

Linking evolutionary and ecological theory illuminates non-equilibrium biodiversity

A. J. Rominger^{1, 2}, I. Overcast³, H. Krehenwinkel¹, R. G. Gillespie¹, J. Harte^{1, 4}, and M. J. Hickerson³

¹Department of Environmental Science, Policy and Management, University of California, Berkeley

²Santa Fe Institute

³Biology Department, City College of New York

⁴Energy and Resource Group, University of California, Berkeley

Corresponding author: Rominger, A.J. (ajrominger@gmail.com).

Keywords: Non-equilibrium dynamics; ecology-evolution synthesis; neutral theory; maximum entropy; next generation sequencing

Abstract

Whether or not biodiversity dynamics tend toward stable equilibria remains an unsolved question in ecology and evolution with important implications for our understanding of diversity and its conservation. Phylo/population genetic models and macroecological theory represent two primary lenses through which we view biodiversity. While phylo/population genetics provide an averaged view of changes in demography and diversity over timescales of generations to geological epochs, macroecology provides an ahistorical description of commonness and rarity across contemporary co-occurring species. Our goal is to combine these two approaches to gain novel insights into the non-equilibrium nature of biodiversity. We help guide near future research with a call for bioinformatic advances and an outline of quantitative predictions made possible by our approach.

1 Non-equilibrium, inference, and theory in ecology and evolution

The idea of an ecological and evolutionary equilibrium has pervaded studies of biodiversity from geological to ecological, and from global to local [1–6]. The consequences of non-equilibrium dynamics for biodiversity are not well understood and the need to understand them is critical with when anthropogenic pressures forcing biodiversity into states of rapid transition [7]. Non-equilibrial processes could profoundly inform conservation in ways only just beginning to be explored [8].

Biodiversity theories based on assumptions of equilibrium, both mechanistic [3, 5, 6] and statistical [see the Glossary; 4, 9] have found success in predicting ahistorical patterns of diversity such as the species abundance distribution [3, 4, 10] and the species area relationship [3, 4]. These theories assume a macroscopic equilibrium in terms of these coarse-grained metrics, as opposed to focusing on details of species identity [such as in 7], although macroscopic and microscopic approaches are not mutually exclusive. Nonetheless, the equilibrium assumed by these theories is not realistic [11], and many processes, equilibrial or otherwise, can generate the same macroscopic, ahistorical predictions [12].

Tests of equilibrial ecological theory alone will not allow us to identify systems out of equilibrium, nor permit us to pinpoint the mechanistic causes of any non-equilibrial processes. The dynamic natures of evolutionary innovation and landscape change suggest that ecological theory could be greatly enriched by synthesizing its insights with inference from population genetic theory that explicitly accounts for history. This would remedy two shortfalls of equilibrial theory: 1) if theory fits observed ahistorical patterns but the implicit dynamical assumptions were wrong, we would make the wrong conclusion about the equilibrium of the system; 2) if theories do not fit the data we cannot know why unless we have a perspective on the temporal dynamics underlying those data.

No efforts to date have tackled these challenges. We propose that combining insights from ecological theory and inference of evolutionary and demographic change from genetic data will allow us to understand and predict the consequences of non-equilibrial processes in governing the current and future states of ecological assemblages. The advent of next generation sequencing (NGS) approaches to biodiversity, from microbes to arthropods [13–23] have made unprecedented data available for synthesizing insights from ecological theory and genetics/genomics. However, we need a tool set of bioinformatic methods (Box 2) and meaningful predictions (section 6) grounded in theory to make use of those data. We present the foundation of this tool set here.

2 Ecological theories and non-equilibrium

Neutral and statistical theories in ecology focus on macroscopic patterns, and equilibrium is presumed to be relevant to those patterns, but not the finer-grained properties of ecosystems. Our goal throughout is not to validate neutral or statistical theories—quite the opposite, we propose new data dimensions, namely genetics, to help better test alternative hypotheses against these null theories, thereby gaining insight into what non-neutral and non-statistical mechanisms are at play in systems of interest.

Non-neutral and non-statistical models [e.g., 5, 6] also invoke ideas of equilibrium in their derivation. However, these equilibria focus on the micro-scale details of species interactions and therefore do not fall within our primary focus, and could in fact be drivers of non-equilibrium and thus interesting alternative hypotheses to test. We focus explicitly on simple yet predictive theories for their utility as null models, not because of a presumption of their realism.

To use these theories as null models, we need a robust measure of goodness of fit. The emerging consensus is that likelihood-based test statistics should be preferred [24]. The “exact test” of Etienne [25] has been extended by Rominger and Merow [26] into a simple

z-score which can parsimoniously describe the goodness of fit between theory and pattern.
We advocate its use in our proposed framework.

The neutral theory of biodiversity [NTB; 3] is a useful null because it assumes that one mechanism—demographic drift—drives community assembly. Equilibrium occurs when homogeneous stochastic processes of birth, death, speciation and immigration have reached stationarity. Thus neutrality in ecology is analogous to neutral drift in population genetics [3].

Rather than assuming any one mechanism dominates the assembly of populations into a community, statistical theories assume all mechanisms could be valid, but their unique influence has been lost to the enormity of the system and thus the outcome of assembly is a community in statistical equilibrium [4, 9]. The mechanistic agnosticism is what makes statistical theories useful nulls. These statistical theories are also consistent with niche-based equilibria [9, 27] if complicated, individual or population level models with many mechanistic drivers were to be upscaled to entire communities.

The maximum entropy theory of ecology [METE; 4] derives its predictions by condensing the many bits of mechanistic information down into ecological state variables and then mathematically maximizing information entropy conditional on those state variables. METE can predict multiple ahistorical patterns, including distributions of species abundance, body size, spatial aggregation, and trophic links [4, 28], making for a stronger null theory [29]. However, multiple dynamics can still map to this handful of metrics [12] and while extensive testing often supports METE’s predictions [4, 10, 30] at single snapshots in time, METE fails to match observed patterns in disturbed and rapidly evolving communities [4, 28]. We cannot know the cause of these failures within the current framework of equilibrium theory testing without adding metrics that capture temporal dynamics.

3 Inferring non-equilibrium dynamics

Unlocking insight into the dynamics underlying community assembly is key to overcoming the limitations of analyzing ahistorical patterns with equilibrial theory. While the fossil record could be used for this task, it has limited temporal, spatial, and taxonomic resolution. Here we instead focus on population/phylogenetic insights into rates of change of populations and species because of the detailed characterization of demographic fluctuations, immigration, selection, and speciation they provide. Bridging ecological theory with models from population/phylogenetics has great potential [31–36] that has yet to be fully realized. How we can best link the inferences of change through time from population/phylogenetics with inferences from macroecology is governed by what insights we can gain from genetic perspectives on demography and diversification.

Coalescent theory [37, 38] is one of the fundamental population genetics tools allowing model-based estimation of complex historical processes. These include population size fluctuations [39], divergence and/or colonization times [40, 41], migration rates [42], selection [43], and complex patterns of historical population structure [44] and gene flow [45, 46]. This approach can also be put in a multi-species, community context via hierarchical demographic models [47–50], even when only small numbers of genetic loci are sampled from populations [51].

These modeled demographic deviations from neutral demographic equilibrium can also be condensed into multi-species summary statistics. For example, Tajima’s D, which measures the strength of non-equilibrium demography in a single population [see Glossary for more details; 52–55], could be averaged over all populations in a sample.

4 Current efforts to integrate evolution into ecological theory

While quantitatively integrating theory from ecology, population genetics, and phylogenetics has not yet been achieved, existing efforts to synthesize perspectives from evolution and ecology point toward promising directions despite being hindered by one or more general issues: 1) lack of a solid theoretical foundation, 2) inability to distinguish multiple competing alternative hypotheses, 3) lack of comprehensive genetic/genomic data, and 4) lack of bioinformatic approaches to resolve species and their abundances.

Phylogenetic information has been incorporated into studies of the NTB to better understand its ultimate equilibrium [56, 57]. However, phylogenetic reasoning also points out the flaws in the NTB’s presumed equilibrium [11]. Attempts to correct the assumed dynamics of NTB through “protracted speciation” [58] are promising, and while their implications for diversification have been considered [59], these predictions have not been integrated with demographic and phylogeographic approaches [e.g., 40, 41, 44] that have the potential to validate or falsify presumed mechanisms of lineage divergence. Such demographic studies, particularly phylogeographic investigations of past climate change [60, 61], have highlighted the non-equilibrium responses of specific groups to perturbations that must be confronted by ecological theory, but no attempt has been made to scale up these observations to implications at the level of entire communities. The recent growth in joint studies of genetic and species diversity [35, 62] have been useful in linking population genetics with ecological and biogeographic concepts. These correlative studies could be bolstered by developing full joint models that link community assembly, historical demography and coalescent-based population genetics combined with NGS.

Studies have also used chronosequences or the fossil record in combination with neutral and/or statistical theory to investigate changes over geologic time in community assembly

mechanisms [28, 63]. While these studies have documented interesting shifts in assembly mechanisms, including departures from equilibrium likely resulting from evolutionary innovations, understanding exactly how the evolution of innovation is responsible for these departures cannot be achieved without more concerted integration with genetic data.

5 What is needed now

A key limitation to using ahistorical theory to infer dynamic mechanisms is that multiple mechanisms, from simple and equilibrial to complex, can map onto the same ahistorical pattern [29, 64]. This means that even when a theory describes the data well, we do not really know the dynamics that led to that good fit [11].

Quantitatively integrating the dynamics inferred from population and phylogenetic approaches with ahistorical, equilibrial ecological theory can break this many-to-one mapping of mechanism onto prediction and contextualize whether a match between ahistorical pattern and theory truly results from equilibrial dynamics or only falsely appears to. There are two complementary approaches to achieve this integration (both discussed further in Box 2):

- Option 1: using dynamics from genetic inference to predict and understand deviations from ahistorical theories. This amounts to separately fitting ahistorical theory to typical macroecological data, while also fitting population genetic and/or phylogenetic models to genetic data captured for the entire community. Doing so requires substantial bioinformatic advances that would allow the joint capture of genetic or genomic data from entire community samples using NGS, while also estimating accurate abundances from NSG output. Separating model fitting avoids assumptions about how macroecological quantities like abundance scale to evolutionary metrics like effective population size; however, this approach does not facilitate the elegance of model comparison as does joint modeling.

- Option 2: building off existing theories, develop new joint models that simultaneously predict macroecological and population genetic patterns. This amounts to building hierarchical models that take genetic data as input and integrate over all possible community states that could lead to these genetic data given a model of community assembly and a model of population coalescence. This approach requires making assumptions about how abundances scale to effective population sizes, but is better suited for comparing competing joint models of evolutionary history and assembly.

5.1 What we gain from this framework

Using our proposed framework, we can finally understand why ahistorical theories fail when they do—is it because of rapid population change, or evolution/long-distance dispersal of novel ecological strategies? We could predict whether a system that obeys the ahistorical predictions of equilibrial ecological theory is in fact undergoing major non-equilibrial evolution. We could better understand and forecast how/if systems out of equilibrium are likely to relax back to equilibrial patterns. With such a framework we could even flip the direction of causal inference and understand ecological drivers of diversification dynamics. This last point bears directly on long-standing debates about the importance of competitive limits on diversification[2, 65]. Conclusions about phylogenetic patterns (e.g. diversification slowdowns) would be more believable and robust if combined with population genetic inference (e.g. declining populations) and community patterns (e.g. deviation from equilibrium).

6 Evo-ecological predictions for systems out of equilibrium

We propose a simple yet powerful way to summarize joint inference into deviations from ecological and evolutionary/demographic equilibrium. Assuming that equilibrial models have

been independently or jointly fit (Box 2) to a dataset of macroecological metrics (such as species abundances) and genetic/genomic variables (such as community-wide polymorphism data) we can then contrast the system’s deviation from ecological equilibrium with its deviation from evolutionary/demographic equilibrium (Fig. 1). Ecological deviations can be measured by, e.g., the previously discussed z-score [26], while evolutionary/demographic deviations can be captured by summary statistics such as community-averaged Tajima’s D. The space of equilibrium and non-equilibrium states that this comparison generates (Fig. 1) can be used to understand a community’s current state, and predict its past and future. Additional predictions from joint eco-evolutionary inference can be tested to further understand a system’s trajectory through phases of equilibrium and non-equilibrium. One particularly useful metric is the relationship between lineage age (colonization or divergence time inferred from molecular data) and lineage abundance (Fig. 2), which is known to be a telling test of the NTB [11, 58]. Comparing different models of assembly and coalescence in a model selection framework can also provide insight.

6.1 Cycles of non-equilibrium

Ecosystems experience regular disturbances which can occur on ecological time-scales, such as primary succession, or evolutionary time scales, such as evolution of novel innovations that lead to new ecosystem processes [66]. We hypothesize that these regular disturbances can lead to cycles of non-equilibrium in observed biodiversity patterns. Using the phase space of equilibrium and non-equilibrium states showing in Figure 1 a clockwise cycle through this space would indicate:

- Panel I \rightarrow II: following rapid ecological disturbance, ecological metrics diverge from equilibrium. The system could potentially relax back to equilibrium (Panel II \rightarrow Panel I), indicating a stationary disturbance process that has no net evolutionary consequences. Conversely,

- Panel II \rightarrow III: ecological non-equilibrium spurs evolutionary non-equilibrium leading to both ecological and evolutionary metrics diverging from equilibrium values
- Panel III \rightarrow IV: evolutionary innovations provide the means for ecological processes to re-equilibrate to their environments
- Panel IV \rightarrow I: finally a potential return to equilibrium on both ecological and evolutionary time scales once evolutionary processes have also relaxed.

Cycles through this space could also occur in a counterclockwise direction, being initiated by an evolutionary innovation. Under such a scenario we hypothesize the cycle to proceed:

- Panel I \rightarrow IV: non-equilibrium evolution (including sweepstakes dispersal) leading to departure from evolutionary equilibrium before departure from ecological equilibrium
- Panel IV \rightarrow III: non-equilibrium ecological response to non-equilibrium evolutionary innovation
- Panel III \rightarrow I: ecological and evolutionary relaxation

We hypothesize that the final transition will be directly to a joint equilibrium in ecological and evolutionary metrics (Panel I) because a transition from panel III to panel II is unlikely, given that ecological rates are faster than evolutionary rates. In general these cycles can be combined arbitrarily depending on the forces and dynamics present in the system. However, transitions where evolutionary rates must operate faster than ecological rates (i.e. Panel III \rightarrow II and Panel IV \rightarrow Panel II) are less likely.

A complete cycle cannot be observed without a time machine, but by combining ahistorical ecological theory and population/phylogenetic inference methods using community-level genetic data we can identify where in this space our focal systems are located. To determine their trajectory through this space we must more deeply explore the joint inference of

community assembly and evolutionary processes. In the following sections we do that for each transition shown in Figure 1 using patterns of lineage age and abundance together with model selection.

6.2 Systems undergoing rapid ecological change

For systems whose metrics conform to demographic equilibrium, but deviate from equilibrium ecological theory (Panel I \rightarrow II), a lack of correlation between lineage age and lineage abundance would indicate that rapid ecological change underlies their dynamics. If slow, equilibrial evolutionary drift is punctuated by regular ecological perturbations, population size would be independent of age (Fig. 2). Actual abundance should similarly be uncorrelated with effective population size in joint genetic-assembly models.

6.3 Ecological relaxation

Ecological relaxation occurs when populations return to steady state. Both ecological (Panel II \rightarrow I) and evolutionary (Panel III \rightarrow IV) mechanisms can facilitate this process (e.g. changes in local population sizes following environmental change [7], or evolution of new species interactions such as host switching [28]). If ecological mechanisms are responsible, age and abundance should again be uncorrelated; if evolutionary mechanics are responsible, age and abundance should be negatively correlated (Fig. 2).

6.4 Non-equilibrium ecological communities fostering non-equilibrium evolution

A lack of equilibrium in an ecological assemblage means that the system will likely experience change in order to re-equilibrate. If ecological relaxation does not occur—by chance, or because no population present is equipped with the adaptations to accommodate the

new environment—then the system is open to evolutionary innovation (Panel II \rightarrow III). Such innovation could take the form of elevated speciation or long-distance immigration. Speciation and sweepstakes immigration/invasion will yield very different phylogenetic signals, however, their population genetic signals in a non-equilibrium community may be very similar (e.g. rapid population expansion). Thus, where non-equilibrium communities foster non-equilibrium diversification (either through speciation or invasion) we expect to see a negative relationship between lineage age and abundance (Fig. 2). Similarly, in a joint genetic-assembly modeling framework, population expansion models should be favored over demographically stationary models.

6.5 Non-equilibrium evolution fostering non-equilibrium ecological dynamics

If evolutionary processes, or their counterpart in the form of sweepstakes immigration/invasion, generate new ecological strategies in a community, this itself constitutes a form of disturbance pushing the system to reorganize (Panel IV \rightarrow III). Evolutionary change would have to be extremely rapid to force ecological metrics out of equilibrium, thus in this scenario we would expect a negative correlation between age and abundance (Fig. 2) and model selection favoring joint genetic-assembly models with highly structured populations and rapid divergence rates. If data become available for large regions of genomes for entire communities, signals of strong selection could also validate non-equilibrium evolution fostering non-equilibrium ecological dynamics (see **Outstanding Questions**).

6.6 Evolutionary relaxation

Evolutionary demographic models average over timescales determined by generation time, population size and mutation/selection balance [37, 38]. Evolutionary relaxation (Panel III \rightarrow I or IV \rightarrow I) means this time-averaged history returns to stationarity, which can occur

if perturbations are absent, or occur on rapid enough time scales (i.e. Panel II \rightarrow I) to be averaged over. By definition, if a system is found in evolutionary demographic equilibrium it has forgotten any non-equilibrium phases in its history. Thus to detect this kind of long-term relaxation we need data from the fossil record (see **Outstanding Questions**).

7 Harnessing evo-ecological measures of non-equilibrium for a changing world

Inference of community dynamics needs to expand the dimensions of data it uses to draw conclusions about assembly of biodiversity and whether/when this is an equilibrial or non-equilibrial process. The need for more data dimensions is supported by others [12]; however, accounting for the complexities of history by explicitly linking theories of community assembly with theories of evolutionary genetics is novel, and made possible by advances in:

1. high throughput sequencing (Box 1) that allow genetic samples to be economically and time-effectively produced on unprecedented scales
2. bioinformatic methods (Box 2) that allow us to make sense of these massive community-wide genetic/genomic datasets
3. theory development (section 6) that provides meaningful predictions to test with our new bioinformatic approaches

This framework is a fertile cross pollination of two fields that, while successful in their own right, are enhanced by their integration. While comparative historical demographic models are advancing [47–50], testing community-scale hypotheses with multi-taxa data would be profoundly improved and enriched if population genetic model were grounded in macroecological theory. What is more, models of community assembly have been overly reliant on ahistorical patterns and assumptions of equilibrium, which are by themselves often

insufficient for distinguishing competing models of assembly [12]. The field is ready to fully merge these two approaches using the wet lab, bioinformatic, and theoretical approaches we advocate here . The time to do so is now, as society faces an increasingly non-equilibrium world, challenging our fundamental understanding of what forces govern the diversity of life and how we can best harmonize human activities with it.

Acknowledgements

We would like to thank L. Schneider for helpful comments. AJR acknowledges funding from the Berkeley Initiative in Global Change Biology and NSF DEB-1241253.

References

- [1] Sepkoski, J.J. (1984) A kinetic model of phanerozoic taxonomic diversity. III. Post-Paleozoic families and mass extinctions. *Paleobiology* 10, 246–267
- [2] Rabosky, D.L. (2009) Ecological limits and diversification rate: alternative paradigms to explain the variation in species richness among clades and regions. *Ecol. Lett.* 12, 735–743
- [3] Hubbell, S.P. (2001) *The unified neutral theory of biodiversity and biogeography*, vol. 32. Princeton University Press
- [4] Harte, J. (2011) *The Maximum Entropy Theory of Ecology*. Oxford University Press
- [5] Chesson, P. (2000) Mechanisms of maintenance of species diversity. *Annu. Rev. Ecol. Syst.* 31, 343–366
- [6] Tilman, D. (2004) Niche tradeoffs, neutrality, and community structure: a stochastic theory of resource competition, invasion, and community assembly. *Proc. Natl. Acad. Sci. U. S. A.* 101, 10854–10861
- [7] Blonder, B. *et al.* (2015) Linking environmental filtering and disequilibrium to biogeography with a community climate framework. *Ecology* 96, 972–985
- [8] Wallington, T.J. *et al.* (2005) Implications of current ecological thinking for biodiversity conservation: A review of the salient issues. *Ecol. Soc.* 10
- [9] Pueyo, S. *et al.* (2007) The maximum entropy formalism and the idiosyncratic theory of biodiversity. *Ecology Letters* 10, 1017–1028
- [10] White, E.P. *et al.* (2012) Characterizing species abundance distributions across taxa and ecosystems using a simple maximum entropy model. *Ecology* 93, 1772–1778

- [11] Ricklefs, R.E. (2006) The unified neutral theory of biodiversity: do the numbers add up? *Ecology* 87, 1424–1431
- [12] McGill, B.J. *et al.* (2007) Species abundance distributions: moving beyond single prediction theories to integration within an ecological framework. *Ecol. Lett.* 10, 995–1015
- [13] Taberlet, P. *et al.* (2012) Towards next-generation biodiversity assessment using dna metabarcoding. *Molecular Ecology* 21, 2045–2050
- [14] Gibson, J. *et al.* (2014) Simultaneous assessment of the macrobiome and microbiome in a bulk sample of tropical arthropods through dna metasytematics. *Proceedings of the National Academy of Sciences* 111, 8007–8012
- [15] Shokralla, S. *et al.* (2015) Massively parallel multiplex dna sequencing for specimen identification using an illumina miseq platform. *Scientific reports* 5, 9687
- [16] Ji, Y. *et al.* (2013) Reliable, verifiable and efficient monitoring of biodiversity via metabarcoding. *Ecology letters* 16, 1245–1257
- [17] Zhou, X. *et al.* (2013) Ultra-deep sequencing enables high-fidelity recovery of biodiversity for bulk arthropod samples without pcr amplification. *Gigascience* 2, 4
- [18] Bohmann, K. *et al.* (2014) Environmental dna for wildlife biology and biodiversity monitoring. *Trends in Ecology & Evolution* 29, 358–367
- [19] Linard, B. *et al.* (2015) Metagenome skimming of insect specimen pools: potential for comparative genomics. *Genome biology and evolution* 7, 1474–1489
- [20] Leray, M. and Knowlton, N. (2015) Dna barcoding and metabarcoding of standardized samples reveal patterns of marine benthic diversity. *Proceedings of the National Academy of Sciences* 112, 2076–2081
- [21] Dodsworth, S. (2015) Genome skimming for next-generation biodiversity analysis. *Trends in plant science* 20, 525–527

- [22] Liu, S. *et al.* (2016) Mitochondrial capture enriches mito-dna 100 fold, enabling pcr-free mitogenomics biodiversity analysis. *Molecular ecology resources* 16, 470–479
- [23] Venkataraman, A. *et al.* (2015) Application of a neutral community model to assess structuring of the human lung microbiome. *MBio* 6
- [24] Baldridge, E. *et al.* (2016) An extensive comparison of species-abundance distribution models. *PeerJ* 4, e2823
- [25] Etienne, R.S. (2007) A neutral sampling formula for multiple samples and an 'exact' test of neutrality. *Ecology letters* 10, 608–618
- [26] Rominger, A.J. and Merow, C. (2017) meter: an r package for testing the maximum entropy theory of ecology. *Methods in Ecology and Evolution* 8, 241–247
- [27] Neill, C. *et al.* (2009) A competitive coexistence principle? *Oikos* 118, 1570–1578
- [28] Rominger, A.J. *et al.* (2015) Community assembly on isolated islands: macroecology meets evolution. *Glob. Ecol. Biogeogr.*
- [29] McGill, B. (2003) Strong and weak tests of macroecological theory. *Oikos* 102, 679–685
- [30] Xiao, X. *et al.* (2015) A strong test of the maximum entropy theory of ecology. *Am. Nat.* 185, E70–E80
- [31] Webb, C.O. *et al.* (2002) Phylogenies and community ecology. *Annu. Rev. Ecol. Syst.* 33, 475–505
- [32] Lavergne, S. *et al.* (2010) Biodiversity and climate change: Integrating evolutionary and ecological responses of species and communities. *Annu. Rev. Ecol. Evol. Syst.* 41, 321–350
- [33] McGaughan, A. (2015) Integrating a population genomics focus into biogeographic and macroecological research. *Front. Ecol. Evol.* 3

- [34] Laroche, F. *et al.* (2015) A neutral theory for interpreting correlations between species and genetic diversity in communities. *Am. Nat.* 185, 59–69
- [35] Papadopoulou, A. *et al.* (2011) Testing the Species–Genetic diversity correlation in the aegean archipelago: Toward a Haplotype-Based macroecology? *Am. Nat.* 178, 241–255
- [36] Dexter, K.G. *et al.* (2012) Historical effects on beta diversity and community assembly in amazonian trees. *Proc. Natl. Acad. Sci. U. S. A.* 109, 7787–7792
- [37] Kingman, J.F.C. (1982) The coalescent. *Stochastic Process. Appl.* 13, 235–248
- [38] Rosenberg, N.A. and Nordborg, M. (2002) Genealogical trees, coalescent theory and the analysis of genetic polymorphisms. *Nat. Rev. Genet.* 3, 380–390
- [39] Kuhner, M.K. *et al.* (1998) Maximum likelihood estimation of population growth rates based on the coalescent. *Genetics* 149, 429–434
- [40] Charlesworth, D. (2010) Don’t forget the ancestral polymorphisms. *Heredity* 105, 509–510
- [41] Edwards, S.V. and Beerli, P. (2000) Perspective: gene divergence, population divergence, and the variance in coalescence time in phylogeographic studies. *Evolution* 54, 1839–1854
- [42] Wakeley, J. (2008) *Coalescent Theory*. Roberts and Company Publishers
- [43] Kern, A.D. and Schrider, D.R. (2016) Discoal: flexible coalescent simulations with selection. *Bioinformatics* 32, 3839–3841
- [44] Prado-Martinez, J. *et al.* (2013) Great ape genetic diversity and population history. *Nature* 499, 471–475

- [45] Beerli, P. and Felsenstein, J. (2001) Maximum likelihood estimation of a migration matrix and effective population sizes in n subpopulations by using a coalescent approach. *Proc. Natl. Acad. Sci. U. S. A.* 98, 4563–4568
- [46] Hey, J. and Nielsen, R. (2004) Multilocus methods for estimating population sizes, migration rates and divergence time, with applications to the divergence of *Drosophila pseudoobscura* and *D. persimilis*. *Genetics* 167, 747–760
- [47] Xue, A.T. and Hickerson, M.J. (2015) The aggregate site frequency spectrum (aSFS) for comparative population genomic inference. *Mol. Ecol.*
- [48] Hickerson, M.J. *et al.* (2006) Test for simultaneous divergence using approximate bayesian computation. *Evolution* 60, 2435–2453
- [49] Carstens, B.C. *et al.* (2016) Community trees: Identifying codiversification in the páramo dipteran community. *Evolution* 70, 1080–1093
- [50] Chan, Y.L. *et al.* (2014) Detecting concerted demographic response across community assemblages using hierarchical approximate bayesian computation. *Mol. Biol. Evol.* , msu187
- [51] Drummond, A.J. *et al.* (2005) Bayesian coalescent inference of past population dynamics from molecular sequences. *Mol. Biol. Evol.* 22, 1185–1192
- [52] Tajima, F. (1989) Statistical method for testing the neutral mutation hypothesis by DNA polymorphism. *Genetics* 123, 585–595
- [53] Jensen, J.D. *et al.* (2005) Distinguishing between selective sweeps and demography using DNA polymorphism data. *Genetics* 170, 1401–1410
- [54] Schrider, D.R. *et al.* (2016) Effects of linked selective sweeps on demographic inference and model selection. *Genetics* 204, 1207–1223

- [55] Stephan, W. (2016) Signatures of positive selection: from selective sweeps at individual loci to subtle allele frequency changes in polygenic adaptation. *Mol. Ecol.* 25, 79–88
- [56] Jabot, F. and Chave, J. (2009) Inferring the parameters of the neutral theory of biodiversity using phylogenetic information and implications for tropical forests. *Ecol. Lett.* 12, 239–248
- [57] Burbrink, F.T. *et al.* (2015) Predicting community structure in snakes on eastern nearctic islands using ecological neutral theory and phylogenetic methods. *Proceedings of the Royal Society B: Biological Sciences* 282, 20151700
- [58] Rosindell, J. *et al.* (2010) Protracted speciation revitalizes the neutral theory of biodiversity. *Ecol. Lett.* 13, 716–727
- [59] Etienne, R.S. and Rosindell, J. (2011) Prolonging the past counteracts the pull of the present: protracted speciation can explain observed slowdowns in diversification. *Systematic Biology* , syr091
- [60] Smith, B.T. *et al.* (2012) Evaluating the role of contracting and expanding rainforest in initiating cycles of speciation across the isthmus of panama. *Proc. Biol. Sci.* 279, 3520–3526
- [61] Hickerson, M.J. and Cunningham, C.W. (2005) Contrasting quaternary histories in an ecologically divergent pair of low-dispersing intertidal fish (xiphister) revealed by multi-locus DNA analysis. *Evolution* 59, 344–360
- [62] Vellend, M. (2005) Species diversity and genetic diversity: parallel processes and correlated patterns. *Am. Nat.* 166, 199–215
- [63] Wagner, P.J. *et al.* (2006) Abundance distributions imply elevated complexity of post-paleozoic marine ecosystems. *Science* 314, 1289–1292

- [64] Engen, S. and Lande, R. (1996) Population dynamic models generating the lognormal species abundance distribution. *Math. Biosci.* 132, 169–183
- [65] Harmon, L.J. and Harrison, S. (2015) Species diversity is dynamic and unbounded at local and continental scales. *The American Naturalist* 185, 584–593
- [66] Erwin, D.H. (2008) Macroevolution of ecosystem engineering, niche construction and diversity. *Trends in Ecology & Evolution* 23, 304–310
- [67] Krehenwinkel, H. *et al.* (2016) A cost-efficient and simple protocol to enrich prey dna from extractions of predatory arthropods for large-scale gut content analysis by illumina sequencing. *Methods in Ecology and Evolution*
- [68] Elbrecht, V. and Leese, F. (2015) Can dna-based ecosystem assessments quantify species abundance? testing primer bias and biomass—sequence relationships with an innovative metabarcoding protocol. *PloS one* 10, e0130324
- [69] Coissac, E. *et al.* (2016) From barcodes to genomes: extending the concept of dna barcoding. *Molecular ecology*
- [70] Nielsen, H.B. *et al.* (2014) Identification and assembly of genomes and genetic elements in complex metagenomic samples without using reference genomes. *Nature biotechnology* 32, 822–828
- [71] Angly, F.E. *et al.* (2014) Copyrighter: a rapid tool for improving the accuracy of microbial community profiles through lineage-specific gene copy number correction. *Microbiome* 2, 11
- [72] Overcast, I.A. and Hickerson, M.J. (in prep.) Integrating community assembly models and comparative population genetics.
- [73] Rosindell, J. *et al.* (2015) Unifying ecology and macroevolution with individual-based theory. *Ecol. Lett.* 18, 472–482

- 465 [74] Kelleher, J. *et al.* (2016) Efficient coalescent simulation and genealogical analysis for
466 large sample sizes. *PLoS Comput Biol* 12, e1004842
- 467 [75] Dawson, A. *et al.* (2016) Quantifying pollen-vegetation relationships to reconstruct an-
468 cient forests using 19th-century forest composition and pollen data. *Quaternary Science*
469 *Reviews* 137, 156–175
- 470 [76] Capo, E. *et al.* (2016) Long-term dynamics in microbial eukaryotes communities: a
471 palaeolimnological view based on sedimentary dna. *Molecular Ecology* 25, 5925–5943

Boxes

Box 1: Wetlab techniques

Next generation sequencing (NGS) technology has ushered in a revolution in evolutionary biology and ecology. The large scale recovery from bulk samples (e.g. passive arthropod traps) of species richness, food web structure, and cryptic species promise unprecedented new insights into ecosystem function and assembly [13–15, 67]. Two approaches, differing in cost and effectiveness, have emerged.

Metabarcoding describes the targeted PCR amplification and next generation sequencing of short DNA barcode markers (typically 300-500 bp) from community samples [16]. The resulting amplicon sequences can be clustered into OTUs or grafted onto more well supported phylogenies. Even minute traces of taxa in environmental samples can be detected using metabarcoding [18]. Amplicon sequencing is cheap, requires a small workload, and thus allows rapid inventories of species composition and species interactions in whole ecosystems [14, 20]. However, the preferential amplification of some taxa during PCR leads to highly skewed abundance estimates [68] from metabarcoding libraries.

Metagenomic approaches, in contrast, avoid marker specific amplification bias by sequencing libraries constructed either from untreated genomic DNA [19, 21], or after targeted enrichment of genomic regions [22]. While being more laborious, expensive and computationally demanding than metabarcoding, metagenomics thus offers improved accuracy in detecting species composition [17]. Moreover, the assembly of high coverage metagenomic datasets recovers large contiguous sequence stretches, even from rare members in a community, offering high phylogenetic resolution at the whole community level [69]. Due to large genome sizes and high genomic complexity, metazoan metagenomics is currently limited to the assembly of short high copy regions. Particularly mitochondrial and chloroplast genomes as well as

nuclear ribosomal clusters are popular targets [21, 69]. In contrast, microbial metagenomic studies routinely assemble complete genomes and characterize gene content and metabolic pathways even from complex communities [70]. This allows unprecedented insights into functional genetic process underlying community assembly and evolutionary change of communities to environmental stress. Such whole genome based community analysis is not yet feasible for macroorganisms. However, considering the ever increasing throughput and read length of NGS technology, as well as growing number of whole genomes, it might well become a possibility in the near future, opening up unprecedented new research avenues for community ecology and evolution.

Box 2: Bioinformatic advances

While species richness can be routinely identified by sequencing bulk samples using high throughput methods, estimating species abundance remains challenging [68] and severely limits the application of high throughput sequencing methods to many community-level studies. We propose two complementary approaches to estimate species abundance from high throughput data. The first approach estimates abundance free from any models of community assembly, the second jointly estimates the parameters of a specific assembly model of interest along with the parameters of a coalescent-based population genetic model.

Model-free abundance estimation. We propose a pipeline (Fig. 1) where raw reads are generated and assembled into a phylogeny using standard approaches, and potentially aided by additionally available sequence data in a super tree or super matrix approach. The numbers of sequences assigned to each terminal tip are then used in a Bayesian hierarchical model which seeks to estimate the true number of organisms representing each terminal tip, accounting for sequencing biases originating from, e.g. primer affinity and copy number differences between taxa. Information on phylogenetic relatedness can inform modeled correlations in biases between taxa [71, e.g. copy number is known to be phylogenetically

conserved at least in microbes]. This approach is particularly tailored to metabarcoding data. In a potentially powerful extension, and thanks to the proposed Bayesian framework, information from sequencing experiments that seek to calibrate metabarcoding studies [e.g., 67] can be used to build meaningfully informative priors and improve model accuracy. Through a simulation study (described in the supplement) we show that true underlying abundances can be accurately estimated (Fig. II).

Joint inference of community assembly and population genetic models. Coupling individual-based, forward-time models of community assembly with backwards-time hierarchical multi-taxa coalescent models permits inference about the values of the parameters in both models. This framework is flexible enough to incorporate multiple refugia, colonization routes, ongoing migration and both neutral and deterministic processes of assembly on time scales of hundreds of thousands of years (Fig. III). A forthcoming implementation [gimmeSAD π ; 72] jointly models a forward-time individual-based neutral community assembly process [73] and corresponding expectations of community level genetic diversity and divergence using the msPrime coalescent simulator [74]. This has been accomplished by rescaling the time dependent local abundance distributions into time dependent effective population size distributions while allowing for heterogeneity in migration and colonization rates. This simulation model can be combined with random forest classifiers and hierarchical ABC to enable testing alternative assembly models, including models that have not yet reached their theoretical equilibria.

Glossary

ahistorical Patterns or theories which do not contain information about the historical processes that gave rise to them

approximate Bayesian computation (ABC) . A method of calculating an approximate posterior sample of parameters in a complex model whose likelihood function cannot be analytically solved by simulating realizations of the model, computing summary statistics from those realizations, and probabilistically accepting or rejecting the parameter values leading to those summary statistics based on their agreement with the observed statistics computed from the real data.

coalescent A stochastic, backwards in time population genetic model in which alleles in the sample are traced to their ancestors under demographic models of interest.

equilibrium Equilibrium is often reserved for systems in thermodynamic equilibrium—which all life violates. By “biodiversity equilibrium” we make an analogy to thermodynamics and say that biodiversity is in equilibrium if its macroscopic state (e.g. richness of species abundance distribution, but not necessarily specific species compositions) is steady, and across arbitrary subsystems, the same steady state applies.

hierarchical model A modeling approach that facilitates complex hypotheses and causal relationships by allowing model parameters at one level to be dependent on parameters at another level.

statistical equilibrium In the context of biodiversity, a description of a steady state arrived at not by the force of one or a few deterministic mechanisms but by the stationary, statistical behavior of very large collections of mechanistic drivers acting on large assemblages of organisms.

Tajima’s D A metric of non-stationary evolution computed as the difference between two distinct derivations of theoretical genetic diversity. If neutral molecular evolution in a

566 constant population holds, both derivations should be equal, and otherwise if assumptions
567 of constant demography and neutral selection are violated, will be unequal.

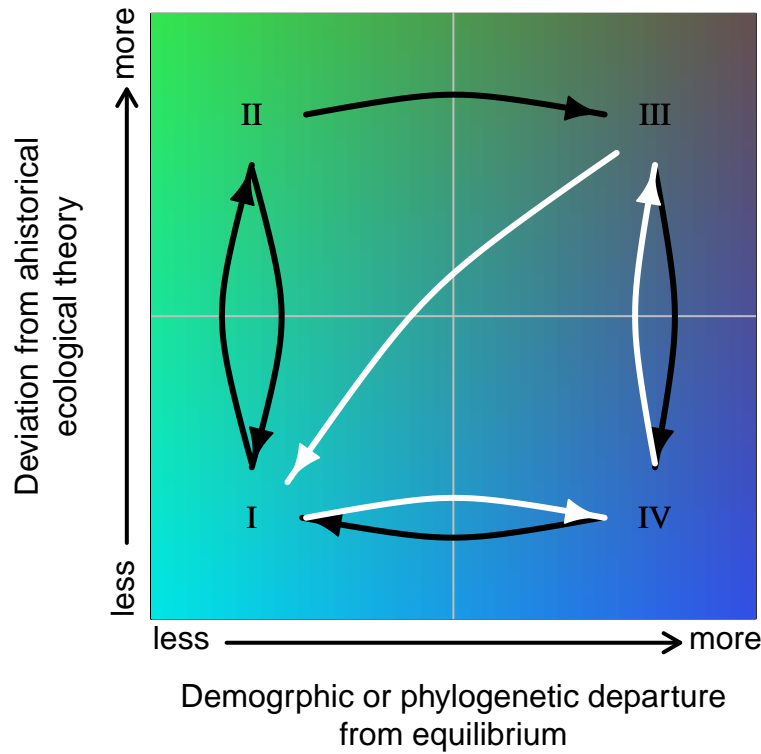


Figure 1: Hypothesized cycles between different states of equilibrium and non-equilibrium in ecological theory (y-axis) and evolutionary demography/diversification (x-axis). Deviations from ecological theory can be quantified by the previously discussed exact tests [25] and z-scores [26], while many statistics are available to quantify departure from demographic/diversification steady state including the previously discussed Tajima's D. Panels I–IV are discussed in the text. Colors correspond to deviation from ahistorical ecological theory and evolutionary equilibrium. Black cycle corresponds to non-equilibrium initiated by ecological disturbance (with potential to continue to evolutionary non-equilibrium or relaxation to equilibrium). White cycle is initiated by evolutionary innovation.

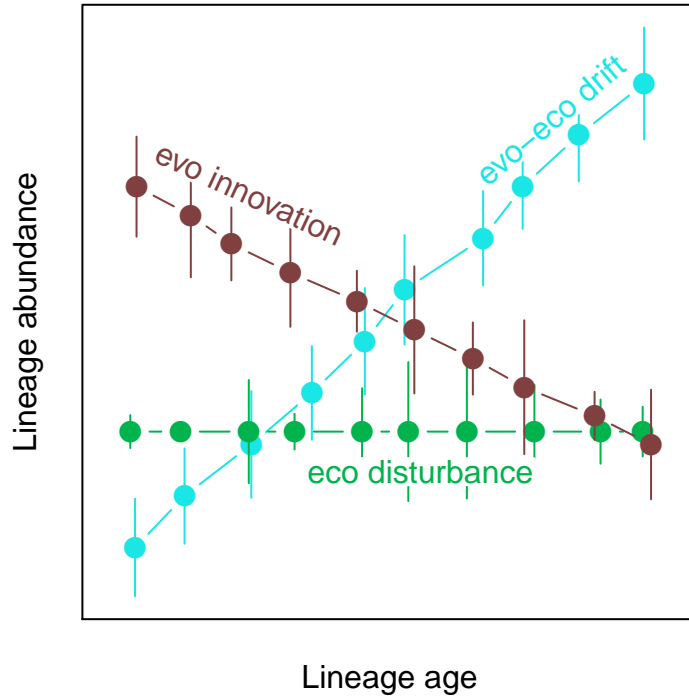


Figure 2: Hypothesized relationships between lineage age and abundance under different evo-ecological scenarios. Colors correspond to panels in Figure 1: teal is evo-ecological equilibrium; green is rapid transition to ecological non-equilibrium following short timescale disturbance; dark brown is non-equilibrium in both ecological and evolutionary metrics.

569 **Box 2** figures

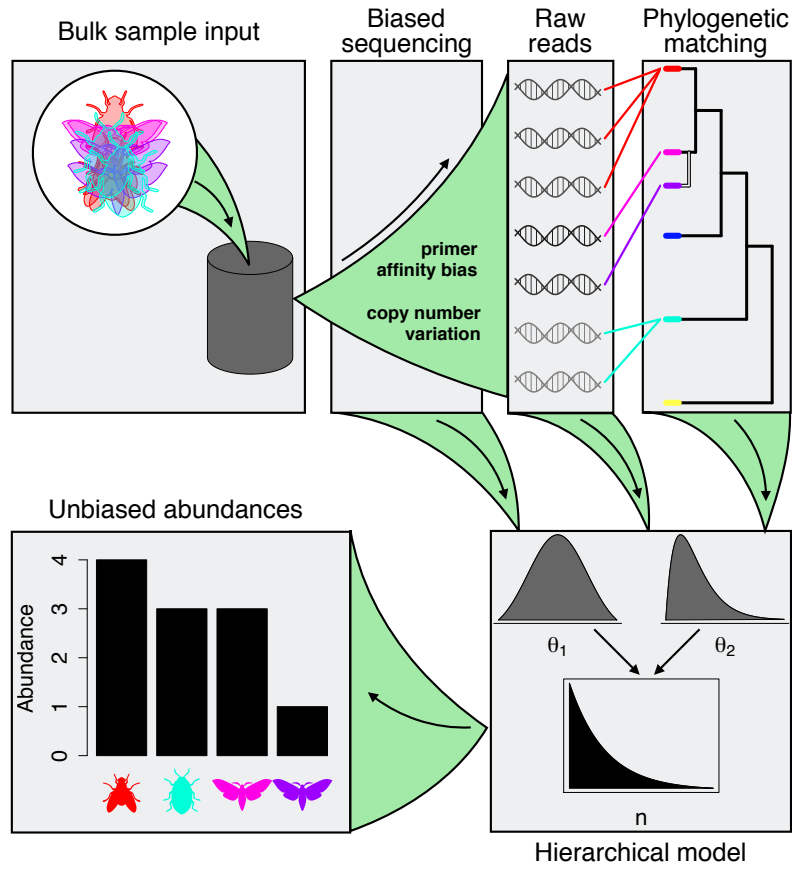


Figure I: Pipeline to estimate true abundances from metabarcoding data. The pipeline follows sequence generation, matching sequences to a phylogeny (generated from the sequences themselves, or better yet from higher coverage data) and finally Bayesian hierarchical modeling leading to abundance estimates.

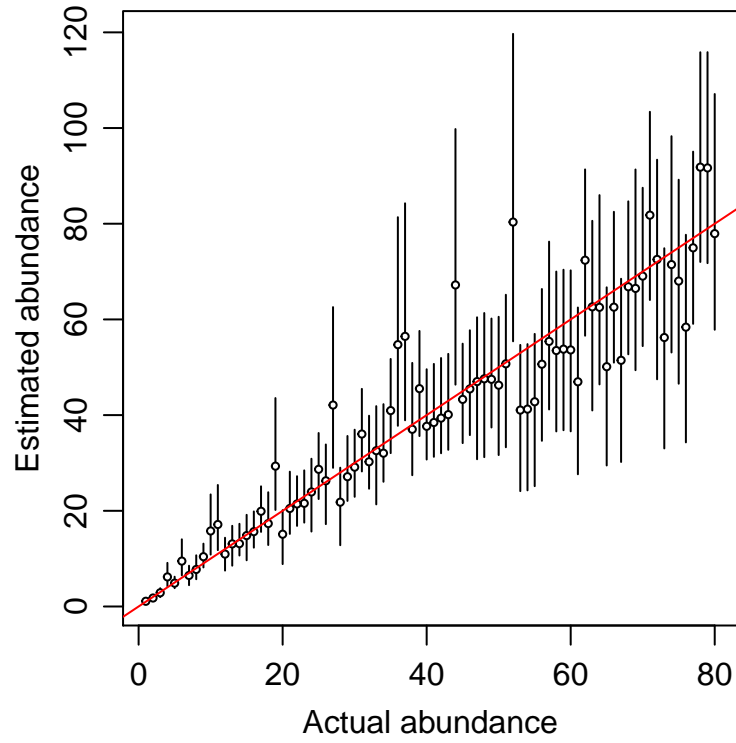


Figure II: Demonstration of agreement between actual and estimated abundances. Actual (simulated) abundances are on the x-axis, which the y-axis shows estimated abundances (error bars are 95% maximum credible intervals). The simulation study is described in the supplement.

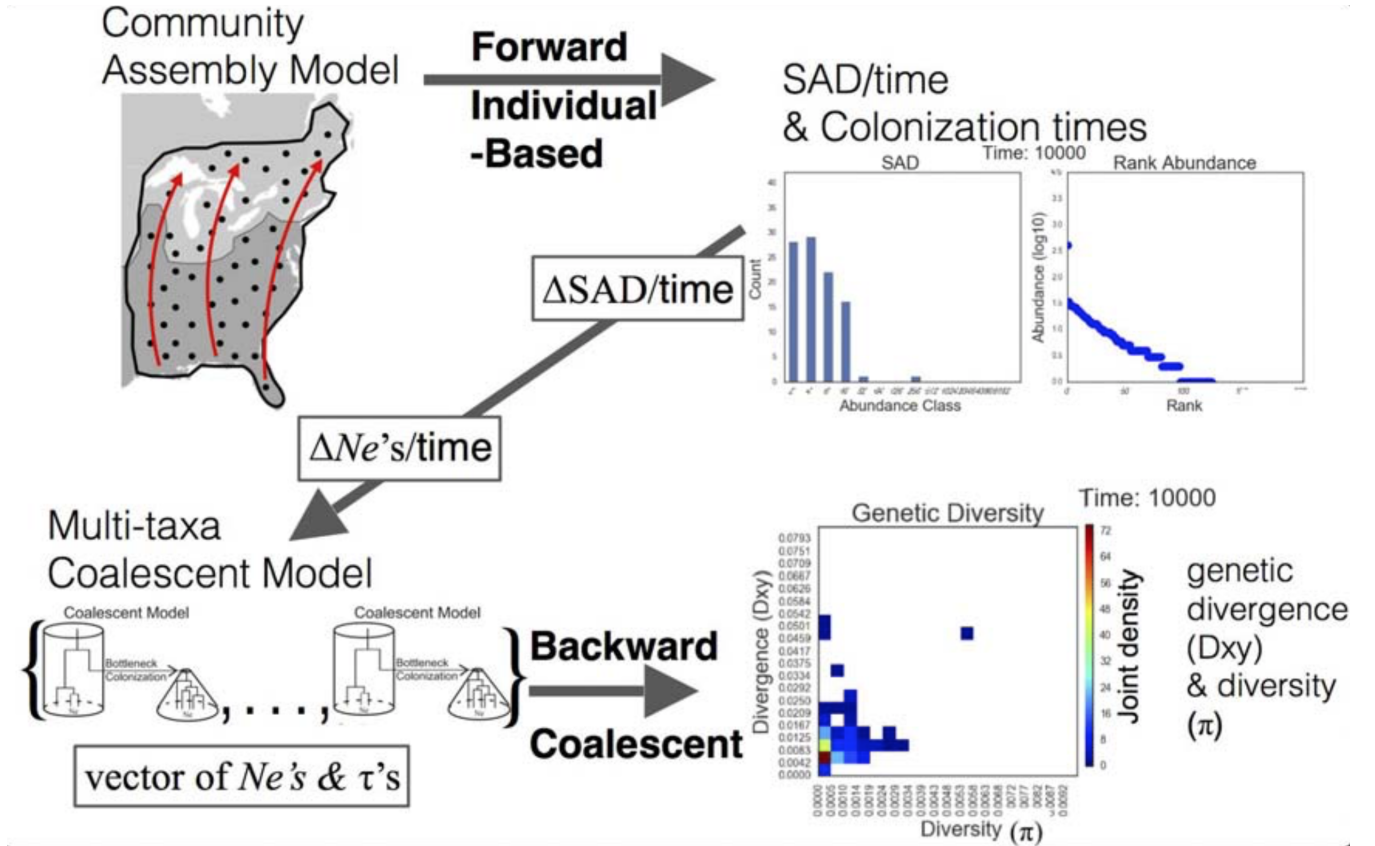


Figure III: The gimmeSAD π pipeline. The forward time models involves multi-regional expansion generating local abundance distributions over time with heterogeneity in colonization times. These temporally dynamic local abundances are re-scaled into local n_e distributions over time to generate multi-species genetic data the the coalescent, which is summarized here with a time-dependent joint spectrum of genetic diversity statistics.