Structure Matched Higher Order Reservoir Computing for Complex System Prediction

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Abstract

Conventional reservoir computing (RC) provides an efficient framework for chaotic time series prediction, but its random input mapping and pairwise reservoir connections do not explicitly reflect the higher order relations that often govern nonlinear dynamical systems. This paper proposes a structure matched higher order RC framework that coordinates two stages of the prediction process. In the input layer, a block structured input matrix is constructed according to the local higher order neighbor sets associated with the predicted variable, so that target related variable couplings are organized before entering the reservoir. In the reservoir layer, higher order node interactions are introduced into the state evolution equation, allowing the structured input information to be further propagated and recombined through nonlinear reservoir dynamics. Experiments on the Lorenz chaotic system show that the proposed framework achieves lower prediction errors. Parameter analysis further shows that prediction performance depends on the coordinated selection of input scaling, node block allocation, and higher order coupling strength. These results indicate that prediction performance in RC can be improved not only by increasing reservoir nonlinearity, but also by coordinating how target related structural information is injected and internally evolved. The proposed framework provides a useful route for incorporating higher order structural information into RC and may support more reliable prediction of complex systems governed by multivariable interactions.

Keywords: Reservoir computer; Higher order interaction; Chaotic time series prediction; Nonlinear dynamical systems

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1. Introduction

Complex dynamical systems are widely present in various natural science and engineering scenarios such as meteorological evolution, biological neural activities, power networks, and nonlinear oscillations [1–3]. These

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systems typically exhibit strong nonlinearity, multivariable coupling, sensitivity to initial conditions, and complex long term evolution behaviors, making their time series modeling and prediction one of the core issues in the study of complex systems. Especially for chaotic systems, although their evolution process follows deterministic dynamical laws, due to the complex variable correlations within the system, high precision prediction still faces significant challenges [4–6]. In recent years, with the development of machine learning methods, directly conducting complex dynamical modeling and prediction based on observational data has become an important research direction in this field [7–10].

Reservoir computing (RC), a computationally efficient recurrent neural network paradigm, has demonstrated strong performance in various tasks, including chaotic time series prediction, nonlinear system identification, and complex dynamical system modeling. Its effectiveness mainly comes from its distinctive training strategy: only the weights of the readout layer are trained, while the recurrent reservoir, which is usually initialized randomly or with structured connectivity, remains fixed during training. This design enables RC to use high dimensional dynamical state spaces for effective temporal feature representation [11–14]. Compared with conventional recurrent neural networks (RNNs), RC retains rich dynamical representation capability while offering practical advantages such as simple architecture, low computational cost, and reduced training complexity. Therefore, it has attracted increasing attention in both theoretical and applied research [15–18]. Recent studies further show that RC is not limited to short term prediction of low dimensional chaotic systems. It has also been successfully applied to high dimensional spatiotemporal chaotic system modeling, complex network dynamics analysis, reconstruction of unobserved state variables, and reproduction of the geometric structures and statistical properties of long term attractors [19–23].

Despite these advances, conventional RC remains limited in exploiting structured variable relations and nonpairwise interactions in complex dynamical systems. First, classical RC usually adopts randomly generated input matrices and reservoir connection matrices. Although this construction has good general applicability, its performance is easily affected by random structures and hyperparameter selection, and it is difficult to explicitly utilize the potential structural relationships among system variables [24–26]. Existing RC improvements can be organized according to the stage at which structural or nonlinear information is introduced. One class of methods mainly improves the input or feature representation, for example through nonlinear input expansion, task dependent input encoding, output enhancement, or local structural embedding [27–30]. These methods improve how external signals are represented or injected into the reservoir. Another class of methods modifies the reservoir itself, such as deep reservoir architectures, physical reservoir implementations, or higher order reservoir interactions, which mainly enrich the internal state evolution and nonlinear transformation capability [31,32]. These two categories improve RC from different perspectives, but they also reveal a remaining gap: the structural information organized at the input stage is often not explicitly matched with the nonlinear interaction mechanism inside the reservoir. In particular, even when local structural information is introduced into RC, existing models usually encode variable dependencies in a pairwise manner, while the evolution of complex dynamical systems can be governed by the joint effects of multiple variables [33,34]. This gap motivates prediction oriented RC models that explicitly organize target related higher order variable relations at the input stage and make this organization compatible with the internal reservoir dynamics.

Higher order interactions have been shown to play an important role in the formation of complex system

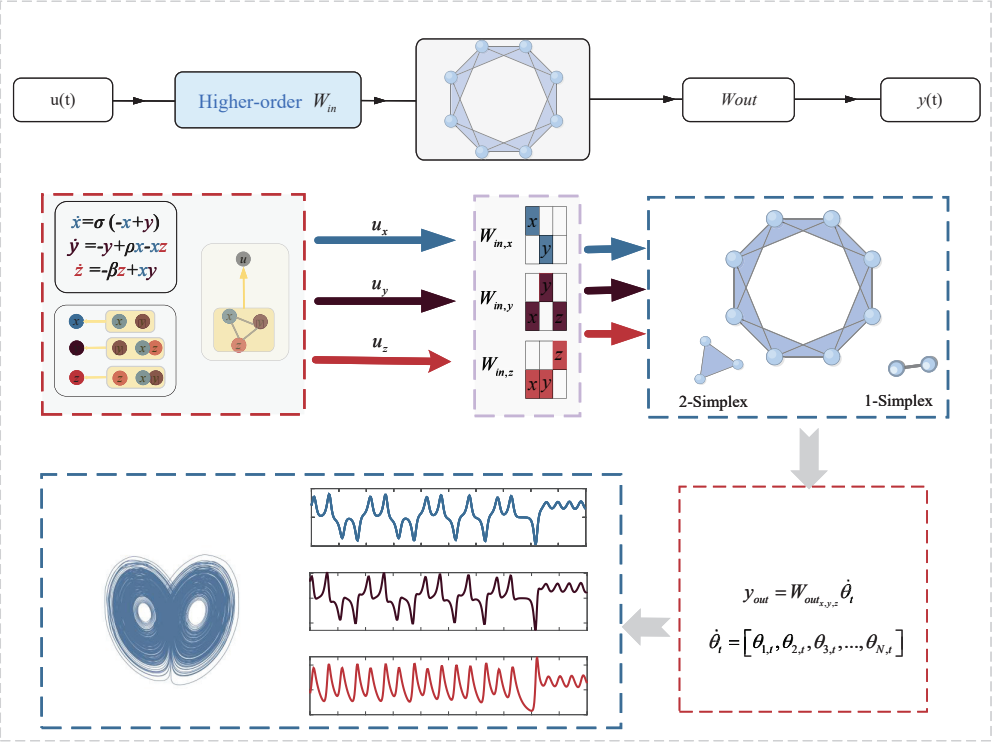


Figure 1: Schematic for the proposed structure matched higher order reservoir computing model.

dynamics. Compared with models based only on pairwise coupling, higher order structures provide a more direct description of the joint effects among multiple variables or nodes, and they can strongly affect collective dynamical behaviors such as diffusion, synchronization, spreading, and evolutionary processes [35–37]. In the RC context, higher order information has been introduced from different perspectives. For example, higher order dynamical information has been used to support complex structure inference and dynamics prediction, while higher order interactions have also been incorporated into reservoir dynamics to enrich nonlinear state evolution [38,39]. These studies demonstrate the potential of higher order information for RC, but they leave an important prediction oriented question insufficiently addressed: how can the target dependent higher order structure used for input injection be made consistent with the higher order interactions that govern reservoir state evolution? To address this question, this paper develops a structure matched higher order RC framework in which a block structured input embedding and a higher order reservoir coupling mechanism act on the input driving and internal evolution stages, respectively. Through this coordinated design, target related structural information is selectively injected into the reservoir and then processed by compatible nonlinear reservoir dynamics.

Compared with the higher order reservoir model in Ref. [39], the present work further introduces a target dependent matched input mask before the reservoir state evolution. The model in Ref. [39] mainly enriches the internal reservoir dynamics through higher order interactions, whereas the input injection does not explicitly distinguish the local multivariable structure associated with the predicted target. In contrast, the proposed method first organizes target related variables through a block structured input matrix and then processes the injected information with higher order reservoir dynamics. Therefore, the main novelty of the proposed framework lies in matching prediction oriented input organization with higher order internal reservoir evolution,

rather than only adding a higher order coupling term to the reservoir.

2. Theory and model

To improve the prediction capability of reservoir computing for complex chaotic time series, this paper constructs a structure matched higher order reservoir computing model, whose overall structure is shown in Fig. 1. It should be noted that the term higher order is used in two related but distinct senses in this work. The higher order input structure describes target dependent multivariable relations in the original dynamical system, whereas the higher order reservoir interaction describes nonlinear nonpairwise interactions among reservoir states. These two higher order objects are therefore not treated as the same mathematical object. Instead, they are designed to act at two different stages of the RC prediction process. The proposed model is based on the conventional RC framework, but it does not treat input mapping and reservoir evolution as two independent design choices. Instead, it organizes target related higher order variable information before input injection and then uses higher order reservoir interactions to process this structured information during state evolution. Specifically, in the input layer, the input matrix is constructed in a block structured manner according to the local higher order neighbor structure related to the target variable. This design allows variable coupling information associated with the prediction target to be embedded before entering the reservoir. In the reservoir layer, higher order node interactions are introduced, so that the internal reservoir states are affected not only by pairwise node connections but also by the joint effects of multiple nodes. As shown in Fig. 1, the higher order structural embedding in the input layer mainly acts on the external signal injection process, while the higher order node interactions in the reservoir layer mainly act on the internal state evolution process. These two mechanisms correspond to the information input and dynamical evolution stages, respectively, and their coordinated design improves the ability of the proposed model to represent nonlinear and nonpairwise dynamical relationships in chaotic time series.

For a dynamical system with m state variables, the input time series at time t is represented as

$$u(t) = [u_1(t), u_2(t), ..., u_m(t)]^T \tag{1}$$

where $u_m(t)$ denotes the mth state variable at time t. In conventional reservoir computing, the input signal is usually mapped to the reservoir nodes through a random input matrix. Although such random mapping provides a generic nonlinear projection, it treats different input variables as statistically interchangeable at the injection stage. For complex dynamical systems, however, the evolution of a target state variable is often determined by a specific subset of variables and their joint effects. A fully random input matrix may therefore dilute the target related structural information before it enters the reservoir, especially when the governing dynamics contain nonpairwise or nonlinear combination terms.

Based on this consideration, a block structured input matrix is adopted in the input layer. For the target variable u_q, its corresponding higher order neighbor set is denoted as:

$$S_q = \{s_{q,1}, s_{q,2}, ..., s_{q,D_q}\} \tag{2}$$

where $s_{q,d}$ represents the dth local variable set related to the target variable u_q, and D_q denotes the number of higher order neighbor sets. The set S_q is target dependent: different predicted variables may correspond

to different local variable groups because their governing dynamics may involve different linear or nonlinear coupling terms. According to this structure, the input matrix is divided into several input blocks:

$$\tilde{W}_{in}^{(q)} = [\psi(s_{q,1})^T, \psi(s_{q,2})^T, ..., \psi(s_{q,D_q})^T]^T \tag{3}$$

Here, $\psi(s_{q,d})$ denotes the input block corresponding to the dth local higher order neighbor set. If an input variable belongs to the set $s_{q,d}$, the corresponding column in the input matrix is assigned random weights. Otherwise, if the variable is unrelated to the current structural block, the corresponding column is set to zero. In this way, the input matrix is no longer a fully random matrix, but a structured matrix composed of random blocks and zero blocks. The purpose of this construction is not only to reduce random input mixing, but also to make the input injection target aware: variables that are dynamically relevant to the predicted component are allocated explicit input channels, whereas unrelated variables are suppressed in the corresponding block. This design enhances the representation of multivariable coupling relationships at the input stage.

In the reservoir layer, a higher order node interaction mechanism is further introduced. Let $\theta_i(t)$ denote the state of the ith reservoir node, and let N be the number of reservoir nodes. Different from a conventional reservoir that only considers pairwise connections between nodes, the proposed model considers both low order pairwise coupling and higher order node coupling. The reservoir state update can be expressed as:

$$\begin{aligned}
\ddot{\theta}_i(t) = (1-\varepsilon)\left[\gamma\dot{\theta}_i(t) + \omega_i - \sin\theta_i(t)\right] \\
+\varepsilon\left[\frac{k_1}{N}\sum_{j=1}^{N} A_{ij}\sin\left(\theta_j(t) - \theta_i(t)\right)\right. \\
+\frac{k_2}{2N}\sum_{j=1}^{N}\sum_{k=1}^{N} B_{ijk}\sin\left(\theta_j(t) + \theta_k(t) - 2\theta_i(t)\right) \\
\left.+\alpha\tanh\left(\left[\widetilde{W}_{in}\mathbf{u}(t) + \beta\right]_i\right)\right].
\end{aligned} \tag{4}$$

Here, ε is the leakage rate, which controls the relative influence of the current input and the historical reservoir state. γ is the damping coefficient, and ω_i denotes the intrinsic frequency or external driving term of the node. A_{ij} represents the pairwise connection between reservoir nodes, while B_{ijk} represents the higher order connection in the reservoir. k_1 and k_2 denote the low order coupling strength and the higher order coupling strength, respectively. α is the input coupling strength, β is the input bias term, and $\tilde{W}_{in}$ denotes the structured input matrix. In this equation, the first term describes the self dynamics of a single reservoir node, the pairwise coupling term describes the interaction between two nodes, and the higher order coupling term describes the joint influence of multiple nodes on the current node state. In the implementation, B_{ijk} is constructed as a sparse random interaction tensor. A binary sparsity mask is first used to select the allowed higher order interaction entries, and the unselected entries are set to zero. The nonzero entries are randomly assigned and then modulated by the coupling strength k_2 in Eq. (4). This sparse construction follows the common RC practice of using sparse internal connections. It also reduces the computational burden of dense higher order coupling and avoids excessive nonlinear mixing among reservoir nodes, which helps maintain stable reservoir dynamics.

As shown in Eq. (4), the proposed model integrates target dependent input embedding and higher order reservoir interactions into a unified state update framework. The connection between the two levels of higher order information lies in their functional roles rather than in a one to one mathematical equivalence. The input

layer determines which target related multivariable information is injected into each structural block, whereas the reservoir layer determines how the injected information is transformed and recombined by pairwise and higher order node interactions. This creates a direct correspondence between the organization of the external driving signal and the nonlinear interaction pattern inside the reservoir. By introducing the higher order coupling term, the internal reservoir states are no longer determined only by simple pairwise connections. Instead, the reservoir can generate richer nonlinear dynamical responses. When the higher order coupling strength k_2 is properly matched with the input structure, the reservoir can more fully characterize multibody coupling relationships in complex systems, thereby improving its representation ability for chaotic time series. Although Eq. (4) is implemented with a Kuramoto like oscillator reservoir in the main experiments, the structure matched design is not restricted to this specific node model; it can also be implemented in other reservoir update forms by retaining the target dependent input mask and the higher order state interaction term.

During the training stage, the normalized chaotic time series is first injected into the reservoir through the structured input matrix. Under the joint influence of low order coupling, higher order coupling, and external input, the reservoir generates high dimensional dynamical states. After discarding the initial transient states, the reservoir state matrix $\boldsymbol{\theta}$ is collected, and the model output is obtained through a linear readout layer:

$$\hat{\mathbf{y}}(t) = W_{out}\boldsymbol{\theta}(t) \tag{5}$$

The output weight matrix W_{out} is solved by ridge regression:

$$W_{out} = Y\boldsymbol{\Theta}^T\left(\boldsymbol{\Theta}\boldsymbol{\Theta}^T + \lambda I\right)^{-1} \tag{6}$$

where $\boldsymbol{\theta}$ is the reservoir state matrix collected during training, Y is the target output matrix, λ is the regularization coefficient, and I is the identity matrix. Since only the output layer weights need to be solved during training, the proposed model retains the advantages of reservoir computing, such as simple training and low computational cost.

To verify the effectiveness of the proposed structure matched higher order reservoir computing model in chaotic time series prediction, the classical Lorenz system is selected as the experimental object. The Lorenz system is a typical three dimensional nonlinear dynamical system, in which the state variables exhibit obvious coupling relationships and complex chaotic evolution under certain parameter settings. Therefore, it is commonly used to evaluate the ability of time series prediction models to learn nonlinear dynamical behaviors. The governing equations of the Lorenz system are given by [40]:

$$\begin{cases} \dot{x} = \sigma(y - x), \\ \dot{y} = \rho x - y - xz, \\ \dot{z} = xy - bz. \end{cases} \tag{7}$$

where x, y, and z are the three state variables of the system, and σ, ρ, and b are system parameters. In this study, the standard chaotic parameter setting is adopted, with $\sigma = 10$, $\rho = 28$, and $b = 8/3$. In the experiments, the three state variables are predicted separately. The conventional reservoir computing model, the input structured RC model, and the proposed structure matched higher order RC model are compared to analyze the effects of higher order structural embedding in the input layer and higher order interaction mechanisms in the reservoir layer on prediction performance.

To ensure a fair comparison among different models, all basic parameters are kept consistent, except for the input layer structural parameters and the higher order interaction parameters in the reservoir layer. The fixed parameters mainly include the number of reservoir nodes, leakage rate, damping coefficient, constant external force, input coupling strength, and input bias term. The parameters in Table 1 are selected according to commonly used settings in reservoir computing and oscillator reservoir studies, together with preliminary tests that ensure stable reservoir responses. Specifically, the leakage rate, damping coefficient, external force, input coupling strength, and input bias are chosen from parameter ranges that allow the reservoir states to remain bounded while preserving sufficient nonlinear response and memory. The number of reservoir nodes is set to $N = 100$ to provide enough state dimensionality while keeping the computational cost moderate. These basic parameters are not independently optimized for each model; instead, they are kept identical for the conventional RC, the input structured RC, and the proposed structure matched higher order RC. Therefore, the performance comparison mainly reflects the effects of structured input embedding and higher order reservoir interaction. The subsequent parameter analysis focuses on the structural parameters directly related to the proposed mechanism, including the input scaling factors, input node block ratio, and higher order coupling strength. The detailed settings are listed in Table 1.

Table 1: Parameter settings of the reservoir model

Symbol	Description	Value
ε	Leakage rate	0.71
γ	Damping coefficient	-1.44
ω	Constant external force	0.7155
N	Number of reservoir nodes	100
α	Input coupling strength	9.06
β	Input bias term	$[-0.989, 0.989]$

3. Results

The main observation from the Lorenz prediction task is that matching target dependent input organization with higher order reservoir dynamics significantly suppresses prediction error fluctuations. As shown in Fig. 2, compared with the conventional RC, the proposed model keeps the prediction errors closer to zero for all three state variables. The conventional RC produces larger error amplitudes and more evident fluctuations, especially when the local evolution of the chaotic trajectory changes rapidly. This behavior is related to the fully random input mapping and pairwise reservoir dynamics in conventional RC, which do not explicitly organize the variable coupling information associated with the prediction target. In contrast, the improvement of the proposed model arises because the target dependent input embedding selectively injects relevant local variable information into the reservoir, while the higher order reservoir interactions further process this information through richer nonlinear state evolution. Therefore, matching input organization with reservoir dynamics reduces prediction errors and improves the stability of chaotic time series prediction.

To evaluate the performance of the model in chaotic time series prediction, a normalized root mean square

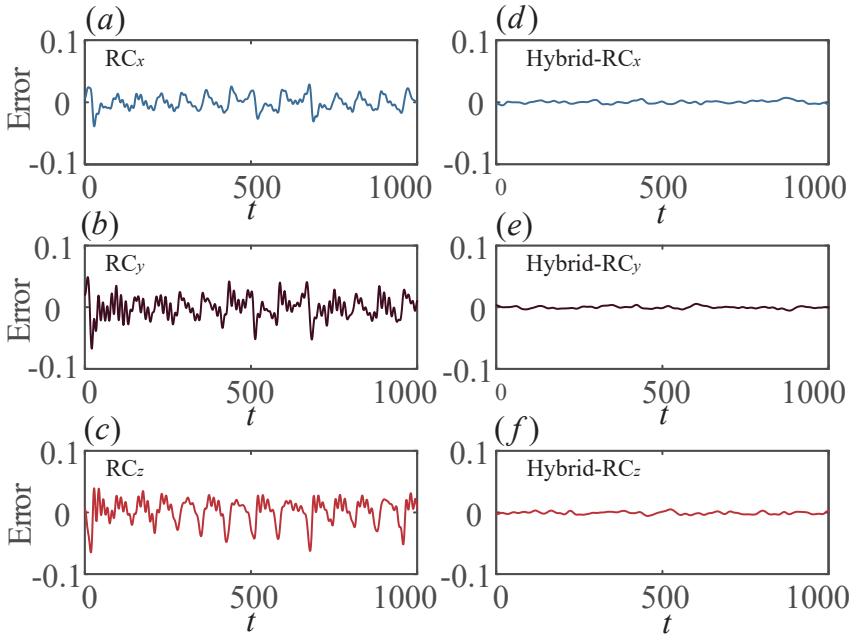


Figure 2: Prediction error comparison between the conventional RC and the proposed structure matched higher order RC on the Lorenz system. (a)–(c) Prediction errors of the conventional RC for the x, y, and z components, respectively. (d)–(f) Prediction errors of the structure matched higher order RC for the x, y, and z components, respectively.

error, denoted by RMS in the figures and tables for brevity, is used as the evaluation metric:

$$RMS = \frac{\sqrt{\left\langle (y(i) - \hat{y}(i))^2 \right\rangle}}{\langle |\hat{y}(i)| \rangle} \tag{8}$$

where i denotes the index of each data point in the time series, $\hat{y}(i)$ is the value predicted by the RC model, $y(i)$ is the target value,and the operator $\langle \cdot \rangle$ denotes the average operation. The normalization by the mean absolute predicted value makes the metric dimensionless. A lower RMS value indicates a smaller deviation between the predicted and true sequences, thereby reflecting better prediction performance.

To further quantitatively compare the prediction performance of different models, Table 2 presents the RMS results for the three state variables x, y, and z. The input structured RC optimizes the input matrix W_{in} while retaining a pairwise reservoir network, whereas the proposed structure matched higher order RC further introduces higher order reservoir interactions. The results show a clear stepwise improvement. Compared with the conventional RC, the input structured RC reduces the RMS errors by organizing W_{in}, which improves target related information injection even though the reservoir network remains pairwise coupled. The proposed model further obtains the lowest errors for all three components, indicating that higher order reservoir interactions provide additional gains beyond input optimization. Thus, the structured input embedding and the higher order reservoir dynamics are complementary: the former improves the information injection stage, while the latter enhances the internal nonlinear state evolution. The component dependent improvement is also consistent with the Lorenz dynamics. The x equation mainly contains linear terms, so the conventional RC can already learn this component with a relatively small error and the additional gain is moderate. In contrast, the y and z

components involve stronger nonlinear coupling through the xz and xy terms, respectively, and their evolution depends more on the joint effects of multiple variables. Therefore, they benefit more clearly from the structured input and higher order reservoir interactions. This result indicates that the proposed structure matched higher order RC is especially effective when the target variable is governed by multivariable cooperative dynamics.

Table 2: Prediction errors of different models on the Lorenz system

Variable	RC	Input structured RC	Proposed RC
x	8.74×10^{-4}	6.05×10^{-6}	2.19×10^{-6}
y	2.00×10^{-3}	7.72×10^{-5}	9.83×10^{-6}
z	6.70×10^{-3}	5.69×10^{-5}	6.46×10^{-6}

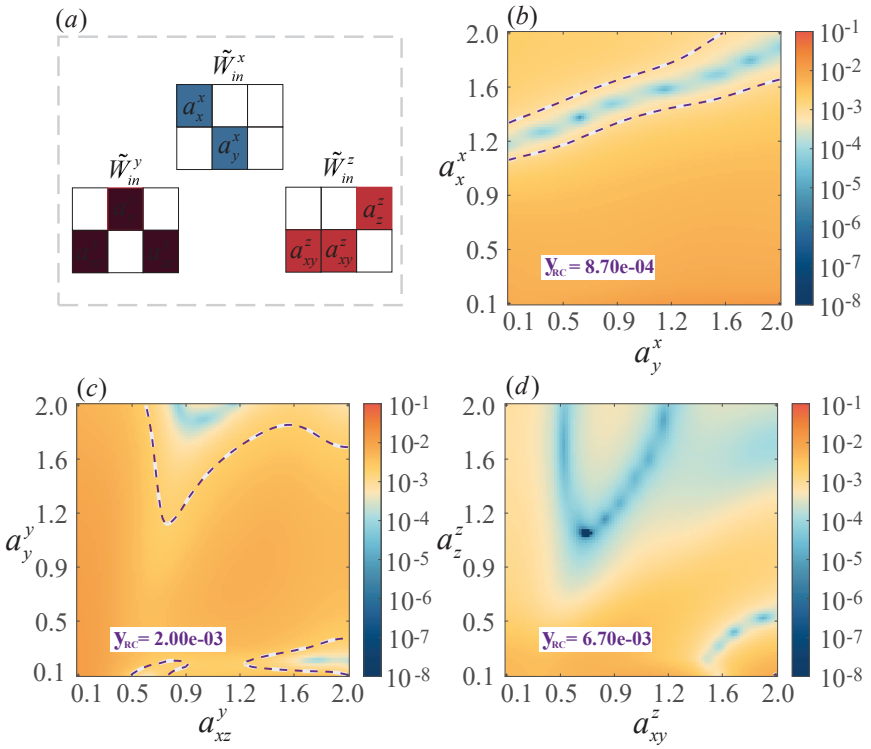


Figure 3: Effects of input weight scaling factors on Lorenz prediction errors. (a) Block structured input matrices for different target variables. (b)–(d) Prediction errors of the x, y, and z components as functions of their corresponding input scaling factors.

The benefit of the structured input layer is target dependent, because different state variables require different relative driving strengths from their associated input blocks. This behavior is illustrated in Fig. 3, where the input weight scaling factors are varied for each prediction target. The three state variables exhibit different low error regions, indicating that input scaling should be selected according to the dynamics of the target variable. For the x component, the low error region in Fig. 3(b) is mainly located near the diagonal of the parameter space. This is consistent with the Lorenz equation, where the x component is mainly governed

by the linear relation between x and y; therefore, balanced injection of the two related input blocks is sufficient for stable prediction. In contrast, the low error regions for the y and z components in Figs. 3(c)-(d) are more scattered because their evolution involves nonlinear coupling terms. These results show that the input scaling factors should be coordinated across structural blocks, rather than tuned independently or increased for a single block.

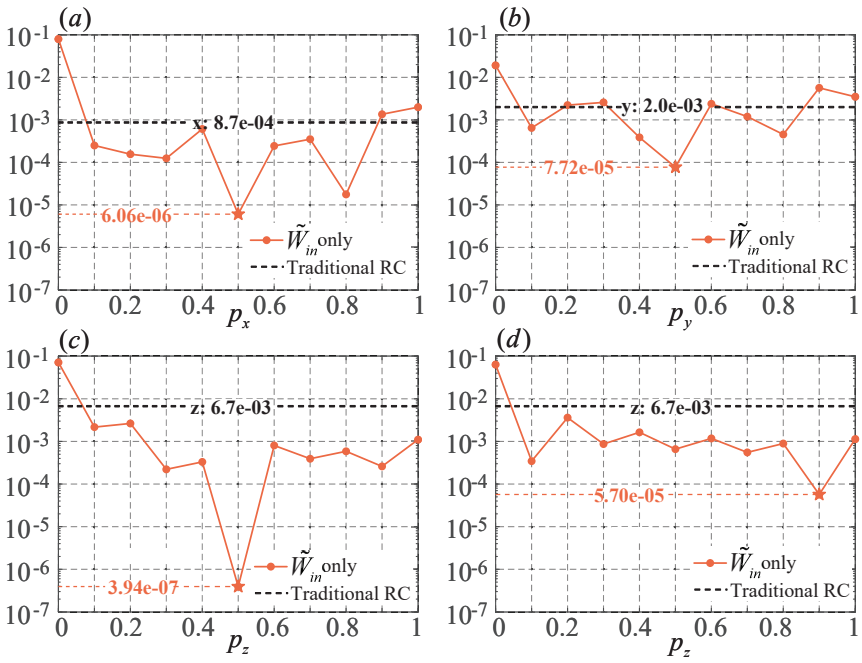


Figure 4: Effects of input node block ratios on Lorenz prediction errors. (a)–(c) Prediction errors of the x, y, and z components under selected input scaling settings. (d) Prediction error of the z component under an alternative input scaling setting. Dashed lines denote conventional RC baselines, and stars mark the minimum errors.

In addition to input scaling, Fig. 4 analyzes the input node block ratio, which controls how reservoir nodes are allocated to different input blocks. Under favorable input scaling settings, Figs. 4(a)-(c) show that lower errors are usually obtained when node resources are allocated without being dominated by a single block. This indicates that each type of target related variable information needs sufficient representation capacity in the reservoir. Fig. 4(d) further shows that the favorable node block ratio changes when the input scaling setting is changed. Therefore, the input weight scaling factor and the node block ratio should be considered together: the former determines the driving strength of each input block, while the latter determines its representation capacity in the reservoir. The structured input layer is effective only when input strength and node resource allocation are properly matched, rather than by simply increasing either the input weight or the number of nodes assigned to one block.

After structured input is injected into the reservoir, higher order interactions among reservoir nodes further affect the state evolution. To examine this effect, high order coupling strength k_2 is varied, as shown in Fig. 5. The prediction error changes nonmonotonically with k_2, indicating that higher order coupling is not simply beneficial when it becomes stronger. Instead, appropriate values of k_2 can enrich the reservoir dynamics,

whereas mismatched values may increase the prediction error. The effect of k_2 varies across variables. For the z component, Fig. 5(c) shows limited improvement, this is because the z component is mainly affected by the nonlinear term xy, and its prediction performance relies strongly on how the input layer organizes the relationship between x and y. When this information has already been effectively injected, changing k_2 alone brings only limited additional improvement. Fig. 5(d) further shows that, after changing the input layer configuration, an appropriate value of k_2 can reduce the prediction error of the z component. This confirms that higher order reservoir interactions do not provide uniform gains under all parameter settings. Their effect depends on whether the internal reservoir dynamics are matched with the structured input. Therefore, the advantage of the proposed model comes from the coordinated action of input layer structural embedding and reservoir layer higher order interactions, rather than from simply adding a second order coupling term.

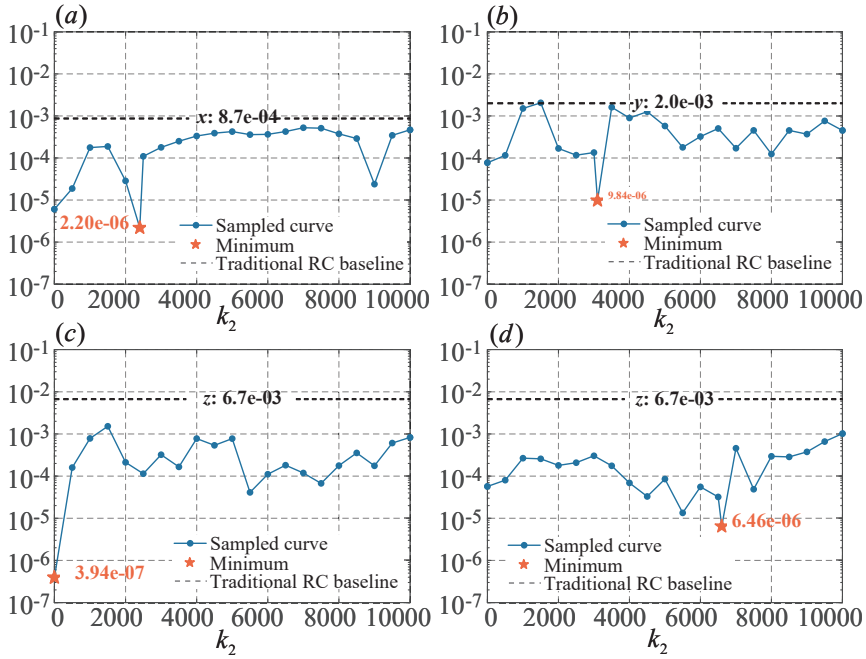


Figure 5: Effects of second order coupling strength k_2 on Lorenz prediction errors. (a)–(c) Prediction errors of the x, y, and z under one input layer configuration. (d) Prediction error of the z component under another input layer configuration. Dashed lines denote conventional RC baselines, and stars mark the minimum errors.

To further evaluate the applicability of the proposed structure matched higher order RC model to different networked dynamical systems, supplementary experiments were conducted based on the UK power grid network structure, as shown in Fig. 6. The purpose of this experiment is to examine whether the proposed framework remains effective when both the node dynamics and the coupling topology are changed. Different from the Lorenz system, which is a low dimensional chaotic system with explicit nonlinear coupling terms, the UK power grid is a networked dynamical system with realistic topology and higher order coupling. Therefore, this experiment provides a complementary test of the proposed method under a different node model and coupling structure. Following the higher order Kuramoto model used in Ref. [38], the grid dynamics are described by a

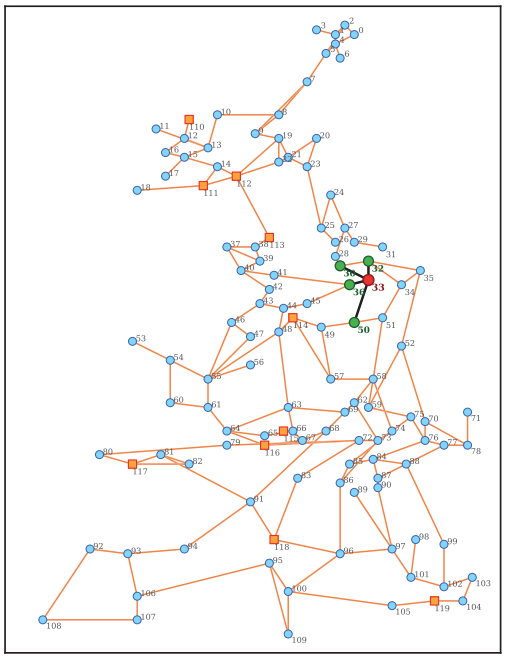


Figure 6: Topological structure of the UK power grid and the local neighborhood of the target node.

Kuramoto model with pairwise and higher order interactions:

$$\begin{aligned}\dot{\theta}_i^{(\mathrm{g})}(t) = \Omega_i^{(\mathrm{g})} + \kappa_1^{(\mathrm{g})} \sum_{j=1}^{N_\mathrm{g}} A_{ij}^{(\mathrm{g})} \sin\Big(\theta_j^{(\mathrm{g})}(t) - \theta_i^{(\mathrm{g})}(t)\Big) \\ + \kappa_2^{(\mathrm{g})} \sum_{j=1}^{N_\mathrm{g}} \sum_{\ell=1}^{N_\mathrm{g}} \mathcal{B}_{ij\ell}^{(\mathrm{g})} \sin\Big(\theta_j^{(\mathrm{g})}(t) + \theta_\ell^{(\mathrm{g})}(t) - 2\theta_i^{(\mathrm{g})}(t)\Big)\,.\end{aligned} \tag{9}$$

Here, $N_\mathrm{g} = 120$ is the number of grid nodes, $\theta_i^{(\mathrm{g})}$ and $\Omega_i^{(\mathrm{g})}$ denote the phase and natural frequency of grid node i, respectively, and $A_{ij}^{(\mathrm{g})}$ and $\mathcal{B}_{ij\ell}^{(\mathrm{g})}$ denote the pairwise adjacency matrix and the third order adjacency tensor of the power grid. The parameters $\kappa_1^{(\mathrm{g})}$ and $\kappa_2^{(\mathrm{g})}$ are the corresponding pairwise and higher order coupling strengths. The superscript (g) distinguishes the power grid quantities in Eq. 9 from the reservoir variables and coupling parameters in Eq. (4), and it is omitted from the axis labels in Fig. 7 for brevity. These power grid quantities specify the physical dynamical system used to generate the prediction data; they are distinct from the adjacency matrix, higher order interaction tensor, and coupling strengths of the reservoir in Eq. (4). Unless otherwise stated, the natural frequency assignment, the constructions of $A_{ij}^{(\mathrm{g})}$ and $\mathcal{B}_{ij\ell}^{(\mathrm{g})}$, the initial conditions, and the numerical integration scheme used for data generation are the same as those used in Ref. [38]. The state variable $\sin\theta_{33}^{(\mathrm{g})}$ of node 33 is selected as the prediction target [41,42]. For this target, the matched input mask is constructed according to the local coupling structure associated with node 33. The input blocks correspond to the target node, its neighboring nodes, and the nodes involved in the higher order coupling structure related to node 33. Thus, the structured input matrix is matched with the higher order coupling relation of the predicted node rather than being randomly generated. Figs. 7(a)-(b) compare the prediction trajectories of the conventional RC and the proposed structure matched higher order RC model, while Figs. 7(c)-(d) show their corresponding prediction errors. The conventional RC can follow the overall trend of the true trajectory, but noticeable deviations remain in some peak and rapidly varying regions. In contrast, the proposed model shows

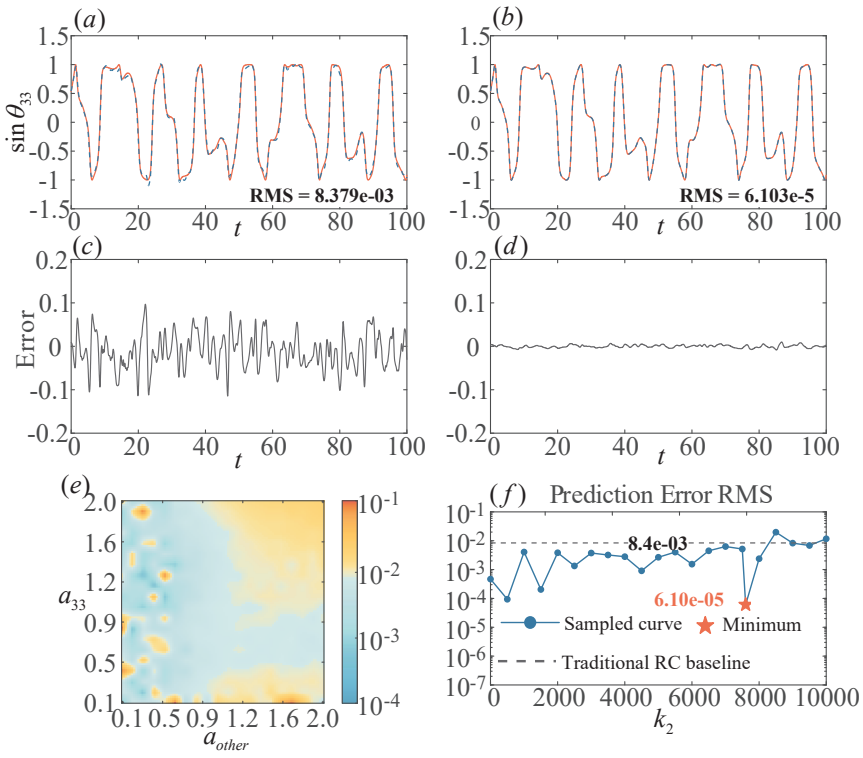


Figure 7: Prediction and parameter analysis for node 33 in the UK power grid. (a) Conventional RC prediction. (b) Structure matched higher order RC prediction. (c) Conventional RC prediction error. (d) Structure matched higher order RC prediction error. (e) Effect of input scaling factors on prediction error. (f) Effect of the reservoir higher order coupling strength k_2 on prediction error. **For the power grid model,** $N_{\mathrm{g}} = 120$**,** $\kappa_1^{(\mathrm{g})} = 5 \times 10^4$**,** $\kappa_2^{(\mathrm{g})} = 3700$**, and the simulation step is** $\Delta t = 0.01$**. The training and testing sequences contain** 8000 **and** 1000 **samples, respectively, and the nonzero input mask entries for node 33 are sampled from** $\mathcal{U}(-1, 1)$**.** Dashed lines denote conventional RC baselines, and stars mark the minimum errors.

better agreement with the true trajectory and produces a much lower prediction error, reducing the RMS from 8.379×10^{-3} to 6.103×10^{-5}. This result indicates that the introduction of structured input and higher order interactions significantly enhances the characterization capability of the model for local network dynamics.

Fig. 7(e) further shows that the structured input matrix can reduce the prediction error by organizing the information from the target node and its neighboring nodes. This result indicates that, for networked dynamical systems, prediction performance can be improved when the input layer explicitly reflects the local structure related to the target node. Fig. 7(f) analyzes the effect of the higher order coupling strength k_2. The reservoir coupling strength k_2 is varied to test how the injected structural information is processed by higher order reservoir dynamics. After introducing higher order coupling into the reservoir, lower prediction errors can be obtained at appropriate parameter values, demonstrating that higher order reservoir interactions can enhance the representation of local dynamical features. Meanwhile, the effect of k_2 depends on its matching with the current input structure and the local dynamic characteristics of the target node. These experimental results demonstrate that the structure matched higher order RC model is not limited to typical low dimensional chaotic systems, but can also achieve good prediction performance in complex networked dynamical systems with realistic network topology.

4. Conclusion and perspectives

This paper proposes a structure matched higher order reservoir computing framework for complex system prediction. In the proposed framework, a target dependent block structured input matrix is first constructed to organize local higher order variable relations before they enter the reservoir. Then, higher order node interactions are introduced into the reservoir state evolution, so that the injected structural information can be further propagated and recombined through nonlinear reservoir dynamics. In this way, the proposed model does not simply increase reservoir complexity, but builds a correspondence between input organization and internal reservoir dynamics. Experiments on the Lorenz chaotic system show that the proposed method achieves lower prediction errors than conventional RC, with more pronounced improvements for state variables governed by stronger nonlinear coupling. Supplementary experiments on the UK power grid further demonstrate that the framework can also improve prediction performance in networked dynamical systems with realistic topology. Parameter analysis shows that the input weight scaling factor, input node block ratio, and higher order coupling strength jointly affect prediction performance, confirming that the advantage of the proposed method comes from the matching between structured input embedding and higher order reservoir interactions. These results provide a useful route for incorporating higher order structural information into reservoir computing and suggest that coordinated input organization and reservoir dynamics are important for predicting complex time series. Future work will extend the framework to higher dimensional chaotic systems, broader networked dynamical systems, and real world complex time series prediction tasks.

Data availability statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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