Inferring Ecosystem Networks as Information Flows

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Abstract

The detection of causal interactions is of great importance when inferring complex ecosystem functional and structural networks for basic and applied research. Convergent cross mapping (CCM) based on nonlinear state-space reconstruction made substantial progress about network inference by measuring how well historical values of one variable can reliably estimate states of other variables. Here we investigate the ability of a developed Optimal Information Flow (OIF) ecosystem model to infer bidirectional causality and compare that to CCM. Results from synthetic datasets generated by a simple predator-prey model, data of a real-world sardine-anchovy-temperature system and of a multispecies fish ecosystem highlight that the proposed OIF performs better than CCM to predict population and community patterns. Specifically, OIF provides a larger gradient of inferred interactions, higher point-value accuracy and smaller fluctuations of interactions and α -diversity including their characteristic time delays. We propose an optimal threshold on inferred interactions that maximize accuracy in predicting fluctuations of effective α -diversity, defined as the count of model-inferred interacting species. Overall OIF outperforms all other models in assessing predictive causality (also in terms of computational complexity) due to the explicit consideration of synchronization, divergence and diversity of events that define model sensitivity, uncertainty and complexity. Thus, OIF offers a broad ecological information by extracting predictive causal networks of complex ecosystems from time-series data in the space-time continuum. The accurate inference of species interactions at any biological scale of organization is highly valuable because it allows to predict biodiversity changes, for instance as a function of climate and other anthropogenic stressors. This has practical implications for defining optimal ecosystem management and design, such as fish stock prioritization and delineation of marine protected areas based on derived collective multispecies assembly. OIF can be applied to any complex system and used for model evaluation and design where causality should be considered as non-linear predictability of diverse events of populations or communities.

44 “But truth is ever incoherent”

45 Astrid Recker

46

47 1 Introduction

48 1.1 Ecosystem Complexity and Predictability

49 The flourishing development of complexity science^{1;2} has shed light on research questions
50 and applications in many interdisciplinary fields, for instance, climate change^{3;4;5}, epidemi-
51 ology^{6;7} and ecosystem sciences at multiple scales^{8;9;10}. In this burgeoning science, complex
52 network models play a central role in the quantitative analysis, synthesis and design (includ-
53 ing predictions) of ecosystems and their visual representation. This is because functional
54 and structural networks – such as species interactions and ecological corridors – are the core
55 elements of ecosystems defining species organization and ecosystem function. When inferring
56 networks, causal inference¹¹ is one of the fundamental steps for ecosystem reconstruction and
57 graphical representation by assessing interactions or interdependencies dynamically or across
58 a period of time – between biota, environment, and among those – that can be conceptual-
59 ized as information flows in a general purview¹². In a quantitative sense, network inference
60 can performed via causality inference based on time series data defining the dynamics of
61 ecosystem components. Causal inference also attracts much attention in some emerging dis-
62 ciplines such as big data science via machine learning since it brings a new set of tools and
63 perspectives for some problems in these areas. However, this issue of causal inference is still
64 an extremely challenging problem due to the intrinsic lack of knowledge or observability of
65 the “true” reality of a system especially for highly complex non-linear systems driven by non-
66 linear environmental forcing. Certainly the objective of causal inference is defining unknowns;
67 however robust model validation must be performed. In order to make causal inference prac-
68 tical and achievable, causality is often replaced with predictability as it is articulated in this
69 paper. A plethora of conceptual approaches, frameworks and algorithmic tools including
70 but not limited to Pearson’s Correlation Coefficient (PCC)^{13;14}, Bayesian Networks (BNs)
71 and Dynamic Bayesian Networks (DBNs)^{15;16;17;18;19}, Neural Networks, Graphical Gaussian
72 Models (GGMs)^{20;21}, Wiener-Granger causality (GC) model²², Structural Equation Mod-
73 eling (SEM)^{23;24;25;26;27;28}, Convergent Cross Mapping (CCM)²⁹ and information-theoretic
74 models^{30;31;32;33} for instance, to tackle causal interactions and infer complex networks in
75 terms of correlation, predictability and probability have been well established; however, most

76 tools are solely tested on low-dimensional systems and some are even untested on ecosystems
 77 at different levels of complexity or simulated ones. The vast majority of these models in
 78 ecosystem science (with the exception of CCM and few others such as PCMCI³⁴) consider
 79 only the inferred causality between species pairs one at a time without the simultaneous con-
 80 sideration of all species pairs for each species that is shaping ecosystem collective behavior
 81 mediated by environmental dynamics. The ensemble of all species causations is representable
 82 as nonlinear dynamical network over the space-time-environmental domain considered. It is
 83 therefore valuable for science to seek for robust models and explore novel methods to identify
 84 and quantify the pattern-oriented causality between variables (such as species) and how this
 85 causality is predictive of target complex system patterns.

87 1.2 Causal Interaction Inferential Models

88 1.2.1 From Granger to Convergent Cross Mapping

89 For quite a long time, correlation has been considered as a heuristic of causal relationship
 90 between variables even though George Berkeley³⁵ always suggested that correlation did not
 91 necessarily or sufficiently imply causation. Especially for ubiquitous nonlinear dynamics, ap-
 92 plying linear correlation to infer causation is cursory and risky. Statements about causation
 93 and correlation actually do not have much to do with each other, particularly when there is
 94 no a-priori knowledge of the studied ecosystem processes. The conceptualization and identifi-
 95 cation of "causality" was originally introduced by Wiener³⁶ who propounded that "causality"
 96 between two variables can be identified by measuring how well one variable facilitates the pre-
 97 dictability of the other. In this broader view causality was already conceptualized correctly
 98 as predictability.

99 In 1969, Granger formalized Wiener's idea³⁶ in terms of autoregression and established
 100 the framework of Wiener-Granger causality (GC) model²² that after lead to the Nobel prize
 101 in economics. Since then, GC approach has become a frequently used advance for causation
 102 and useful to infer causal interactions between strongly coupled variables. According to the
 103 concept of GC model, a variable is said to "GC cause" a second variable if knowledge of
 104 the current value of the first variable helps in predicting that of the second variable. This
 105 notion of causality was substantially based on the predictability of time series, although
 106 strictly speaking Granger causality is about conditional independence of variables rather
 107 than predictability. The key requirement of GC model is separability that is a feature of

108 purely linear and stochastic systems²², and provides a way to understand the system as sum
 109 of components rather than as a whole non-linear entity composed by multiple components
 110 difficult to separate. Separability means that the second variable can be independently and
 111 uniquely forecasted by the first variable; an assumption that reflects how studied systems
 112 are interpreted as linear systems and that is certainly not the case of real complex systems.
 113 Additionally, states in the past of some variables in dynamical systems can be inherited
 114 through time, which means that the behavior of dynamical systems has memory. Yet, both
 115 cause and effect are embedded in a non-separable higher dimension trajectory. Space-time
 116 separability therefore becomes extremely hard to satisfy in systems that can be described
 117 as complex networks where each node (variable) influences several nodes or even all nodes
 118 in the entire system simultaneously, resulting in a non-random propagation of information
 119 through the network. In this sense ecosystems can be thought that information machines
 120 where separability is only possible by fixing thresholds of significance for the patterns to
 121 investigate. As a consequence, GC model might be problematic while using in nonlinear
 122 dynamical systems with deterministic settings and weak to moderate interaction. In attempt
 123 to solve the causality inference problem in complex ecosystems, Sugihara et al. (2012)²⁹
 124 developed the Convergent Cross Mapping (CCM) model²⁹, and successfully applied this
 125 model to a coupled non-linear mathematical predator-prey model and a real-world sardine-
 126 anchovy-temperature ecosystem. Later on, Ushio et al. (2018)³⁷ applied CCM to a complex
 127 fish ecosystems with 15 species after removing seasonality from abundance data in order to
 128 assess “true” or biological interactions.

129 In dynamic systems two variables (X and Y for instance) are causally linked if they are
 130 generated by one system and share a common attractor manifold. It implies that each variable
 131 can be used to recover (predict) the other one. CCM is the method capable of quantifying
 132 this kind of correspondence between two variables. CCM does so by measuring the extent
 133 to which the states of one variable (considering values rather than probability distributions)
 134 can be reliably estimated by the other one with time lags. In practice, CCM take values
 135 of variables X and Y, a time lag embedding is derived from the time series of Y, and the
 136 ability to estimate the states of variable X from the time lag embedding quantifies how much
 137 signature of X is encoded in the time series of Y. This principle was termed as “Cross Map-
 138 ping”, and it was suggested that the causal effect of X on Y is determined by how well Y
 139 “cross maps” X. Sugihara et al. (2012)²⁹ noted that CCM had drawbacks, although some
 140 of these are disputable. For instance for the phenomenon of “generalized synchrony” as a
 141 result of exceptionally strong unidirectional causation (X strongly “cross maps” Y, but Y
 142 does not causes X). In such a case, both directions (X “cross maps” Y, Y “cross maps” X) of

the causal relationship can be observed from CCM's results, resulting in a "misleading" bidirectional causality³⁸. This was perceived as a limitation of CCM in distinguishing between bidirectional causality and strong unidirectional causality because of the synchrony. Misleading is however not a correct definition since we believe any variable has always non-zero interdependencies due to unaccounted factors and chance that interactions may appear at least once in the ecosystem considered. Yet, asymmetrical interdependence is a norm rather than a numerical artifact. Another key property, and potentially a drawback, of CCM is convergence that is stable predictability (ρ) after a critical library size defining the minimum information for reliable inference. However, datasets are not always long enough especially for real-world applications. Yet, convergence might be limited by the finite size of time series data. Lastly, CCM suffers from the high computational complexity in terms of model parameters and computation speed. Despite these drawbacks CCM is used in this study as a benchmark for evaluating our proposed model.

1.2.2 From Information Flow to Transfer Entropy

Most natural and artificial systems composed of a large number of interacting elements can be represented as networks. Networks, functional and structural, are the backbone of ecosystems. In order to untangle such networks, the primary mission is to identify and quantify causations between elements and then to infer the networks for analysis and visualization. These networks are information fluxes representing ecosystems via non-linear dynamic interactions. Ecosystems can be identified in terms of network topology as collective dynamics and as a function of macroecological indicators as entropy/energy states. Variables in information theory including Shannon entropy, Mutual Information (MI) and Transfer Entropy (TE) have been recently used in complex network science to characterize ecosystems at different scales³⁹. Herein, TE coined by Thomas Schreiber⁴⁰ is an information-theoretic quantity measuring the asymmetric bidirectional information transfer (vs. information flow as in Lizier et al. (2010)⁴¹ when conditional entropies are used to exclude indirect pairs of species whose interactions is of second order importance) between two variables⁴². In a conceptual and practical view, besides GC and CCM, TE can be an appropriate candidate to infer the causality between interacting elements in complex ecosystems.

As mentioned above, GC model may be problematic in complex systems due to highly nonlinear dynamics, and CCM may not be suitable for distinguishing well bidirectional or strong unidirectional interactions, the requirement convergence, the lack of consideration of

176 probability distribution functions (pdfs), and numerical sensitivity due to high computa-
 177 tional complexity. By contrast, TE, as a non-parametric, model-free information-theoretic
 178 variable defined from nonlinear dynamics of Markov chain process (mappable as stochastic
 179 pdf propagation equivalently), it provides a directed measure to detect asymmetric dynam-
 180 ical information transfer between two time-varying variables. TE is particularly convenient
 181 because, on the contrary of other models such as CCM, is a “first principle” variable defined
 182 without assuming any particular functional/process or numerical model to identify the inter-
 183 actions in studied systems⁴³. For this reason, TE is the elementary block of complex systems
 184 represented as information processing machines where uncertainty or information shapes sys-
 185 tems’ collective behavior driven by non-linear convolution of intrinsic system’s properties and
 186 external noise (e.g. biology and environment, respectively). Thus, TE has been considered
 187 as an important and powerful tool to analyze causal relationships in nonlinear complex sys-
 188 tems⁴⁴ and numerical methods are just used to calculate TE from its analytical form (such
 189 as the choice of pdf binning and entropy discretization). It is worth noting that for Gaussian
 190 random processes TE is equivalent to Granger causality⁴⁵ but these are rare processes in
 191 nature. The vast majority of natural process are multimodal and non-Gaussian.

192 Although, in its basic formulation, TE has already been widely used for causality infer-
 193 ence, general principles, unified frameworks, and models, and further developments based on
 194 TE are still lacking. More importantly no work hitherto has been done to give systematic val-
 195 idations for TE-based causality inference models with mathematically synthetic data, as well
 196 as real-world ecosystems, to elucidate how TE behaves dependent on dynamics and complex-
 197 ity. Razak et al. (2014)⁴⁶ made progress on this issue by using classical and amended Ising
 198 models which are mathematical models of ferromagnetism in statistical mechanics; Duan
 199 et al., (2013)⁴⁷ provided a theoretical and experimental systemic validation of a TE-based
 200 model; and finally Runge et al. (2018)⁴⁸ explored TE and other models with synthetic data.
 201 However, these studies are applied to complex systems with a limited number of variables or
 202 whose dynamics is well defined; yet, they did not validate the model for realistic ecosystems
 203 in its full complexity, driven also by data fallacies, as seen in nature. Therefore, specific
 204 applications of TE-based models lack of a rigorous performance assessment that thus re-
 205 mains elusive. On one side low complexity well-known ecosystems can validate the inferred
 206 pairwise interactions, while highly complex ecosystems can validate the whole systemic in-
 207 teraction network predictability on some patterns such as biodiversity indicators over time.
 208 The former problem deals more with accurate causality between pairs, while the latter deals
 209 more with ecosystem predictability.

1.3 Optimal Information Flow and Predictability

In this study, to overcome limitations of CCM and TE inference models estimating species pairs independently of each other, as well as to revise and validate “causality” in a predictive sense, we propose the Optimal Information Flow (OIF) model based on previously developed models by our group^{49;39}. Specifically, the proposed OIF model involves four main steps: (i) MI-based optimal time delay assessment that maximizes the predictability of variables and focus on extreme or rare interactions³⁹; (ii) TE computation considering data probabilistic dynamics; (iii) coupled maximization of uncertainty reduction and removal of indirect links; and (iv) selection of optimal TE threshold for predicting selected patterns (e.g. α -diversity). The optimal threshold on TE is not necessarily within the scale-free maximum uncertainty reduction range (describing ecosystem collective dynamics) because predicted patterns define the pattern-specific salient TE. Technically, in this paper we offer a different estimation of TE than Li and Convertino (2019)³⁹ (based on JIDT Kernel estimator suitable for power-law distributed data⁴²), and we explore all TEs (without TE thresholding) with the aim of capturing all differences between TEs and CCM interaction matrices and their ability to predict fluctuations in macroecological patterns considering connected species a posteriori. In addition, OIF is improved with respect to Li and Convertino (2019)³⁹ by considering its extension over time to reconstruct dynamical information networks, and the time-dependent Markov order (self-memory) of each species. Note that in this paper we consider all inferred TEs without any redundancy check and removal of indirect interactions as in Servadio and Convertino, (2018)⁴⁹ because we wish to characterize the full interaction matrix without any assumptions on biological interactions or methodological criteria of subordinate interactions. This is particularly important when no knowledge is available a priori about biological interactions, whether the biomarker used (e.g. abundance) is reflective of the interactions of interest (physical, biomass conversion, hormonal interactions, etc.), and when indirect weak interactions are quite important (and this is quite common for small organisms, e.g. microbes).

The performance of OIF is assessed by applying it to three prototypical case studies including mathematical deterministic and real-world ecosystems. One is a biologically inspired mathematical model that can generate synthetic two-coupled time-series variables describing dynamics similar to predator-prey dynamics²⁹. Two parameters (β_{xy} and β_{yx}) in the equations underlying the model are describing the strength of true interdependence between two simulated variables and they can be free varied. Other two case studies are real-world ecosystems: the case of externally forced poorly coupled species (sardine-anchovy-

temperature system)²⁹ and the one of highly complex interacting species (fish community in Maizuru bay)³⁷ (Fig. 1). The well-documented CCM method is also used for these three cases and the results from CCM, despite its known drawbacks of convergence, strong asymmetrical causality miscalculation, and computational complexity, were somewhat considered as benchmark interactions due to the lack of other estimates.

OIF is not perceived as a competitor with other already published models, including GC and CCM, but rather it aims at providing an alternative and hopefully more precise assessment to predictive inference in cases not completely covered by previous models. Theoretically, leaving aside systematic data issues, OIF is expected to give a better performance than other models in interdependence assessment owing to the aforementioned fine properties of TE for nonlinear dynamics. Besides, given the relationship between entropy and diversity⁵⁰ (specifically Shannon and Transfer entropy and α - and β -diversity), OIF provides a potential advantage to predict the information about macroecological indicators of ecosystems. In consideration of these features, TE causality is proposed as *non-linear predictability* of both population fluctuations of species (in this case abundance fluctuations) and community macroecological indicators, simultaneously.

The fundamental principle about OIF is anchored into the idea of systemic uncertainty reduction (leading to maximum predictive accuracy) that is by itself a form of quantitative validation considering aleatoric uncertainty in species variables. Certainly systematic uncertainty (of models and algorithms) and biological ignorance are two other important elements to consider for a complete validation, and we tried to address those to a certain extent but further studies are required. It should be kept in mind that Interactions are always specific to a target outcome, e.g. biomass variation, that is likely reflected by the species biomarker as model inputs. For this reason we emphasize that the inferred interactions are generally *predictive causal relationships* which maximize predictive accuracy of multivariate time series and not "absolute" species interactions (for an interesting semantics discussion on species interactions see Nakazawa (2020)⁵¹).

2 Results

2.1 Two Species Unidirectional Coupling Ecosystem

This bio-inspired ecosystem $S(\beta_{xy} = 0, \beta_{yx})$ describing the unidirectional coupling is run for 1000 time steps for reaching stationarity, generating a set of 1000 points long time-series dependent on β_{yx} . This means that species X has an increasing effect on Y with the increase of β_{yx} , but Y has no effect on X. Both CCM and the proposed OIF model are separately used to quantify the potential causality between species X and Y. The inferred causality dependent on β_{yx} only (as a physical interaction) is shown in Fig. 2A. β , ρ and TE have different units; specifically β and ρ are dimensionless while TE is measured in bits or nats (a logarithmic unit of information or entropy). Therefore, any comparison is done considering gradients of change when these variables vary together rather than making comparisons between absolute values which are meaningless. Figure 2A shows that under the condition of $\beta_{xy}=0$, results of "Y to X" (i.e. the estimated effect on Y on X) is close to 0 for the OIF model ($TE_{Y \rightarrow X}(\beta_{yx})$) that precisely describe the no-effect of Y on X. "X to Y" ($TE_{X \rightarrow Y}(\beta_{yx})$) well tracks the increasing strength of the effect of X on Y for increasing values of the physical interaction β_{yx} embedded into the mathematical model. However, considering results of the CCM model, "Y to X" ($\rho_{Y \rightarrow X}(\beta_{yx})$) presents non obvious (and likely wrong) non-zero values with higher fluctuations compared to $TE_{Y \rightarrow X}(\beta_{yx})$ especially for lower values of β_{yx} . This erroneous estimates of CCM is likely related to the need of CCM for convergence. For CCM, "X to Y" ($\rho_{X \rightarrow Y}(\beta_{yx})$) shows an increasing trend for increasing values of β_{yx} and decreasing when β_{yx} is greater than ~ 0.5 non-trivially. In consideration of these results for the unidirectional coupling ecosystem, the OIF model performs better over CCM in terms of unidirectional causality inference.

2.2 Two Species Bidirectional Coupling Ecosystem

In this case, the effect between two species is bidirectional. Species X has an effect on species Y and vice versa. The univariate dynamical systems $S(0.2/0.5/0.8, \beta_{yx})$ are run for 1000 time steps under the same conditions determined by β_{xy} . Certainly this situation is fictional since in real ecosystems the interaction strength is changing when other interacting species change their interactions. Thus, keeping one interaction fixed around one value is a strong unrealistic simplification (analogous of one-factor at-a-time sensitivity analyses) but it is a

toy model that allows to verify the power of network inference models. These models generate three sets of 1000 points long time-series dependent of β_{yx} for each fixed β_{xy} . OIF and CCM are used to infer “causality” between X and Y – in the form of ρ and TE – and compare that against the real embedded interaction β_{yx} and β_{xy} shown in Fig. 2BCD. Considering all results of Figure 2 corresponding to fixed β_{xy} s, the correlation coefficient ρ yielded from CCM and TE from OIF are both able to track the strength of causal trajectories. However, TE seems to perform better in term of ability to infer fine-scale changes in interactions. In particular, considering Fig. 2D (right plot), higher TE_{yx} higher for low β_{yx} makes sense because $\beta_{xy} > \beta_{yx}$ that means Y has a larger influence on X than vice versa and then Y is able to predict X. Additionally, TE does not suffer of convergence problems; specifically, considering Fig. 2A (left plot), higher ρ for small β_{yx} is not sensical and that is likely related to convergence problems of CCM.

Considering all results of Figure 2 corresponding to fixed β_{xy} s, the correlation coefficient ρ yielded from CCM and TE from OIF are both able to track the strength of causal trajectories. Ideally, the causality from Y to X is a constant since β_{xy} is a fixed value for each case. In this figure, the red curve in the right panel representing the OIF-inferred (TE-based) causality from Y to X is higher for greater β_{xy} s, while red curves representing CCM-inferred (ρ) causality in the left panel present higher fluctuations especially for lower β_{yx} . For the causality from X to Y determined by β_{yx} in the mathematical model, theoretically speaking, the causality from X to Y should monotonously grow when β_{yx} increases from 0 to 1. In Figure. 2, blue curves in the right panel representing the OIF-inferred (TE-based) causality from X to Y present monotonously increasing features as a whole with the increasing β_{yx} , while those from CCM model (ρ) do not and show considerable fluctuations. Therefore, OIF outperforms CCM in terms of the ability to infer the fine-scale changes in causality. In particular, considering Fig. 2D (right plot), higher TE_{yx} higher for low β_{yx} makes sense because $\beta_{xy} > \beta_{yx}$ that means Y has a larger influence on X than vice versa and then Y is able to predict X. Additionally, TE does not suffer of convergence problems; specifically, considering Fig. 2A (left plot), higher ρ for small β_{yx} is not sensical and that is likely related to convergence problems of CCM.

Additionally, $\rho_{Y \rightarrow X}(\beta_{yx})$ shows higher fluctuations on average especially for the condition of lower β_{yx} s compared to $TE_{Y \rightarrow X}(\beta_{yx})$. When considering the effect of X on Y that is a function of β_{yx} for CCM, $\rho_{X \rightarrow Y}$ reaches an extreme value at around $\beta_{yx} = 0.5$ and then declines for larger values of β_{yx} . This is not consistent with the expected effect of X on Y that should be proportional to β_{yx} embedded into the mathematical model. The ability of

ρ to reflect the proportional relationship between the effect of X on Y (manifested by β_{yx}) vanishes for high β_{xy} s due to unexpected and somewhat inconspicuous changes in $\rho_{X \rightarrow Y}$ for larger β_{yx} . In simple words, the expected increasing trend of ρ is lost for larger β_{yx} that is counterintuitive. On the other side, $TE_{X \rightarrow Y}(\beta_{yx})$ invariably maintains an increasing trend for increasing values of β_{yx} . OIF is also performing better than CCM when predicting higher average values of $TE_{Y \rightarrow X}$ for increasing values of β_{xy} (red curves in Fig. 2ABCD, right plots) as expected by the fixed effect in the mathematical model of Y on X. These results suggest that when compared to ρ of CCM, TE can track well the causal interactions over β_{yx} with higher performance and without considering the convergence requirement of CCM. CCM needs to consider the length of time series that makes $\rho_{X \rightarrow Y}(\beta_{yx})$ convergent to a stable value, but uncertain for large differences in time-series length of (X,Y) and sensitive to short time series.

In more realistic settings for real ecosystems (and in analogy to global sensitivity analyses) when β_{xy} and β_{yx} are both considered as arguments of the two-variable (X,Y) bio-inspired model, the simulated ecosystem becomes a truly bivariate system, yet yielding complexity but more interest into the causality inference (Fig. 3). The dynamical system $S(\beta_{xy}, \beta_{yx})$ was generated for 800 time steps under the same conditions mentioned above. We generated the datasets that allowed us to study linear and non-linear predictability indicators for inferring the embedded physical interactions. Specifically, we measure undirected linear correlation coefficient $corr_{X;Y}(\beta_{xy}, \beta_{yx})$, non-linear undirected mutual information $MI_{X;Y}(\beta_{xy}, \beta_{yx})$, directed non-linear correlation coefficient $\rho_{X \rightarrow Y}(\beta_{xy}, \beta_{yx})$ and $\rho_{Y \rightarrow X}(\beta_{xy}, \beta_{yx})$, and non-linear directed transfer entropy $TE_{X \rightarrow Y}(\beta_{xy}, \beta_{yx})$ and $TE_{Y \rightarrow X}(\beta_{xy}, \beta_{yx})$ as shown in Fig. 3. These 2D phase-space maps in Fig. 3 show strikingly similar patterns for classical linear correlation coefficients, MI, ρ of CCM and TE of OIF which underline the fact that all methods are able to infer the interdependence patterns of interacting variables explicitly defined by β_{xy} and β_{yx} . The color of phase-space maps is proportional to the inferred interaction between X and Y when the mutual physical interactions are varying according to the mathematical model in Eq. 5.1. In Fig. 3, even though phase-space maps of undirected $corr_{X;Y}(\beta_{xy}, \beta_{yx})$ and $MI_{X;Y}(\beta_{xy}, \beta_{yx})$ present similar patterns (in value organization and not value range) to those of directed ρ and TE, neither $corr_{X;Y}(\beta_{xy}, \beta_{yx})$ and $MI_{X;Y}(\beta_{xy}, \beta_{yx})$ provide information about the direction of causality. As expected MI shows the opposite pattern of the average TE due to the fact that MI is the amount of shared information (or similarity) versus the amount of divergent information (divergence and asynchronicity) between X and Y.

In a biological sense TE should be interpreted as the probability of likely uncooperative

dynamics (leading to or driven by environmental or biological heterogeneity) while MI as the probability of cooperative dynamics (leading to or driven by homogeneity). Here we refer to cooperative and uncooperative interactions based on the similarity or dissimilarity in pair dynamics manifested by species abundance fluctuations. For instance divergence and asynchronicity (that define TE) in pair species dynamics manifest uncooperative interactions. The balance of cooperative and uncooperative interactions can result into net interactions at the ecosystem scale manifesting neutral patterns, or net interactions may lead to niche patterns biased toward strong environmental or biological factors⁵². Certainly, cooperation in a biological sense should be interpreted on a case by case basis. In a broader uncertainty propagation perspective⁴⁹, “cooperation” between variables means that variables contribute similarly to the uncertainty propagation, while “competition” means that one variable is predominant over the other in terms of magnitude of effects since TE is proportional to the magnitude rather than the frequency of effects. For the former case the total entropy of the system is higher than the latter case. Interestingly, correlation $\text{corr}(\beta)$, ρ and TE show similar patterns in both organization and value range (but not in singular values of course), which sheds some important conclusions about the similarity and divergence of these methods as well as their capacity and limitations in characterizing non-linear systems.

When comparing the phase-space patterns from CCM and OIF (displaying ρ and TE) a more colorful and informative pattern is revealed by OIF. This means that TE gives a better gradient when tracking the increasing strength of causality for increasing values of β_{xy} and β_{yx} . When comparing the phase-space patterns for the two causal directions of “ $X \rightarrow Y$ ” and “ $Y \rightarrow X$ ”, phase-space maps from CCM are very similar, while those from TE present apparent differences in the strength of effects for the two opposite direction of interaction. ~~Therefore, TE model is much more sensitive to the direction compared to CCM when detecting the directional causality.~~ Therefore, OIF is more sensitive to the direction of interaction compared to CCM when detecting directional causality.

These results imply that TE performs better to distinguish directional embedded physical interactions (that are dependent on direct interactions β -s, species growth rate r_x and r_y , and contingent values $X(t)$ and $Y(t)$ determining the total interaction as seen in the model of Eq. 5.1) in the species causal relationships. It should be emphasized how all linear and non-linear interaction indicators are inferring the total interaction and not only those exerted by β -s. In a broad uncertainty purview⁴⁹ the importance of these three factors (β -s, r -s and $X(t)/Y(t)$) depends on their values and probability distributions that define the dynamics of the system; dynamics such as defined by the regions identified by patterns in Fig. 3 for the

406 predator-prey system in Eq. 5.1. In principle, the higher the difference between these three
407 interaction factors in the species considered, the higher the predictability and sensitivity of
408 OIF. Fig. 4 highlights three different dynamics corresponding to the TE blue, green and red
409 regions in Fig. 3.

410 In all dynamical states represented by Fig. 3, species are interacting with different mag-
411 nitude and this defines distinct network topologies. Three prototypical dynamics are show in
412 Fig. 4 with colors representative of ρ and TE in Fig. 3. The “blue” deterministic dynamics
413 has very high synchronicity and no divergence considering variable fluctuation range (the gap
414 is deterministic and related to the numerically imposed $u = 1$), as well as no linear correlation
415 between non-lagged variables. In perfect synchrony one would have one point in the phase-
416 space. Thus, absence of correlation does not imply complete decoupling of species but it can
417 be a sign of small interactions. The “green” dynamics shows a relatively high synchronicity
418 and medium divergence. In the phase-space of synchronous values of X and Y a correlation is
419 observed with relatively small fluctuations because the divergence is small. Lastly, the “red”
420 dynamics shows a relatively high asynchronicity and divergence. The stochasticity is higher
421 than previous dynamics and the “mirage correlation” in the phase space has higher variance.
422 Time-dependent mirage correlations in sign and magnitude mean that correlation (that may
423 suggest common dynamics in a linear framework) does not imply similarity in dynamics for
424 the two species. Non-linearity is higher from blue to red dynamics as well as predictability
425 but lower absolute information entropy. Then, it is safe to say that linear dynamics (or small
426 stochasticity) does not imply higher predictability.

427

428 2.3 Real-world Sardine-Anchovy-Temperature Ecosystem

429 CCM and proposed OIF model are also used for a real-world fishery ecosystem to infer
430 potential causal interactions between Pacific sardines (*Sardinops sagax*) landings, Northern
431 anchovies (*Engraulis mordax*) and Sea-Surface Temperature (SST) recorded at Scripps Pier
432 and Newport Pier, California. Sardines and anchovies do not interact physically (or the
433 interaction is low in number), while both of them are influenced by the external environmental
434 SST that is the external forcing. To quantify the likely causal interactions between species
435 and SST based on real data, we use CCM considering the length of time series for convergence
436 of ρ , as well as OIF considering a set of time delays for acquiring stable values of inferred
437 interactions TEs.

Results from CCM in Fig. 5A (plots from top to bottom) show that no significant interaction can be claimed between sardines and anchovies, as well as from sardines or anchovies in the SST manifold which expectedly indicates that neither sardines nor anchovies affect SST. This latter results, considering its biological plausibility should be taken as one validation criteria of predictive models, or complimentary as a test for anomaly detection of spurious interactions. The reverse effect of SST on sardines and anchovies can be quantitatively detected with the correlation coefficient ρ as well as TE. Although the calculated causations between SST and sardines or anchovies are moderate, CCM is able to provide a good performance in causality inference when the length of time series used is long enough due to convergence requirement.

Figure 5B shows OIF's results of inferred causal interactions between sardines, anchovies and SST dependent on the time delay u . For sardines and anchovies, OIF exposes bidirectional interactions that are actually biologically plausible, especially when both populations coexist in the same habitat, versus the results of CCM that infer $\rho = 0$. Ecologically speaking, even though fish populations do not directly influence sea temperature, we can find some clues about SST in fish populations influenced by SST. These clues can be interpreted as information of SST encoded in fish populations over abundance time records. So, observations of fish populations can be used to inversely predict the change of SST; this can be interpreted as "reverse predictability" (or "biological hindcasting") in a similar way of when predicting historical climate change from ice cores. This information is captured by OIF, leading to nonzero values of TE from fish populations to SST. In this regard, we emphasize the distinction between direct and indirect (reverse) information flow, where direct information flow is most of the time larger and signifies causality (e.g. of SST for sardine and anchovies), and indirect (reverse) information flow that is typically smaller and signifies predictability (e.g. sardine and anchovies for ocean fluctuations). It is possible – especially for linear systems where an effect is observed immediately after a change – that information of SST encoded in fish populations is high if the interdependence, represented by the functional time delay u , of the environment-biota is small. However, for highly non-linear systems such as fishes and the ocean, changes in temperature may take a while before being encoded into fish population abundance⁵³. Thus, it is correct that the highest values of TE are for high u . Values of TE for small u -s are numerical artifacts related to systematic errors. Thus, for the effect of external SST on sardines and anchovies, OIF model gives unstable causal interactions with bias for lower time delays due to known dependencies of TE on u (such as cross-correlation for instance) that establishes the temporal lag on which the dependency between X and Y is evaluated. In a sense, plots in Figure 5B are like cross-variograms for the pairs of variables

considered. TE becomes stable when the time delay is located in an appropriate range. It means that OIF requires an optimal time delay that makes results of the causality inference robust and that is related to optimal TEs (as highlighted in Li and Convertino (2019)³⁹ and Servadio and Convertino (2018)⁴⁹) that defines the most likely interdependency between variables for the u with the highest predictability. The fact that TE of sardine and anchovies to SST is high for some small ranges of u may be also a byproduct of data sampling, i.e., fish and SST sampling locations are different (fish abundance is actually about fish landings) and that can introduce spurious correlations/causation. Overall, these findings suggest that the OIF model provides more plausible results, but it requires careful selection of optimal time delays.

Figure S1 shows the relationships between normalized ρ and TE estimated for all selected values of L and u of pairs in Fig. 5 (sardine-anchovy, sardine and SST, anchovy and SST). These plots show opposite results than the proportionality between ρ and TE in Fig. 3 because non-optimal values are used, that is non-convergent ρ -s and suboptimal TE during the interaction inference procedure (Fig. S1). TE for too small u -s determines overestimation of interactions due to the implicit assumptions that variables have an immediate effect on each other and that is not always the case as highlighted by the vast time-lagged determined non-linear regions in Fig. 3. If “transitory” values of ρ for small L are disregarded, as well as TEs for small u -s, the relationship between ρ and TE shows a correct linear proportionality.

2.4 Real-world Multispecies Ecosystem

Interactions between fish species living in the Maizuru bay are intimately related to external environmental factors of the ecosystem where they live, the number of species living in this region considering also the unreported ones) and biological species interactions, which leads to a complex dynamical nonlinear system. In Fig. 6 the network of observed fish species (Table S1) is reported where only the interactions considered in Ushio et al. (2018)³⁷ for the CCM are reported. This is because the goal is to compare the CCM inferred network to the TE-based one based on abundance. Fig. 7 shows the temporal fluctuations of abundance and the functional interaction matrices of ρ and TE. In this paper we study and compare average ecosystem networks for the whole time period considered but dynamical networks can also be extracted via time-fluctuating ρ and TE as shown in Fig. S3. These dynamical networks can be useful for studying how diversity is changing over time and ecosystem stability (Figs. S4, S6-S7) as well as understanding the relationship between ρ and TE (Fig. S5). In the network

of Fig. 6 the color and width of links is proportional to the magnitude of TE (Table S2); for the former a red-blue scale is adopted where the red/blue is for the highest/lowest TEs. The diameter is proportional to the Shannon entropy of the species abundance pdf (Table S3). The color of nodes is proportional to the structural node degree, i.e. how many species are interconnected to others after. Therefore, the network in Fig. 6 is focusing on uncooperative species whose divergence and/or asynchronicity (that is a predominant factor in determining TE over divergence) is large. Yet, the connected species are rarely but strongly interacting in magnitude rather than frequently and weakly (i.e., cooperative or similar dynamics). Additionally, the species with the smallest variance in abundance are characterized by the smallest Shannon entropy (smallest nodes) and more power-law distribution although the latter is not a stringent requirement since both pdf shape and abundance range (in particular maximum abundance) play a role in the magnitude of entropy. Average entropy such as average abundance are quantities with limited utility in understanding the dynamics of an ecosystem as well as ecological function. Nonetheless, species with high average abundance (e.g. species 5) have a very regular seasonal oscillations and the largest number of interactions with divergent species. A result that is expected considering the size of the population and the ability of the species to follow regular environmental fluctuations.

Figure S2 shows that the strongest linear correlation is for the most divergent and asynchronous species (from species 4 to 9) for which both ρ and TE are the highest (Fig. 7 B and C). This confirms the results of Fig. 3 and the fact that competition (or dynamical diversity more generally) increases predictability. This also highlights the fact that linear correlation among state variables does not imply synchronicity or dynamic similarity as commonly assumed. The interaction matrices in Fig. 7 B and C confirm that TE has the ability to infer a larger gradient of interactions than ρ and the total entropy of the TE matrix is lower than ρ . Pairwise the inferred interaction values by CCM and OIF are different but ρ and TE patterns appear clearly similar and yet proportional to each other.

CCM and OIF models are applied to calculate the potential interactions between all pairs of species. Fig. 7B and C show interaction matrices describing the normalized ρ from CCM and TE from OIF model of all pairwise species, respectively. The greater the strength of likely interaction, the warmer the color. These results demonstrate that CCM and OIF model present similar patterns for the interaction matrices in terms of interaction distribution, gradient and magnitude in order of similarity. This indicates that both CCM and OIF are able to infer the potentially causal relationships between species. Compared to the CCM interaction heatmap the OIF heatmap presents larger gradients of inferred interactions that

highlight the divergence and asynchrony in fish populations of species 4-9 from other species. This difference can be observed in Figure S2 that shows the strongest linear correlations for the most divergent and asynchronous species (4-9). It is worth noting that species 4-8 are all native species (See Table S1). Therefore, despite the patterns of interactions of CCM and TE are similar, CCM allows one a better identification of clusters of species with similar or distinct interaction ranges. Additionally TE estimates some weak observed interactions such as of species 2 (*E. japonicus*) with others, while CCM essentially consider null interactions for these species.

Precisely, the most interacting species (4-9) are the most divergent and asynchronous species (with respect to the whole community) as well as diverse in terms of values of abundance; these species form the "collective core" that is likely determining the stability of the ecosystem. Interestingly the number of these species is relatively small and it confirms results of other studies (see ^{54;55;56;57;39}) showing that the number of species with weak interactions is much larger. Theory suggests that this pattern promotes stability as weak interactors dampen the destabilizing potential of strong interactors⁵⁴. Mediated cooperation (e.g. by many "weakly" interacting competitors) as shown by Tu et al (2019)⁵² promotes biodiversity and diversity increases stability. When considering abundance values (at same time steps) of collective core species (Fig. S2) these species are linearly related and this increases their mutual predictability by either using linear or non-linear models based on correlation coefficient and TE. This proves that non-linearity increases predictability.

The choice of the optimal u that maximizes MI leads to the optimal TE model and resultant interaction network. The observed u over time is really small (Fig. S9) and this signifies how likely the ecosystem has small memory and responds quickly to rapid changes, or the information of change is carried over time by ecosystem's interactions which leads to accurate short-term forecasting. In other words, temperature-induced changes may take long time but the information of change is replicated at short time periods. The chosen time delay $u = 1$ corresponds to the species sampling of two weeks. Note that values of u are also dependent on the data resolution and they are strongly related to fluctuations rather than absolute α -diversity value. Thus, while biodiversity may fluctuate rapidly in time, value of α -diversity for seasons or longer time periods can be more stable and manifesting higher memory (representative of u for the whole ecosystem) than the one between species pairs (related to pair's u). Short-term catastrophic dynamics (for instance related to dramatic habitat change, sudden invasions, extinctions or rapid adaptations) may lead to irreversible shifts in interactions (strength and sign); this, in turn can affect biodiversity patterns that are completely uninformed by past dynamics. Thus, there is certainly a limit to predictability and to the validity

of time delays which can change very rapidly. However, we insist in emphasizing that models are *predictive tools* and predictions is not necessarily causality reflecting the many and highly complex underlying processes. Yet, interpretation of results must be done with care.

We also study temporally dynamical networks for the fish ecosystem community (see Section 2.3). CCM and OIF model are applied to quantify the causality between all possible pairs of species at each time period by calculating ρ and TE, respectively. Estimated effective α -diversity (Eq. 2.8) from CCM- and TE-based inferred networks at each time point can be obtained and then compared to the taxonomic (or "real") α -diversity. Results are shown in Fig. 8 and Fig. S6. In the whole time period, the estimated α -diversity from CCM is constant, whereas the global trend of the estimated α -diversity from OIF model slightly decreases over time that is consistent with the global trend of real α -diversity. CCM always predicts a non-zero interaction for all species (including negative values) whereas OIF predicts zero interactions for some species that are then not making part of the estimated effective α -diversity.

Figure 8 shows the effective α diversity from CCM and OIF for an optimal threshold of ρ and TE (i.e., 0.2 and 0.3) that maximizes the correlation coefficient and Mutual Information (MI) between α_{CCM} or α_{TE} and the taxonomic α , respectively. The maximization of the correlation coefficient and MI guarantees that the estimated effective α are the closest to the taxonomic α . Figure S6 shows effective α for unthresholded interactions and other thresholds. Note that the threshold on TE does not coincide with the value of TE that maximizes the total network entropy (Fig. 8) and then some of the reported species may not be part of the ecosystem strongly. Thus, this threshold method is also useful to identify species that are truly forming local diversity vs. transient species. Considering the pattern of fluctuations of effective α -diversity from CCM they are poorly unrelated to the real α -diversity, while those from OIF are much more synchronous with seasonal fluctuations of real α -diversity. However, α_{TE} is a bit higher than the average taxonomic α . Both CCM and TE predicts a decrease in α in time that corresponds to an increase in SST. As shown in Fig S6, OIF is attributing higher sensitivity to SST for small interaction species because α fluctuations show seasonality that happens when species follow environmental dynamics closely. Vice versa, CCM is predicting a broader sensitivity for all positively interacting species. These results reveal that OIF gives an effective tool to measure meaningful interdependence relationships between species for constructing temporally dynamical networks where the number of nodes over time (estimated $\alpha(t)$) can reflect closely the taxonomic α -diversity. This allow us to find more reliably how changes of environmental factors (e.g. SST) affect biodiversity in ecosys-

tems. The establishment of thresholds on interactions is also useful for exploring ranges of interdependencies and associated effective α -diversity with respect to the average taxonomic diversity. β effective diversity is another very important macroecological indicator informing about ecosystem changes; for instance in Li and Convertino (2019)³⁹ β -diversity identified distinct ecosystem health states. However, α and β (effective diversity) variability are highly linked to each other and yet looking into one or another would provide equivalent results. The difference between taxonomic and effective β -diversity may provide some information about invasive or rare species have weak influence on the ecosystem since they are characterized by low TEs. Supplementary Information contains further elaborations on results.

3 Discussion

In the paper the proposed Optimal Information Flow (OIF) model was validated by considering the problem of causality inference of species interactions for ecosystems with different level of complexity and systemic uncertainty: a deterministic mathematical model of predator-prey dynamics, the real Sardine-Anchovy-Temperature triplet ecosystem in the Pacific, and a real multispecies fish ecosystem in Japan. These three case studies are epitomic example of deterministic, low and high complexity dynamics. The mathematical model can be generalized as a model for interaction dynamics between individual or communities of the same species or between two generic variables X and Y. The quantification of interactions was compared to the well-documented CCM model.

Early method of correlation were proved to be neither necessary nor sufficient to estimate the causal relationship between time series variables (mostly due to the fact that any association does not prove causality because models are not surrogate of reality and scale-dependent data are just a sample of ecosystem dynamics), even though it remains a common and heuristic notion^{35 29}. Despite these views we prove the power and limitations of correlation methods with respect to non-linear methods (such as OIF and CCM), dynamics of the complex ecosystem considered, and target patterns to predict that define whether correlation is able to measure interactions. As for the latter, for instance we show how even highly non-linear systems show linearity when non-linear "causal" variables are considered at the same time step (as a virtue of non-linear asynchronicity). Therefore, the scale of analysis considering also the space-time domain with the explicit consideration of lag effects, determines the dynamics that is visible and the model that can be used for predictions.

Granger causality is the primary framework that uses predictability especially for identifying causation, however it is problematic in highly nonlinear systems even with some deterministic states or components. Sugihara et al. (2012)²⁹ managed to deal with the problem and introduced the CCM model. CCM was well documented and successfully applied to bio-inspired mathematical models, as well as real-world ecosystems²⁹. Despite interactions among species or variables, or interdependencies more generally defined, are rarely completely zero and related to patterns of different processes to capture, Sugihara et al. (2012)²⁹ maintains the view of a deterministic single-value causality. In our opinion calculating causality in an absolute sense between variables is always not only very hard, but also meaningless because the resulting values are dependent on data and models used as well as the predicted patterns for which interactions are calculated for. The very first question should be causality about what? After that the evaluation of the dynamics of the ecosystem coupled to the target patterns to map should drive model selection. Causality is actually predictability of patterns of interest and predictability can be close to true causality for systems with low complexity and noise. The basic principles to interpret predictability are uncertainty reduction and accuracy that can be quantified as the probability of an event to occur given another one (as predictands and predictors, respectively).

From the perspective of information theory that has attracted attention in complex networks research, entropy is the information-theoretic description for uncertainty or more precisely lack of organization rather than absolute uncertainty. Uncertainty is in fact also information about the diversity of values of a complex system (see e.g. Jost (2006)⁵⁰ that demonstrated how entropies are reasonable indices of diversity) and the distribution of these values determines entropy. The fundamental work of studying complex networks is to untangle complex interdependencies comprising a large number of potential causations between all pairwise nodes (variables), that allows one to predict the collective behavior of complex systems. The intuitive and heuristic notion for this problem in information theory is transfer entropy that measures the uncertainty reduction (or information flow) between nodes (variable). From this conceptual perspective we name the OIF model for inferring potential causality seen as sets of uncertainty reduction networked fluxes. Multiple transfer entropies for one single variable as a function of all others determine non-linearity that cannot be overlooked even when variable interaction is deterministic. Considering entropy as diversity also implies that OIF provides reflections of temporal changes in diversity (e.g. biodiversity) determined by changes in information fluxes.

The bio-inspired mathematical model generates a clean inter-species interaction ecosystem

without any noise, that allow us to estimate “true” causality between synthetic species X and Y. The so-called “true” causality means the causation embedded numerically in the parameters in the dynamical equations 2.1 (β_{xy} and β_{yx}). When β_{xy} is fixed as zero only the unidirectional causality ($X \rightarrow Y$) exists between species X and Y. Then, any estimator of predictive causality closer to the physical causality β defines the accuracy of the model. Results from Fig. 2 shows how OIF model outperforms CCM.

Depending on the values of the parameters the model may capture some biological dynamics such as amensalism and commensalism (when β_{xy} or β_{yx} are zero), or predation, competition and mutualism (when both β_{xy} and β_{yx} are different than zero). Biologists define amensalism (i.e. a strong asymmetrical competition) is a type of biological relationship between species in which one species (e.g. X) has a potential negative effect on another (Y), but the second species Y has no detectable effect on the first species X. Biologically speaking, commensalism is another type of biological relationship in which one species (Y) gets benefits while the other one (X) is neither helped or harmed.

In a broad complex dynamic perspective it is easier to talk about “cooperation” or “competition” between variables meaning that variables contribute similarly to the uncertainty propagation of the whole ecosystem, or that one variable is predominant over the other in terms of magnitude vs. frequency of effects. Similarly to brain function⁵⁸, cooperation is typically driven by excitatory interactions leading to synchronization in biomass fluctuations, where species are characterized by power-law distributions; vice versa competition is driven by inhibitory interactions leading to asynchronization, where species are characterized by exponential or non-fat tail distributions of abundance. The generic dynamical characterization allows to avoid pitfalls of the categorical classification of interactions in biology that suffers from the lack of knowledge about true and meaningful values of interactions that distinguish one biological dynamics from another; this is also considering change in biological interactions over time driven by environmental changes and/or evolution. Depending on the ecosystem state, interactions might range between “positive” and “negative” with no clear cuts between them: e.g.³⁹ showed that network topology and interactions among the same microbial species change for different ecosystem states. We also caution to use numerical estimates of interactions to replace empirical biological knowledge because data-inferred interactions are always much more complex than experimental values (e.g. about highly controlled lab tests) and interactions are certainly highly affected by the environmental context, measurement technology, and biomarker considered (e.g. abundance or others). The similar pattern of inferred interactions of the predator-prey system shows that all methods

(correlation, MI, CCM and OIF) can work for inferring causality between two variables with different level of granularity. However, considering our definition of predictive causality, as non-linear predictability of diverse events from independent predictors, OIF outperforms all other models due to the explicit consideration of asynchronicity, divergence and diversity of events that define model sensitivity, uncertainty and complexity. All these considerations further emphasize the need to distinguish biological interactions and model-driven inferred interdependencies (or predictive interactions) as also emphasized by other authors⁵¹.

To analyze OIF performance for "low complexity" ecosystems we considered the ambiguous dynamics of sardines and anchovies in oceans. On multidecadal time scales, sardines and anchovies present alternating dominance across global fisheries. Although in appearance a ecological competition seems to exist between these two species (due to the inversely proportional and synchronized abundance changes), the simultaneous fluctuations of sardine and anchovy stocks suggest that they are also influenced by the ocean temperature.

Incompatible hypotheses have been advanced to try to give explanations for this pattern of alternating dominance, unfortunately leaving aside many other species that clearly exist in the ocean and interacting with sardines and anchovies. Some supposed that these two species act in direct and clear competition⁵⁹, while others argued that this pattern is just a result of different or opposite fish dynamics in response to common global environmental forces⁶⁰. Results in Baumgartner (1992)⁶¹ revealed that in longer time series not only the negative cross-correlation observed in the 20th century disappears, but the correlation with global environmental forces also has been ambiguous. This lack of correlation is however only related to the fact that species are synchronous and environment→species effects are characterized by relatively small lags. Yet, lack of evident correlation exist but that does exclude causation. Jacobson and MacCall⁶² applied two models to this issue and proposed a relationship that SST influences the behavior and population of sardines and anchovies; however, this relationship vanished when applying the analysis to stock assessments from 1992 to 2009. Although all these possible explanations from different points of view are competing, or even unstable, such results can illustrate that causal interactions among sardines, anchovies and SST present features of nonlinear dynamics. Nonetheless, and more importantly, the conclusion is that both species are weakly interacting and majorly affected by the environment. All interdependencies exist and they just change in terms of normalized magnitude without neglecting the fact that intrinsic interspecies interaction is also modulated by the environment. As shown by the predator-prey mathematical model (Fig. 3) and real data (Fig. 5 and 7), synchronized species are certainly affected by a third variable (e.g. the

environment and other species) that is forcing both in fluctuating at the same time.

Heuristically, it is also very unlikely that two species (or variables more generally) are perfectly synchronized unless they are identical. What Fig. 4 shows is somewhat very affine to the Heisenberg’s uncertainty principle that marks a clear break from the classical deterministic view of the universe. We cannot know the present state of the world in full detail (such as for the “red” dynamics), let alone predict the future with absolute precision. Determinism, driven by synchrony, allows us to know the current state of the system if that is unaltered but not to predict future states. Vice versa, uncertainty-driven asynchronicity and divergence allow us to predict likely future more than actual present and that appears to be in contradiction to deterministic views but not to realistic probabilistic (or relativistic) view of system dynamics. For this sardines-anchovies “problem” unfortunately the whole complexity of ecosystems has never been considered despite other species may have a dominant effect on their abundance. This underlines the importance of space-time and biological scale (where biological scale is define by the number of interdependent species at the same or different trophic levels) in framing the problem and bounding conclusions to model results: any “causation” is in reality an interdependence between species constrained to the chosen scales, data resolution, as well as model analytics and biomarkers used for inferring interdependencies. For instance, lack of large environmental disturbances (or coarse resolution sampling) affecting rapidly small organism change may reduce the information flow, and yet affecting the inferred interaction network.

In addition to testing OIF on the simplified sardine-anchovy ecosystem, we apply OIF and CCM to a multispecies ecosystem in which 14 dominant fish and 1 jellyfish species were monitored in an abundance census in the Maizuru Bay, Japan. In this ecosystem, all species can be interconnected, leading to an intricate causality system that is extremely hard to estimate considering intrinsic biological species interactions, interactions related to environmental influence, and biological interaction mediated by the environment. “True causality” assessment is also extremely hard because there is no knowledge of which ecological or biological marker can capture all these interaction types. However, when causality is shifted to predictability of patterns of interest, the issue of inferring causality becomes practical and meaningful. Predictive causality between species X and Y, for instance, depends on whether X can assist in predicting the future of Y beyond the extent to which Y itself predicts its own future, and complementarily whether the model can predict the collective behavior of the system which can be reflected by macroecological indicators dependent on all predictive causality. In this case study, both CCM and OIF models are effective for causality detection

777 from different points of view and they majorly differ considering interaction gradient and
778 computational complexity. As for the latter OIF and CCM have 3 and 20 parameters to
779 populate and the speed of inference assessment for the Maizuru 15 species ecosystem is 2
780 and 15 minutes, respectively. An already published work used the same time-series data to
781 study how to infer the network and forecast the system stability for the fish community using
782 CCM³⁷.

783 Ushio et al. (2018)³⁷ used a “S-map” model (i.e., sequential locally weighted global linear
784 map model) to track dynamical interactions over causally related species over time where
785 causality between species is estimated a-priori via CCM. S-map does so by predicting future
786 values of species abundance from the reconstructed multivariate state-space vector (where
787 species are interdependent by inference). Before CCM a “phase-lock twin surrogate” method
788 removes seasonality from abundance data; this method generates time series that preserve
789 the shape of a species attractor but exhibit no causal relationship with a target (seasonality)
790 time series. Other predictive models other than S-map have been proposed such as the
791 multiview embedding model⁶³ (in a “Empirical Dynamic Modeling” suite of models⁶⁴) that
792 is combining multiple species embeddings (with different time delays) and that is superior in
793 forecasting skill than multivariate (e.g. S-map) and univariate embedding (used by CCM for
794 reconstructing the attractor of each species individually and later on the cross-mapping skill
795 ρ of each other is evaluated).

796 Here we believe that any environmental forcing is important to be captured and affect
797 non-linearly and in an unpredictable way the interactions among species; pure biological
798 interactions are utopianly impossible to measure (leading to the “curse of environment sep-
799 arability” from biota) and they are always context dependent (i.e. the geographical area
800 considered although universality in biological dynamics may be expected). While it may be
801 true that synchronization driven by seasonality can lead to misidentification of “biological”
802 or “true” causality (false negative without the consideration of time lags, or false positive
803 as in Ushio et al. (2018)³⁷ if lags are considered in the phase-space), we believe that the
804 environment is precisely the common identifiable cause of synchronization of species (or of
805 other asynchronous effects impacting species differently) in a predictive causality purview.
806 Additionally our is a more realistic analysis of ecosystems where the environment is central
807 in shaping interconnected populations, and then community patterns, via complex non-linear
808 function vs. simple assumed sinusoidal seasonality (homogeneous for all species). Lastly, in
809 our opinion another pitfall of the “phase-lock twin surrogate” model of Ushio et al. (2018)³⁷
810 is the fact that seasonality importance is weighted for each species in isolation whereas sea-

sonality is also affecting interactions of species pairs in ecosystems. Interactions that arguably should be inferred from data as they are since data contain hardly separable non-linear effects of environment and other species dependencies in addition to single species adaptation and evolution.

OIF, through the inference of a better gradient of systemic interaction “causality”, predicts how biodiversity changes over time with average value, fluctuations and trend that is closer to the taxonomic α -diversity. This is for effective α diversity with the optimal threshold on interactions maximizing the similarity with observed α (via maximization of Mutual Information). The concept of effective α is very useful because it allows to see which set of interactions is determining levels of α diversity that is potentially more or less sensitive to environmental forcing. For example, S6 shows that high interaction species form a small portion of community diversity that is increasing over time vs. the systemic decrease in diversity (observed in Fig. 8). More importantly, the increasing fluctuations of estimated α from OIF show the potential way in which climate and/or other anthropogenic changes negatively affects biodiversity in the region considered in relation to intensified interspecies interactions as suggested also in other studies^{65;66;67}. These results are certainly beneficial for fishery resources management and habitat protection aiming to preservation of the fish community with ecological, economic and social outcomes. Thus, models like OIF should be evaluated in this bigger perspective of ecosystem utility or ecological engineering with multiple utilities rather than just seeing these models for the hard inference of pure “biological” interaction causality. Supplementary Information contains further discussions about CCM, TE causality inference, predictability, ecosystem organization and stability.

4 Conclusions

Causality detection is a fundamental step in the inference of complex networks with the aim of understanding processes of observed complex systems. This is incredibly important for poorly observable large scale ecosystems whose structural and functional networks are their backbone. However, quantifying the “truly causal” interactions in complex systems is illusory and perhaps impossible to achieve due to data and model limitations (e.g. sampling over space and time), partial ignorance about underlying processes, the strong unmeasurable influence of environmental dynamics, and more importantly their relativity dependent on the scale of analysis and the patterns for which interactions are relevant for. Nonetheless, when

causality is shifted to predictability, this issue becomes practical and useful because it links causal *predictable* interactions to some patterns to predict. Patterns that are defining the socio-ecological outcomes of interest for which interactions are signatures of the underlying processes. In this paper we propose the Optimal Information Flow (OIF) model and assess its validity and performance in causality inference by comparing OIF to well-documented CCM and correlation model. This is done for a deterministic predator-prey mathematical model, a data-driven sardine-anchovy species dynamics, and an observed multiple fish species ecosystem. We show that OIF, like CCM, is able to effectively identify asymmetric causal interactions between any pair of species. Moreover, OIF performs better than CCM because it provides: (i) a larger gradient of interaction values, yet defining interactions at higher resolution with better definition of asymmetrical interdependencies; (ii) smaller fluctuations around the estimated interaction values for any time delay u , yet a less uncertain inference; (iii) the estimated memory of one and pairs of species in terms of time delay (without considering future modifications of CCM⁶⁸); (iv) independence on the length of historical data and no requirement for convergence, as well as lower computational complexity (leading to lower sensitivity and uncertainty in state estimates); and, (v) more accurate predictions of temporal changes in macroecological indicators of ecosystems such as for the effective α -diversity after optimal MI-based threshold selection. However, OIF requires the identification of the optimal u value as shown in³⁹ but this is easily automated by exploring the delay that maximizes MI. Even though a time delay can be defined for any pair of species, we show the the average time delay, derived from analyzing all species pairs, can be a global optimum providing accurate macroecological predictions for the ecosystem considered. Thus, the assumption-free information-theoretic OIF is a strong candidate model for the inference of predictable causality in complex ecosystems. A model that is itself an ecosystem mimicking the information flow constituting the backbone of real ecosystems of any nature, from environmental to socio-technological systems. The complexity of real world systems might be higher than the ones studied in this paper, considering the velocity of transitions in rapidly changing systems. Nonetheless, we believe that the dynamics encompassed in our study reflects the fundamental stochastic processes observable in the real world, particularly at stationarity but changes in network topology can be mapped by inferring dynamical networks over time. In a broader uncertainty propagation perspective interactions should be considered as “cooperation” and “competition” between species (or variables more generally) meaning that they contribute in a similar or opposite way to the uncertainty (or information) propagation. Competition means that one variable is predominant (or very diverse) over the other in terms of magnitude of interactions since TE is proportional to the magnitude rather than the frequency of

878 interactions. Interactions that are specifically proportional to the divergence and asynchrony
879 of variables/species which leads to higher predictability. In conclusion, our model can find
880 useful applications in research and applied work for ecosystems at multiple biological scales.
881 A myriad of other models have been proposed in literature, and these can be used simultane-
882 ously in real-life applications, to provide the full range of possible states of interactions and
883 average systems' patterns trajectories. As causality is considered as non-linear predictability
884 of diverse events of populations or communities, we believe OIF is the optimal model able to
885 predict the largest divergence of trajectories due to the full consideration of ecosystem states
886 via species probability distribution functions. Predictive causality is a convenient definition
887 for any ecosystem, or data science problem more generally. However, for investigations of
888 causality aiming to learn underlying physical processes of observed patterns, or for solving
889 pressing issues of real complex ecosystems, a more in depth inquiry of complexity and dy-
890 namics (in relation to the target objectives), system learning and stakeholder collaboration
891 are of paramount importance since data and models alone cannot reveal the full picture nor
892 identify realistic and optimal solutions.

5 Materials and Methods

5.1 Ecosystems Models

5.1.1 Bio-inspired Two Species Mathematical Model

In Sugihara et al. (2012)²⁹, a mathematical model was introduced to generate coupled nonlinear sequences for testing the CCM presented in that study. The model consists of two diffusively coupled logistic maps describing a simple bio-inspired dynamics without any external environmental effects on both species. It is analytically formulated as:

$$\begin{aligned} X(t+1) &= X(t)[r_x - r_x X(t) - \beta_{xy} Y(t)] \\ Y(t+1) &= Y(t)[r_y - r_y Y(t) - \beta_{yx} X(t)] \end{aligned} \quad (5.1)$$

where X and Y are two random variables linked by factors β_{xy} and β_{yx} that establish the strength of their interactions. It gives possibility to estimate the "true" causality in an absolutely numerical sense and this model can be therefore indicated as $S(\beta_{xy}, \beta_{yx})$. If β_{xy} is fixed as 0 and β_{yx} is fixed as non-zero or varied free, that is, X causes Y , but not vice versa. If β_{xy} and β_{yx} are both non-zero, X causes Y and vice versa. These conditions generate two different kinds of coupling variables that respectively represent unidirectionally and bidirectionally interactive species-species systems described as the case 1 in Fig. 1. r_x and r_y are the intrinsic growth rates for each variable.

In this study, we focus on both unidirectionally and bidirectionally interactive species-species systems. For unidirectional coupling, β_{xy} is fixed as 0, but β_{yx} is free varied within the range of $[0,1]$, leading to a simplified model as $S(0, \beta_{yx})$. This unidirectional model $S(0, \beta_{yx})$ is exploited to generate coupled sequences of two random variables X and Y where X affects Y , but not vice versa. For bidirectional coupling, we study two different conditions. On the one hand, we consider a system $S(\beta_{xy}, \beta_{yx})$ in which β_{xy} is fixed as 0.2, 0.5 and 0.8, β_{yx} is free varied within the range of $[0,1]$. This model can be indicated as a univariate model $S(0.2/0.5/0.8, \beta_{yx})$ and is used to generate interdependent coupled time-series variables where the effect of X on Y changes over β_{yx} , while the effect of Y on X is stabilized due to the fixed non-zero β_{xy} s. On the other hand, we consider a bivariate system $S(\beta_{xy}, \beta_{yx})$ in which both β_{xy} and β_{yx} are free varied. This model indicated as $S(\beta_{xy}, \beta_{yx})$ generates coupled time series of variables X and Y where X and Y randomly interact with each other. For all these conditions mentioned here, $S(0, \beta_{yx})$, $S(0.2/0.5/0.8, \beta_{yx})$ and $S(\beta_{xy}, \beta_{yx})$ are run under the conditions of which initial $x(1) = 0.4$, $y(1) = 0.2$ and intrinsic growth rates of

variables r_X and r_Y respectively are 3.8, 3.5 as used in²⁹. These time series of variables X and Y generated by the models for example can be time-series data of species abundance.

5.1.2 Sardine-Anchovy-Temperature Ecosystem

As a real-world ecosystem case study, yearly time-series data of Pacific sardine landings, northern anchovy landings and sea surface temperature (SST) obtained at Scripps Pier and Newport Pier, California are used here. Sardines and anchovies seldom interact with each other because of geographical distribution. External environmental factors including SST affect sardines and anchovies, but not vice versa. It is a typical example of unidirectional causal relationship in real-world ecosystems and such tripartite relationship can be described as the case 2 in Fig. 1. Sugihara et al. (2012)²⁹ also studied this fishery ecosystem and successfully inferred the weak causal interactions between sardines, anchovies and SST with the CCM method. We remake the experiments Sugihara et. al did, and apply our proposed OIF model to do the same work as well, thereby validate the OIF model by comparing results to those from CCM.

5.1.3 Fish Community in the Maizuru Bay Ecosystem

Long-term time-series data counting the observations of the fish community collected along the coast of the Maizuru Fishery Research Station of Kyoto University³⁷ are used in the multispecies case study described as the case 3 in Fig. 1 for OIF model validation. Underwater direct visual censuses were conducted approximately once every two weeks from January 1, 2002 to April 2, 2014, totally generating 285 time points sequences during about 12 years long census. Dominant fish species (that is, with a total observation count was larger than 1,000) were considered, because rare species that were sporadically observed during most of the census term have many zero values, and yet there were not suitable for the time-series analysis. Information of rare species dynamics is typically very small within other species and their inclusion does not change results about the whole ecosystem interaction topology beyond just adding poorly or not interacting species as found in Ushio et al, (2018)³⁷. Therefore, only 14 dominant fish species and 1 jellyfish species were selected in this dataset. 1 Jellyfish species was selected in the dataset because this species was abundant in this area and was thought to have considerable influences on the community and ecosystem dynamics.

953 Accordingly, both OIF and CCM model are exploited to measure causal interactions among
954 14 dominant fish species and 1 Jellyfish setting up the dynamical complex multispecies system.
955

956 5.2 Interactions Inference Models

957 5.2.1 Linear Correlation Model

958 The linear correlation between non-lagged random variables X and Y is given by:

$$\text{corr}(X, Y) = \frac{\sum_{t=1}^L (x_t - \bar{X})(y_t - \bar{Y})}{\sqrt{\sum_{t=1}^L (x_t - \bar{X})^2 \sum_{t=1}^L (y_t - \bar{Y})^2}} \quad (5.2)$$

959 where $\bar{X} = \frac{1}{L} \sum_{t=1}^L x_t$ and $\bar{Y} = \frac{1}{L} \sum_{t=1}^L y_t$. L is the length of time-series of X and Y.
960

961 5.2.2 Convergent Cross Mapping Model

962 The principle of CCM model involves state space reconstruction from two variables and
963 quantifies the potentially causal (asymmetrical) relationship between these variables using
964 the method of nearest neighbor forecasting. Nearest neighbor forecasting method is an appli-
965 cation of Takens' Theorem called simplex projection. States of a system are reconstructed by
966 applying successive time lags of time-series variable underlying the method of time lag em-
967 bedding^{29;38}. Interestingly, this method has been originally applied to describe the transition
968 to turbulence of fluids^{69;70}.

969 In the case where X causes Y, Takens' theorem indicates that there should exist a "causal"
970 relationship between states of X and the contemporaneous states of Y. CCM quantifies this re-
971 lationship using the simplex projection to predict time-series X from reconstructed Y. Specif-
972 ically, a manifold M_X ("reconstructed", "shadow" or predictor manifold) is constructed from
973 lags of variable X (i.e., $X(t - \tau)$ with the time lag τ) and used to estimate contemporaneous
974 values of $Y(t)$. M_X is an approximation that will display convergence up to the level set
975 by observational error and process noise. At convergence the approximated $\hat{Y}(t)|M_X$ will be
976 close to $Y(t)$. The relationship between $Y(t)$ and $Y(t - \tau)$ is on the target manifold. To
977 explore the opposite "causality" CCM explores the convergence of $\hat{X}(t)|M_Y$ to $X(t)$ where
978 M_Y is the predictor manifold. Thus, CCM determines how well local neighborhoods (defined

by $E + 1$ points, that is the minimum number of points needed for a bounding simplex in an E -dimensional space) on the manifold M_X correspond to local neighborhoods on M_Y .

Pearson’s correlation coefficients ρ (originally defined as Eq. 5.2 considering non-time lagged variables) between predicted time series and observations of X (or Y) are calculated. The non-linear correlation coefficient is considered as the indicator of cross-mapping skill, that is the “causality” between species X and Y . The non-linear ρ is defined as:

$$\begin{aligned}\rho(X \rightarrow Y) &= \frac{\text{cov}(Y(t), \hat{Y}(t)|M_X)}{\sigma_Y \sigma_{\hat{Y}(t)|M_X}} \\ \rho(Y \rightarrow X) &= \frac{\text{cov}(X(t), \hat{X}(t)|M_Y)}{\sigma_X \sigma_{\hat{X}(t)|M_Y}}\end{aligned}\tag{5.3}$$

where cov and σ are the covariance and standard deviation. $\hat{X}(t)|M_Y$ and $\hat{Y}(t)|M_X$ are the predicted values of $X(t)$ and $Y(t)$ considering the attractor manifolds of lagged Y and X . Considering the relationship between the calculated cross-mapping skill and the length of time series L , ρ increases with L until a convergent stable value. ρ is always larger the longer L and that indicates causality according to Sugihara et al. (2012)²⁹. Typically, no less than 30 points in the time-series data should be used for CCM analyses⁷¹. Further details about the use of CCM for this study are provided in Supplementary Information. CCM codes are available at <https://github.com/HokudaiNexusLab/net-valid>.

5.2.3 Optimal Information Flow Model: TE Inference

OIF requires time-series data of variable biomarkers (e.g. abundance) as input, and produces a Transfer entropy (TE) matrix quantifying interactions between all pairs of variables. Therefore, the primary output of OIF is a functional interaction network for the ecosystem considered. In this paper we consider all inferred TEs without any redundant interaction removal as in Servadio and Convertino, (2018)⁴⁹. All OIF codes are available at <https://github.com/HokudaiNexusLab/net-valid>. TE is a non-parametric statistic in information theory that estimates the amount of information that a source variable contains about a destination variable considering destination’s current and historical states⁴⁰. It measures how much directed (time-asymmetric) information transfers between two variables, giving an incentive to quantify the causal relationship between two variables with TE. Here

1005 it can be calculated as:

$$TE_{Y \rightarrow X}^{(k,l)} = \sum_{x,y} p(X_t, X_{t-u}^{(k)}, Y_{t-u}^{(l)}) \log \frac{p(X_t | X_{t-u}^{(k)}, Y_{t-u}^{(l)})}{p(X_t | X_{t-u}^{(k)})}, \quad (5.4)$$

1006 where, X and Y denote two random variables, k and l refer to the Markov orders of
 1007 variables X and Y , implying that we need to at least consider k (l) time points of variable
 1008 X (Y) in the past for the estimation in order to capture all relevant information in the past
 1009 of X (Y). Here we assume that the time-series analysis here obeys a memoryless Markov
 1010 process. Hence, parameters k and l are fixed as 1, that is to say, the next states of X and Y
 1011 are only dependent on the current states and not on states in the past. u is the source-target
 1012 time delay establishing lagged influence and is free varied. Servadio and Convertino (2018)⁴⁹
 1013 proposed a framework of optimal information networks (OIN) to select TEs that maximize
 1014 the total entropy for inferred networks. Probability distribution functions associated to the
 1015 network with maximum entropy are considered as the most predictive distributions fitting
 1016 observations (where power-laws have the lowest entropy but highest uncertainty reduction
 1017 when compared to other distributions). TE in Eq. 5.4 is estimated until the selected time t
 1018 with incremental time series data whose minimum resolution is g (equal to 30 time points,
 1019 that is 60 weeks) that defines the minimum number of points required for robust inference
 1020 (see Supplementary Information section S1.3).

1021 In this paper, OIF is improved by incorporating the well-documented JIDT toolkit⁴² in
 1022 computing TE. The JIDT toolkit provides users with multiple alternatives for pdf estimation
 1023 including discrete, binned, Gaussian, Kraskov (KSG) and Kernel models that cover most data
 1024 types (from uniform to power-law). Therefore, OIF with JIDT is more flexible in relation to
 1025 diverse ecosystems and datasets.

1026 JIDT-Kernel as model-free estimator calculates joint pdf by discretizing data into bins.
 1027 A classical approach called Kernel estimation uses equal-width bins specified by a bin-width
 1028 parameter. The joint pdf can be written as:

$$p(\mathbf{x}) = \frac{1}{N} \sum_{n=1}^N \Theta(|\mathbf{x} - \mathbf{x}_n| - r), \quad (5.5)$$

1029 where Θ is a step kernel such that $\Theta(x \leq 0) = 1$ otherwise equals zero, $|\mathbf{x} - \mathbf{x}_n|$ is the
 1030 maximum distance between variable $\mathbf{x}$ and observation measurement $\mathbf{x}_n$ for $n = 1, 2, \dots, N$.

1031 The parameter r is the specified bin width. Note that the estimation is sensitive to the choice
1032 of parameter, and the number of bins can be different between variables. After calibration
1033 we selected the optimal bin-width as 0.25.

1034 In this study we also investigate the optimal TE that provides a clearer detection and
1035 more accurate quantification for causal relationships between two variables by choosing an
1036 appropriate time delay u in a specified range. The choice of the optimal u within the range
1037 leads to the optimal TE model and resultant network inference while considering the minimum
1038 computational complexity. As shown in our previous work about microbiome³⁹, time delay u
1039 used to calculate TE between species is the one who minimizes the distance from one species
1040 to another in the inferred network.

1041 The distance can be calculated by³¹:

$$d(X, Y) = e^{-MI(X(t \pm u); Y(t))} \quad (5.6)$$

1042 where MI is the mutual information of variables X and Y. MI of two random variables X and
1043 Y, is given by:

$$MI(X(t \pm u); Y) = \sum \sum p(x(t \pm u), y) \log \frac{p(x(t \pm u), y)}{p(x)p(y)}, \quad (5.7)$$

1044 where $p(x)$ and $p(y)$ are the marginal distributions of random X and Y, and $p(x(t \pm u), y)$
1045 is the joint probability distribution that is the pdf affected by the time-delay. The time delay
1046 u that is chosen is exactly the one that maximizes the MI of the two variables, because that
1047 is the one that minimizes the uncertainty. MIs is calculated using a range of time delays u
1048 (defining temporal entropy reduction parameters) and then the time delay corresponding to
1049 the maximum MI is selected before the calculation of TE. The choice of using the time delay
1050 u that maximizes MI is focusing on the highest predictability rather than the investigation
1051 of true causality. For example, two species may have a relatively low average interaction,
1052 except for a limited time period when the interaction is very high due to seasonal predation
1053 or sudden environmental disturbances (e.g., intense fishing or water pollution). Thus, by
1054 considering the maximum MI the focus is on extreme interactions (leading to the highest
1055 predictability) vs. average most likely mutual interactions, or more precisely it is focused on
1056 the magnitude of potential interactions rather than the interaction frequency. Yet, extreme
1057 accidental interactions are also captured by the choice of $MI(u = u_{max})$, although very
1058 limited interactions may exist on average. This is equivalent to the approach of extended

1059 CCM³⁸ for which the time delay that maximizes predictability (convergence) is chosen. The
 1060 existence of a time delay explicitly takes into account delayed interaction effects, for example,
 1061 due to delays in biomass conversion in case of predation; interestingly these model-inferred
 1062 delays should be used when assessing predator-prey abundance scaling laws⁷² (fingerprinting
 1063 ecosystem metabolic function) whose exponent is affected. In addition, we also compare the
 1064 results of the linear cross-correlation estimates and the non-linear MI estimates for species
 1065 interactions. Mutual information is a distance between two probability distributions while
 1066 correlation is a linear distance between two random variables. This is done to detect the
 1067 causal relationships between variables in the non-linear mathematical predator-prey model
 1068 (where the two variable X and Y can be also belong to the same species) also to detect the
 1069 performance of linear vs. non-linear interaction inference models. On the contrary of the
 1070 asymmetric TE (that measures directed interdependencies between variables), MI, as well
 1071 as cross-correlation, provides a symmetric measure for inferring mutual interdependencies
 1072 unable to identify the direction of potential causal interactions.

1073 5.3 Predicted Ecosystem Biodiversity Patterns

1074 Details about the calculations of taxonomic and effective α -diversity are contained in the
 1075 Supplementary Information.

1076

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Author Contribution

M.C. idealized the study, wrote the manuscript, and prepared all final figures. J.L. performed all calculations and created the preliminary figures.

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Figure Captions

Figure 1. Studied ecosystem complexity. Epitomes of increasing ecosystem complexity are shown from left to right where nodes are representing variables (e.g. species or other socio-environmental features). Case 1 shows two basic cases: unidirectional and bidirectional interactions where true interaction strength is known because embedded into a mathematical model. Case 2 is about environment-mediated interactions with no knowledge of "true" interactions. Case 3 is a multispecies ecosystem with multiple bidirectional interactions with no knowledge of "true" interactions.

Figure 2. Inferred predictable causality via CCM and TE for embedded true causality. CCM correlation coefficient (ρ , left plots) and Transfer Entropy (TE, right plots) are shown for the bio-inspired mathematical model in Eq. 5.1 representing bidirectional interactions. The mathematical model indicated as $S(\beta_{xy}, \beta_{yx})$ is simplified as a univariate function because β_{xy} is fixed while β_{yx} is free and varying within the range $[0, 1]$. β_{xy} and β_{yx} are establishing true causality while ρ and TE are indicators of predictable causality. Y's causal effects on X is theoretically fixed as a stable value corresponding to each β_{xy} . The greater β_{xy} the stronger Y affects X (estimated by ρ_{yx} and TE_{yx} in red lines). (A) $\beta_{xy} = 0$ means that Y does not affect X and then X dynamics is only related to stochastic dynamics due to birth-death process as in the model (Eq. 2.1). X's effects on Y depends on the value of β_{yx} , theoretically leading to increasing functions ρ_{xy} and TE_{xy} (blue lines) when β_{yx} increases; (B) $\beta_{xy} = 0.2$; (C) $\beta_{xy} = 0.5$; and (D) $\beta_{xy} = 0.8$.

Figure 3. Phase-space maps of normalized coupling predictive causation via correlation, mutual information, CCM and OIF for varying true causal interactions. Both true causal interactions β_{xy} and β_{yx} are free varying within the range $[0, 1]$, indicating a bivariate model $S(\beta_{xy}, \beta_{yx})$ where both species (or variables more generally) are interacting with each other with different strength. (A) normalized correlation coefficient; (B) normalized mutual information; (C) and (E) normalized CCM correlation coefficient (ρ) for interaction directions of $X \rightarrow Y$ and $Y \rightarrow X$; (D) and (F) normalized transfer entropy (TE) from OIF model for interaction directions of $X \rightarrow Y$ and $Y \rightarrow X$.

Figure 4. Dynamics of abundance and predictability for the bidirectional two species ecosystem model. (A) plots refer to the species abundance in time for the mathe-

1314 matical model in Eq. 2.1 for different predictability regimes associated to different interaction
 1315 dynamics from low to high complexity ecosystem associated to low and high predictability.
 1316 Blue, green and red refer to a range of predictable interactions as in Fig. 3: specifically,
 1317 Blue is for $(\beta_{yx}, \beta_{xy})=(0.18, 0.39)$ (small mutual interaction, and predominant effect of Y
 1318 on X), Green is for $(0.64, 0.57)$ (high mutual interactions, and slightly predominant effect
 1319 of X on Y), and Red for $(0.94, 0.34)$ (high mutual interactions, and predominant effect of
 1320 X on Y). (B) phase-space plots showing the non-time delayed associations between X and
 1321 Y corresponding to synchronous and homogeneous, mildly asynchronous and divergent, and
 1322 asynchronous and divergent dynamics. The transition from synchronous/small interactions
 1323 to asynchronous/high interaction lead to a transition from modular to nested ecosystem in-
 1324 teractions when more than one species exist (Fig. 6).

1325
 1326 **Figure 5. Inferred predictive causality for the sardine-anchovy-Sea Surface**
 1327 **Temperature ecosystem.** CCM correlation coefficient (ρ) and OIF predictor (TE) are
 1328 shown in the left and middle plots for different pairs considered (sardine-anchovy, sardine
 1329 and SST, anchovy and SST from top to bottom).

1330
 1331 **Figure 6. Part of the estimated species interaction network for the Maizuru**
 1332 **Bay ecosystem.** Species properties are reported in Table S1. The color and width of links
 1333 is proportional to the magnitude of TE (Table S2); for the former a red-blue scale is adopted
 1334 where the red/blue is for the highest/lowest TEs. The diameter is proportional to the Shan-
 1335 non entropy of the species abundance (Table S3) that is directly proportional to the degree of
 1336 uniformity of the abundance pdf and the diversity of abundance values (e.g., the higher the
 1337 zero abundance instances the lower the entropy). The color of nodes is proportional to the
 1338 structural node degree, i.e. how many species are interconnected to others after considering
 1339 only the CCM derived largest interactions (see Ushio et al. (2018)³⁷ and Fig. 7). Other
 1340 interactions exist between species as reported in Fig. 7. TE is on average proportional to ρ
 1341 (Fig. S4 and S5).

1342
 1343 **Figure 7. Normalized species interactions matrices inferred by CCM and OIF**
 1344 **models for Maizuru Bay ecosystem.** In the census of the aquatic community, 15 fish
 1345 species were counted in total. Interaction inferential models use time lagged abundance mag-
 1346 nitude (CCM) or pdfs of abundance (OIF) shown in A. (B) normalized CCM correlation
 1347 coefficients (ρ) between all possible pairs of species. (C) normalized transfer entropies (TEs)

1348 between all pairs of species from the OIF model. Both CCM and OIF predict that the most
 1349 interacting species (in terms of magnitude rather than frequency) are 7, 8 and 9 on average.
 1350 Thus, interaction matrices are more proportional to the asynchronicity than the divergence
 1351 of species in terms of abundance pdf, although abundance value range defines the uncertainty
 1352 (and diversity) for each species that ultimately affects entropy and interactions (e.g., if one
 1353 species have many zero abundance instances or many equivalent values, such as species 2,
 1354 TEs of that species are expected to be low due to lower uncertainty despite the asynchrony
 1355 and divergence).

1356

1357 **Figure 8. Predicted α -diversity via optimal interaction threshold for CCM's ρ**
 1358 **and OIF's TE versus taxonomic diversity.** Effective α diversity from CCM and OIF are
 1359 shown (blue and red) for an optimal threshold of ρ and TE (i.e., 0.2 and 0.3) that maximizes
 1360 the correlation coefficient and Mutual Information (MI) between α_{CCM} or α_{TE} and the tax-
 1361 onomic α , respectively. The maximization of the correlation coefficient and MI guarantees
 1362 that the estimated effective α are the closest to the taxonomic α . g is the resolution of the
 1363 network inference determined by the minimum number of points required to construct pdfs
 1364 and infer TE robustly (see Supplementary Information section S1.3).

1365

Figure 1:

Figure 2:

Figure 3:

Figure 4:

Figure 5:

Figure 6:

Figure 7:

Figure 8: