Supplementary Information: Regularized S-map for inference and forecasting with noisy ecological time series

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S1 Equivalence of SVD and least-square solution

Here we report a standard and straightforward proof that may be useful to the reader. We want to show that the solution of the weighted least-square problem is equivalent to the solution of a SVD as discussed in the main text (Methods section). Let us consider the linear system $B = A \cdot C$ with $B = WX_{t+1} = WY$ and $A = WX_t$. The solution of the weighted ordinary least square is:

$$(X^T WX)^{-1} X^T WY = X^{-1} W^{-1} X^{-T} X^T WY = X^{-1} Y \tag{S1}$$

Equivalently, if we call $\tilde{X} = WX_t$, the SVD solution for the linear system is

$$(\tilde{V}\tilde{\Sigma}^{-1}\tilde{U}^T)WY = \tilde{X}^{-1}WY = (WX)^{-1}WY = X^{-1}Y. \tag{S2}$$

Then, $(X^T WX)^{-1} X^T WY = (\tilde{V}\tilde{\Sigma}^{-1}\tilde{U}^T)WY$.

S2 Derivation of the stochastic dynamics

In this section, we show how we derived the model used in the main text to test the reconstructing performance of the S-map. It is important to provide the details of the model because the comparison of the analytical and stochastic Jacobian matrix needs particular care.

All the following are standard computations in stochastic dynamics, but we show them here for clarity to the reader that is not familiar with the theory of stochastic processes. To derive the stochastic dynamics we write down the master equation, which in its most general form is written as:

$$\frac{\partial p(\vec{n}, t)}{\partial t} = \sum_{l=1}^{\text{num of reactions}} [\underbrace{T_l(\vec{n}|\vec{n} - \vec{\mu}_l)p(\vec{n} - \vec{\mu}_l, t)}_{\text{gain}} - \underbrace{T_l(\vec{n} + \vec{\mu}_l|\vec{n})p(\vec{n}, t)}_{\text{loss}}], \tag{S3}$$

where $\vec{n} = (n_1, \dots, n_d)$ is the state vector, $p(\vec{n}, t)$ is the probability of observing a system in state $\vec{n}$ and $\vec{\mu}_1 = (a, b, c), \dots, \vec{\mu}_{\text{num of reactions}}$ are stoichiometric coefficients (Constable & McKane, 2015). The stoichiometric coefficients are introduced for a notational convenience that will be clear in Eq. (S7).

The solution of the master equation provides us with the probability distribution of observing a state $\vec{n}$ at time t. The reaction rate can be written easily in terms of chemical reactions. As an example take the reaction $A + B \rightarrow A + A$ that takes place at rate $\mathcal{A}_{AB}$. Then, if we call n_A and n_B the number of reactant A and B, respectively, the reaction term reads:

$$T_\alpha(n_A + 1, n_B - 1 | n_A, n_B) = \mathcal{A}_{AB} \frac{n_A n_B}{V^2}, \tag{S4}$$

where we have assumed mass action on the reaction rates and V is a measure of system size. Obviously, the solution of the master equation in a closed analytical form is extremely challenging to find. Therefore, following standard methods of stochastic dynamics, we take the Van Kampen system size expansion of the master equation to recover the Fokker-Plank equation (Van Kampen, 1992; Gardiner, 2004):

$$\frac{\partial p(\vec{x}, \tau)}{\partial \tau} = -\sum_{i=1}^{d} \frac{\partial}{\partial x_i} D_i(\vec{x}) p(\vec{x}, \tau) + \frac{1}{2V} \sum_{i,j=1}^{d} \frac{\partial}{\partial x_i \partial x_j} \mathcal{T}_{ij}(\vec{x}) p(\vec{x}, \tau), \tag{S5}$$

where we have used the change of variable: $\vec{x} = (n_1/V, \ldots, n_d/V)$ and $\tau = t/V$.

The drift and diffusion term of the Fokker-Plank equation (i.e., first and second term on the right hand side of Eq. (S5)) can be written explicitly following (McKane et al., 2014; Constable & McKane, 2015):

$$D_i(\vec{x}) = \sum_{k=1}^{R} \mu_{i,k} T_k(V\vec{x} + \mu_k | V\vec{x}) \tag{S6}$$

$$\mathcal{T}_{ij}(\vec{x}) = \sum_{k=1}^{R} \mu_{i,k} \mu_{j,k} T_k(V\vec{x} + \mu_k | V\vec{x}) \tag{S7}$$

Using the stoichiometric coefficients and the equations above (Eq. (S7)), we can write down the stochastic dynamics explicitly in term of an Ito stochastic differential equation as Eq. (**??**) in the main text:

$$\dot{\vec{x}} = \mathcal{D}(\vec{x}) + \frac{1}{\sqrt{V}} \xi(\vec{x}, \tau), \tag{S8}$$

where $\mathcal{D}(\vec{x})$ will be the deterministic vector field and $\xi(\vec{x}, \tau)$ is a Gaussian random variable with $\langle \xi(\vec{x}, \tau) \rangle = 0$ and $\langle \xi_i(\vec{x}, \tau) \xi_j(\vec{x}, \tau') \rangle = \mathcal{T}_{ij}(\vec{x}) \delta(\tau - \tau')$. In the numerical solution of Eq. (S8) we will use a vector of independent Wiener processes to simulate the noise.

In the next short section we write down the model explicitly. Following the main text the subscript $\gamma = 1, 2, 3$ correspond to predator-prey, RPS and chaotic dynamics respectively.

A. Cyclic Lotka-Volterra

Here we considered a cyclic Lotka-Volterra dynamics (i.e., the classic rock-paper-scissor game). The SDE reads:

$$\dot{\vec{x}} = -\vec{x} \mathcal{A}_2 \vec{x} + \frac{1}{\sqrt{V}} \xi_2(\vec{x}, \tau), \tag{S9}$$

where the interaction matrix $\mathcal{A}$ reads:

$$\mathcal{A}_2 = \begin{bmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{bmatrix} \tag{S10}$$

The covariance matrix of the Gaussian noise is derived from Eq. (S7):

$$\mathcal{T}(\vec{x}) = \begin{bmatrix} x_1(||\mathcal{A}_{12}||x_2 + ||\mathcal{A}_{13}||x_3) & -||\mathcal{A}_{21}||x_1x_2 & -||\mathcal{A}_{31}||x_1x_3 \\ -||\mathcal{A}_{12}||x_1x_2 & x_2(||\mathcal{A}_{21}||x_1 + ||\mathcal{A}_{23}||x_3) & -||\mathcal{A}_{32}||x_2x_3 \\ -||\mathcal{A}_{13}||x_1x_3 & -||\mathcal{A}_{23}||x_2x_3 & x_3(||\mathcal{A}_{31}||x_1 + ||\mathcal{A}_{32}||x_2) \end{bmatrix}$$

and V is the system size. Now we can just take the partial derivative of Eq. (S9) to recover the analytical Jacobian matrix and use it to compare exactly the analytical and numerical results.

B. Predator-prey and Chaotic Lotka-Volterra

Following the same calculation as before, we can write down the noise for the predator-prey and chaotic Lotka-Volterra dynamics:

$$\dot{\vec{x}} = \vec{x}(\vec{r}_\gamma - \mathcal{A}_\gamma \vec{x}) + \frac{1}{\sqrt{V}}\xi_\gamma(\vec{x}, \tau) \tag{S11}$$

The interaction matrices that generates the predator-prey and chaotic trajectories in a Lotka-Volterra dynamics are:

$$\mathcal{A}_1 = \begin{bmatrix} 0 & -0.3 \\ 0.5 & 0 \end{bmatrix} \tag{S12}$$

$$\mathcal{A}_3 = \begin{bmatrix} 1 & 1.09 & 1.52 & 0 \\ 0 & 0.72 & 0.316 & 0.98 \\ 3.56 & 0 & 1.53 & 0.72 \\ 1.53 & 0.64 & 0.44 & 1.27 \end{bmatrix} \tag{S13}$$

and $\vec{r}_1 = [1, -0.5]$ $\vec{r}_3 = [1, 0.72, 1.53, 1.27]$. These set of parameters for the chaotic trajectories are taken from (Vano et al., 2006). A simple computation of Eq. (S7) leads to a covariance matrix of the noise that is diagonal with element $\mathcal{T}_{ii}(\vec{x}) = x_i(r_i + \sum_j \mathcal{A}_{ij}x_j)$ for both predator-prey and chaotic dynamics.

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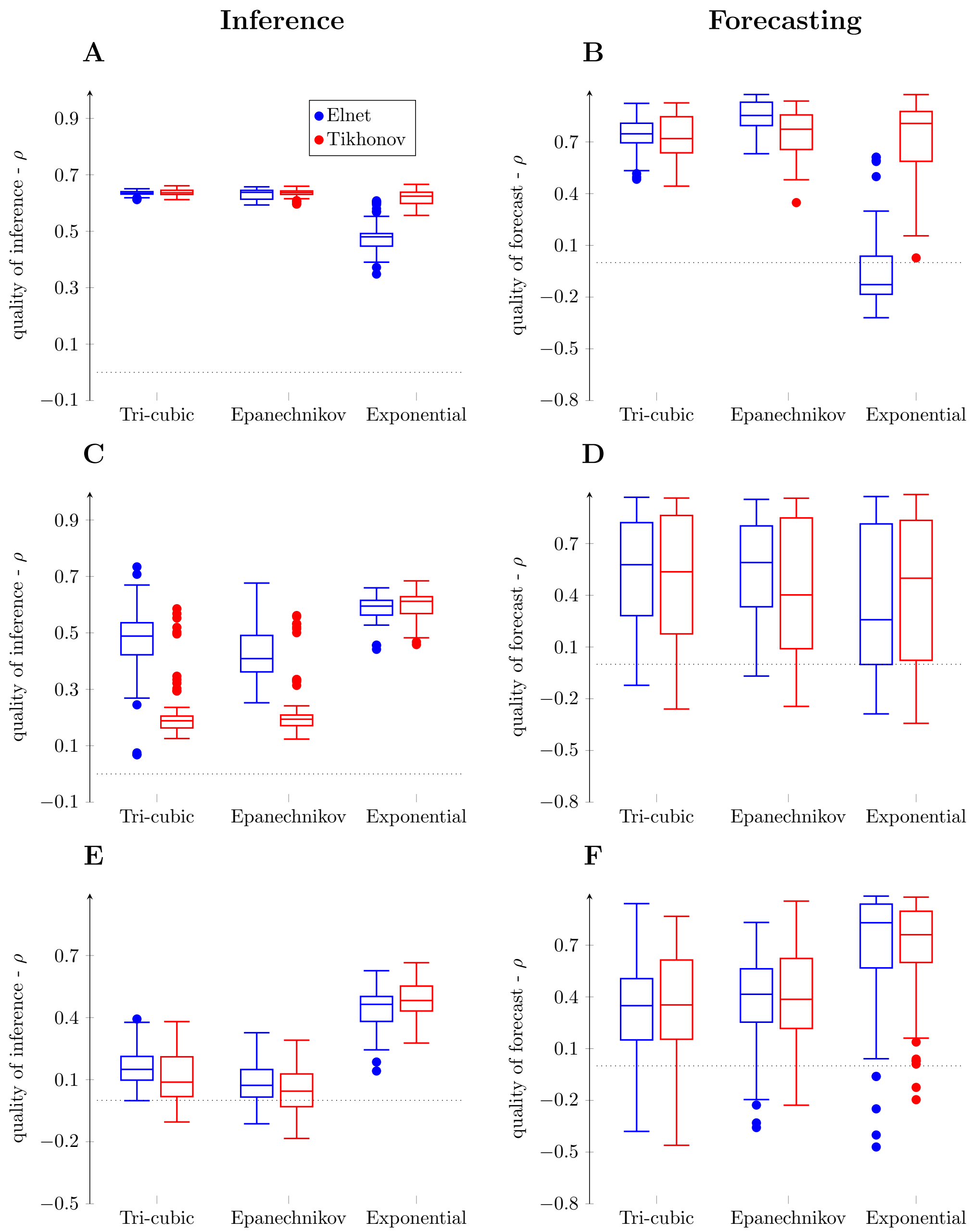

Figure S1: [Supplementary Figure] **Inference and forecasting skills in terms of correlation coefficients.** The figure is equivalent to Figure 2 in the main text, but the results are expressed in terms of ρ.

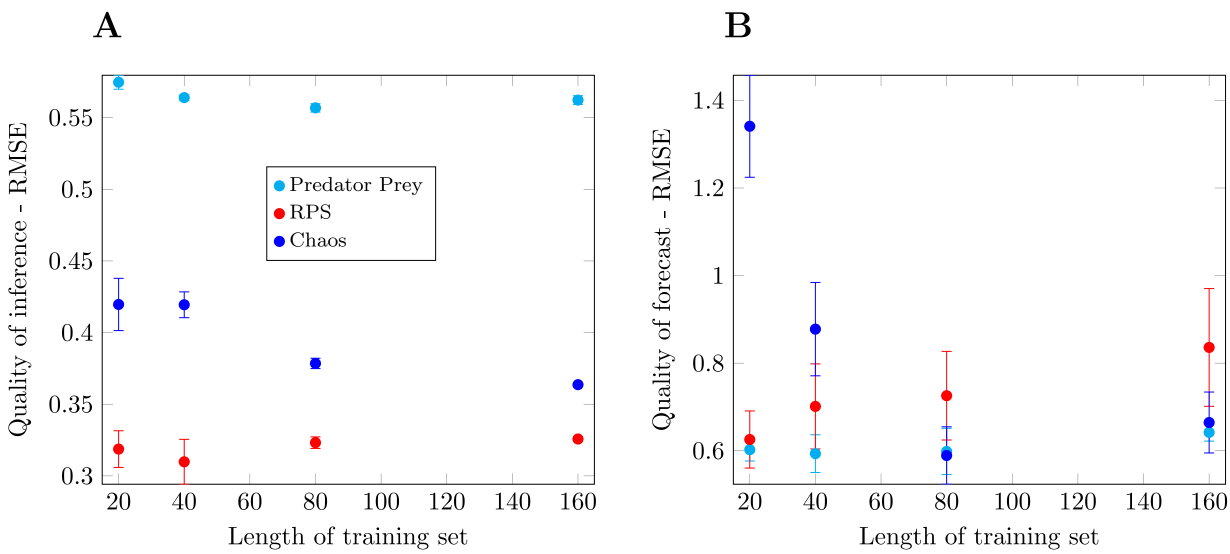

Figure S2: **Robustness of the regularized S-map to the length of the training set**. For each of the three models analyzed, the figure shows that both the inference and the forecasting skills of the regularized S-map are robust to the number of data points used to train the algorithm. The performance is reported as RMSE.

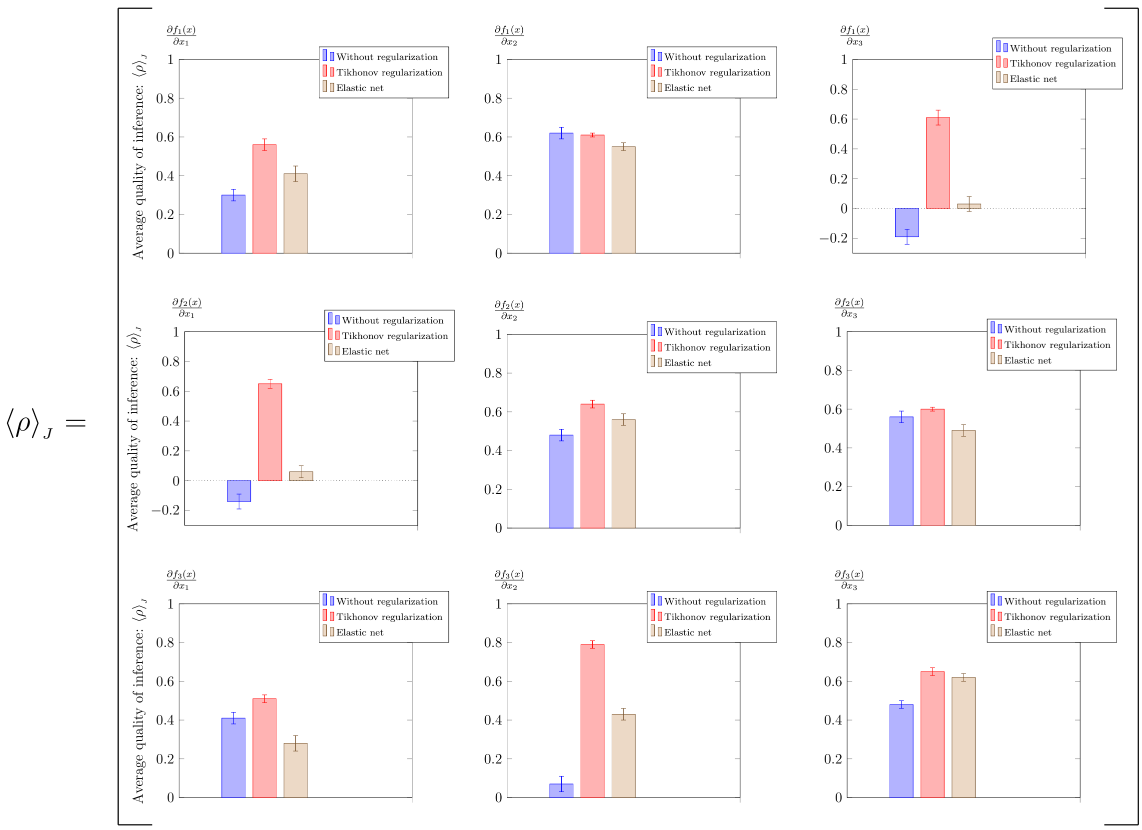

Figure S3: [Supplementary Figure] **Quality of the reconstruction of the Jacobian coefficients for the rock-paper-scissor model.** Parameters are inferred using a training set of 100 data points. As discussed in the main text, the figure shows that the quality of the reconstruction varies significantly across the matrix particularly using the standard S-map.

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