

A Dual Koopman Approach to Low-order Modeling of Ensemble Weather Simulations

Zhicheng Zhang and Yoshihiko Susuki

Department of Electrical Engineering, Kyoto University



Summary

- ❖ Methodologies for **low-order modeling** and **anomaly detection** of **ensemble weather simulations** are developed.
- ❖ A **dual Koopman approach** to **deviation dynamics** is introduced for our development as a new mathematical framework.
- ❖ An **explicit formula** characterizing the **accuracy** of the low-order modeling is derived, which is computationally tractable using DMD methods (e.g., kernel EDMD).

Motivation

Given: Ensemble (a collection of trajectories from M initial conditions $x_0^1, x_0^2, \dots, x_0^M$)

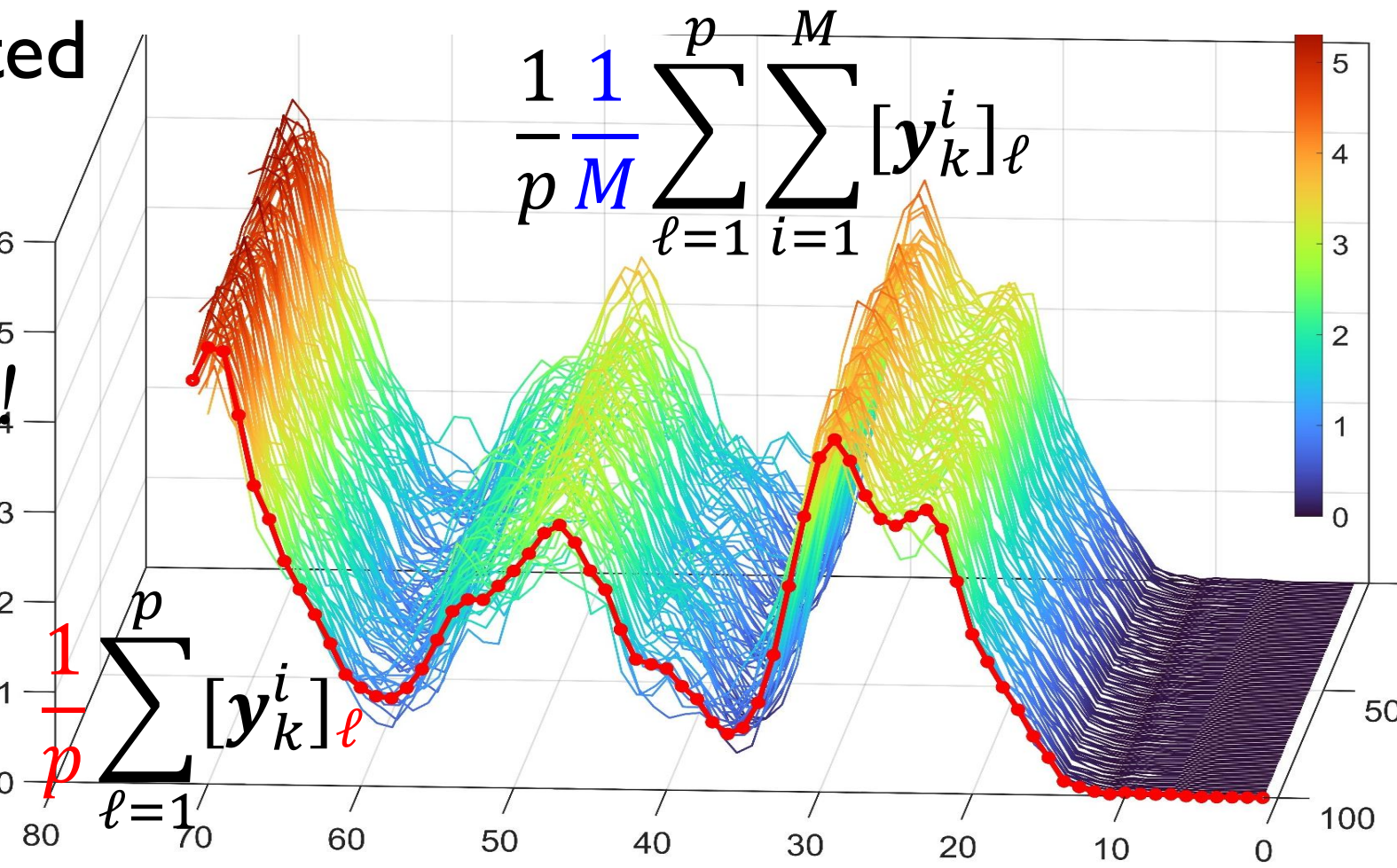
Goal: To establish methodologies and tools to
(1) develop a low-order model representing the given ensembles, and
(2) detect anomalous members (possibly related to bad weather conditions, e.g., heavy rainfall).

Key Idea: Focus on “deviation dynamics” between an ensemble and their **ensemble mean**.

Method: Dual Koopman acting on **kernel sections** decodes ensemble members via $\kappa_{x_0^i}$.

(i.e., the **RKHS feature representation** of the point x_0^i).

$$\begin{bmatrix} y_0^1 & y_0^2 & y_0^3 & \dots & y_0^{M-1} \\ y_1^1 & y_1^2 & y_1^3 & \dots & y_1^{M-1} \\ y_2^1 & y_2^2 & y_2^3 & \dots & y_2^{M-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_{N-1}^1 & y_{N-1}^2 & y_{N-1}^3 & \dots & y_{N-1}^{M-1} \end{bmatrix}$$



Koopman and its Dual Koopman Approach

❑ Koopman and its Dual Koopman Mode Decomposition on RKHS [1]

Standard Koopman on RKHS:

$$U^k f = \sum_{j=1}^{\infty} \lambda_j^k \psi_j \langle \phi_j, f \rangle, f \in \mathcal{H}$$

Koopman (X): In-Distinguish

the ensemble member between any x_0^i using the **same observable** f .

Dual Koopman on RKHS:

$$(U^k)^* g = \sum_{j=1}^{\infty} \bar{\lambda}_j^k \phi_j \langle \psi_j, g \rangle, g \in \mathcal{H}$$

Let $g = \kappa_{x_0^i} \in \mathcal{H}$ (RKHS)

$$(U^k)^* \kappa_{x_0^i} = \sum_{j=1}^{\infty} \bar{\lambda}_j^k \phi_j \langle \psi_j, \kappa_{x_0^i} \rangle, \psi_j(x_0^i)$$

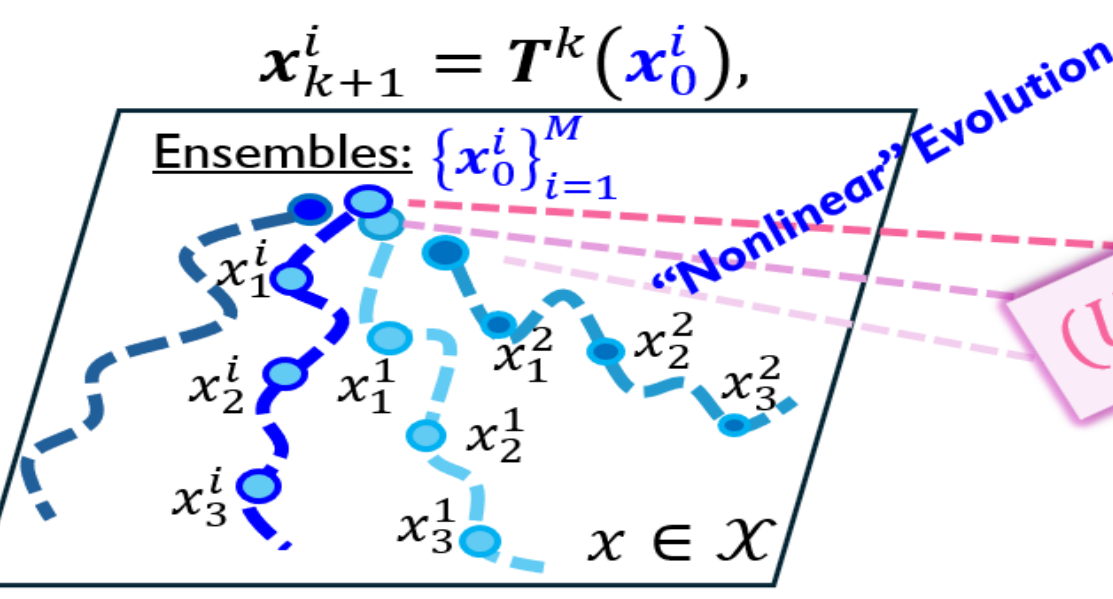
Koopman & its Dual:

$$\langle f, (U^k)^* g \rangle_{\mathcal{H}} = \langle U^k f, g \rangle_{\mathcal{H}}$$

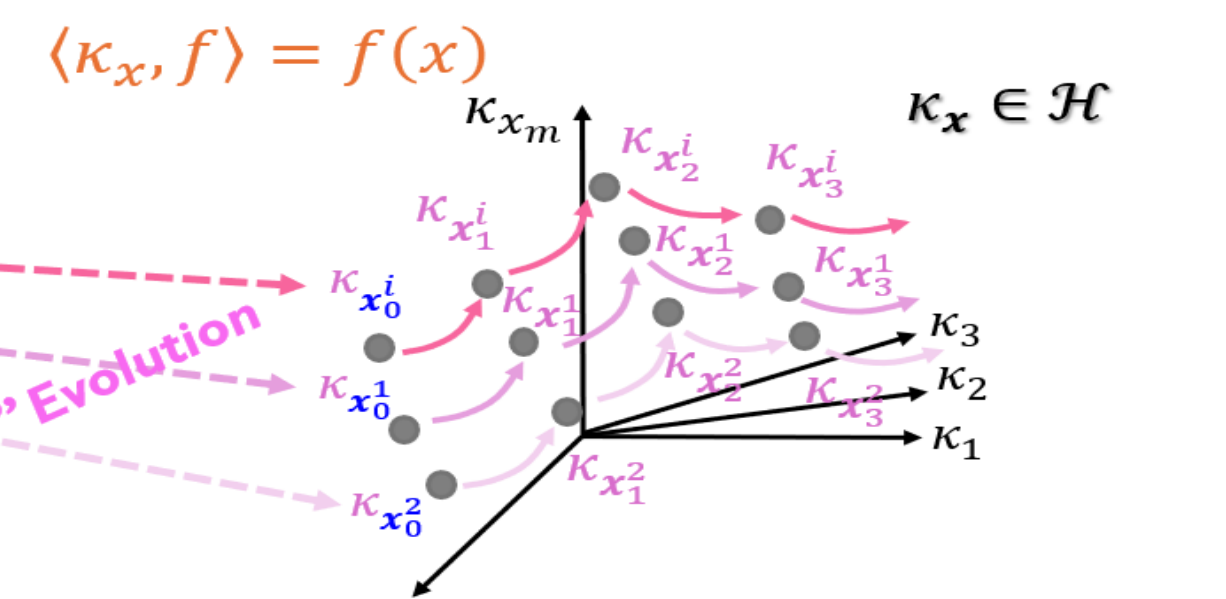
Dual Koopman (✓): Distinguish

the ensemble member between any x_0^i using the **kernel sections** $\kappa_{x_0^i}$.

State Space



Reproducing Kernel Hilbert Space



Data Space: $y_k^i = f(x_k^i)$

$$U \psi_j = \lambda_j \psi_j$$

$$\langle (U^k)^* \kappa_{x_0^i}, f \rangle = \langle \kappa_{x_0^i}, U^k f \rangle = U^k f(x_0^i)$$

$$y_k^i \approx \sum_{j=1}^r \bar{\lambda}_j^k \langle \psi_j, \kappa_{x_0^i} \rangle \langle \phi_j, f \rangle = \langle (U^k)^* \kappa_{x_0^i}, f \rangle$$

$$\mathcal{H}_r = \text{span}\{\phi_1, \dots, \phi_r\}$$

$$(U^k)^* \kappa_{x_0^i} = \sum_{j=1}^r \bar{\lambda}_j^k \phi_j \langle \psi_j, \kappa_{x_0^i} \rangle$$

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Dual Koopman Theory to Deviation Dynamics

Assumption: All ensemble members (trajectories) converge to a **common attractor**.

Assumption (Invariant subspace) Let evaluation functional (or kernel section) $\kappa_{x_0^i} \in \mathcal{H}$ on RKHS. Assume there exists a finite dimensional Koopman-invariant subspace, spanned by the leading dual Koopman eigenfunctions $\mathcal{H}_r = \text{span}\{\phi_1, \dots, \phi_r\}$.

Proposition 1 (Dual KMD Viewpoint of Problem 1): Dual KMD provides an explicit formula to quantify the deviation from the vector-valued **ensemble trajectory** and its **ensemble mean trajectory**, $y_k^i - \langle y_k \rangle$, in the ensemble members, which can be reformulated as the **deviation of kernel sections (or evaluation functionals) in RKHS**:

$$y_k^i - \langle y_k \rangle := \mathcal{C}_f \mathcal{E}_k^i = \left\langle (U^k)^* (\kappa_{x_0^i} - \bar{\kappa}_{x_0}), f \right\rangle = \sum_{j=1}^r \bar{\lambda}_j^k \langle \psi_j, \kappa_{x_0^i} - \bar{\kappa}_{x_0} \rangle \langle \phi_j, f \rangle$$

$$\|R_k^i\| \leq \sum_{j=r+1}^{\infty} |\bar{\lambda}_j^k| \left| \langle \psi_j, \kappa_{x_0^i} - \bar{\kappa}_{x_0} \rangle \right| |\mathcal{C}_j| \approx \sum_{j=r+1}^{\infty} \bar{\lambda}_j^k \left| \langle \psi_j, \kappa_{x_0^i} - \bar{\kappa}_{x_0} \rangle \right| \mathcal{C}_j + R_k^i$$

❖ If for some ensemble index $i \in \{1, \dots, M\}$, the residual R_k^i is small, then it gives the surrogate model $\mathcal{H}_r = \text{span}\{\phi_1, \dots, \phi_r\}$ by the dominant dual Koopman KEFs, which well captures the **ensemble mean dynamics**.

Preliminaries and Problem Formulation

❑ **Ensemble dynamics with different initial realizations (i.e., nonlinear evolution)**

$$x_{k+1}^i = T(x_k^i) := T^k(x_0^i), x_k \in \mathcal{X}, i = 1, \dots, M$$

$$y_k^i = f(x_k^i), f: \mathcal{X} \rightarrow \mathbb{R}^p, f \in \mathcal{F}$$

❑ **Ensemble Mean Dynamics** (i.e., ensembles M)

$$\langle y_k \rangle := \frac{1}{M} \sum_{i=1}^M y_k^i = \frac{1}{M} \sum_{i=1}^M U^k f(x_0^i), \Rightarrow (U^k)^* \bar{\kappa}_{x_0} := \frac{1}{M} \sum_{i=1}^M (U^k)^* \kappa_{x_0^i} = (U^k)^* \left(\frac{1}{M} \sum_{i=1}^M \kappa_{x_0^i} \right)$$

Linear evolution!

Problem 1 (Ensemble Trajectories vs. Ensemble Mean Trajectory): Can we provide an explicit formula to quantify the deviation from the vector-valued ensemble mean $y_k^i - \langle y_k \rangle$ in the ensemble, that is, multiple trajectories.

Numerical Experiment: PREC Deviation Analysis

Return to Ensemble Data Space:

$$\langle (U^k)^* \kappa_{x_0^i}, f \rangle_{\mathcal{H}} = U^k f(x_0^i) = y_k^i$$

$$y_k^i - \langle y_k \rangle \approx \sum_{j=1}^r \bar{\lambda}_j^k \left\langle \kappa_{x_0^i} - \bar{\kappa}_{x_0}, \phi_j \right\rangle \langle \phi_j, f \rangle + R_k^i$$

Ensemble Precipitation Weather data:

- Dual Koopman amplitudes with time evolution:
- $\mathbf{Y}^i \in \mathbb{R}^{20860 \times 71}$
- Weather simulation region: 127--132 E, 30--34 N,
- Snapshots $N=71$, $p=20860$, Ensembles $M=100$

$$\alpha_j^i(k) := \bar{\lambda}_j^k \psi_j(x_0^i) = \bar{\lambda}_j^k \langle \psi_j, \kappa_{x_0^i} \rangle$$

$$\bar{\alpha}_j(k) = \bar{\lambda}_j^k \langle \psi_j, \bar{\kappa}_{x_0} \rangle$$

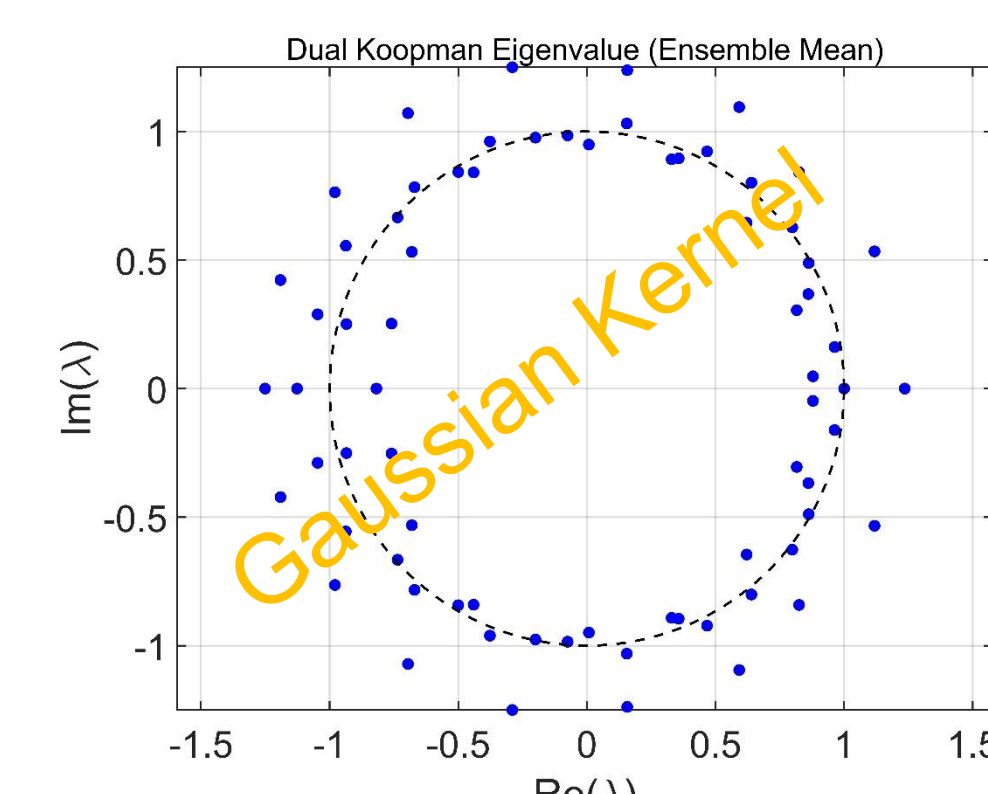


Fig. 1: Dual Koopman Eigenvalues and its absolute values

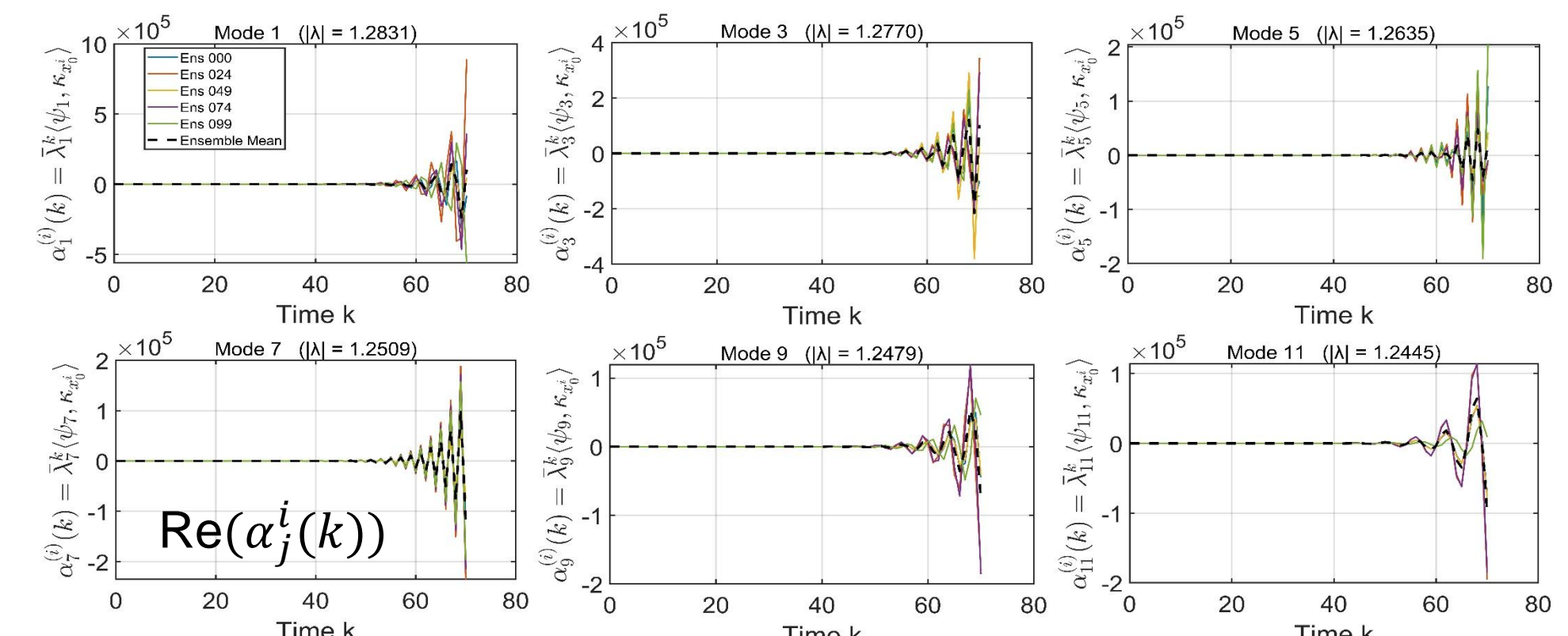


Fig. 2: Time-evolved dual Koopman amplitudes act on kernel sections (Gaussian)

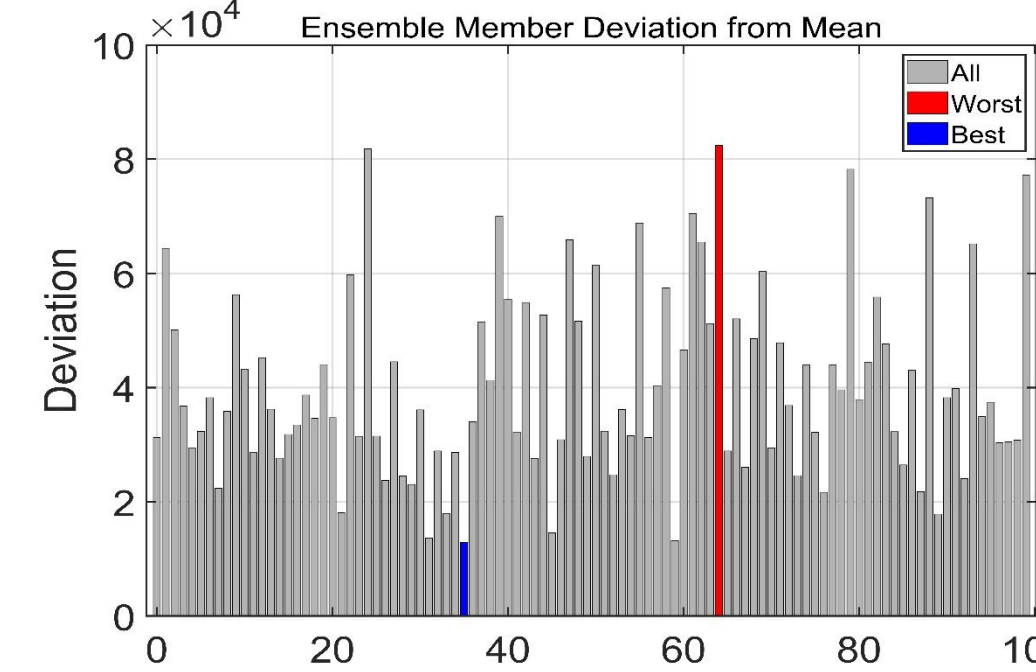


Fig. 3: Detect the worst/best case of ensembles to achieve Goal (2)

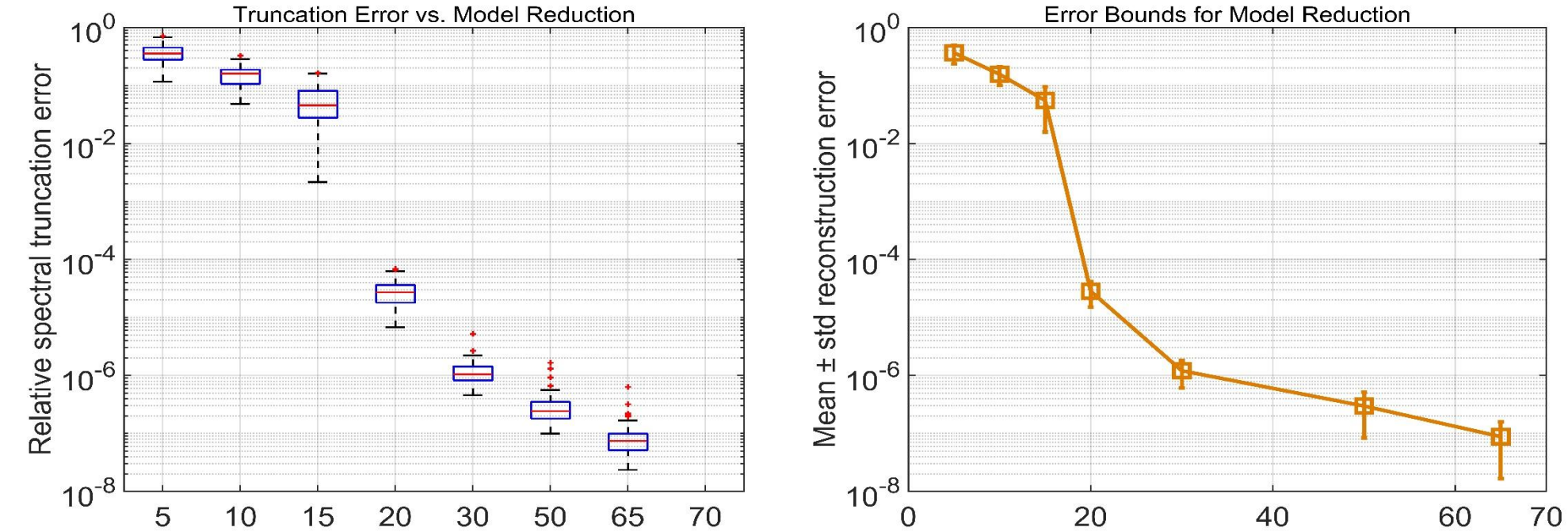
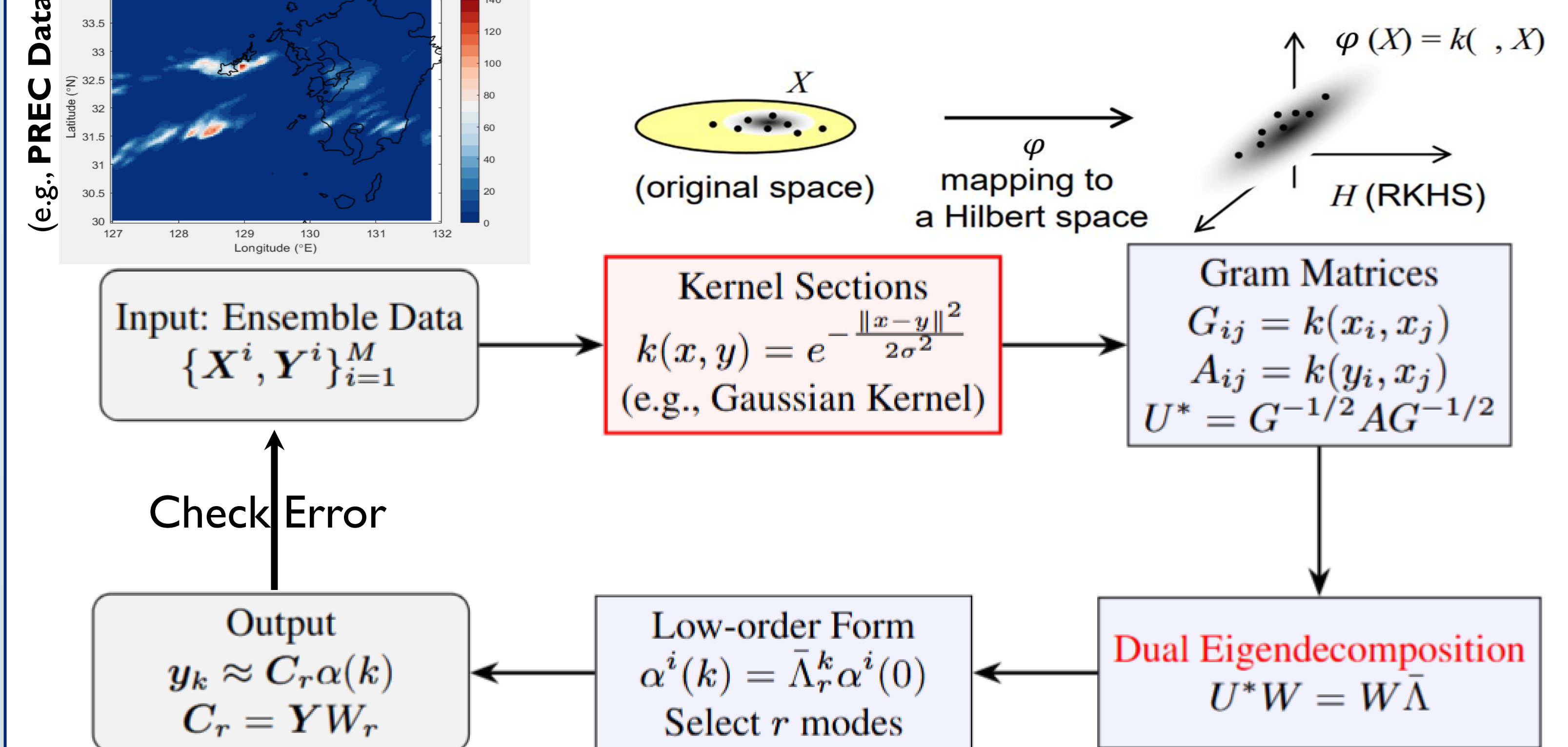


Fig. 4: Provide model-reduction and error bound to achieve Goal (1)

Pipeline: Dual Koopman in Practice with Data



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