNODA_{SM}$.

We found that nestedness has a negative relationship with maximum dissimilarity and the number of clusters. To see how each of the components varies as function of these same variables we built GLMs. Then, using the predicted values between $WNODA_{SM}$ and $WNODA_{DM}$ we plot the expected ratio between them as function of maximum dissimilarity and number of clusters.

Nestedness $_{SM}$

Model

Method: Generalized Linear Model
Family: Quasibinomial
Link function: Logit
Response variable: Nestedness between nodes belonging to the same module ($WNODA_{SM}$)
Explanatory variables on the full model: 1- Maximum dissimilarity (*maxdis*), 2- Number of

clusters (*nclust*), 3- Interaction (variables 1 and 2)

N: 268

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			267	12.52		
maxdis	1	6.13	266	6.39	267.65	0.0000
nclust	2	0.15	264	6.25	3.20	0.0422
maxdis:nclust	2	0.10	262	6.15	2.18	0.1149

All explanatory variables were statistically significant. We maintained the full model.

Estimates on the minimum model

	Estimates
(Intercept)	1.7942
maxdis	-0.4812
nclust2	0.1821
nclust4	-0.2015
maxdis:nclust2	-0.0238
maxdis:nclust4	0.1039

Nestedness $_{\text{DM}}$

Model

Method: Generalized Linear Model

Family: Quasibinomial

Link function: Logit

Response variable: Nestedness between nodes belonging to different modules (WNODA-DM)

Explanatory variables on the full model: 1- Maximum dissimilarity (*maxdis*), 2- Number of clusters (*nclust*), 3- Interaction (variables 1 and 2)

N: 268

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			267	82.15		
maxdis	1	53.59	266	28.55	981.97	0
nclust	2	13.65	264	14.90	125.06	0
maxdis:nclust	2	1.90	262	13.00	17.43	0

All explanatory variables were statistically significant. We maintained the full model.

Estimates on the minimum model

	Estimates
(Intercept)	1.7942
maxdis	-0.4812
nclust2	0.1821
nclust4	-0.2015
maxdis:nclust2	-0.0238
maxdis:nclust4	0.1039

Plot

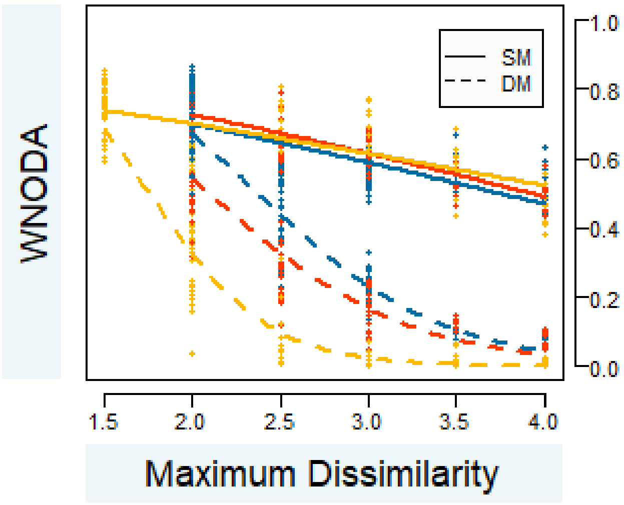


Figure S11. Nestedness (WNODA) between nodes belonging to the same module (SM) and nestedness between nodes belonging to different modules (DM) as functions of maximum dissimilarity (horizontal axis) and number of clusters (colors: blue= 1 cluster, red= 2 clusters, and yellow= 4 clusters).

Predicted ratio between WNODA$_{SM}$ and WNODA$_{DM}$

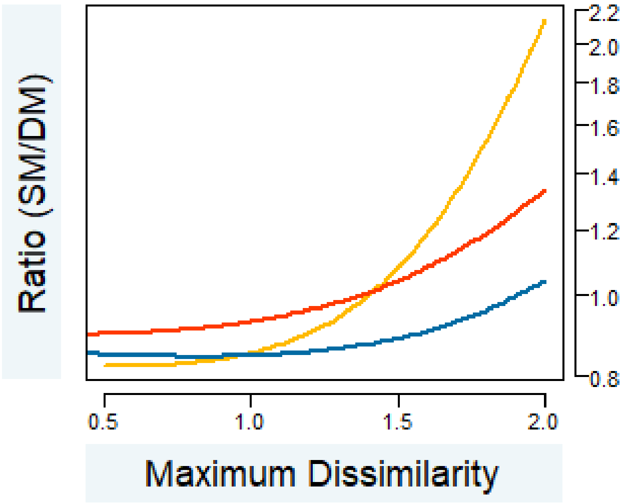


Figure S12. Predicted ratio between nestedness $_{SM}$ and nestedness $_{DM}$ as functions of maximum dissimilarity (horizontal axis) and number of clusters (colors). Ratio was calculated by dividing the GLM predictions for WNODA$_{SM}$ and WNODA$_{DM}$.

Section S9. Network Topologies

Rationale of the analysis

Here, we considered three network topologies: modular, nested, and compound. To categorically define which topology was shown by each simulated network, we used the approach proposed by Felix et al. (2017) based on null model analysis.

First, we tested for nested and modular topologies using free null models (null models that do not conserve the modular structure of the matrix). In the free models, each randomized matrix was generated using a modified version of the method proposed by Vázquez et al. (2007).

Their method creates a null matrix conserving the original connectance and the total number of interactions, and probabilistically conserving the marginal sums. To this end, the algorithm first defines the binary structure of the null matrix, assigning interactions according to probabilities based on the marginal sums of the original matrix. However, to prevent reducing the size of the matrix, the algorithm requires that each species has at least one interaction. After that, the remaining interactions are distributed among the filled cells, following again probabilities based on marginal sums.

This method, however, is not fully adequate for our simulated matrices, as their interaction weights are not counts, but continuous. Therefore, the procedure results in null matrices with very different marginal sums from the original matrix, especially in matrices with many weak interactions. To deal with this, we modified the algorithm so that it does not fill the matrices by distributing unitary interactions (including and summing 1s) but by distributing a smaller value: 0.1.

For each simulated network, we generated a free null model with 500 randomized matrices and performed a Z-test to test whether the observed value of each metric was significantly different from the distribution of values of the null matrices. A network was considered modular when its value of Barber modularity was significantly higher than the randomized values. Similarly, a network was considered nested, when it had a significant WNODA value. To avoid excessively low consumer richness in each module, which would prejudice statistical analysis, we excluded the networks with less than 50 consumer species and kept 415 simulated networks for this and subsequent analysis.

Null model analysis was performed in the Sagarana High-Performance Computing cluster from the High-Performance Processing Center, Institute of Biological Sciences, Federal University of Minas Gerais, Brazil.

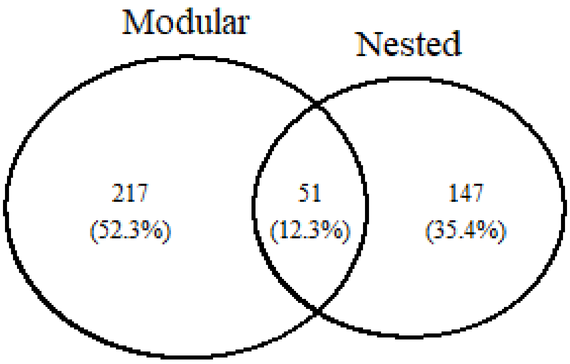


Figure S13. Veen Diagram for the number of simulated networks presenting modular, nested, and both topologies. There was no network not presenting any of those two topologies. Topology was defined by a null model approach using a free null model, following the Vaznull algorithm (available at bipartite package). Number of simulated networks considered: 415.

Then, we used GLMs to test whether the model parameters affects the chance of a network having nested and modular topologies.

Nested networks

Model

Method: Generalized Linear Model

Family: Quasibinomial

Link function: Logit

Response variable: Nested or non-nested (binary variable)

Explanatory variables on the full model: 1- Maximum dissimilarity (*maxdis*), 2- Initial matrix (*initial_matrix*), 3- Number of clusters (*nclust*), 4- Resource richness (*Sres*), 5- Consumer richness (*Scon*), 6- Interaction (variables 1 and 2), 7- Interaction (variables 1 and 3), 8- Interaction (variables 2 and 3), 9- Interaction (variables 1, 2, and 3)

N: 415

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			414	574.44		
maxdis	1	388.36	413	186.09	2719.94	0.0000
initial_matrix	2	2.86	411	183.22	10.02	0.0001
nclust	2	46.59	409	136.64	163.14	0.0000
Sres	1	1.53	408	135.10	10.75	0.0011
Scon	1	46.73	407	88.37	327.30	0.0000
maxdis:initial_matrix	2	4.33	405	84.04	15.17	0.0000
maxdis:nclust	2	6.96	403	77.08	24.39	0.0000
initial_matrix:nclust	4	20.79	399	56.28	36.41	0.0000
maxdis:initial_matrix:nclust	4	0.87	395	55.41	1.53	0.1931

We removed the triple interaction (between variables 1, 2, and 3). Then we tested the new model (Model 2) against the full model using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Full model	395	55.41				
Model 2	399	56.28	-4	-0.87	1.53	0.1931

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			414	574.44		
maxdis	1	388.36	413	186.09	2537.78	0.0000
initial_matrix	2	2.86	411	183.22	9.35	0.0001
nclust	2	46.59	409	136.64	152.22	0.0000
Sres	1	1.53	408	135.10	10.03	0.0017
Scon	1	46.73	407	88.37	305.38	0.0000
maxdis:initial_matrix	2	4.33	405	84.04	14.15	0.0000
maxdis:nclust	2	6.96	403	77.08	22.76	0.0000
initial_matrix:nclust	4	20.79	399	56.28	33.97	0.0000

Estimates on the minimum model

	Estimates
(Intercept)	27.2312
maxdis	-18.1443
initial_matrixall1	171.1757
initial_matrixrnorm	13.4517
nclust2	-11.5511
nclust4	0.9234
Sres	0.0098
Scon	0.0692
maxdis:initial_matrixall1	-74.4046
maxdis:initial_matrixrnorm	-3.9343
maxdis:nclust2	5.8598
maxdis:nclust4	-3.9111
initial_matrixall1:nclust2	-19.8149
initial_matrixrnorm:nclust2	-4.2742
initial_matrixall1:nclust4	-58.4090
initial_matrixrnorm:nclust4	-7.8739

Plots

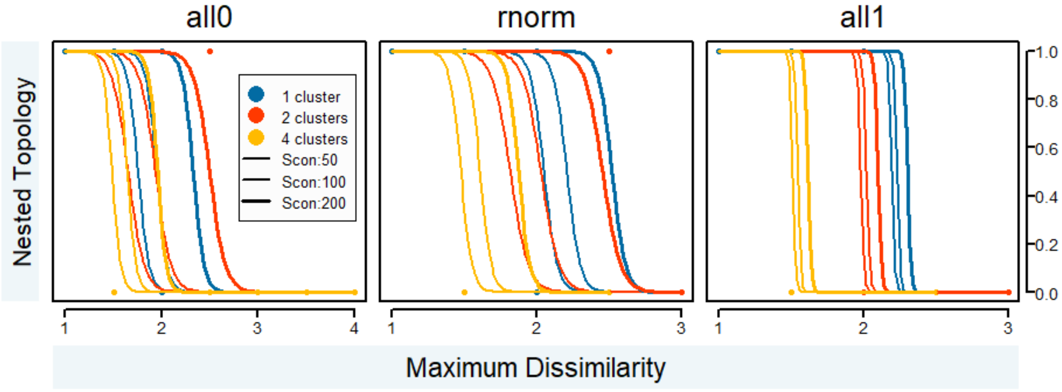


Figure S14. Chance of a simulated networks presenting a nested topology (binary variable) as a function of parameters maximum dissimilarity (horizontal axis), number of clusters (colors), consumer richness (line widths), and initial matrix (plots). The average value of resource richness was used to draw the curves.

Modular networks

Model

Method: Generalized Linear Model

Family: Quasibinomial

Link function: Logit

Response variable: Modular or non-modular (binary variable)

Explanatory variables on the full model: 1- Maximum dissimilarity (*maxdis*), 2- Initial matrix (*initial_matrix*), 3- Number of clusters (*nclust*), 4- Resource richness (*Sres*), 5- Consumer richness (*Scon*), 6- Interaction (variables 1 and 2), 7- Interaction (variables 1 and 3), 8- Interaction (variables 2 and 3), 9- Interaction (variables 1, 2, and 3)

N: 415

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			414	539.51		
maxdis	1	418.60	413	120.91	3624.98	0.0000
initial_matrix	2	0.34	411	120.58	1.46	0.2346
nclust	2	61.03	409	59.55	264.23	0.0000
Sres	1	3.40	408	56.15	29.48	0.0000
Scon	1	2.66	407	53.49	23.06	0.0000
maxdis:initial_matrix	2	3.30	405	50.19	14.28	0.0000
maxdis:nclust	2	0.00	403	50.19	0.00	1.0000
initial_matrix:nclust	4	1.95	399	48.24	4.23	0.0023
maxdis:initial_matrix:nclust	4	0.00	395	48.24	0.00	1.0000

We removed the triple interaction (between variables 1, 2, and 3). Then we tested the new model (Model 2) against the full model using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Full model	395	48.24				
Model 2	399	48.24	-4	0		

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			414	539.51		
maxdis	1	418.60	413	120.91	3661.69	0.0000
initial_matrix	2	0.34	411	120.58	1.47	0.2312
nclust	2	61.03	409	59.55	266.91	0.0000
Sres	1	3.40	408	56.15	29.78	0.0000
Scon	1	2.66	407	53.49	23.29	0.0000
maxdis:initial_matrix	2	3.30	405	50.19	14.43	0.0000
maxdis:nclust	2	0.00	403	50.19	0.00	1.0000
initial_matrix:nclust	4	1.95	399	48.24	4.27	0.0021

We removed the interaction between the variables Maximum dissimilarity and Number of clusters. Then we tested the new model (Model 3) against the old model (Model 2) using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Model 2	399	48.24				
Model 3	401	48.24	-2	0	0	1

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			414	539.51		
maxdis	1	418.60	413	120.91	3680.04	0.0000
initial_matrix	2	0.34	411	120.58	1.48	0.2295
nclust	2	61.03	409	59.55	268.25	0.0000
Sres	1	3.40	408	56.15	29.92	0.0000
Scon	1	2.66	407	53.49	23.41	0.0000
maxdis:initial_matrix	2	3.30	405	50.19	14.50	0.0000
initial_matrix:nclust	4	1.95	401	48.24	4.29	0.0021

Estimates on the minimum model

	Estimates
(Intercept)	-142.7717
maxdis	82.9170
initial_matrixall1	-26.7035
initial_matrixrnorm	47.5277
nclust2	0.0000
nclust4	21.5650
Sres	-0.0108
Scon	-0.0094
maxdis:initial_matrixall1	3.7301
maxdis:initial_matrixrnorm	-32.9231
initial_matrixall1:nclust2	20.2145
initial_matrixrnorm:nclust2	0.0000
initial_matrixall1:nclust4	21.1084
initial_matrixrnorm:nclust4	2.5071

Plots

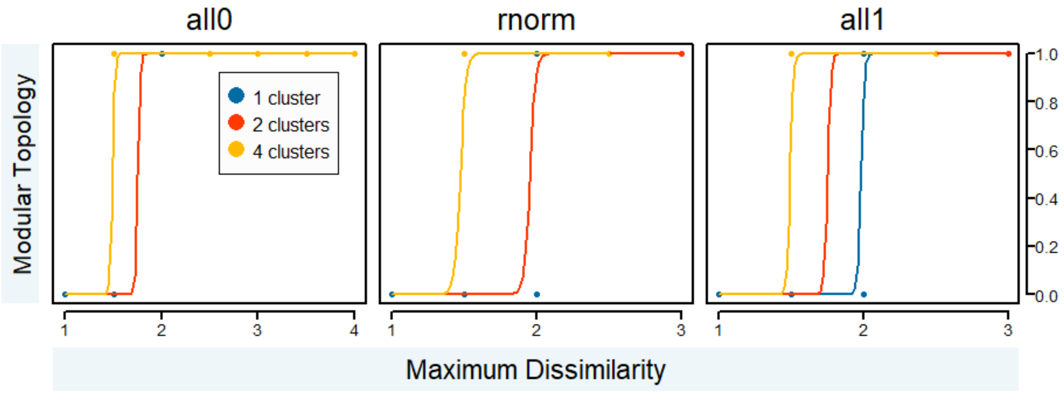


Figure S15. Chance of a simulated networks presenting a modular topology (binary variable) as a function of maximum dissimilarity (horizontal axis), number of clusters (colors), and initial matrix (plots). Average values of consumer and resource richness were used to draw the curves.

Compound topology

A network was considered as having a compound topology, when it was significantly modular and presented a significant $\mathrm{WNODA_{SM}}$ (i.e., a modular network with modules internally nested). To test the significance of $\mathrm{WNODA_{SM}}$ in each simulated network we used restricted null models (Felix et al. 2017). A restricted null model is one that conserves the modular structure of the matrix when generating the randomized matrices. As, by definition, nodes in the same modules overlap more than nodes in different modules, not conserving the modular structure of the randomized matrix (i.e., using a free null model) would result in an inflated type I error ratio for $\mathrm{WNODA_{SM}}$.

Of the 268 modular networks, 142 (53%) presented a compound topology. Then, we used GLMs to test whether the model parameters affects the chance of a modular network presenting a compound topology.

Model

Method: Generalized Linear Model
Family: Quasibinomial
Link function: Logit
Response variable: Compound or non-compound (binary variable)
Explanatory variables on the full model: 1- Maximum dissimilarity (*maxdis*), 2- Initial matrix (*initial_matrix*), 3- Number of clusters (*nclust*), 4- Resource richness (*Sres*), 5- Consumer richness (*Scon*), 6- Interaction (variables 1 and 2), 7- Interaction (variables 1 and 3), 8- Interaction (variables 2 and 3), 9- Interaction (variables 1, 2, and 3)
N: 268

Variance analysis and model reduction

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			267	370.57		
maxdis	1	54.98	266	315.59	54.51	0.0000
initial_matrix	2	0.98	264	314.61	0.49	0.6150
nclust	2	2.90	262	311.71	1.44	0.2392
Sres	1	0.09	261	311.61	0.09	0.7612
Scon	1	123.18	260	188.44	122.13	0.0000
maxdis:initial_matrix	2	0.20	258	188.23	0.10	0.9046
maxdis:nclust	2	0.50	256	187.74	0.25	0.7808
initial_matrix:nclust	4	2.21	252	185.52	0.55	0.7007
maxdis:initial_matrix:nclust	4	4.60	248	180.92	1.14	0.3380

We removed all the interactions between explanatory variables. Then we tested the new model (Model 2) against the full model using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Full model	248	180.92				
Model 2	260	188.44	-12	-7.51	0.62	0.8239

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			267	370.57		
maxdis	1	54.98	266	315.59	56.70	0.0000
initial_matrix	2	0.98	264	314.61	0.51	0.6031
nclust	2	2.90	262	311.71	1.50	0.2258
Sres	1	0.09	261	311.61	0.10	0.7565
Scon	1	123.18	260	188.44	127.04	0.0000

We removed the variable Resource richness (*Sres*) and tested the new model (Model 3) against the old model (Model 2) using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Model 2	260	188.44				
Model 3	261	188.44	-1	0	0	0.9765

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			267	370.57		
maxdis	1	54.98	266	315.59	56.83	0.0000
initial_matrix	2	0.98	264	314.61	0.51	0.6024
nclust	2	2.90	262	311.71	1.50	0.2251
Scon	1	123.27	261	188.44	127.43	0.0000

We removed the variable Initial matrix (*initial_matrix*) and tested the new model (Model 4) against the old model (Model 3) using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Model 3	261	188.44				
Model 4	263	190.81	-2	-2.37	1.23	0.2954

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			267	370.57		
maxdis	1	54.98	266	315.59	56.74	0.0000
nclust	2	2.03	264	313.56	1.05	0.3526
Scon	1	122.76	263	190.81	126.69	0.0000

We removed the variable Number of clusters (*nclust*) and tested the new model (Model 5) against the old model (Model 4) using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Model 4	263	190.81				
Model 5	265	195.35	-2	-4.54	2.34	0.0981

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			267	370.57		
maxdis	1	54.98	266	315.59	59.81	0
Scon	1	120.24	265	195.35	130.82	0

Estimates on the minimum model

	Estimates
(Intercept)	3.4925
maxdis	-2.7650
Scon	0.0357

Plots

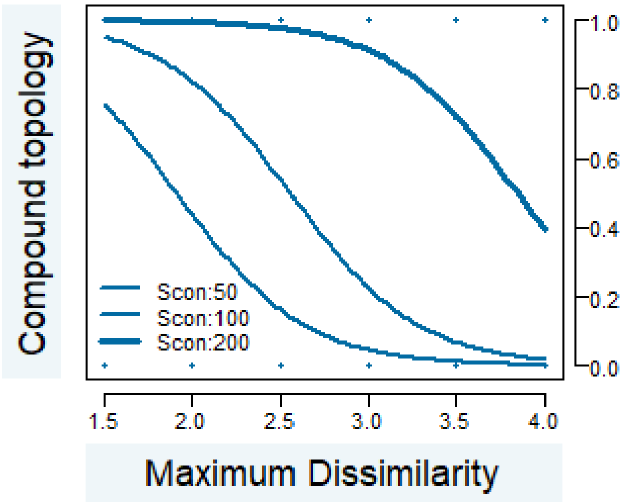


Figure S16. Chance of a modular simulated networks presenting a compound topology (binary variable) as a function of maximum dissimilarity (horizontal axis) and consumer richness (line widths). Compound topologies were detected by using restricted null models: null models that conserves the modular structure in the randomized matrices. Only modular networks were used in this analysis (n=268).

Consumer richness and nestedness significance

Consumer richness had minor effects on nestedness (WNODA) values, but moderate effects on the chance that a network was detected as nested. Similarly, it affected the chance of a modular network being detected as having a compound topology. These results may indicate that, rather than affecting the emergence of nestedness, consumer richness affects it detection.

To check this possible bias, we plotted nestedness (WNODA) and nestedness between species in the same module (WNODA$_{SM}$) as function of consumer richness, and distinghished networks with significative and non-significative nestedness (Figure S17). Indeed, higher nestedness is necessary for a smaller network to be considered nested, and so, despite consumer richness not affecting the nestedness value of a network, it affected whether these values are significative.

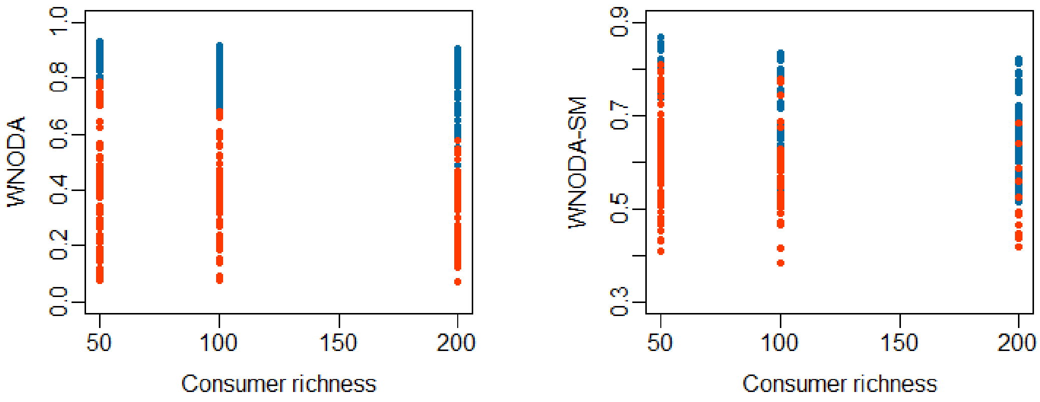


Figure S17. Consumer richness affects the detection of significative nestedness and significative nestedness SM in simulated networks. For a same value of nestedness, larger networks are more likely detected as significantly nested. Blue dots: significative nestedness; red dots: non-significative nestedness. Analysis for nested topologies (WNODA) were conducted only in simulated networks with at least 50 consumers (n=415). Analysis for compound topologies (modular networks with significative WNODA SM) were conducted only in the modular simulated networks (n=268).

Section S10. Relationship between performance and generalism of consumers

Rationale of the analysis

For each consumer in each network, we calculated its mean performance, the average of the consumer's performance on all its resources. We also calculated two generalism indices: 1) basic generalism, the richness of resources exploited by it, and 2) structural generalism, the diversity of resources exploited by it, measured by Shannon index. Then we calculated the Spearman correlations between performance and generalism indices, in each network. For last, we built GAMs to test whether simulations parameters explains the relationship between consumers' performance and generalism. **Important observation**: It is not possible to calculate correlations using basic generalism in completely filled matrices, since values are equal for all consumers.

Performance *vs.* basic generalism

Model

Method: Generalized Additive Model
Family: Gaussian
Link function: Identity
Response variable: Correlation between performance and basic generalism
Explanatory variables on the maximum model: Parametric terms: 1- Initial matrix (*initial_matrix*), 2- Number of clusters (*nclust*), 3- Resource richness (*Sres*), 4- Consumer richness (*Scon*); Smooth terms: 5- Maximum dissimilarity (*maxdis*)
N: 437

Variance analysis and model reduction

	df	F	p-value
initial_matrix	2	1.18	0.3085
nclust	2	24.23	0.0000
Sres	1	9.59	0.0021
Scon	1	14.50	0.0002

	edf	Ref.df	F	p-value
s(maxdis)	3.55	3.89	62.72	0

We removed the variable Initial matrix (*initial_matrix*). Then we tested the new model (Model 2) against the full model using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Full model	426.11	37.64				
Model 2	428.10	37.83	-1.99	-0.19	1.06	0.3455

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	df	F	p-value
nclust	2	23.36	0.0000
Sres	1	9.34	0.0024
Scon	1	14.91	0.0001

	edf	Ref.df	F	p-value
s(maxdis)	3.58	3.9	65.69	0

```
## [1] "Deviance Explained: 0.4"

## [1] "R-sq.(adj): 0.39"
```

Estimates on the minimum model

	Estimates
(Intercept)	-0.3879
nclust2	-0.1385
nclust4	-0.2555
Sres	0.0007
Scon	-0.0008
s(maxdis).1	-0.2492
s(maxdis).2	0.0257
s(maxdis).3	-0.3144
s(maxdis).4	-0.4268

Plot

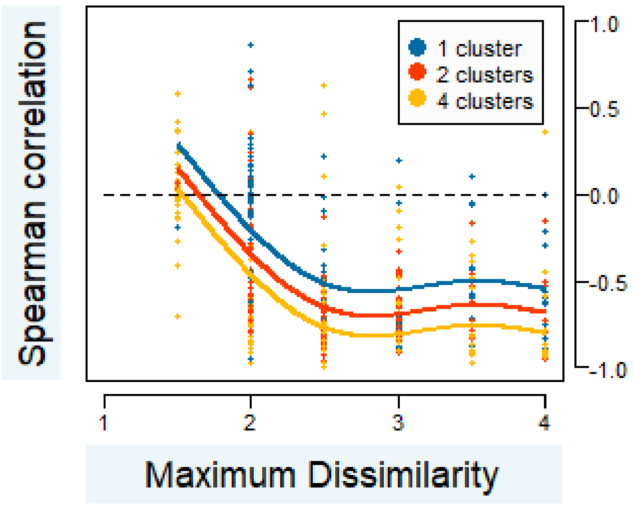


Figure S18. Relationship between consumers' mean performance and basic generalism in each simulated network (measured by Spearman correlations) as a function of maximum dissimilarity (horizontal axis) and number of clusters (colors). Average values of consumer and resource richness were used to draw the curves.

Performance *vs.* structural generalism

Model

Method: Generalized Additive Model
Family: Gaussian
Link function: Identity
Response variable: Correlation between mean performance and structural generalism
Explanatory variables on the maximum model: Parametric terms: 1- Initial matrix (*initial_matrix*), 2- Number of clusters (*nclust*), 3- Resource richness (*Sres*), 4- Consumer richness (*Scon*); Smooth terms: 5- Maximum dissimilarity (*maxdis*)
N: 672

Variance analysis and model reduction

	df	F	p-value
initial_matrix	2	0.39	0.6795
nclust	2	8.44	0.0002
Sres	1	26.09	0.0000
Scon	1	7.55	0.0062

	edf	Ref.df	F	p-value
s(maxdis)	3.97	4	174.17	0

We removed the variable Initial matrix (*initial_matrix*). Then we tested the new model (Model 2) against the full model using ANOVA.

	Resid. Df	Resid. Dev	Df	Deviance	F	Pr(>F)
Full model	661	69.84				
Model 2	663	69.92	-2	-0.08	0.39	0.677

There was no significant difference in the deviance explained by the two models. We maintained the reduced model.

	df	F	p-value
nclust	2	8.63	0.0002
Sres	1	26.11	0.0000
Scon	1	7.50	0.0063

	edf	Ref.df	F	p-value
s(maxdis)	3.97	4	190.2	0

```
## [1] "Deviance Explained: 0.55"

## [1] "R-sq.(adj): 0.54"
```

Estimates on the minimum model

	Estimates
(Intercept)	-0.2160
nclust2	-0.0944
nclust4	-0.1212
Sres	0.0010
Scon	-0.0005
s(maxdis).1	-0.5446
s(maxdis).2	-1.2471
s(maxdis).3	0.9505
s(maxdis).4	-0.0543

Plot

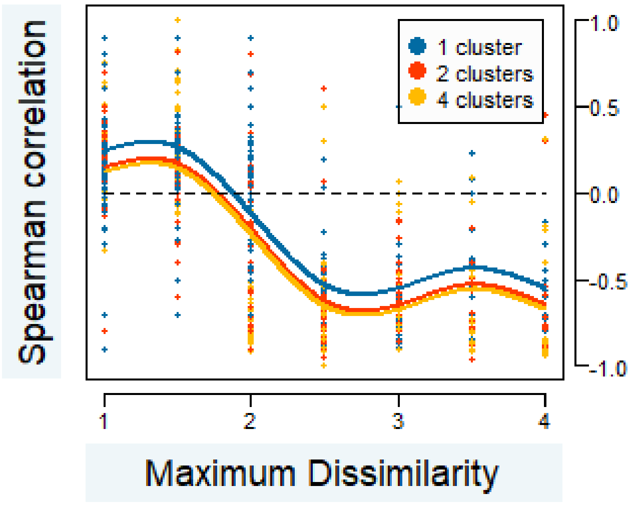


Figure S19. Relationship between consumers' mean performance and structural generalism in each simulated network (measured by Spearman correlations) as a function of maximum dissimilarity (horizontal axis) and number of clusters (colors). Average values of consumer and resource richness were used to draw the curves.

Section S11. Relationship between performance and between-modules generalism of consumers

Rationale of the analysis

In each one of the 268 modular networks, we calculated the the participation coefficient (P) (Guimera & Nunes Amaral 2005) for all consumers. P is a measure of how much the consumer’s links are distributed between different modules; therefore, it represents between-module generalism.

We also developed a weighted version of P. Instead of accounting for the distribution of links, the weighted P measures the distribution of weights between modules.

Then, we calculated Spearman correlations between consumers’ mean performances and between-module generalism (for both binary and weighted P). Following the IHS predictions, we would expect correlations to be mostly negative.

Results

In most of the modular networks, the performance of consumers has a negative relationship with between-module generalism (P): 75% of the networks for the binary metric and 84% for the weighted metric.

The following figures present the density of such correlations for the binary and weighted P.

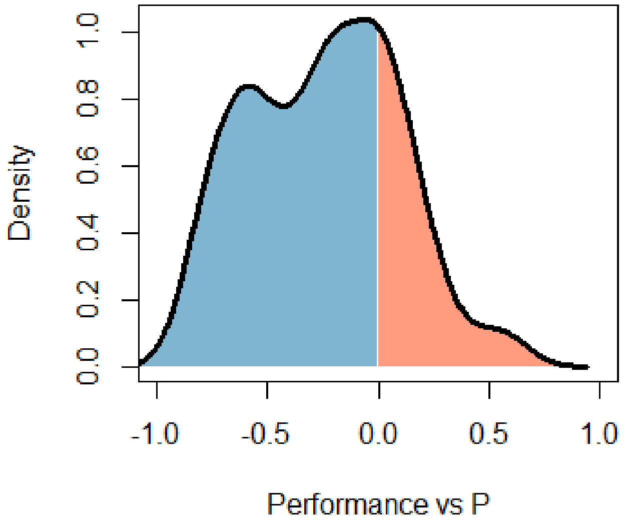


Figure S20 Density plot for the Spearman correlations between performance and the participation coefficient (P) of consumers in modular networks. As expected, most correlations are negative.

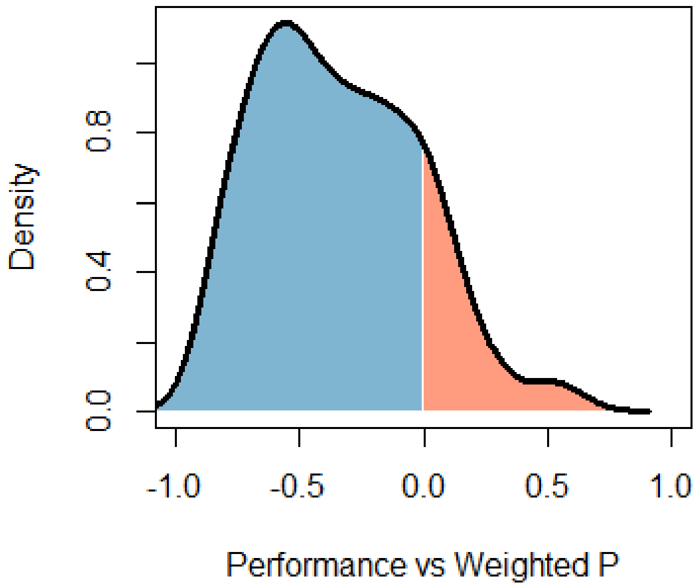


Figure S21. Density plot for the Spearman correlations between performance and the weighted participation coefficient (WP) of consumers in modular networks. As expected, most correlations are negative.

Appendix S3. Weighted nestedness based on overlap and decreasing abundance (WNODA).

Rafael Barros Pereira Pinheiro, Gabriel Moreira Félix Ferreira, Carsten F. Dormann, Marco Aurelio Ribeiro Mello. A new model explaining the origin of different topologies in interaction networks.

NODF

NODF (nestedness based on overlap and decreasing fill) is one of the most popular metrics for calculating nestedness in binary bipartite networks (Almeida-Neto et al. 2008). NODF is calculated by averaging values of N, a score calculated for each pairwise comparison between columns or between rows. To calculate N for columns, each column is compared against all columns to its left on the matrix. If the right column has higher or equal degree than the left column, N is 0. However, if the right column has a lower degree, N is the pairwise overlap (PO). Pairwise overlap is defined as the percentage of 1's in the right columns that are also present in the same position on the left column. To calculate N for rows, each row is compared against all rows above it, using the same logic. By averaging values of N it is possible to calculate NODF for columns, for rows, and for the entire matrix.

One important detail is that NODF depends on the order of rows and columns in the matrix. If the matrix is sorted by decreasing rows and columns degrees before the procedure, so that rows with higher degrees are in the top of the matrix and columns with higher degrees are in the left, the value of NODF is maximized: NODF_{MAX} (Beckett et al. 2014). This is the most common procedure for calculating NODF, and it is almost always done this way, even when not explicitly indicated.

WNODF

WNODF (weighted nestedness based on overlap and decreasing fill) is a weighted version of NODF (Almeida-Neto and Ulrich 2011). WNODF is based on the averaging of N values that are calculated through pairwise comparisons of columns and rows, as well as NODF. WNODF is also based on binary decreasing fill, so when the right column (or the down row) in the comparison has equal or higher binary degree, N = 0. However, when the right column (or the down row) has lower degree in the comparison, N is defined as the percentage of non-zero elements in the right column (or the down row) that have lower values than its correspondents in the left column (or in the top row) (i.e., weighted pairwise overlap).

To maximize WNODF, the matrix must be sorted by decreasing binary degree in the same way that maximizes NODF.

WNODA

WNODA (weighted nestedness based on overlap and decreasing abundance) is a new metric that we created to estimate the nestedness of weighted bipartite networks. Similarly, as NODF and WNODF, WNODA is calculated by averaging scores (N) calculated by pairwise comparison of rows and of columns. To calculate N, in each pairwise comparison, first we check whether there is decreasing abundance by comparing the marginal totals (MT), and then we calculate the weighted pairwise overlap.

For each pair of columns *i* and *j*, in which j is a column at right of *i*, if MT_j is higher or equal to MT_i, N = 0 (i.e., there is no decreasing abundance). However, if MT_j is lower than MT_i, N is the weighted pairwise overlap. As well as in WNODF, the weighted pairwise overlap is defined as the percentage of non-zero elements in *j* that have lower values than its correspondent on *i*. N for rows is calculated using this same logic (with *j* being a row bellow *i*). WNODA is the mean of N values and can be calculated for columns, rows, and the entire matrix.

WNODA depends on matrix order. To maximize WNODA, rows and columns must be sorted by decreasing marginal totals, so that rows and columns with higher summed weights are in the top left corner of the matrix. WNODA varies from 0 (perfectly non-nested) to 100 (perfectly nested).

Comparing NODF, WNODF, and WNODA

To help understand the differences between WNODA, WNODF, and NODF, we provide some examples. In those examples, matrices presented are organized by decreasing marginal totals, but when calculating NODF and WNODF they were reorganized to maximize the index, as previously explained. For simplicity, we will only analyze the nestedness of columns, but all arguments presented are equally valid for rows and the entire matrix.

EXAMPLE I

	C1	**C2**	**C3**	**C4**
R1	100	90	80	70
R2	90	80	70	60
R3	80	70	60	50
R4	70	60	50	40
R5	60	50	40	30
R6	50	40	30	20
R7	40	30	20	10
R8	30	20	10	5

$NODF_{col} = 0$
$WNODF_{col} = 0$
$WNODA_{col} = 100$

In this case, we have a completely filled matrix, i.e., all rows interact with all columns. As a result, there is no binary decreasing fill, and therefore, $NODF_{col}$ and $WNODF_{col}$ are equal to 0. However, since there is decreasing abundance and the weights of the columns with lesser marginal totals are always a lesser value than the correspondent weights in the columns with greater marginal total, $WNODA_{col}$ is 100.

EXAMPLE II

	C1	**C2**	**C3**	**C4**
R1	100	90	80	70
R2	90	80	70	60
R3	80	70	60	50
R4	70	60	50	40
R5	60	50	40	30
R6	0	40	30	20
R7	0	0	20	10
R8	0	0	0	5

$NODF_{col} = 100$
$WNODF_{col} = 0$
$WNODA_{col} = 77.6$

In this second example, binary and weighted overlap go in opposite directions: the columns with high weights are the ones with lower degrees. Once NODF is not affected by the weights, $NODF_{col} = 100$. However, as WNODF depends on both binary decreasing fill and overlap of weights, $WNODF_{col} = 0$.

In this matrix, the only elements that deviate from the nestedness pattern of example I are the 0's in the left bottom of the matrix. $WNODA_{col}$ is affected by then in a very proportional way, reducing from 100 to 77.6.

EXAMPLE III

	C1	**C2**	**C3**
R1	100	90	80
R2	90	80	70
R3	80	70	60
R4	70	60	50
R5	60	50	40
R6	50	40	0
R7	40	0	0
R8	0	1	1
R9	0	0	1

$NODF_{col} = 0$
$WNODF_{col} = 0$
$WNODA_{col} = 76.2$

In this third example, most of the matrix is perfectly binary and weighted nested (R1 to R7). If we consider just this portion of the matrix, $NODF_{col}$, $WNODF_{col}$, and $WNODA_{col}$ would be 100. However, the addition of two rows (R8 and R9) with very weak links in an opposite pattern is sufficient to reduce $NODF_{col}$ and $WNODF_{col}$ to zero. This kind of effect is expected for binary metrics, like NODF, as they do not distinguish between strong and weak links, but it is undesirable for weighted metrics in which the inclusion of weak links should have small effects. WNODA is affected by the inclusion of these weak links in a much more moderated extent: $WNODA_{col}$ reduces from 100 to 76.2.

$WNODA_{SM}$ and $WNODA_{DM}$

Lewinsohn *et al.* 2006 proposed that highly diverse ecological networks likely present a compound topology: a modular network with internally nested modules. Recently, compound topologies were found in real-world ecological networks (Flores et al. 2013, Felix et al. 2017, Mello et al. 2018).

In order to test for a compound topology, Felix *et al.* 2017 proposed a new method (adapted from the method of Flores *et al.* 2013) that consists in computing separately the nestedness between nodes of the same module from the nestedness between nodes of different modules. Both studies used the NODF metric to measure nestedness, however, this approach can be used with any metric based on pairwise node comparisons, including WNODA.

This can be done using WNODA by distinguishing N values calculated for comparison of nodes of the same module from N values calculated for comparison of nodes of different modules. The averaging of N values from each of these two groups results, respectively, in $\mathrm{WNODA}_{\mathrm{SM}}$ and $\mathrm{WNODA}_{\mathrm{DM}}$. In a matrix with a compound topology, we expect $\mathrm{WNODA}_{\mathrm{SM}}$ to be much higher than $\mathrm{WNODA}_{\mathrm{DM}}$.

The function nest.smdm

An R function (nest.smdm) to measure nestedness and its components DM and SM, using NODF, WNODF, and WNODA is now available at bipartite package for R (Dormann et al. 2008).

References:

Almeida-Neto, M., P. Guimarães, P. R. Guimarães, R. D. Loyola, and W. Ulrich. 2008. A consistent metric for nestedness analysis in ecological systems: reconciling concept and measurement. Oikos 117:1227–1239.

Almeida-Neto, M., and W. Ulrich. 2011. A straightforward computational approach for measuring nestedness using quantitative matrices. Environmental Modelling & Software 26:173–178.

Beckett, S. J., C. A. Boulton, and H. T. P. Williams. 2014. FALCON: a software package for analysis of nestedness in bipartite networks. F1000Research 3:1–14.

Dormann, C. F., B. Gruber, and J. Fründ. 2008. Introducing the bipartite Package: Analysing Ecological Networks. R News 8:8–11.

Felix, G. M., R. B. P. Pinheiro, R. Poulin, B. R. Krasnov, and M. A. R. Mello. 2017. The compound topology of a continent-wide interaction network explained by an integrative hypothesis of specialization. bioRxiv.

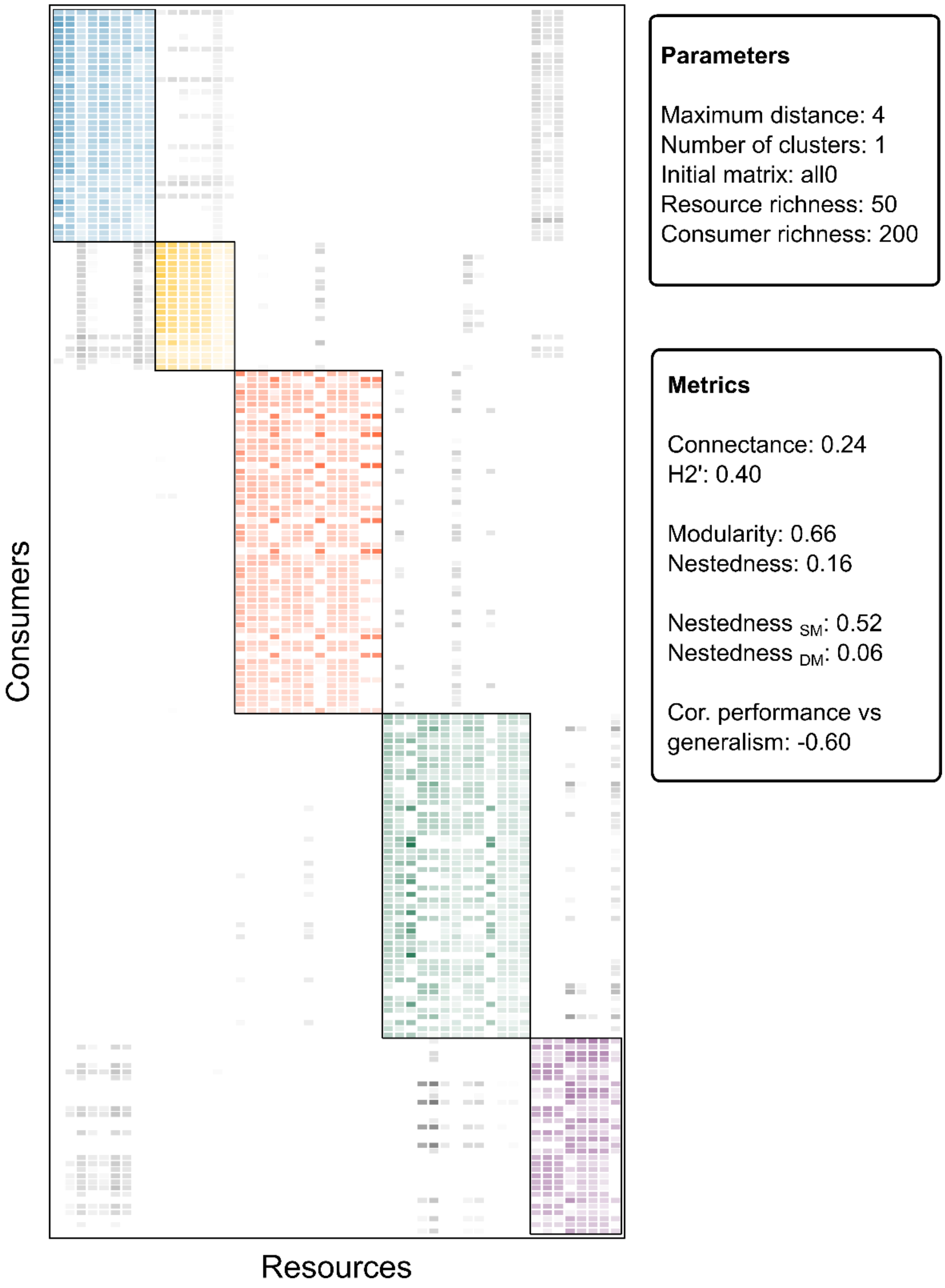
Flores, C. O., S. Valverde, and J. S. Weitz. 2013. Multi-scale structure and geographic drivers of cross-infection within marine bacteria and phages. The ISME Journal 7:520–532.

Lewinsohn, T. M., P. Inácio Prado, P. Jordano, J. Bascompte, and J. M. Olesen. 2006. Structure in plant-animal interaction assemblages. Oikos 113:174–184.

Mello, M. A. R., G. M. Felix, R. B. P. Pinheiro, R. L. Muylaert, C. Geiselman, S. E. Santana, M. Tschapka, N. Lotfi, F. A. Rodrigues, and R. D. Stevens. 2018. Insights on the assembly rules of a continent-wide multilayer network. bioRxiv.

Appendix S4. Modularity emergence without resource dissimilarity discontinuities.

Rafael Barros Pereira Pinheiro, Gabriel Moreira Félix Ferreira, Carsten F. Dormann, Marco Aurelio Ribeiro Mello. A new model explaining the origin of different topologies in interaction networks.



Parameters

Maximum distance: 4
Number of clusters: 1
Initial matrix: all0
Resource richness: 50
Consumer richness: 200

Metrics

Connectance: 0.24
H2': 0.40

Modularity: 0.66
Nestedness: 0.16

Nestedness $_{SM}$: 0.52
Nestedness $_{DM}$: 0.06

Cor. performance vs generalism: -0.60

Figure S1. Modularity emergence without resource dissimilarity discontinuities. Originally, we hypothesized that modularity in the interaction network would only reflect the discontinuities already existing on the resource dissimilarity. It is, then, remarkable that even in simulations without clusters in the resource dissimilarity structure (number of clusters = 1), highly modular simulated networks were produced. Here, we present a simulated network to exemplify these results. Rows are consumers, columns are resources, colors represent modules, and the tones represent the weight of each interaction. Basic generalism (the richness of resources exploited) was used to calculate the correlation presented.

MATERIAIS SUPLEMENTARES DO CAPÍTULO 2

A NOVEL PERSPECTIVE ON NESTEDNESS AND A THEORY-ORIENTED PROCEDURE FOR THE USE OF NULL MODELS

Figure S1. Marginal sum distributions of binary and weighted matrices.

Figure S2. Simulated matrices.

Appendix S1. Efficiency of metrics to distinguish between weighted random and nested matrices.

Appendix S2. Efficiency of metrics to distinguish between binary random and nested matrices.

Figure S1. Marginal sum distributions of binary and weighted matrices.

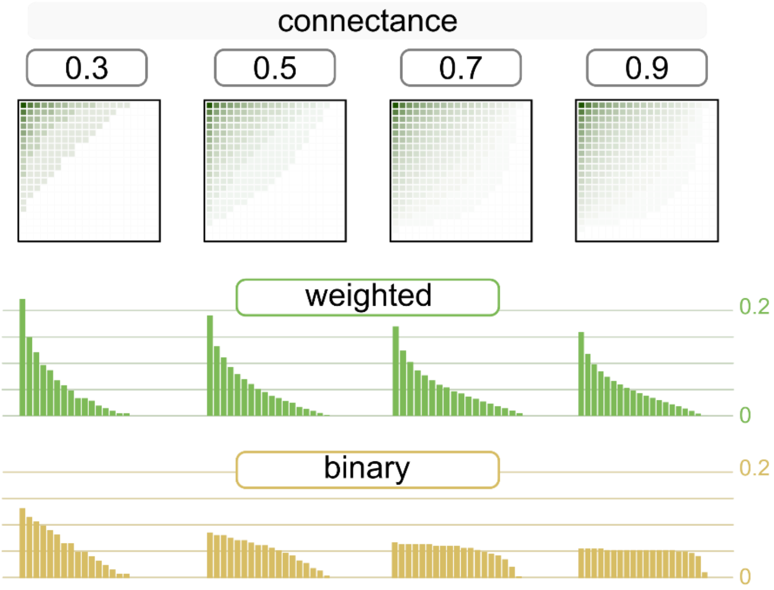


Fig. S1. Marginal sum distributions of binary matrices are contingent on matrix dimensions and connectance. They are, therefore, poor proxies for the weighted marginal sum distributions, especially in highly connected matrices. Matrices were produced following a log-normal distribution on marginal sums. Relative marginal sums on bars. For simplicity we did not remove the empty rows and columns on the matrices, which would modify the connectance (actual connectances are 0.47, 0.62, 0.78, and 0.9).

Figure S2. Simulated matrices.

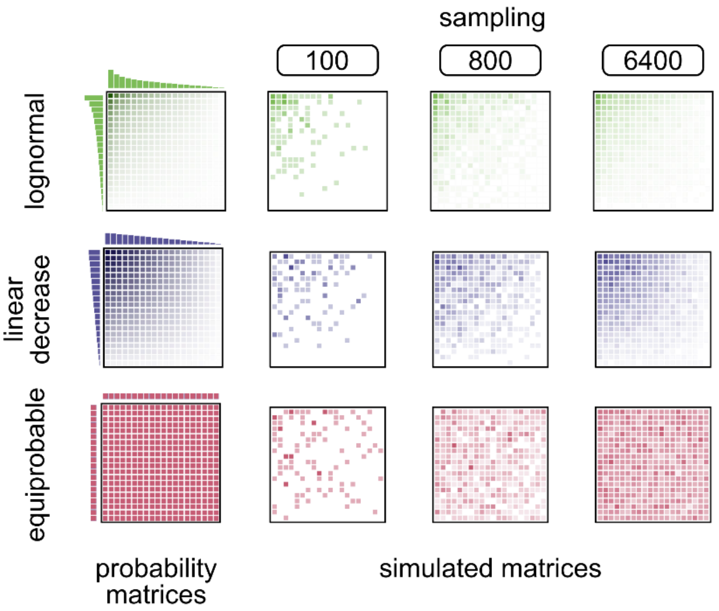


Fig. S2. To check whether nestedness metrics are efficient in distinguishing matrices with different topologies, we simulated matrices following different probability distributions. First, we produced probability matrices with three different distributions of node probabilities: log-normal, linear decrease, and equiprobable. Then, we generated randomized matrices with different total sums (sampling) following cell probabilities.

Appendix S1. Efficiency of metrics to distinguish between weighted random and nested matrices

Pinheiro, R.B.P., Dormann,C.F., Felix, G.M.F, and Mello, M.A.R.

METHODS

In our novel perspective, the main function of a nestedness metric is to distinguish between matrices with randomly distributed cell values (non-significant nestedness, equiprobable null model), matrices in which cell values are partially defined by the marginal sums (significant nestedness), and matrices in which cell values are fully determined by marginal sums (nested matrices, proportional null model). Here, we analyzed the capacity of several indices in distinguishing these topologies.

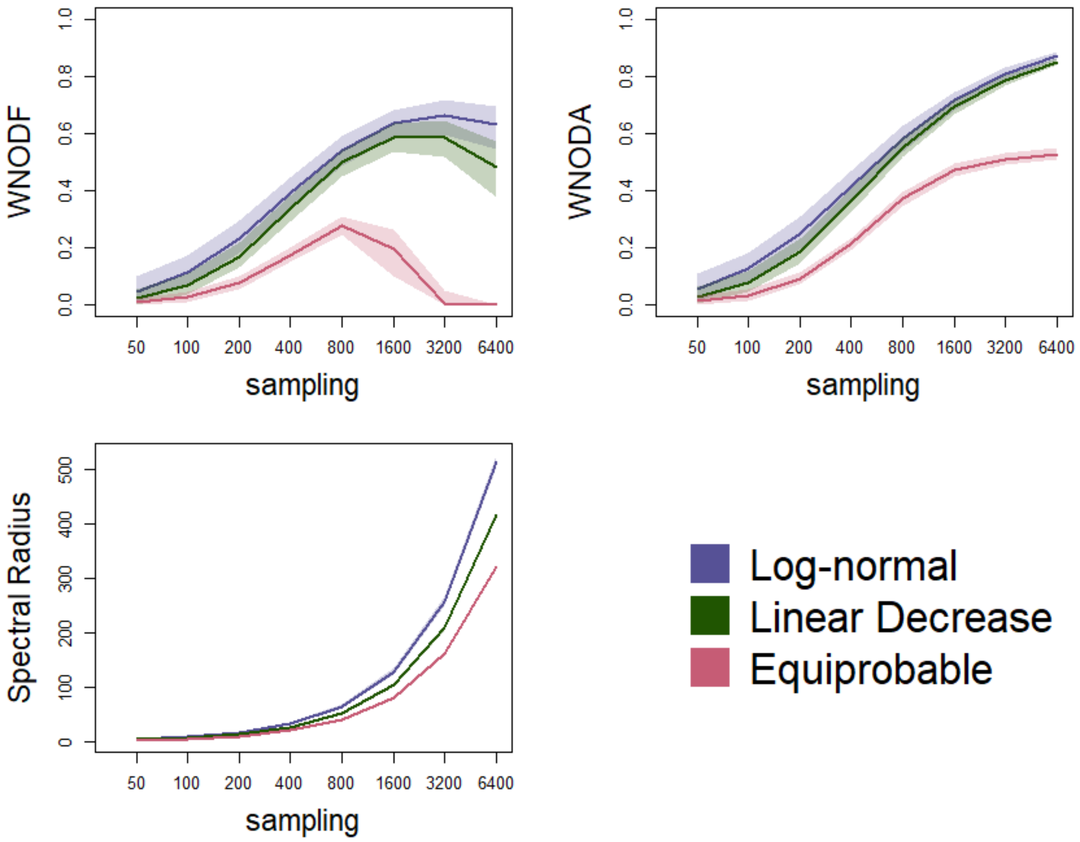
We produced probability matrices with dimensions: 5x5, 10x10, and 20x20, based on three different marginal probabilities: lognormal, linear decrease, and equiprobable. Then, we generated matrices from these probability matrices with different total samplings: 50, 100, 200, 400, 800, 1600, 3200, and 6400. For each unique setup we produced 10,000 matrices. For each matrix we calculated a set of nestedness indices (Table 1 in Methods).

In this analysis we used both weighted and binary indices. However, the models were always produced using the weighted information, and indices are compared between matrices with fixed sampling (instead of connectance). For a comparison of binary indices in matrices with fixed connectances, see Appendix S2.

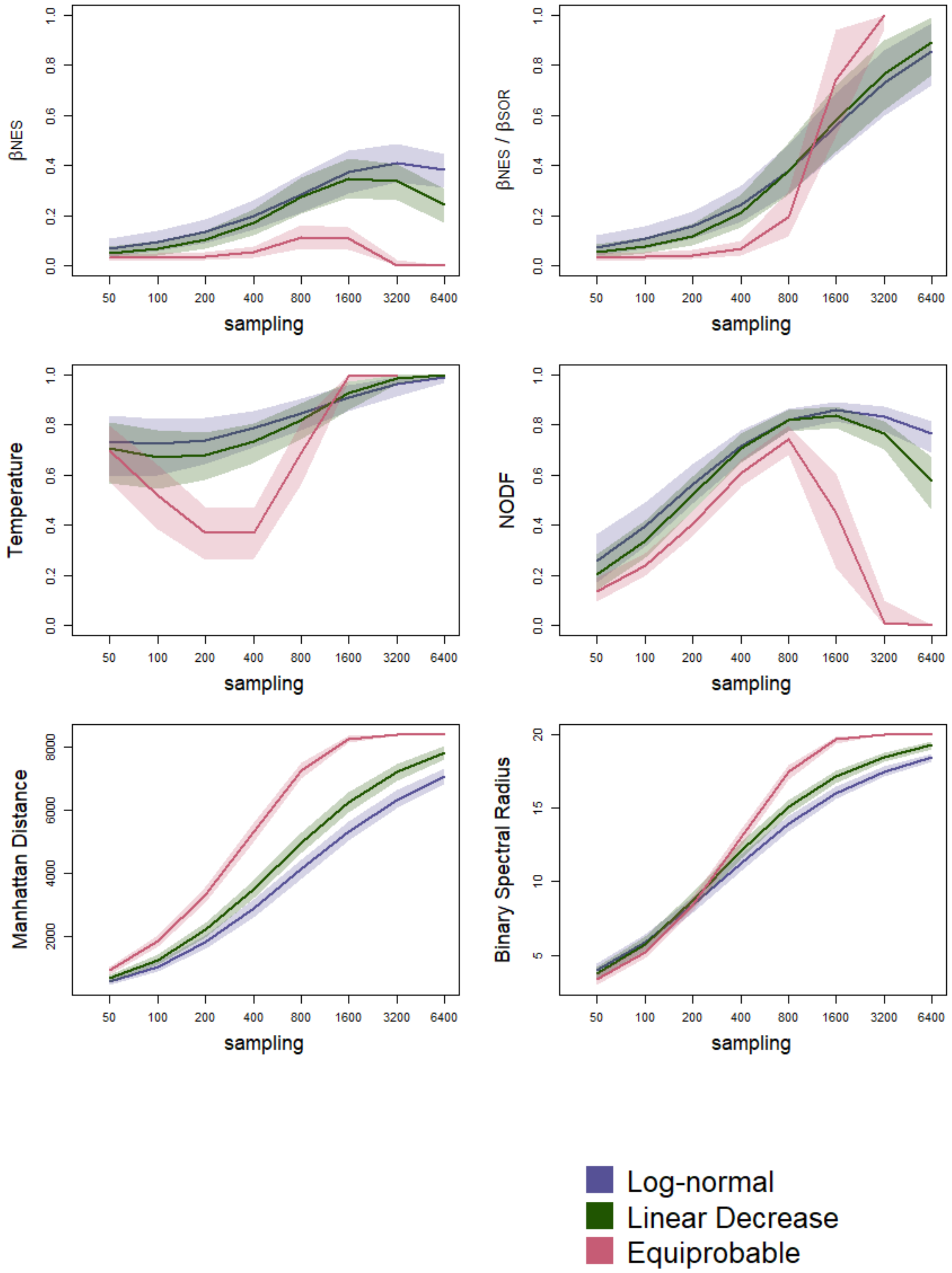
Here we present plots for a graphycal evaluation of the capacity of binary indices to separate between the proportional (lognormal and linear decrease) and the equiprobable null models. Indices in the y-axis and sampling (total weights on the matrix) on the x-axis. Each plot present median and intervals containing 95% of points. NODF, WNODF and WNODA values were divided by 100. For temperature we present 1 minus the raw value divided by 100 (so that it is directly related to nestedness).

MATRIX SIZE: 20 x 20

Weighted indices

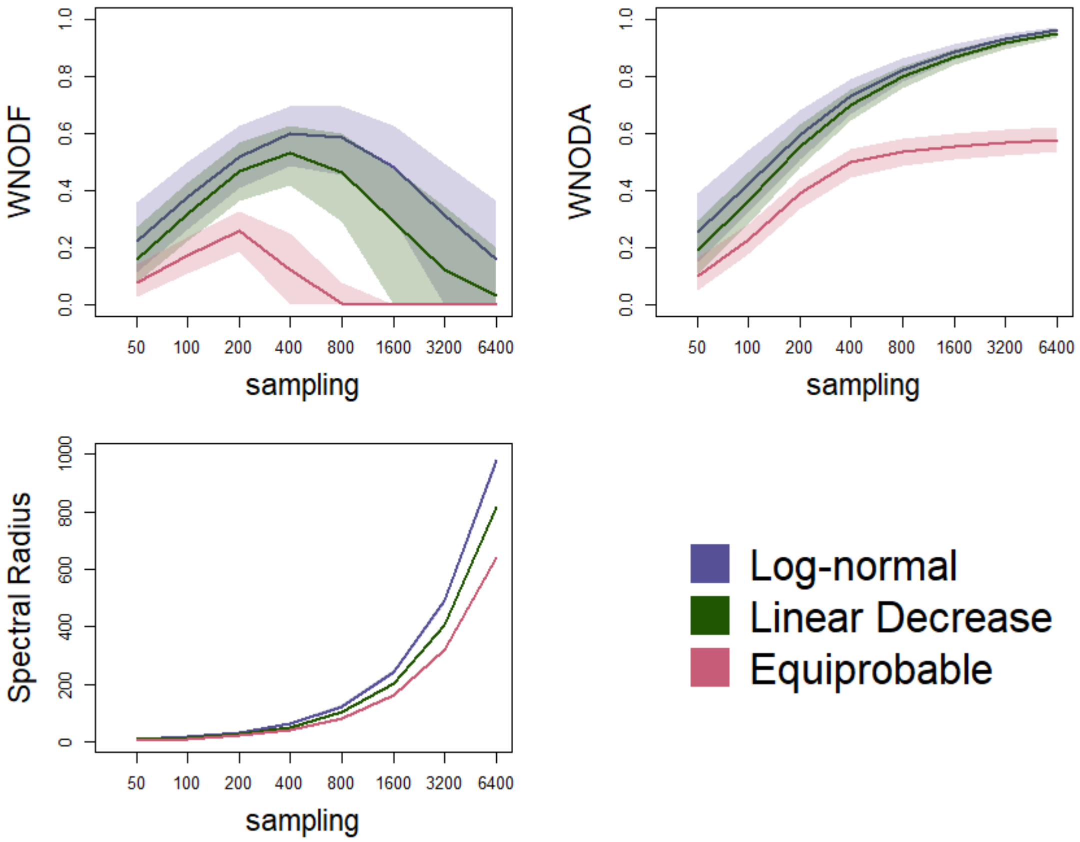


Binary indices

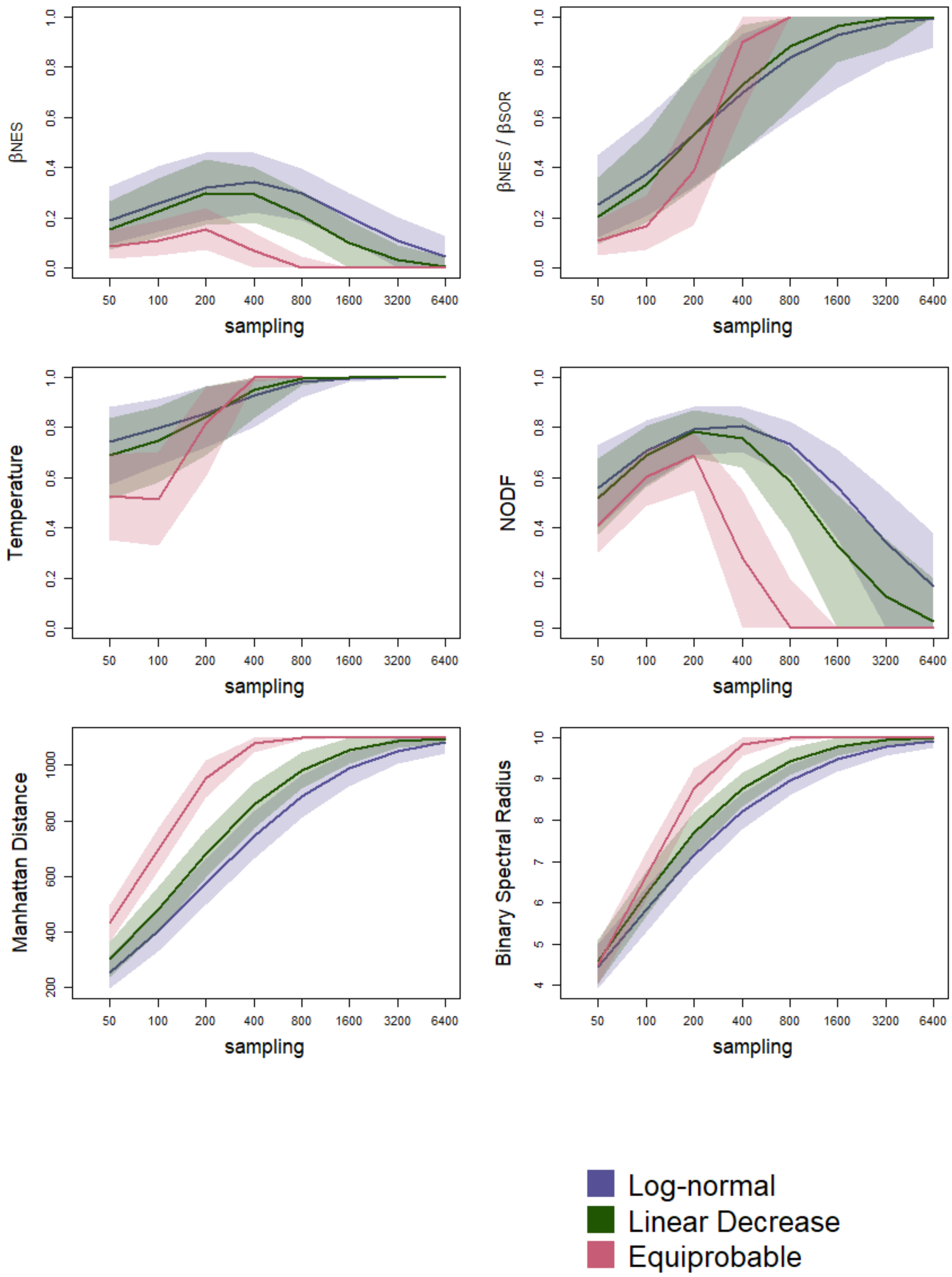


MATRIX SIZE: 10 x 10

Weighted indices

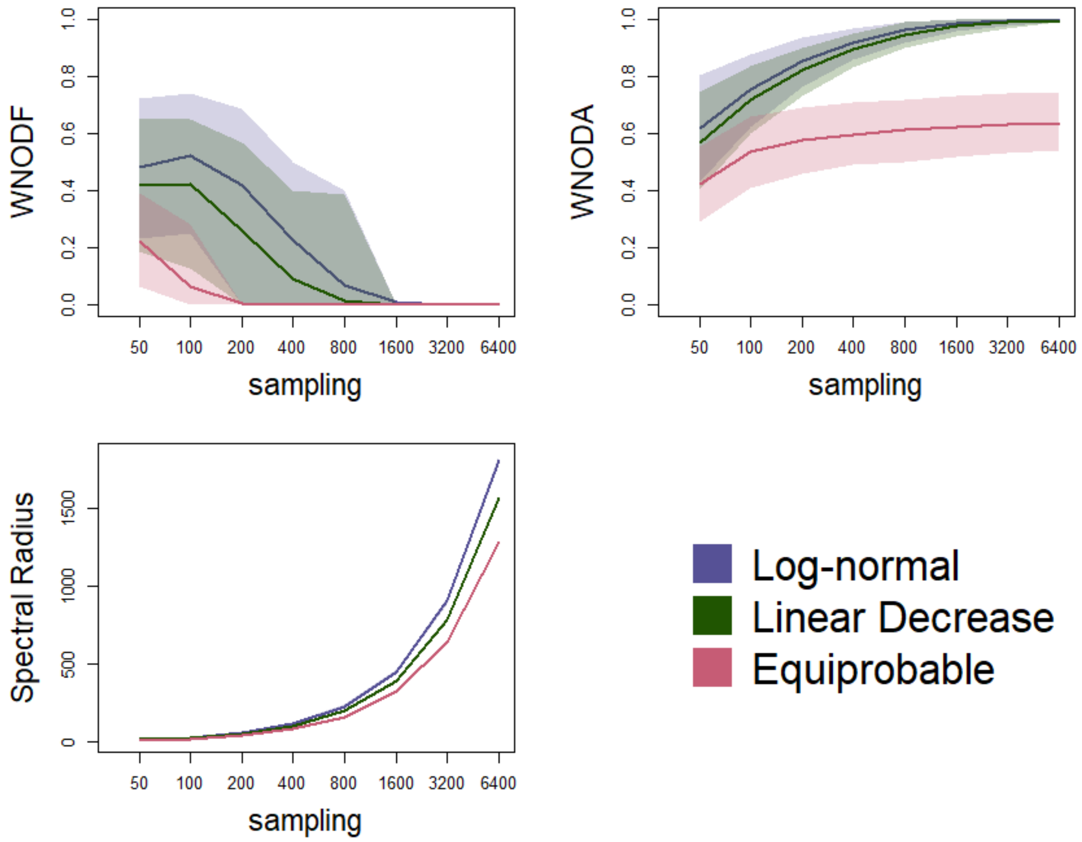


Binary indices

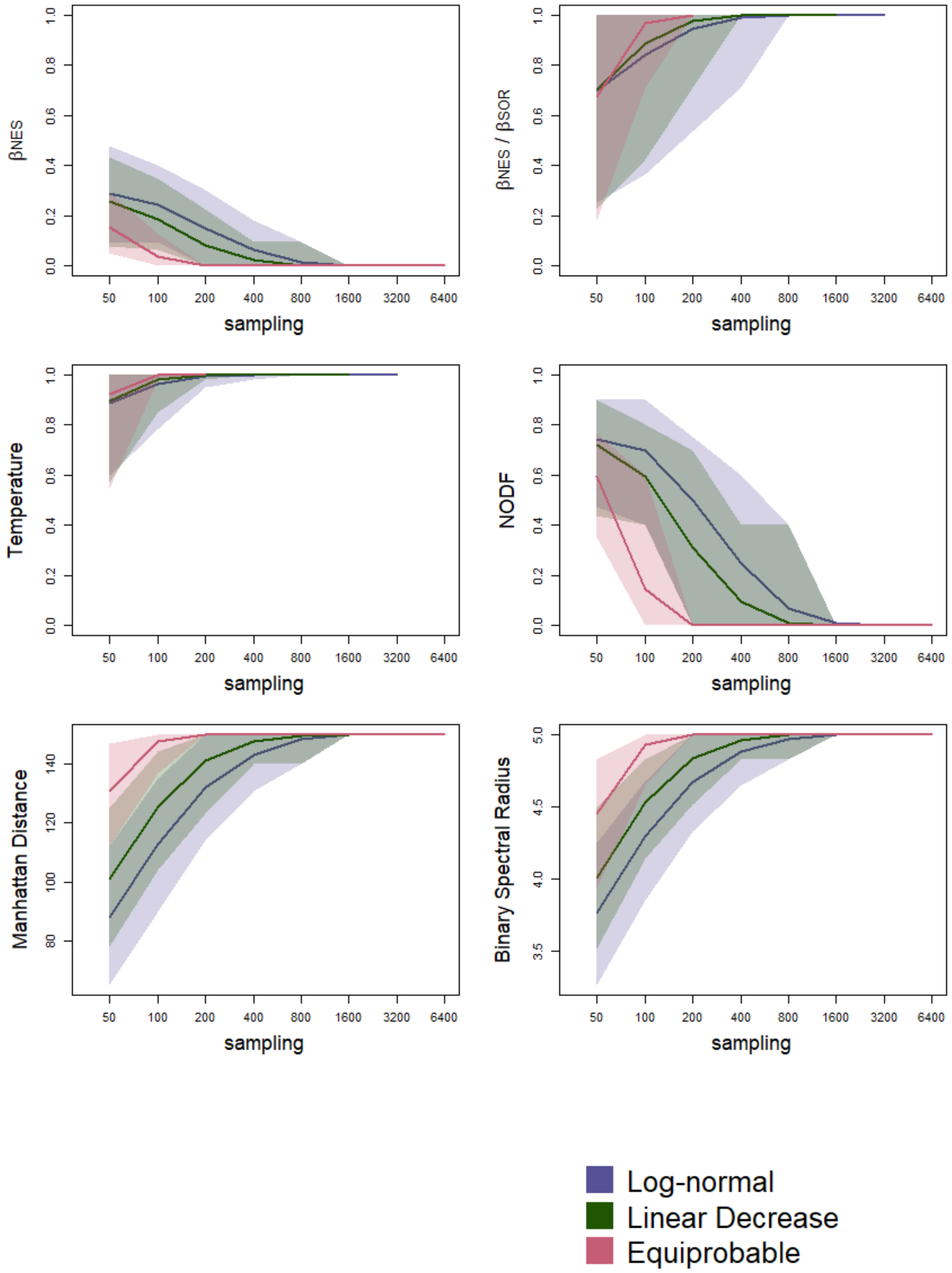


MATRIX SIZE: 5 x 5

Weighted indices



Binary indices



Appendix S2. Efficiency of metrics to distinguish between binary random and nested matrices

Pinheiro, R.B.P., Dormann,C.F., Felix, G.M.F, and Mello, M.A.R.

METHODS

In our novel perspective, the main function of a nestedness metric is to distinguish between matrices with randomly distributed cell values (non-significant nestedness, equiprobable null model), matrices in which cell values are partially defined by the marginal sums (significant nestedness), and matrices in which cell values are fully determined by marginal sums (nested matrices, proportional null model). Here, we analyzed the capacity of several indices in distinguishing these topologies.

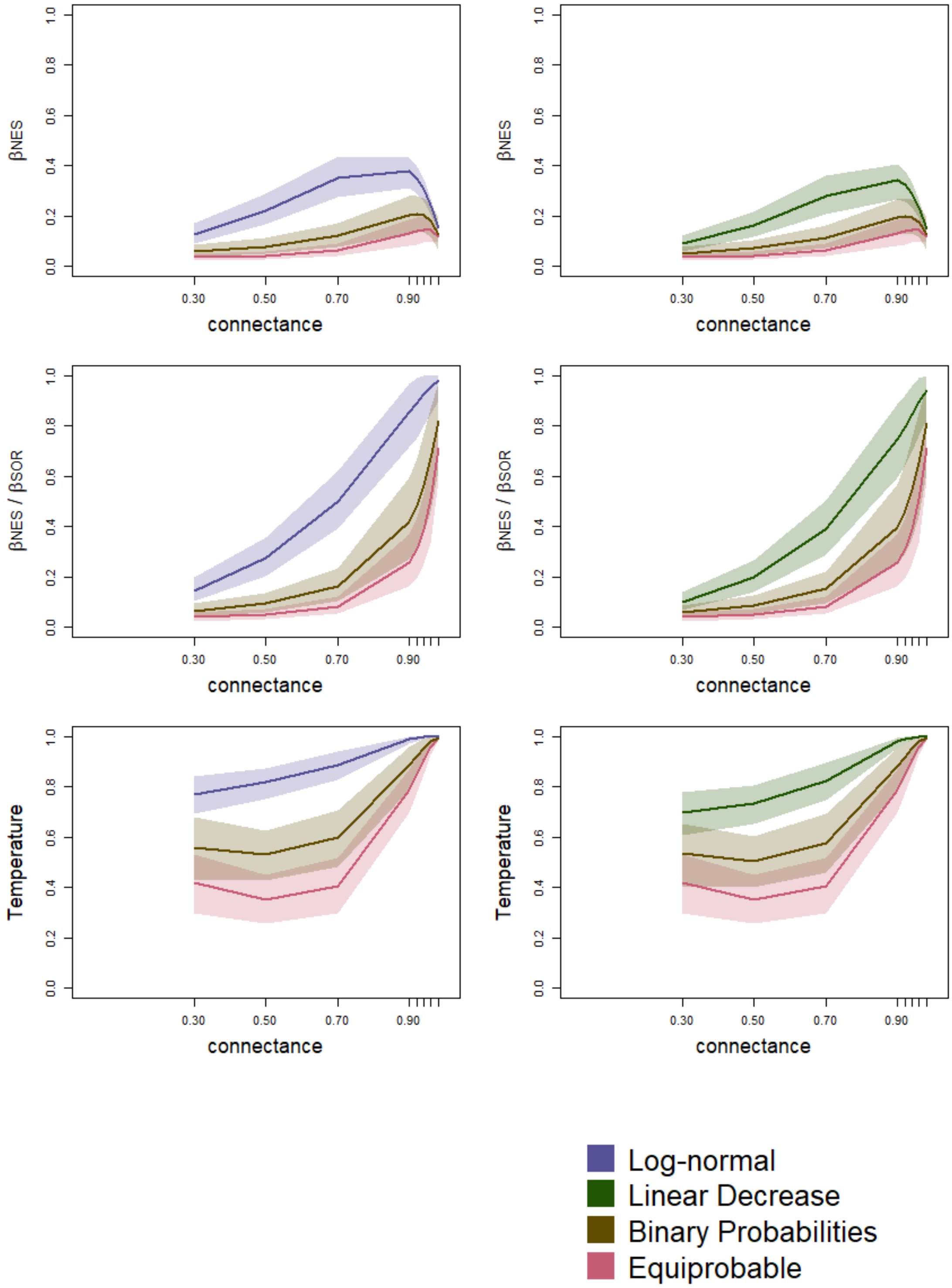
We produced probability matrices with dimensions: 5x5, 10x10, and 20x20, based on three different marginal probabilities: lognormal, linear decrease, and equiprobable. In Appendix S1 we generated weighted matrices from these probability matrices with fixed total sampling. Here, we produced binary matrices for a more appropriate comparison of binary metrics.

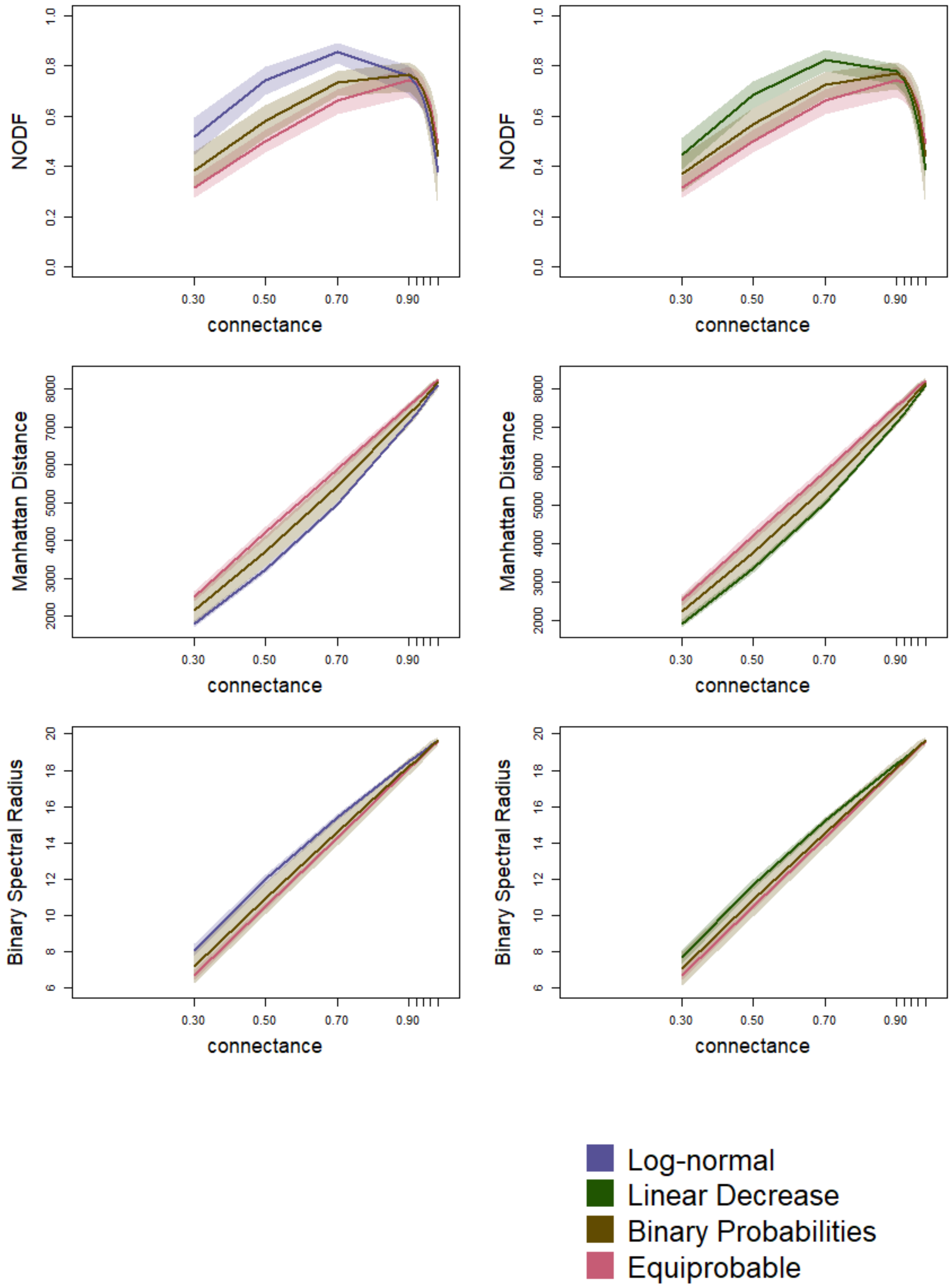
As binary matrices do not present weighted information we can only fix the connectance. We produced binary matrices with connectances: 0.3, 0.5, 0.7, 0.9, 0.92, 0.94, 0.96, and 0.98. For each matrix we calculated a set of binary nestedness indices (Table 1 in Methods).

Moreover, in analysis of binary matrices, we cannot know the original marginal probabilities, only the binary marginal sums (node degrees). To inspect the distortion caused by this approximation, for each matrix produced with fixed connectance, we produced a randomized matrix using a proportional algorithm based on binary marginal sums (binary proportional).

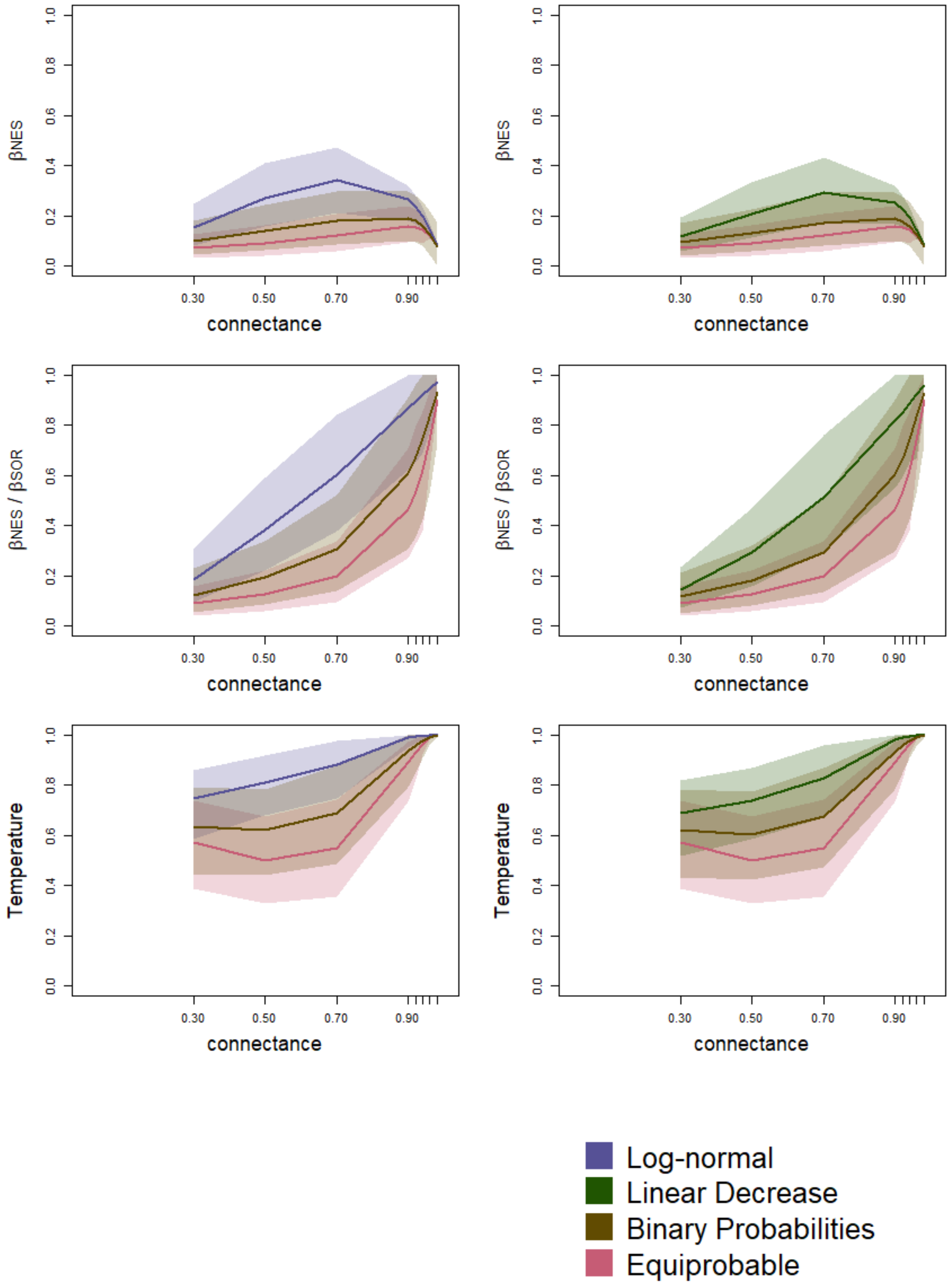
Here we present plots for a graphycal evaluation of the capacity of binary indices to separate between the proportional (lognormal and linear decrease) and the equiprobable null models. We also present values of the binary proportional null model. Indices in the y-axis and connectance on the x-axis. Each plot present median and intervals containing 95% of points. NODF values were divided by 100. For temperature we present 1 minus the raw value divided by 100 (so that it is directly related to nestedness).

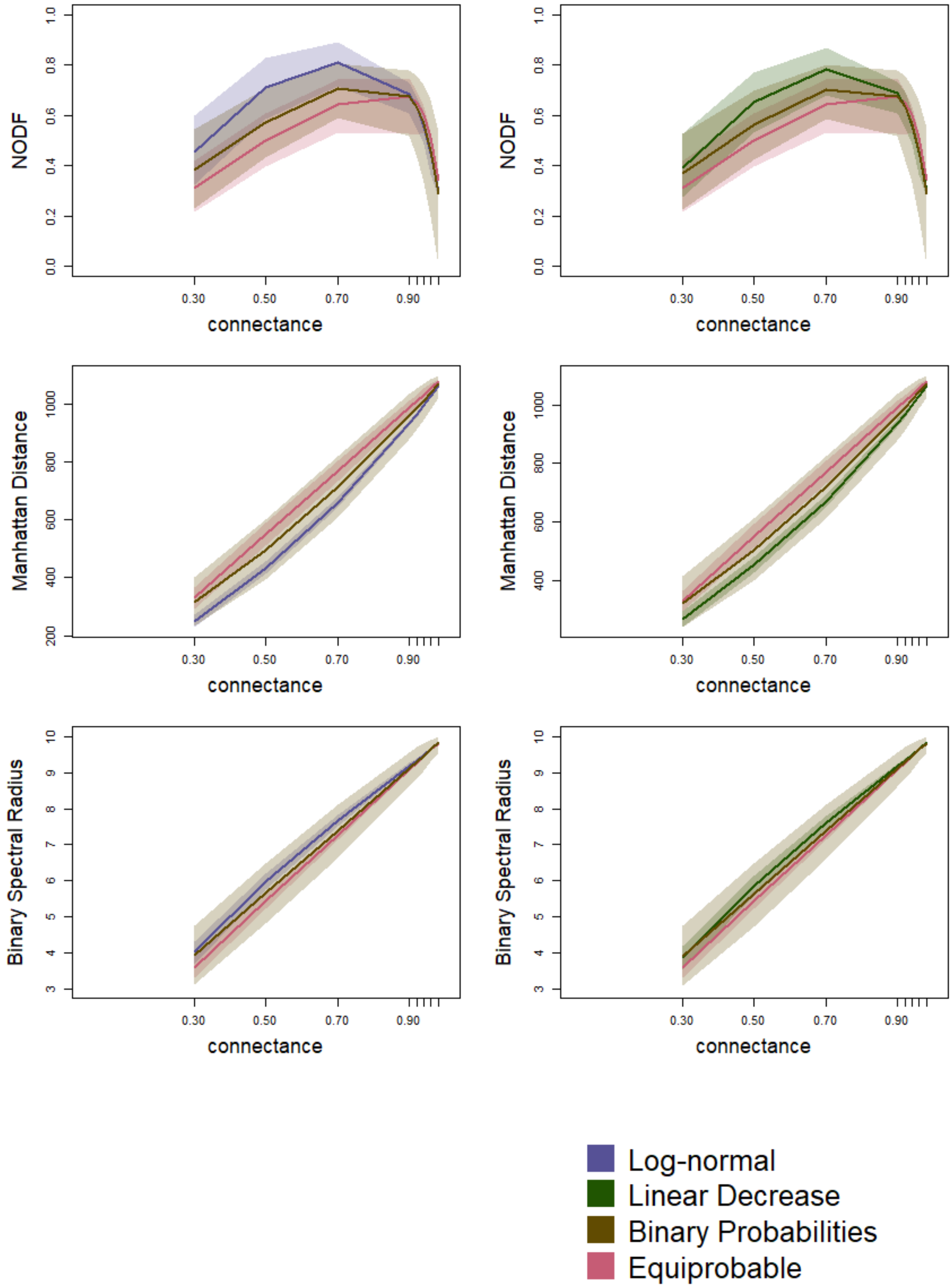
MATRIX SIZE: 20 x 20



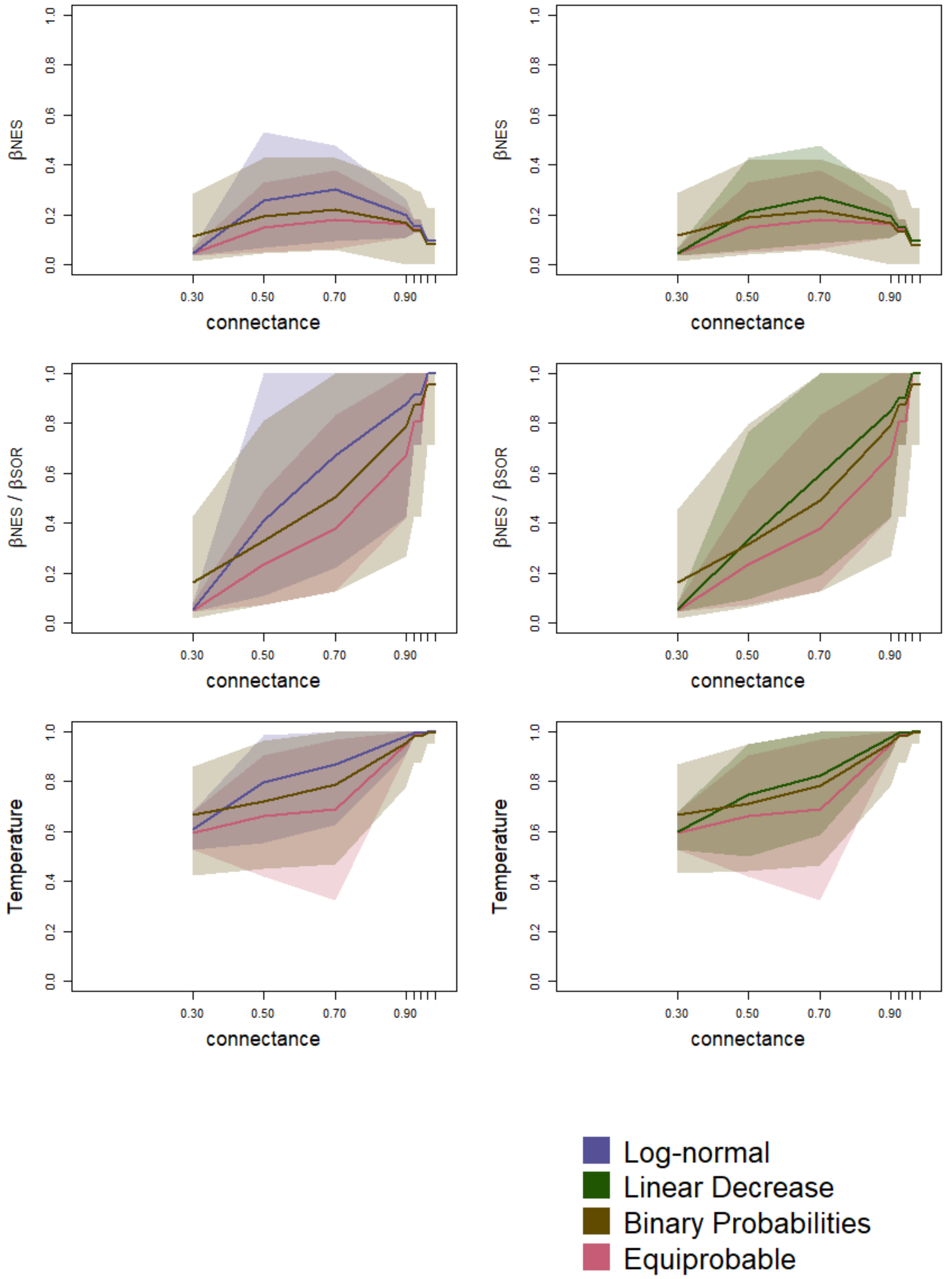

NODF
1.0
0.8
0.6
0.4
0.2
0.0
0.30
0.50
0.70
0.90
connectance
Manhattan Distance
8000
7000
6000
5000
4000
3000
2000
Binary Spectral Radius
20
18
16
14
12
10
8
6
Log-normal
Linear Decrease
Binary Probabilities
Equiprobable

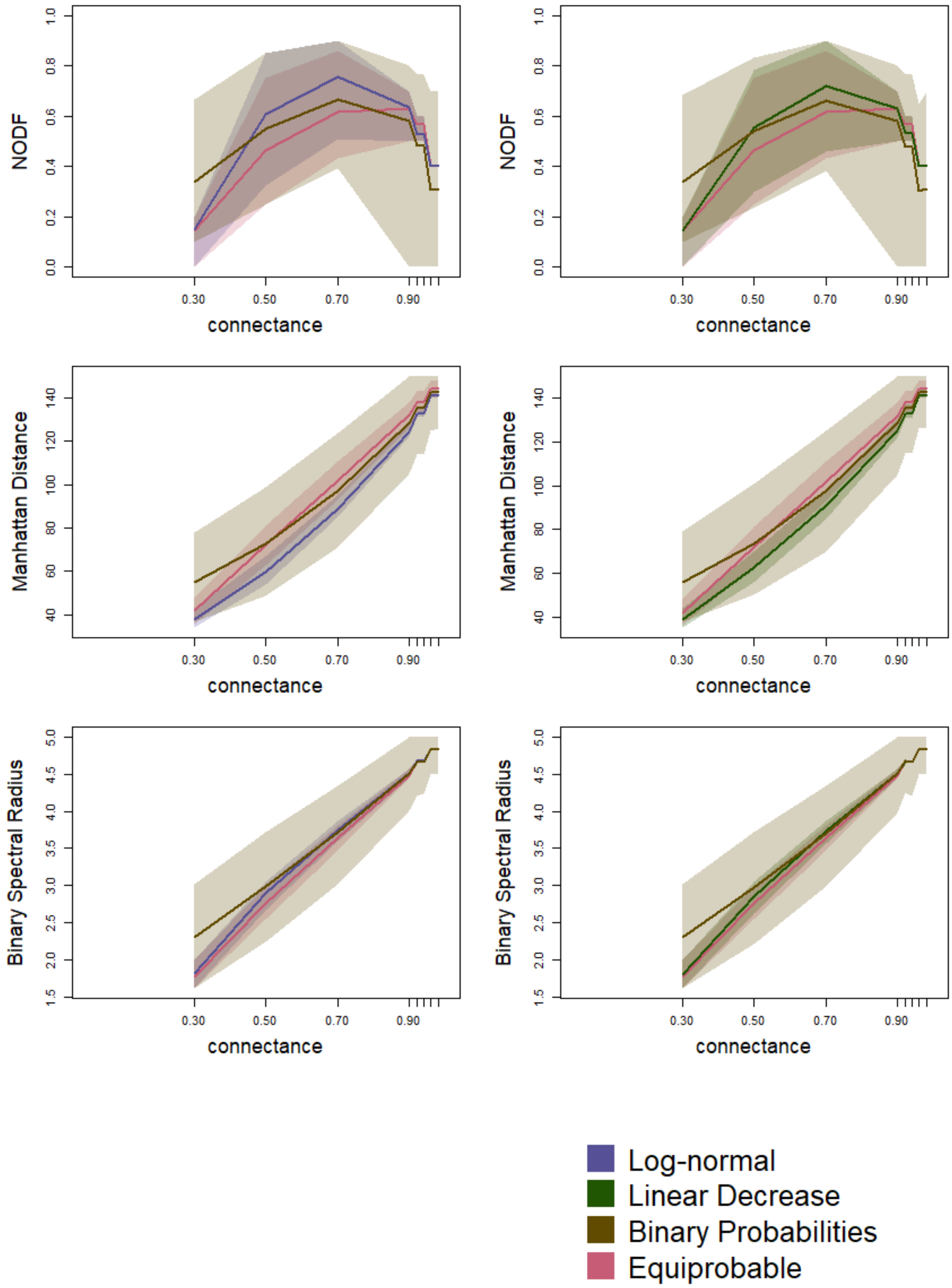
MATRIX SIZE: 10 x 10




NODF
0.0
0.2
0.4
0.6
0.8
1.0
connectance
0.30
0.50
0.70
0.90
Manhattan Distance
200
400
600
800
1000
Binary Spectral Radius
3
4
5
6
7
8
9
10
Log-normal
Linear Decrease
Binary Probabilities
Equiprobable

MATRIX SIZE: 5 x 5




NODF
0.0
0.2
0.4
0.6
0.8
1.0
0.30
0.50
0.70
0.90
connectance
Manhattan Distance
40
60
80
100
120
140
Binary Spectral Radius
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
Log-normal
Linear Decrease
Binary Probabilities
Equiprobable