RESEARCH ARTICLE

Methods in Ecology and Evolution | BRITISH ECOLOGICAL SOCIETY

Scaling up uncertain predictions to higher levels of organisation tends to underestimate change

James A. Orr[1] | Jeremy J. Piggott[1] | Andrew L. Jackson[1] | Jean-François Arnoldi[1,2]

[1]Zoology Department, School of Natural Sciences, Trinity College Dublin, Dublin, Ireland

[2]Theoretical and Experimental Ecology Station, CNRS Moulis, Moulis, France

Correspondence
James A. Orr
Email: james orr: jaorr@tcd.ie

Abstract

1. Uncertainty is an irreducible part of predictive science, causing us to over- or underestimate the magnitude of change that a system of interest will face. In a reductionist approach, we may use predictions at the level of individual system components (e.g. species biomass), and combine them to generate predictions for system-level properties (e.g. ecosystem function).

2. Here we show that this process of scaling up uncertain predictions to higher levels of organisation has a surprising consequence: it tends to systematically underestimate the magnitude of system-level change, an effect whose significance grows with the system's dimensionality. This stems from a geometric observation: in high dimensions there are more ways to be more different, than ways to be more similar.

3. We focus on ecosystem-level predictions generated from the combination of predictions at the species level. In this setting, the ecosystem's relevant dimensionality is a measure of its diversity (and not simply the number of species). We explain why dimensional effects do not play out when predicting change of a single linear aggregate property (e.g. total biomass), yet are revealed when predicting change of nonlinear properties (e.g. absolute biomass change, stability or diversity), and when several properties are considered at once to describe the ecosystem, as in multi-functional ecology.

4. As an application we discuss the consequences of our theory for multiple-stressor research. This empirical field focuses on interactions between stressors, defined as the error made by a prediction based on their observed individual effects. Our geometric approach can be visualised and explored with a web application (https://doi.org/10.5281/zenodo.4611133), and we provide pseudocode outlining how our theory can be applied. Our findings highlight and describe the counterintuitive effects of scaling up uncertain predictions, effects that can occur in any field of science where a reductionist approach is used to generate predictions.

KEYWORDS

dimensionality, diversity metrics, ecological complexity, mechanistic prediction, multifunctionality, multiple stressors, reductionism

1 | INTRODUCTION

In natural sciences, uncertainty of any given prediction is ubiquitous (Dovers & Handmer, 1992). When considering predictions of change, uncertainty has directional consequences: uncertain predictions will lead to either over- or underestimation of actual change. The reductionist approach to complex systems is to gather and use knowledge about individual components before scaling up predictions to the system level (Levins & Lewontin, 1985; Wu et al., 2006). Although scaling up to higher levels of organisation is general to the study of any complex systems, it is particularly well-defined in ecology. In this field, knowledge about the components at lower levels of organisation (individuals, populations) is commonly used to understand the systems at higher levels of organisation (communities, ecosystems; Loreau, 2010; Woodward et al., 2010).

An unbiased prediction of an individual component is one that makes no systematic bias towards over- or underestimation for that component (Box 1). But what happens when we scale up unbiased predictions to higher levels of organisation? If we do not systematically underestimate the change of individual components, will this still be true when considering many components at once? When addressing this question, one must be wary of basic intuitions as the problem is inherently multi-dimensional, thus hard to properly visualise.

As a thought experiment, consider two ecological communities, one species poor (low dimension) and the other species rich (high dimension). Both communities experience perturbations that change species biomass, and we assume that we have an unbiased prediction for this change, up to some level of uncertainty. We then scale up our predictions to the community level, focusing on the change in Shannon's diversity index, caused by the perturbations. By comparing predicted and observed change we can quantify the degree of underestimation of our predictions, at the species and community level. If we simulate this thought experiment (Figure 1a; Appendix S5) we observe the following puzzling results, which motivate our subsequent analysis. Predictions of species biomass change may be unbiased (bottom row of Figure 1a), but when scaled up to the system level for the species-rich community, but not the species-poor community, we see a clear bias towards underestimation of change (top right corner of Figure 1a). In fact, we can generalise this in silico experiment and see that for various ways of measuring change (Euclidean distance, difference in Shannon's diversity index, difference in invariability of total biomass), but not for others (difference in total biomass), this bias towards underestimation grows with species richness, that is, with the dimension of the system (Figure 1b).

As we shall explain in depth, the reason for this emergent bias is that *in high dimensions there are more ways to be more different, than ways to be more similar*. Our goal is to make this statement quantitative and generally relevant to ecological problems. We start from a geometric approach showing that, in two dimensions, our claim can be visualised to reveal a positive relationship between magnitude of uncertainty and underestimation of change. Visualisation is only possible in low dimensions, but a more abstract reasoning

---

BOX 1 Lexicon of concepts

Reductionist view of complex systems

- *Components*: Individual variables B_i that together form a system (e.g. biomass of S species and abiotic compartments forming an ecosystem).
- *System state*: Point in *state space*, represented as a vector $\boldsymbol{B} = (B_1, \ldots, B_S)$ jointly describing all system components.
- *Difference (or magnitude of change) between states*: Euclidean distance $\lVert \boldsymbol{B} - \boldsymbol{B}' \rVert$ between two joint states $\boldsymbol{B}$ and $\boldsymbol{B}'$.

Scaling up uncertain predictions

- *Relative error*: Magnitude of error caused by uncertainty relative to the magnitude of predicted change.
- *Aggregate system-level property*: Scalar function of the joint state (e.g. total biomass or diversity index)
  - *Linear aggregate property*: Linear function of joint state variables (e.g. total biomass).
  - *Nonlinear property*: Nonlinear function of joint state variables (e.g. diversity index).
- *Scaled up prediction:* A prediction made for the joint state, or a scalar property of the joint state, based on individual predictions for components.
- *Unbiased prediction:* A prediction that, despite uncertainties, does not systematically overestimate or underestimate the magnitude of change (of a joint state, a system component or an aggregate property).

Multi-functional view of complex systems

- Multivariate description of a complex system, based on multiple aggregate properties, or *functions* (production, diversity, respiration) instead of individual components (species biomass and abiotic compartments). The state of the system is the joint state $\boldsymbol{F} = (F_1, \ldots, F_{S_F})$ of S_F functions. Difference between states is the distance between two joint functional states $\boldsymbol{F}$ and $\boldsymbol{F}'$.

---

demonstrates that as dimensionality increases so does the bias towards underestimation, which is further strengthened by larger uncertainty. We note that dimensionality is not necessarily an integer value. We propose that the effective dimensionality most relevant to ecological upscaling of predictions is not the number of species, but instead is a specific diversity metric, the inverse participation ratio (IPR; Suweis et al., 2015; Wegner, 1980), comparable (but not equivalent) to Hill's diversity indices (Hill, 1973).

We then explain why the effect of dimensionality depends on how change is measured at the system level (Box 1). If a single linear
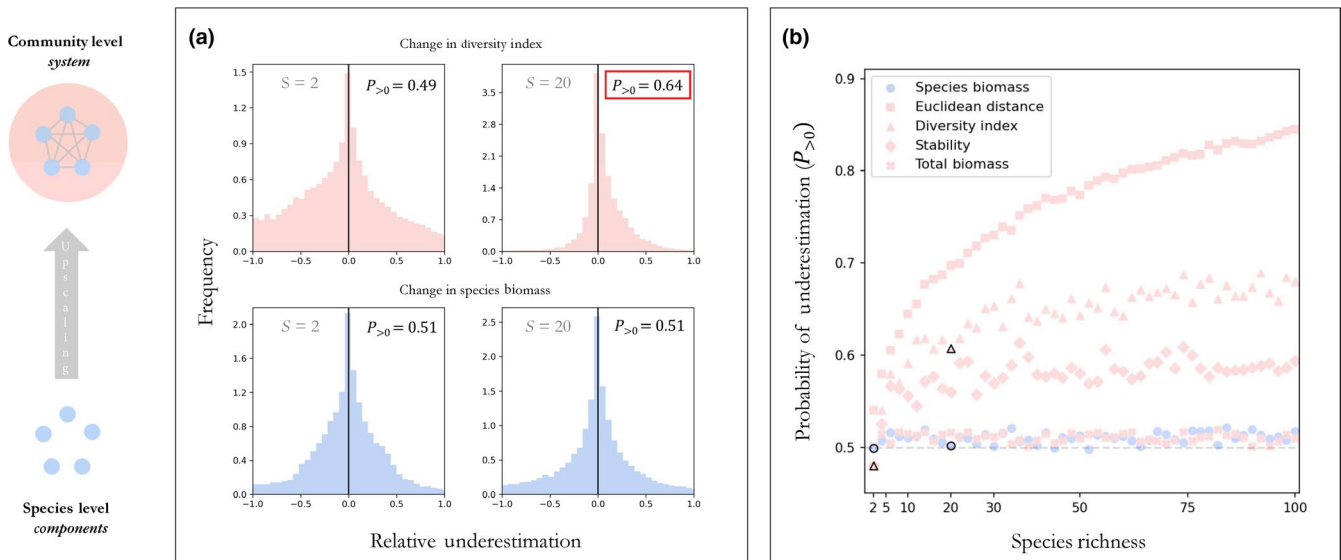
FIGURE 1 (a) Simulated communities of 2 species (left) and 20 species (right) experienced many simulated perturbations (change in species biomass), for which we assume unbiased predictions at the species level. Uncertainty around those predictions is simulated as random terms of zero mean, independent across species. Histograms show the distribution of relative underestimation, defined as the difference between realised and predicted change expressed relatively to the predicted magnitude of change. The probability of underestimation, the probability of relative underestimation being positive, is shown in each plot. By construction, there is no bias towards underestimation at the species level (bottom row). We then scale up our predictions to the community level to generate predictions for Shannon's diversity index (top row). For the first, species-poor community, this upscaling does not generate any bias. However, for the species-rich community a bias emerges as 64% of realisations show an underestimated magnitude of change. (b) An extension of these simulations to many different communities ranging from 2 to 100 species shows that this bias towards underestimation grows with the dimensionality of the system for some aggregate properties (Euclidean distance, diversity index, stability measured as invariability of biomass) but not others (total biomass). The four points outlined in black correspond to the four histograms in part (a)

function is used to aggregate components (e.g. total biomass), dimensionality has no effect. An unbiased prediction for individual components trivially scales up to produce an unbiased system-level prediction. But this is not true in general. Nonlinear functions (e.g. Shannon's diversity index as in Figure 1), can remain sensitive to dimensional effects. Predictions of change of these properties, even if constructed from unbiased predictions of individual components can be systematically underestimated. The significance of this effect will depend on the relative significance of nonlinearities in the function of interest.

On simulated examples we will examine the behaviour of common ecosystem-level properties: diversity, stability and total biomass (the archetypal measure of ecosystem functioning (Loreau et al., 2001)). More generally, we emphasise that dimensional effects will occur as soon as system-level change is measured as a change in multiple properties at once (whether they are linear or not), as is the case in multi-functional descriptions of ecosystems (Manning et al., 2018).

As a seemingly different kind of ecological case study, we then revisit core questions of multiple-stressor research in the light of our theory. In this field, there is a clear prediction (additivity of stressor effects), a high prevalence of uncertainty about the way stressors interact (resulting in non-additivity) and, ultimately, great interest in the ecosystem-level consequences of non-additive stressor interactions (synergism or antagonism; Côté et al., 2016; Jackson et al., 2016; Piggott et al., 2015). Expressed in this context, our theory predicts

the generation of bias towards synergism when multiple-stressor predictions are scaled up to higher levels of organisation.

Research has primarily focused on the causes of uncertainty, working hard to reduce it (Petchey et al., 2015). Here we take a complementary approach by investigating the generic consequences of uncertainty, regardless of the nature of the system studied or the underlying causes of uncertainty. Our theory becomes more relevant as the degree of uncertainty increases, which makes it particularly relevant for ecological problems. But, in fact, our findings could inform any field of science that takes a reductionist approach in the study of complex systems (e.g. economics, energy supply, demography, finance—see Appendix S4), demonstrating how dimensional effects can play a critical role when scaling up predictions.

2 | GEOMETRIC APPROACH

The central claim of this article is that *in high dimensions there are more ways to be more different, than ways to be more similar*. We propose an implication: *a system-level prediction based on unbiased predictions for individual components, tends to underestimate the magnitude of system-level change*.

To understand these statements, it is useful to take a geometric approach to represent the classic reductionist perspective, starting in two dimensions (Figure 2a). Picture two intersecting circles in a system's state space (one blue, one red in Figure 2). The
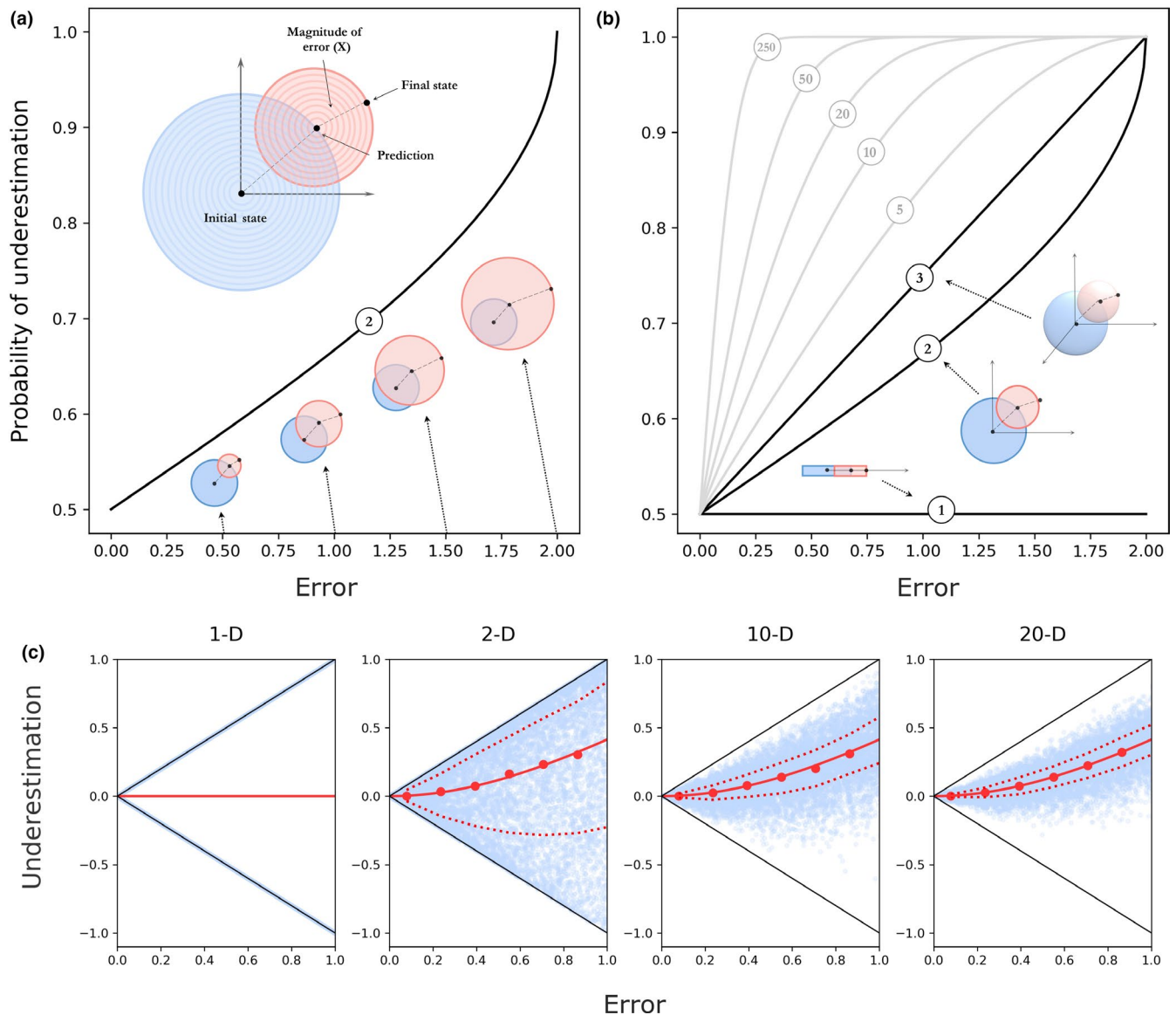
FIGURE 2 (a) Already in two dimensions, the probability of underestimation increases as uncertainty increases. The centre of the blue circle is the initial state (its actual value is irrelevant) and its radius is defined by the predicted magnitude of change. The point at the centre of the red circle corresponds to the predicted state, while its radius represents the magnitude of error made by the prediction. By definition, final states thus fall on the edges of the red circle. If a final state falls inside the blue circle then there has been an overestimation of change (it is closer to the initial state than what was predicted). If a final state falls outside the blue circle (as in the figure) then there has been an underestimation of change (it is farther from the initial state than what was predicted). When uncertainty (thus error) is small, the radius of the red circle is small, and the probability of underestimation is close to 0.5. As error increases, however, there is increasing bias towards underestimation. Eventually when error is twice as large as the prediction only underestimation is possible. (b) This relationship between uncertainty and underestimation is strengthened by dimensionality. As dimensions increase there become even more ways to be more different than ways to be more similar. Each curve corresponds to the probability of underestimation as a function of error for different dimensions labelled as circled numbers. For a fixed amount of error the probability of underestimation will increase with dimension. (c) The relationship between the relative magnitude of error (x) and the relative magnitude of underestimation (y) based on uniform sampling of 1-D, 2-D, 10-D and 20-D intersecting hyper-spheres defined by unbiased but uncertain predictions. The boundaries of this relationship are plotted in black and the median expectation $\tilde{y} = \sqrt{x^2 + 1} - 1$ as derived from Equation (4) is plotted in red (except for 1-D where it does not apply). Blue points are simulated results, red points are the actual median values and dashed lines show the quantiles for vertical subsets of the simulated data. As dimensionality increases the width of the distribution decreases and converges towards its median, which effectively increases the probability of underestimation (b)

first, blue circle is centred on the system's initial state and its radius corresponds to the predicted magnitude of change. The second, red circle is centred at the predicted state (which lies on the

blue circle) and its radius corresponds to the magnitude of realised error of the prediction, in other words, the realised outcome of the uncertainty associated with the prediction (red circle in Figure 2).

The actual final state is thus somewhere on that red circle. If it falls inside the blue circle, the prediction has overestimated the magnitude of change. If, however, it falls outside the blue circle, the prediction has underestimated the magnitude of change. The proportion of the red circle lying outside the blue circle measures the proportion of possible configurations that will lead to an underestimation of change. In other words, for a given magnitude of error caused by uncertainty, this portion of the circle represents the states that are more different from the initial state than predicted. As the relative magnitude of error increases (as the red circle's diameter becomes larger, relative to that of the blue circle) this proportion grows (Figure 2a).

In three dimensions these two intersecting circles become two intersecting spheres. The proportion of interest is the surface of the spherical cap lying outside of the sphere centred on the initial state. Here, a non-intuitive phenomenon occurs: with the same radii as in the 2D case, in 3D there are now more configurations leading to underestimation. As dimensions increase this proportion increases, until the vast majority of possible states lie in the domain where change is underestimated (Figure 2b). This result can be made quantitative from known expressions for the surface of hyper-spherical caps. This gives us an analytical expression for the proportion of configurations leading to an underestimation of change, as a function of the relative magnitude of error (x) and dimension (S):

$$P_{>0}(x) = 1 - \frac{1}{2} I_{1-\frac{x^2}{4}} \left(\frac{S-1}{2}; \frac{1}{2} \right); x = \frac{\|error\|}{\|prediction\|}. \quad (1)$$

In the above equations $\|\cdot\|$ stands for the standard Euclidean norm of vectors,[1] and $I_s(a, b)$ is the cumulative function of the β-distribution (Appendix S2). This is what we mean by *in high dimensions there are more ways to be more different, than ways to be more similar*. To see how this relates to the scaling up of unbiased predictions of individual components (Box 1), we now take a statistical approach. Suppose we uniformly sample the intersecting circles, spheres and hyper-spheres defined above and drawn in Figure 2. The proportion (Equation [1]) becomes a probability, the probability of having underestimated change. This uniform sampling is precisely what happens if the uncertainty of individual variables is independent random normal variables with zero mean (a particular case of an unbiased uncertainty at the component level, see Appendix S2). This justifies our second claim: *a system-level prediction based on unbiased predictions for individual components, tends to underestimate the magnitude of change of the system state*.

This reasoning is geometric and relies on a computation of the surface of classic shapes, such as hyper-spheres and spherical caps. But, the core mechanism behind the behaviour of the probability of underestimation is more general and, in a sense, simpler. To see that,

let us take a step back and analyse the relative magnitude of underestimation, defined as:

$$y = \frac{\|response\| - \|prediction\|}{\|prediction\|}. \quad (2)$$

Given an angle θ between prediction and error vectors (resp. the vectors that point from initial to predicted state, and from predicted state to realised state) we can rearrange Equation (2) as:

$$y(x, \theta) = \sqrt{x^2 + 2x\cos(\theta) + 1} - 1. \quad (3)$$

the term $\cos\theta$ can take any values between -1 and $+1$. For the sake of simplicity, in what follows we will suppose that its mean and median are zero. This is the case if the errors associated with individual variables are drawn from independent symmetric distributions centred on zero (unbiased and unskewed predictions at the component level). In this case the median relationship between error (x) and underestimation (y) is:

$$\tilde{y} = \sqrt{x^2 + 1} - 1. \quad (4)$$

which is strictly positive as soon the error x is non-zero. This holds true in all dimensions greater than one, which can be seen in Figure 2c. The median underestimation $\tilde{y}$ does not depend on dimension, but the probability of underestimation, $P(y > 0; x)$, does. Indeed, $P(y > 0; x)$ is driven by the distribution of the random term $\cos\theta$ in Equation (3). If this distribution is narrow, realisations of y will fall close to $\tilde{y}$. Because the latter is positive and increases predictably with x, so will the probability of any realised y to be positive. Our framework assumes that the difference between two states, regardless of the system's dimensionality, is described by a single number. For multi-dimensional systems this allows for the counter-intuitive scenario where an uncertain prediction can nonetheless accurately predict the magnitude of system-level change.

A known fact from random geometry is that, given a random isotropic vector (i.e. a vector whose direction is uniformly distributed on the sphere), its angle θ with any other given vector satisfies.

$$\mathbb{E}(\cos\theta) = 0; \text{ and } Var(\cos\theta) = \frac{1}{S}. \quad (5)$$

In other words, in high dimensions random vectors are approximately orthogonal, up to a variance inversely proportional to the dimension of state space. In our context, this corresponds to normal i.i.d. distributions of errors, a particular case of independent unbiased and unskewed predictions. This explains why the probability of underestimation increases in Figure 2b with both dimension S and error x. In what follows we use the expression for the variance in Equation (5) as a *definition* of *effective dimension*. In doing so, we can free ourselves from the strict Euclidean representation of Figure 2, and generalise the theory beyond i.i.d. normal error distributions. This will be useful when

---

[1]This is the most convenient norm for our geometric approach but other norms would give similar results.

applying our theory to ecological problems, where components are the biomass of species, and their contributions to ecosystem change are not equivalent, thus errors not i.i.d. Our geometric approach can be explored using the web application at https://doi.org/10.5281/zenodo.4611133.

3 | RELEVANCE TO ECOLOGY

3.1 | Effective dimensionality

We now assume that the axes that define state space represent the biomass of the species that form an ecological system. These species may have very different abundances, and thus will not all contribute equally to a given change. For instance, in response to environmental perturbations, biomass of species typically change in proportion to their unperturbed values (Arnoldi et al., 2018; Lande et al., 2003). The more abundant species (in the sense of higher biomass) will thus likely contribute more to the ecosystem-level change. Thus, if we use species richness as a measure of dimensionality, as the above section would suggest, we will surely exaggerate the importance of rare (i.e low biomass) species. But using Equation (5) to *define dimensionality*, we can resolve that issue. In doing so we show that the relevant dimension when applying our ideas to ecological problems is really a measure of diversity of the community prior to the change, which may not be an integer, and will typically be smaller than the number of individual components.

In fact (Appendix S3), if a species contribution to change is statistically proportional to its biomass B_i the effective dimensionality of a system is the IPR of the biomass distribution,[2] which reads:

$$\text{IPR} = \frac{\left(\sum_{i=1}^{S} B_i^2 \right)^2}{\sum_{i=1}^{S} B_i^4}. \tag{6}$$

This non-integer diversity metric was developed in quantum mechanics to study localisation of electronic states (Wegner, 1980). The IPR approaches 1 when a single species is much more abundant than the others, and approaches S when species have similar abundance—see Suweis et al. (2015) where this metric is used in an ecological context. Note that the IPR is closely related (but not equivalent) to Hill's (1973) evenness measure $^2D = (\sum_i B_i)^2 / \sum_i B_i^2$ (see Appendix S3).

We can show that it is indeed the IPR that determines the variance (over a sampling of predictions and associated uncertainties of species biomasses) of the term $\cos\theta$ in Equation (3) so that:

$$\text{Var}(\cos\theta) = \frac{1}{\text{IPR}}. \tag{7}$$

An uneven biomass distribution thus increases the width of the distribution of underestimation y therefore reducing the probability of

a given realisation of change to have been underestimated. If species richness accurately predicted the width of the distribution of underestimation and therefore the probability of underestimation, the two simulated communities in Figure 3 would behave in the same way. However, the probability of underestimation is lower than expected based on richness, particularly for the community with a more uneven biomass distribution. Indeed, replacing richness S by the IPR in Equation (1) provides an excellent approximation of the behaviour of the probability of underestimation (Figure 3).

3.2 | Aggregate properties and nonlinearity

When scaling up predictions, there are different ways of measuring system-level change (Box 1). The classic reductionist approach is to quantify change via the Euclidean distance in state space, thus keeping track of the motion of joint configurations. This is what we have done so far. Ecologically, this could correspond to measuring the absolute biomass change of a community. Here, by construction, our theory is directly relevant.

But other, non-reductionist, ways of quantifying change at the system level are possible. In ecology, this could correspond to measuring changes in the diversity, stability or functioning of the ecosystem. Yet, if differences in these properties between two states correlate with the distance in the reductionist state space, then our theory will remain relevant. As can be seen in Figure 4, this can be the case for diversity (Shannon's index) and stability (invariability of total biomass, Haegeman et al., 2016). Our theory thus applies to those ecosystem-level properties. This leads us to the conclusion that their degree of change may be systematically underestimated by predictions built from species-level predictions.

On the other hand, changes in total biomass (ecosystem functioning) do not correlate well with state-space Euclidean distance. This is due to the fact that total biomass is a linear function of species biomass (i.e. the sum). In fact, quantifying system-level change via a linear function acts as a projection from the state space onto a one-dimensional space defined by the function. Thus, despite the fact that the ecosystem might be constituted of many species (intrinsically high dimensional) the problem of scaling up predictions is essentially one dimensional. This is why bottom-up predictions of change of total biomass show no additional bias towards underestimation.

More generally, when the linear part of the aggregate property of interest is dominant, dimensional effects are obscured. However, as soon as we consider changes of multiple properties at once, as in multi-functionality approaches in ecology (Box 1), dimensional effects will play out—even if all aggregate properties are essentially linear.

3.3 | Multi-functionality

Scaling up predictions from individual components to an aggregate property can lead to a bias towards underestimation, due to

---

[2]Our theory allows other choices of statistical relationships between biomass and contribution to change, leading to other diversity metrics, which can be seen as generalisation of the inverse participation ratio.
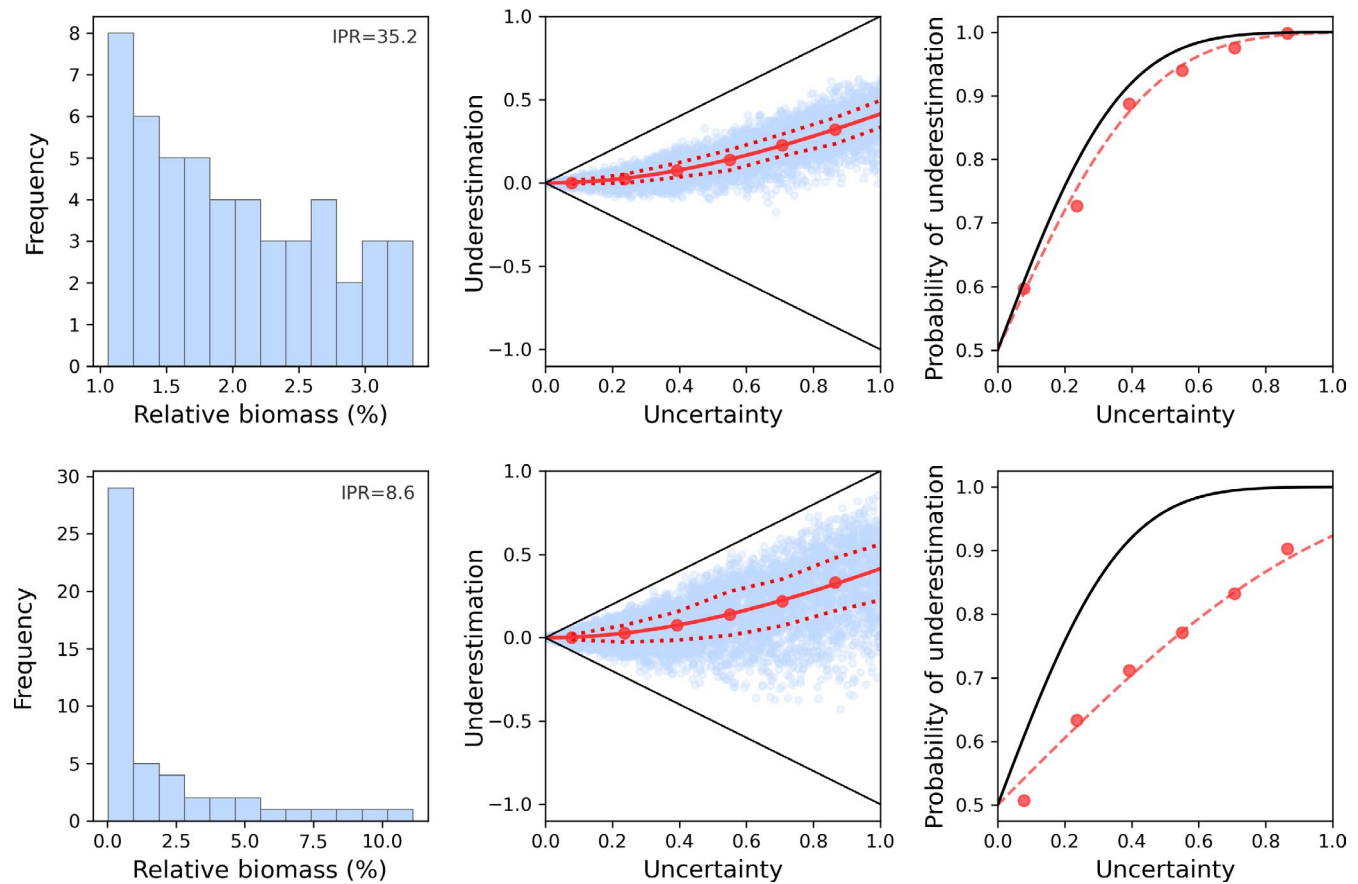
FIGURE 3 Each row corresponds to simulations of 50 species communities with uneven biomass distributions that have experienced perturbations. The first column shows the biomass distributions of these communities. The two communities have inverse participation ratio (IPR), and therefore effective dimensionality, of 35.2 and 8.6. The second column shows the relationship between error and underestimation of these two communities when unbiased predictions of biomass change are scaled up to change in state-space distance. As the biomass distribution becomes more uneven the variance around the median increases (dashed lines are quantiles), which effectively reduces the probability that a given change was underestimated. This can be seen in the third column where predictions using the dimension of state space (50, black curves) are outperformed by predictions using the IPR (35.2 and 8.6. red curves). Red points show the actual probabilities of underestimation for vertical subsets of the simulated data and are accurately predicted using the IPR

dimensional effects. We explained that this occurs for nonlinear aggregate properties, but not linear ones (such as total biomass). Is this to say that our theory is only relevant when predicting the change of nonlinear system-level properties? Yes, but only in the restricted realm of one-dimensional approaches to complex systems.

Using a single function, for example a diversity index, to describe an ecosystem reduces the complexity of the system down to a single number and will potentially hide important details (Hurlbert, 1971). Consequently, there is a growing interest in multi-functionality approaches in ecology (Manning et al., 2018). These approaches are multivariate descriptions of ecosystems, an alternative to the reductionist perspective to account for the multidimensional nature of ecological systems (Box 1). By considering the change of multiple functions at once, even if these functions are essentially linear, dimensional effects will resurface.

To be clear, we still assume that we scale up predictions from the species to the ecosystem level. Only now we scale up predictions from species to several system-level properties at once,

that describe the ecosystem's state from a multi-functional point of view (Box 1). Let us suppose, for simplicity, that those aggregate properties (or functions) are linear. We have seen that considering a single linear function, in terms of upscaling of predictions, effectively reduces the problem to a single dimension. Likewise, considering multiple linear functions essentially reduces the effective dimensionality to the number of functions. Subtleties arise when the number of functions (S_f) and the dimensionality of the underlying system (e.g. IPR) are similar, and/or if the considered functions are collinear (see Appendix S3). For S_f independent functions measured on a community we find that the effective dimensionality (the one that determines the probability of underestimation of change) is:

$$S_{\text{eff}} \approx \frac{1}{\frac{1}{\text{IPR}} + \frac{1}{S_f}}. \tag{8}$$

For example, if the change of an ecosystem with an IPR of 10 is measured using 10 linear functions at once, the effective dimensionality
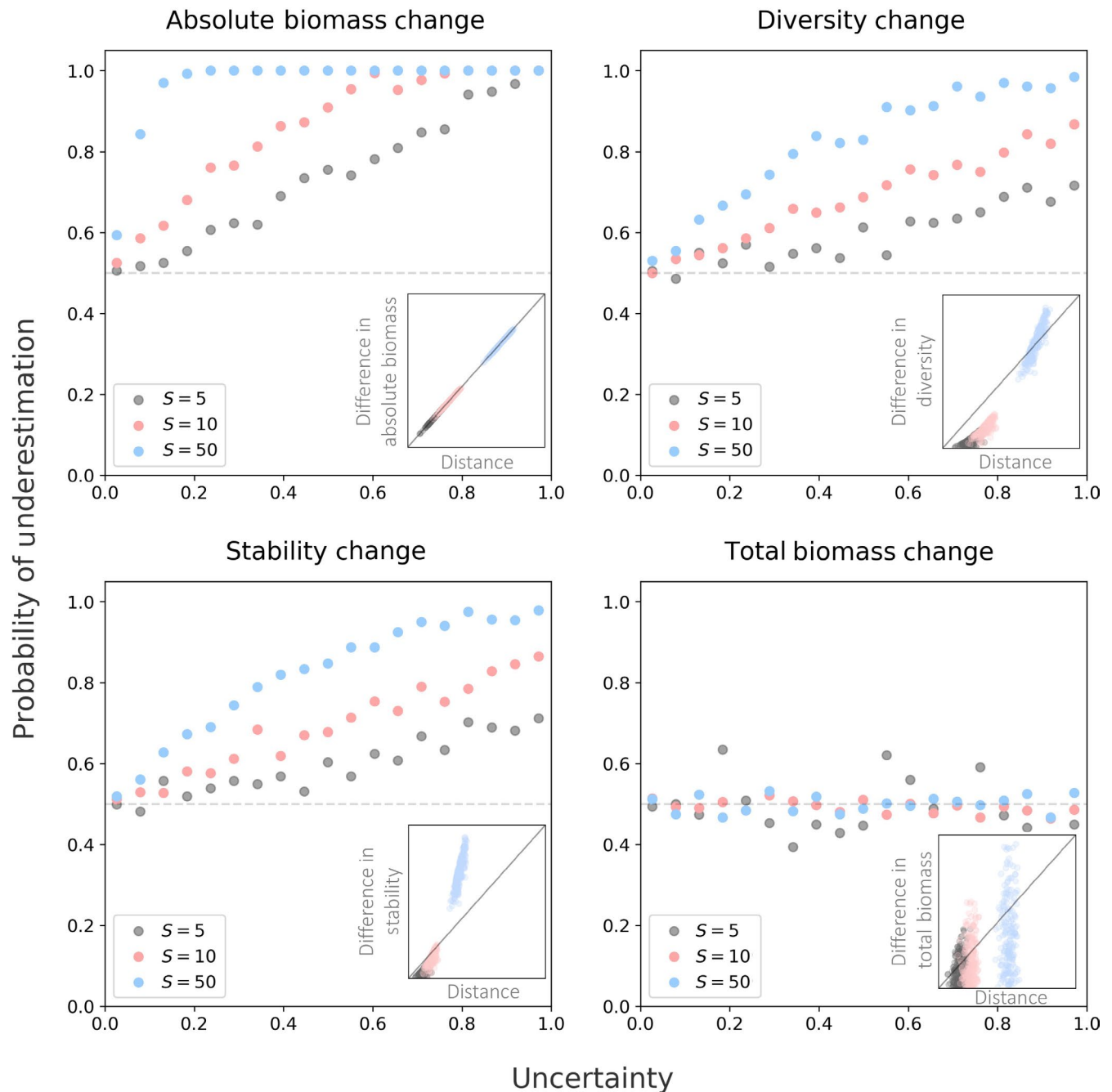
FIGURE 4 Simulated communities of 5 (grey), 10 (red) and 50 (blue) species experienced some change in their biomass. Unbiased predictions of species' biomass change were scaled up to predictions of change in ecosystem-level aggregate properties. The relationship between uncertainty and the probability of underestimation is show for changes in: (1) absolute biomass, (2) diversity, specifically the Shannon index, (3) stability, specifically invariability and (4) total biomass. Subplots show the relationship between changes in each aggregate property and changes in Euclidean distance. Absolute biomass change is analogous to Euclidean distance. Diversity and stability (nonlinear functions) show some correlation with Euclidean distance and are therefore sensitive to dimensional effects. Total biomass (linear function) does not correlate with Euclidean distance so scaled up predictions of change of this aggregate property remain unbiased

is ~5 (Figure S1). If functions are collinear the effective dimensionality will be even lower than S_f. This is to be expected, especially when thinking of an extreme case: if we measure the same function multiple times we should see no dimensional effects. In summary, in a multivariate description of complex systems, dimensional effects will inevitably play out, in more or less intricate ways, whenever a prediction is scaled up from individual components to the system level.

4 | DISCUSSION

Our work demonstrates that a bias towards underestimation of change emerges when unbiased predictions of individual components (e.g. species biomass) are scaled up to the system level (e.g. ecosystem function). Our geometric approach reveals a direct relationship between the probability of underestimation, the magnitude

of error caused by uncertainty and a system's effective dimensionality. This effective dimensionality is not necessarily the number of individual components that form a system, but rather a measure of diversity sensu Hill (1973). In essence, these results come from the fact that *in high dimensions there are more ways to be more different, than ways to be more similar* (Figure 5).

Importantly, it is nonlinear aggregate properties (e.g. absolute biomass change, stability or diversity) that are sensitive to dimensional effects (Figure 5). For linear properties (e.g. total biomass), scaling up does not generate bias. Yet, even in this case, dimensional effects do play out when several functions are considered at once to describe the ecosystem, as in multi-functional approaches in ecology.

Natural systems are intrinsically complex and the way that we describe them is necessarily multivariate (Loreau, 2010). It is generally accepted in ecology that there is a need for mechanistic predictive models, built from individual components and scaled up to the ecosystem level (Harfoot et al., 2014; Mouquet et al., 2015; Poff, 1997; Woodward et al., 2010). We have shown that dimensional effects

will play out in this scaling up, generating additional bias towards underestimation of any predicted system-level change. This is not to say that scaling up predictions is a faulty approach, rather that one must keep track of dimensional effects when doing so.

Our theory provides a generic expectation for the consequences of uncertainty when predictions are scaled up from individual components to the system as a whole. By construction our results are based on 'non-complex' behaviour, in the sense that we assume no correlations between unbiased prediction errors of individual components. Our theory can therefore be thought of as a baseline, a null model of what to expect if only dimensional effects are at play, against which we can test biological (or other) effects. Indeed, interactions between components (e.g. species interactions) may introduce systematic correlations between the prediction errors for each component, which we have assumed independent. This might in turn add further biases towards over- or underestimation, on top of the biases due to dimensional effects. Viewed this way, our research highlights a delineation between statistical and natural
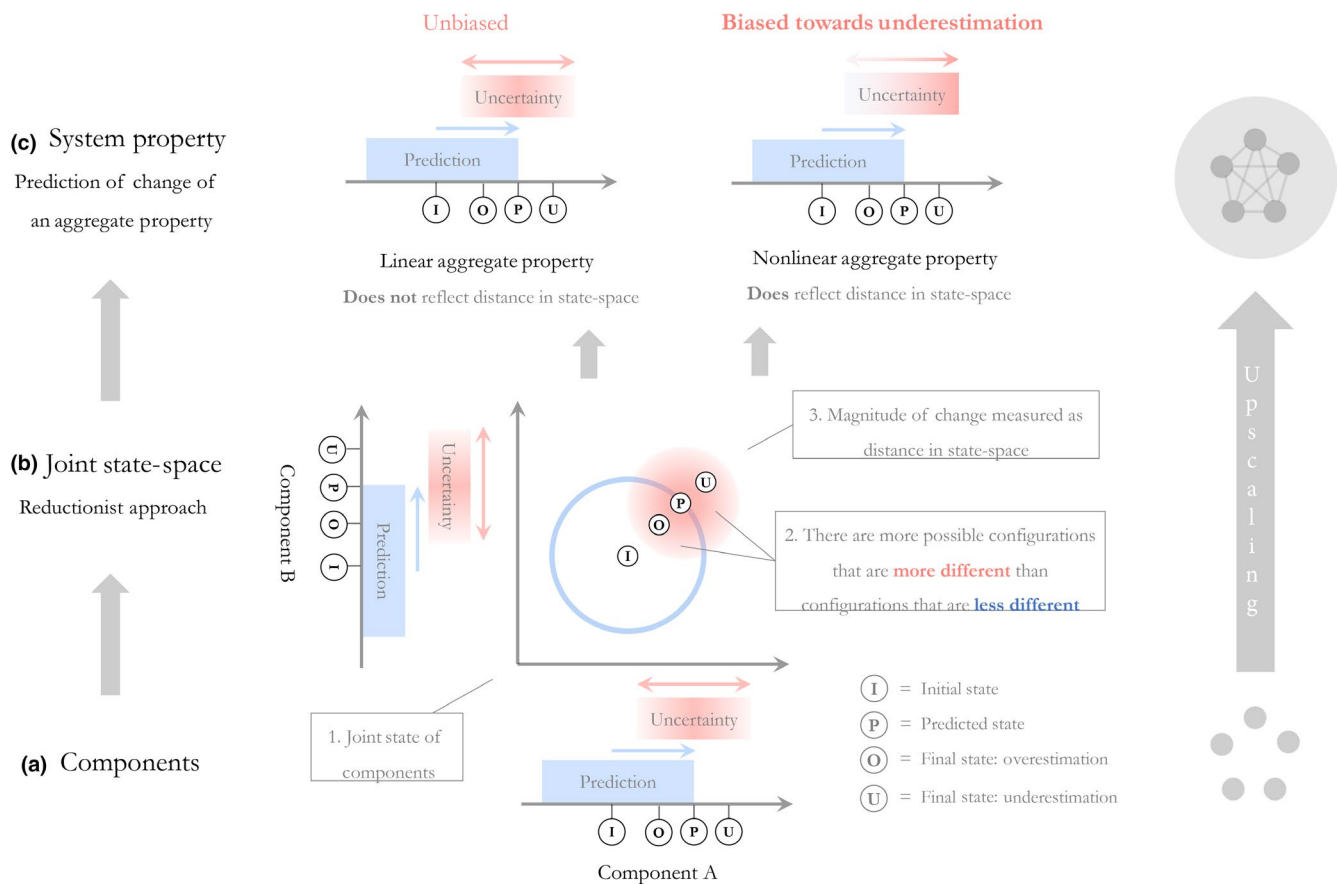
FIGURE 5 An overview of our main findings. (a) Two components, A and B are (b) considered at once to define a joint state (I). Suppose this state changes and falls near a predicted state (P). Then there are more ways for this state to be more different from (I), than ways to be more similar; more of the red disc is outside the blue circle than inside. Consequently, when predictions of change (blue) for individual components are scaled up to predictions of change of their joint state, unbiased uncertainties (red) become biased towards underestimation. In Section 2 we quantified these surprising dimensional effects and investigate beyond the basic two-dimensional case shown here. (c) Magnitude of system-level change can be measured as distance in state space or by some other aggregate property. If an aggregate property is sensitive to changes in distance of the underlying state space, dimensional effects, and therefore a bias towards underestimation, will be conserved. As we explained in Section 3.2, it is the nonlinear part of an aggregate property that controls its sensitivity to changes in state-space distance and thus the tendency of its change to be underestimated by upscaled predictions

mechanisms controlling the behaviour of complex systems (Nekola & Brown, 2007).

We considered two levels of organisation: the level where predictions are made and the level where predictions are scaled up to. In principle, intermediate levels could be considered. For instance, given the increasing resolution of ecological data, predictions of change may originally be based at the level of individual organisms and could first be scaled up to species-level predictions and subsequently scaled up to ecosystem-level predictions. Here, if nonlinear aggregate properties are used, dimensional effects will bias species-level predictions towards underestimation and will further increase this bias for ecosystem-level predictions. With an ever-increasing resolution of data, scaling predictions across multiple levels of organisation, and potentially introducing dimensional effects at multiple levels, may become more common. Consequently, we provide pseudocode explaining how our theory can be applied to empirical data moving forward (Figure 6).

Our work is theoretical and, in essence abstract. Yet it may be relevant for highly practical domains of ecology. To make this point, we now discuss some implications of our theory to multiple-stressor ecological research, an essentially empirical field that explicitly deals with considerable uncertainty of predictions and holds great interest in its consequences.

4.1 | Multiple-stressor research

In the light of our theory, we propose to revisit a seemingly unrelated problem of wide ecological interest: what is the combined effect of multiple stressors on a given ecosystem? By translating our theory into the language of multiple-stressor research we aim to highlight some implications and to inspire further generalisation.

The combined effect of stressors on an ecological system is generally predicted based on the sum of their isolated effects, that is, an 'additive null model' (Folt et al., 1999; Schäfer & Piggott, 2018). Uncertainty around this additive prediction, which is ubiquitous in empirical studies (Crain et al., 2008; Holmstrup et al., 2010; Jackson et al., 2016), causes prediction errors called 'non-additivity'. Uncertain predictions will either overestimate or underestimate the combined effect of stressors, respectively creating 'antagonism' and 'synergism' (Folt et al., 1999; Piggott et al., 2015). This translation of stressor interactions in terms of prediction uncertainty and under- or overestimation leads us to the conclusion that scaling up uncertain multiple-stressor predictions generates bias towards synergism.

Here, scaling up predictions refers to multiple-stressor predictions (e.g. an additive model) at one level (e.g., individuals, populations) being used to build multiple-stressor predictions at higher levels of biological organisation (e.g. communities, ecosystems), an approach for which there is growing interest (Bracewell et al., 2019; Griffen et al., 2016; Kroeker et al., 2017; Orr et al., 2020; Thompson et al., 2018). To be clear, scaling up predictions is not equivalent to simply scaling up investigations; our theory does not predict greater synergism at higher levels of organisation. In fact, we are not making predictions about how stressors will behave at higher levels of organisation. What we claim instead is that, if we have a model for the combined effect of stressors at one level of organisation and use that model to deduce their combined effect at higher levels, the process of scaling up the model will introduce a bias towards an observed synergy between stressors, even if no systematic synergy was observed at the lower level.

Our theory has consequences for the interpretation of stressor interactions and is therefore relevant to the debate surrounding multiple-stressor null models (De Laender, 2018; Griffen et al., 2016; Liess et al., 2016; Schäfer & Piggott, 2018). Our findings are especially relevant to the *Compositional Null Model*, which employs a reductionist approach to the construction of multiple-stressor predictions (Thompson et al., 2018). In such an approach, the baseline against which biological effects are tested must be shifted. Dimensional effects, quantified by the effective dimensionality of the underlying system and the nonlinearity of aggregate properties, need to be accounted for to decipher a biological synergism from merely a statistical synergism.

4.2 | Conclusions

In this paper we have addressed a subproblem of the reductionist program (Levins & Lewontin, 1985; Loreau, 2010; Wan, 2013). We investigated the consequences of uncertainty when unbiased

```
Pseudocode to implement our theory

1)  v = predictions     # input vector with predictions for each component

2)  σ = sd_errors      # input vector with standard deviation of error for each component

3)  Compute effective dimensionality (S_eff) using v and σ (Eq. A)     # can be non-integer

4)  Compute mean error (x) using v and σ (Eq. B)    # mean error relative to prediction

5)  Compute the probability of underestimation at S_eff (Eq. C)    # as a function of error

6)  Evaluate this function for the probability or underestimation at x
```

Equation A:

$$1/S_{eff} = \frac{\sum_i v_i^2 \sigma_i^2}{\sum_i v_i^2 \sum_j \sigma_j^2}$$

Equation B:

$$\bar{x} = \sqrt{\frac{\sum_i \sigma_i^2}{\sum_i v_i^2}}$$

Equation C:

$$\mathbb{P}(y \geq 0 : x) = 1 - \frac{1}{2} I_{1 - \frac{x^2}{2}} \left(\frac{S_{eff} - 1}{2} ; \frac{1}{2} \right)$$

FIGURE 6 Pseudocode describing how our theory can be applied to empirical data. With a vector containing the predictions for each component and a vector with the corresponding standard deviation of prediction errors, the effective dimensionality of the system, and therefore the probability of underestimation, can be computed. Code to implement Equation C is available at https://doi.org/10.5281/zenodo.4611133

predictions of individual components are scaled up to predictions of system-level change. Due to a geometric observation that *in high dimensions there are more ways to be more different, than ways to be more similar*, scaling up uncertain predictions tends to underestimate system-level change. Although we have primarily focused on ecology, and in particular on the response of ecosystems to perturbations; our general findings could inform any field of science where predictions about whole systems are constructed from joint predictions on their individual components, such as economics, finance, energy supply and demography (Appendix S4).

Given the generality of these results, why have these dimensional effects gone unnoticed until now? First, we stress that these effects will only manifest when a reductionist approach is used to study complex systems *and* when distance in state space or some other nonlinear aggregate property is used to measure change at the system level. Second, even when these conditions are met, dimensional effects may be obscured by the natural effects that also contribute to the overall probability of over- or underestimation. Nonetheless, with increasing data quantity and resolution, scenarios where our theory is relevant could become increasingly common. If this is the case, understanding the generic dimensional effects that emerge when uncertain predictions are scaled up will be paramount to better predict the behaviour of complex systems.

ACKNOWLEDGEMENTS

AUTHORS' CONTRIBUTIONS

J.-F.A. developed the theoretical framework; J.A.O. with support from J.-F.A. carried out the simulations and produced the figures; J.A.O. wrote the first draft of the manuscript with support from J.-F.A. All authors contributed to the revision of the manuscript.

PEER REVIEW

The peer review history for this article is available at https://publons.com/publon/10.1111/2041-210X.13621.

DATA AVAILABILITY STATEMENT

All data were simulated. Code is available in a Jupyter Notebook on Zenodo https://doi.org/10.5281/zenodo.4611133 (Orr et al., 2021).

ORCID

James A. Orr https://orcid.org/0000-0002-6531-5623

Jean-François Arnoldi https://orcid.org/0000-0001-9373-4051

REFERENCES

Arnoldi, J.-F., Bideault, A., Loreau, M., & Haegeman, B. (2018). How ecosystems recover from pulse perturbations: A theory of short-to long-term responses. *Journal of Theoretical Biology*, *436*, 79–92. https://doi.org/10.1016/j.jtbi.2017.10.003

Bracewell, S., Verdonschot, R. C., Schäfer, R. B., Bush, A., Lapen, D. R., & Van den Brink, P. J. (2019). Qualifying the effects of single and multiple stressors on the food web structure of dutch drainage ditches using a literature review and conceptual models. *Science of the Total Environment*, *684*, 727–740. https://doi.org/10.1016/j.scitotenv.2019.03.497

Côté, I. M., Darling, E. S., & Brown, C. J. (2016). Interactions among ecosystem stressors and their importance in conservation. *Proceedings of the Royal Society B: Biological Sciences*, *283*(1824), 20152592.

Crain, C. M., Kroeker, K., & Halpern, B. S. (2008). Interactive and cumulative effects of multiple human stressors in marine systems. *Ecology Letters*, *11*(12), 1304–1315. https://doi.org/10.1111/j.1461-0248.2008.01253.x

De Laender, F. (2018). Community-and ecosystem-level effects of multiple environmental change drivers: Beyond null model testing. *Global Change Biology*, *24*(11), 5021–5030. https://doi.org/10.1111/gcb.14382

Dovers, S. R., & Handmer, J. W. (1992). Uncertainty, sustainability and change. *Global Environmental Change*, *2*(4), 262{276. https://doi.org/10.1016/0959-3780(92)90044-8

Folt, C., Chen, C., Moore, M., & Burnaford, J. (1999). Synergism and antagonism among multiple stressors. *Limnology and Oceanography*, *44*(3part2), 864–877. https://doi.org/10.4319/lo.1999.44.3_part_2.0864

Griffen, B. D., Belgrad, B. A., Cannizzo, Z. J., Knotts, E. R., & Hancock, E. R. (2016). Rethinking our approach to multiple stressor studies in marine environments. *Marine Ecology Progress Series*, *543*, 273–281. https://doi.org/10.3354/meps11595

Haegeman, B., Arnoldi, J.-F., Wang, S., de Mazancourt, C., Montoya, J. M., & Loreau, M. (2016). Resilience, invariability, and ecological stability across levels of organization. *bioRxiv*, 085852.

Harfoot, M. B. J., Newbold, T., Tittensor, D. P., Emmott, S., Hutton, J., Lyutsarev, V., Smith, M. J., Scharlemann, J. P. W., & Purves, D. W. (2014). Emergent global patterns of ecosystem structure and function from a mechanistic general ecosystem model. *PLoS Biology*, *12*(4), e1001841. https://doi.org/10.1371/journal.pbio.1001841

Hill, M. O. (1973). Diversity and evenness: A unifying notation and its consequences. *Ecology*, *54*(2), 427–432. https://doi.org/10.2307/1934352

Holmstrup, M., Bindesbøl, A.-M., Oostingh, G. J., Duschl, A., Scheil, V., Köhler, H.-R., Loureiro, S., Soares, A. M. V. M., Ferreira, A. L. G., Kienle, C., Gerhardt, A., Laskowski, R., Kramarz, P. E., Bayley, M., Svendsen, C., & Spurgeon, D. J. (2010). Interactions between effects of environmental chemicals and natural stressors: A review. *Science of the Total Environment*, *408*(18), 3746–3762. https://doi.org/10.1016/j.scitotenv.2009.10.067

Hurlbert, S. H. (1971). The nonconcept of species diversity: A critique and alternative parameters. *Ecology*, *52*(4), 577–586.

Jackson, M. C., Loewen, C. J., Vinebrooke, R. D., & Chimimba, C. T. (2016). Net effects of multiple stressors in freshwater ecosystems: A meta-analysis. *Global Change Biology*, *22*(1), 180–189. https://doi.org/10.1111/gcb.13028

Kroeker, K. J., Kordas, R. L., & Harley, C. D. (2017). Embracing interactions in ocean acidification research: Confronting multiple stressor scenarios and context dependence. *Biology Letters*, *13*(3), 20160802.

Lande, R., Engen, S., & Saether, B. E. (2003). *Stochastic population dynamics in ecology and conservation*. Oxford University Press on Demand.

Levins, R., & Lewontin, R. C. (1985). *The dialectical biologist*. Harvard University Press.

Liess, M., Foit, K., Knillmann, S., Schäfer, R. B., & Liess, H.-D. (2016). Predicting the synergy of multiple stress effects. *Scientific Reports*, *6*, 32965. https://doi.org/10.1038/srep32965

Loreau, M. (2010). *From populations to ecosystems: Theoretical foundations for a new ecological synthesis (mpb-46)* (Vol. 46). Princeton University Press.

Loreau, M., Naeem, S., Inchausti, P., Bengtsson, J., Grime, J., Hector, A., Hooper, D. U., Huston, M. A., Raffaelli, D., Schmid, B., Tilman, D., & Wardle, D. A. (2001). Biodiversity and ecosystem functioning: Current knowledge and future challenges. *Science*, *294*(5543), 804–808.

Manning, P., van der Plas, F., Soliveres, S., Allan, E., Maestre, F. T., Mace, G., Whittingham, M. J., & Fischer, M. (2018). Redefining ecosystem multifunctionality. *Nature Ecology & Evolution*, *2*(3), 427–436. https://doi.org/10.1038/s41559-017-0461-7

Mouquet, N., Lagadeuc, Y., Devictor, V., Doyen, L., Duputié, A., Eveillard, D., Faure, D., Garnier, E., Gimenez, O., Huneman, P., Jabot, F., Jarne, P., Joly, D., Julliard, R., Kéfi, S., Kergoat, G. J., Lavorel, S., Le Gall, L., Meslin, L., … Loreau, M. (2015). Predictive ecology in a changing world. *Journal of Applied Ecology*, *52*(5), 1293–1310.

Nekola, J. C., & Brown, J. H. (2007). The wealth of species: Ecological communities, complex systems and the legacy of frank preston. *Ecology Letters*, *10*(3), 188–196. https://doi.org/10.1111/j.1461-0248.2006.01003.x

Orr, J. A., Piggott, J. J., Jackson, A. L., & Arnoldi, J.-F. (2021, March). Data from: Scaling up predictions: Simulations and shiny application. *Zenodo*, https://doi.org/10.5281/zenodo.4611133

Orr, J. A., Vinebrooke, R. D., Jackson, M. C., Kroeker, K. J., Kordas, R. L., Mantyka-Pringle, C., Van den Brink, P. J., De Laender, F., Stoks, R., Holmstrup, M., Matthaei, C. D., Monk, W. A., Penk, M. R., Leuzinger, S., Schäfer, R. B., & Piggott, J. J. (2020). Towards a unified study of multiple stressors: Divisions and common goals across research disciplines. *Proceedings of the Royal Society B: Biological Sciences*, *287*(1926), 20200421.

Petchey, O. L., Pontarp, M., Massie, T. M., Kéfi, S., Ozgul, A., Weilenmann, M., Palamara, G. M., Altermatt, F., Matthews, B., Levine, J. M., Childs, D. Z., McGill, B. J., Schaepman, M. E., Schmid, B., Spaak, P., Beckerman, A. P., Pennekamp, F., & Pearse, I. S. (2015). The ecological forecast horizon, and examples of its uses and determinants. *Ecology Letters*, *18*(7), 597–611. https://doi.org/10.1111/ele.12443

Piggott, J. J., Townsend, C. R., & Matthaei, C. D. (2015). Reconceptualizing synergism and antagonism among multiple stressors. *Ecology and Evolution*, *5*(7), 1538–1547. https://doi.org/10.1002/ece3.1465

Poff, N. L. (1997). Landscape filters and species traits: Towards mechanistic understanding and prediction in stream ecology. *Journal of the North American Benthological Society*, *16*(2), 391–409. https://doi.org/10.2307/1468026

Schäfer, R. B., & Piggott, J. J. (2018). Advancing understanding and prediction in multiple stressor research through a mechanistic basis for null models. *Global Change Biology*, *24*(5), 1817–1826. https://doi.org/10.1111/gcb.14073

Suweis, S., Grilli, J., Banavar, J. R., Allesina, S., & Maritan, A. (2015). Effect of localization on the stability of mutualistic ecological networks. *Nature Communications*, *6*, 10179. https://doi.org/10.1038/ncomms10179

Thompson, P. L., MacLennan, M. M., & Vinebrooke, R. D. (2018). An improved null model for assessing the net effects of multiple stressors on communities. *Global Change Biology*, *24*(1), 517–525. https://doi.org/10.1111/gcb.13852

Wan, P.-Y.-Z. (2013). Dialectics, complexity, and the systemic approach: Toward a critical reconciliation. *Philosophy of the Social Sciences*, *43*(4), 411–452. https://doi.org/10.1177/0048393112441974

Wegner, F. (1980). Inverse participation ratio in 2+ ε dimensions. *Zeitschrift für Physik B Condensed Matter*, *36*(3), 209–214.

Woodward, G., Perkins, D. M., & Brown, L. E. (2010). Climate change and freshwater ecosystems: Impacts across multiple levels of organization. *Philosophical Transactions of the Royal Society B: Biological Sciences*, *365*(1549), 2093–2106.

Wu, J., Jones, B., Li, H., & Loucks, O. L. (2006). *Scaling and uncertainty analysis in ecology*. Springer.

SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section.

How to cite this article: Orr JA, Piggott JJ, Jackson AL, Arnoldi J-F. Scaling up uncertain predictions to higher levels of organisation tends to underestimate change. *Methods Ecol Evol*. 2021;00:1–12. https://doi.org/10.1111/2041-210X.13621