

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



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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).

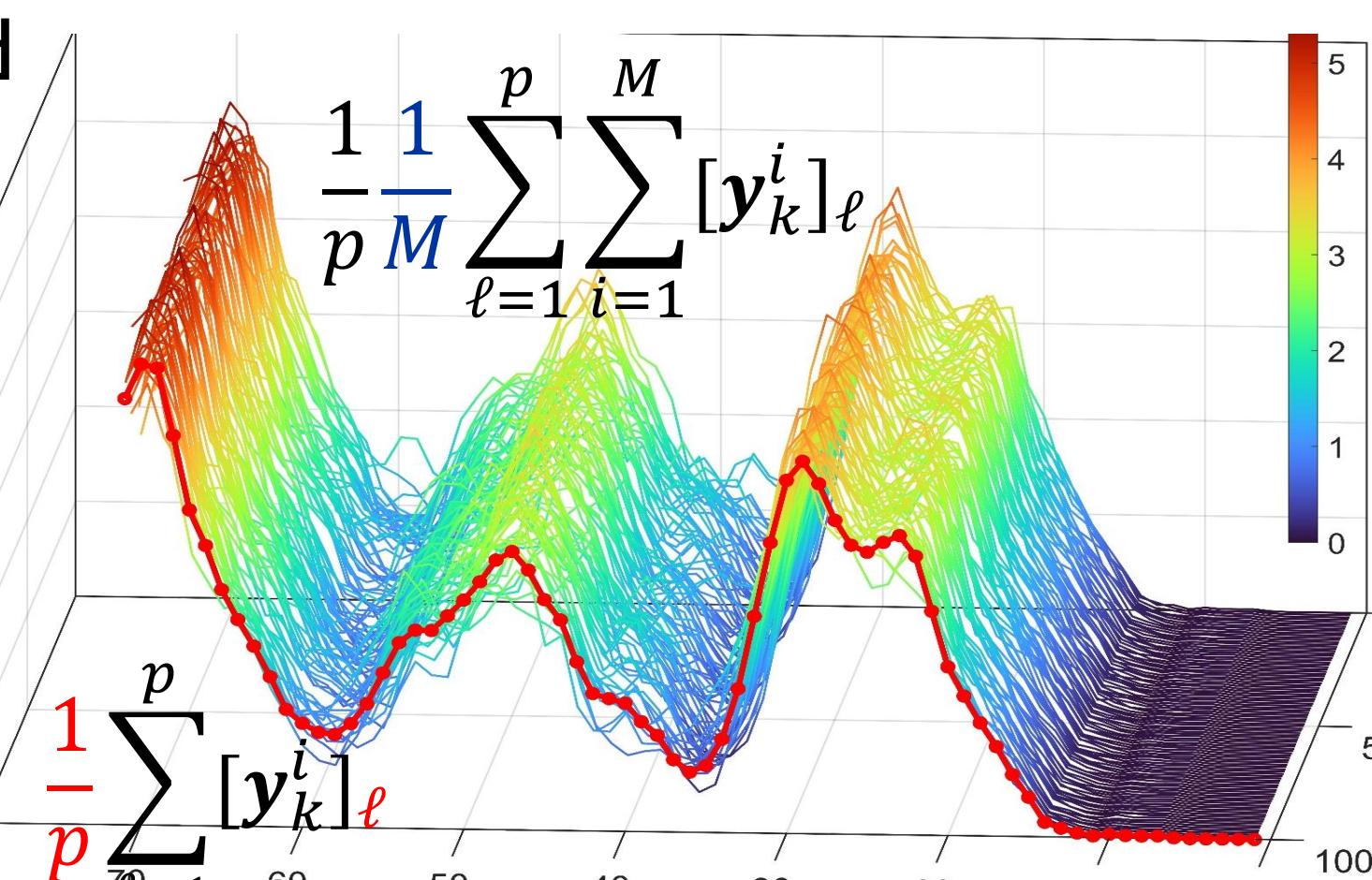
Key Idea: Focus on “deviation dynamics” between an ensemble and their **ensemble mean**

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)

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



Koopman and its Dual Koopman Approach

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

Standard Koopman on RKHS:

$$U^k f = \sum_{j=1}^{\infty} \bar{\lambda}_j^k \psi_j \frac{\langle \phi_j, f \rangle}{\psi_j(x_0)}, f \in \mathcal{H}$$

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)

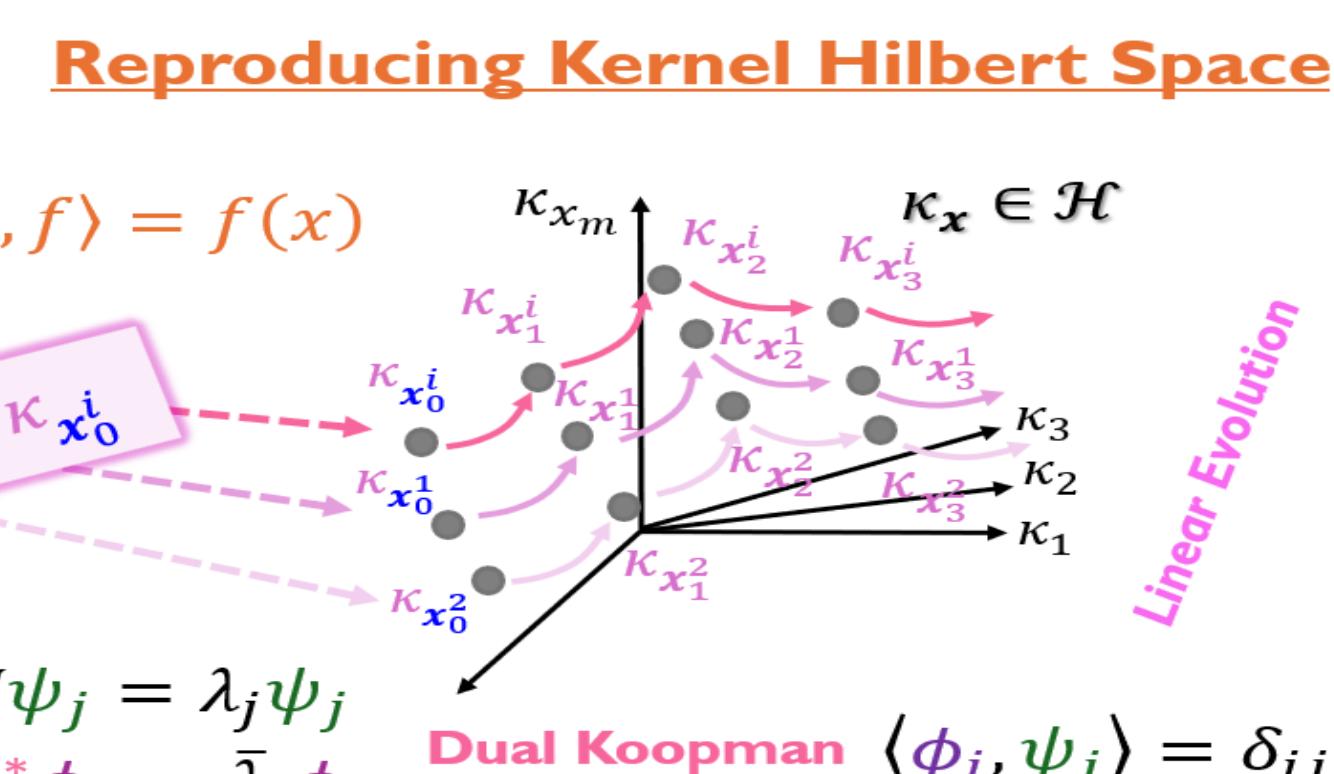
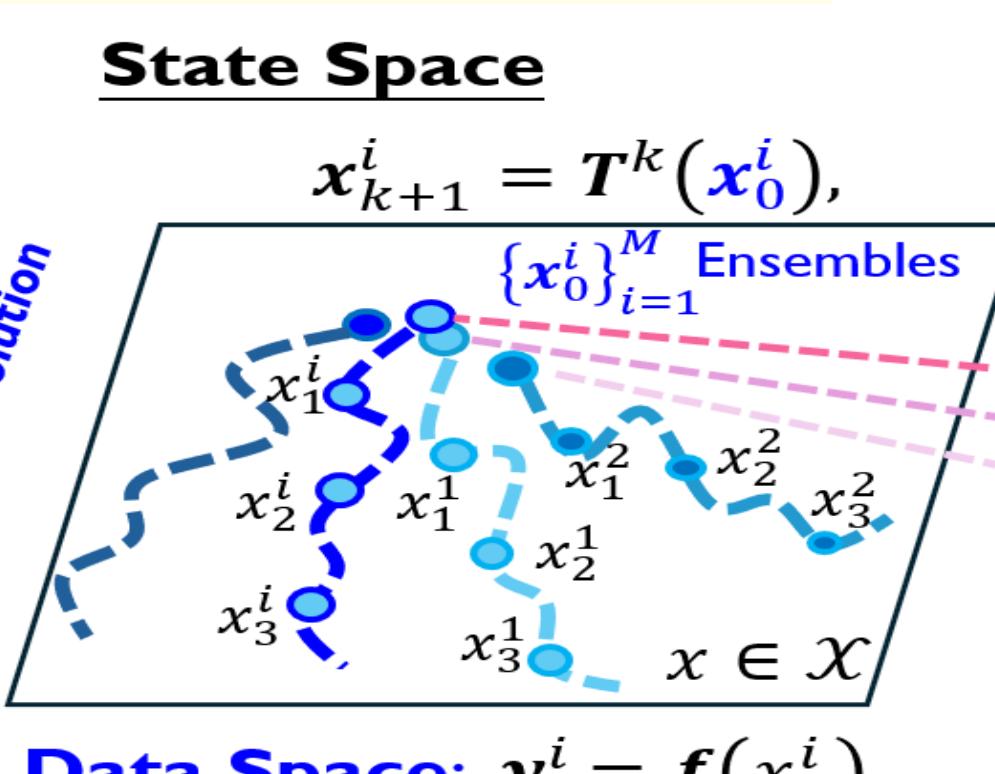
$$(U^k)^* \kappa_{x_0^i} = \sum_{j=1}^{\infty} \bar{\lambda}_j^k \phi_j \frac{\langle \psi_j, \kappa_{x_0^i} \rangle}{\psi_j(x_0^i)},$$

Koopman (X): In-Distinguish
the ensemble member between any x_0^i using the **same observable** f .

$$\langle \phi_i, \psi_i \rangle = \delta_{ij}$$

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** $\kappa_{x_0^i}$.



$$\begin{aligned} U\psi_j &= \lambda_j \psi_j \\ U^*\phi_j &= \bar{\lambda}_j^k \phi_j \\ \text{Dual Koopman } \langle \phi_i, \psi_j \rangle &= \delta_{ij} \\ (U^k)^* \kappa_{x_0^i} &= \kappa_{T^k(x_0^i)} = \kappa_{x_k^i} \end{aligned}$$

Sketch of Dual Koopman

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

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 I (Dual KMD Viewpoint of Problem I): 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**:

$$\begin{aligned} y_k^i - \langle y_k \rangle &:= C_f \mathcal{E}_k^i = \langle (U^k)^* (\kappa_{x_0^i} - \bar{\kappa}_{x_0}), f \rangle = \sum_{j=1}^{\infty} \bar{\lambda}_j^k \langle \psi_j, \kappa_{x_0^i} - \bar{\kappa}_{x_0} \rangle \frac{\langle \phi_j, f \rangle}{c_j} \\ \|R_k^i\| &\leq \sum_{j \geq r+1} |\bar{\lambda}_j|^k \left| \langle \psi_j, \kappa_{x_0^i} - \bar{\kappa}_{x_0} \rangle \right| |C_j| \\ &\approx \sum_{j=1}^r \bar{\lambda}_j^k \langle \psi_j, \kappa_{x_0^i} - \bar{\kappa}_{x_0} \rangle C_j + R_k^i \end{aligned}$$

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)

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

Distinguishable? VS.

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

$$U^k f = f \circ T^k$$

$$(U^k)^* \kappa_{x_0^i} = \kappa_{T^k(x_0^i)}$$

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 I (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:

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

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

Ensemble Precipitation Weather data:

- Dual Koopman amplitudes with time evolution: $\alpha_j^i(k) := \bar{\lambda}_j^k \psi_j(x_0^i) = \bar{\lambda}_j^k \langle \psi_j, \kappa_{x_0^i} \rangle$, $\bar{\alpha}_j(k) = \bar{\lambda}_j^k \langle \phi_j, \bar{\kappa}_{x_0} \rangle$
- Weather simulation region: 127--132 E, 30--34 N,
- Snapshots $N=71$, $p=20860$, Ensembles $M=100$

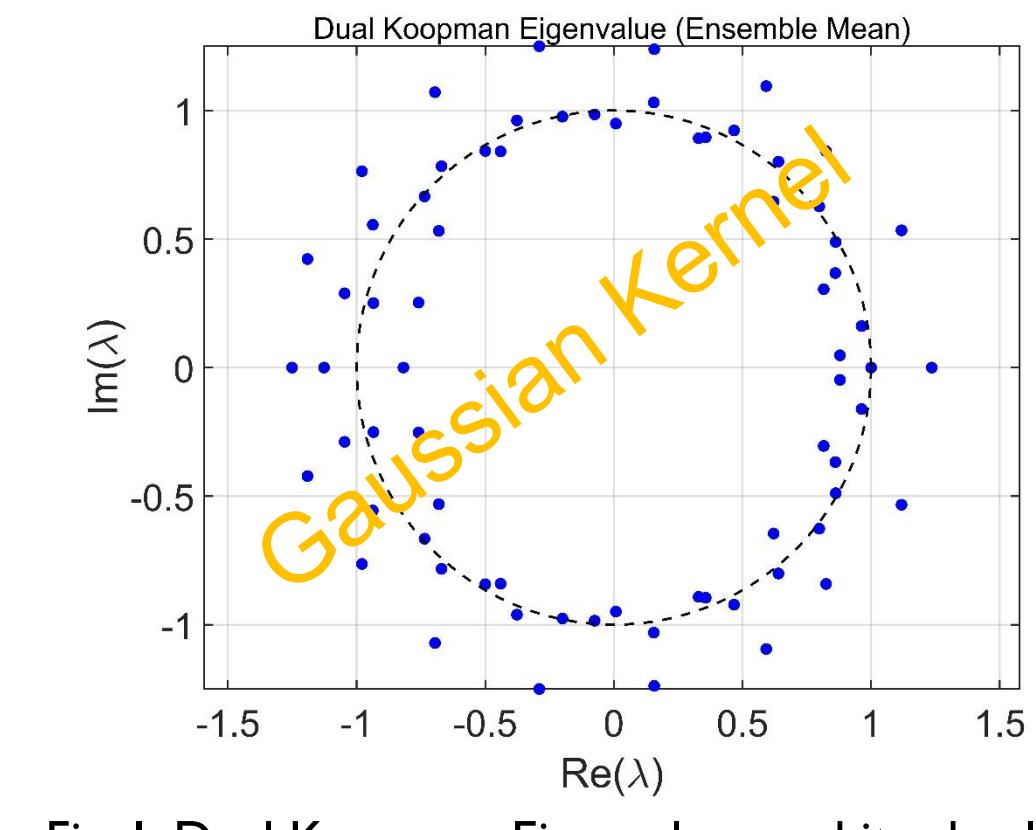


Fig. 1: Dual Koopman Eigenvalues and its absolute values

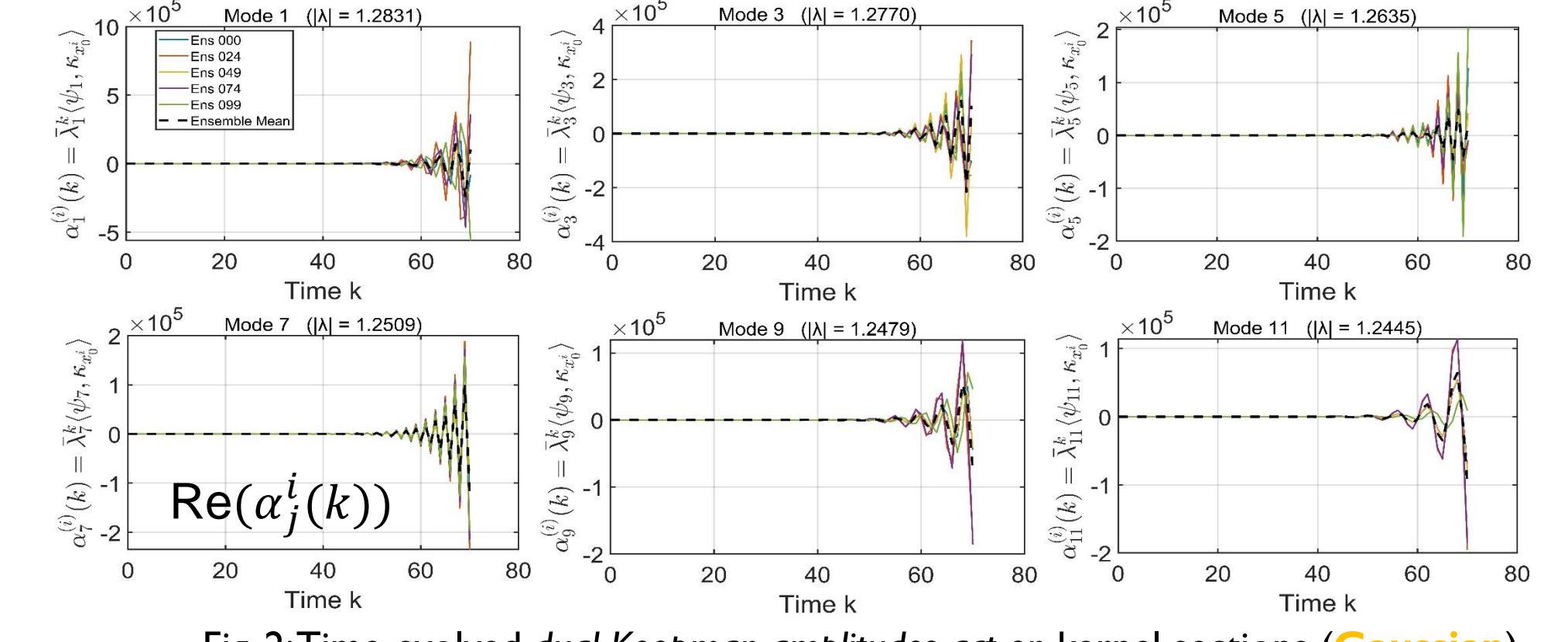


Fig. 2: Time-evolved dual Koopman amplitudes act on kernel sections (Gaussian)

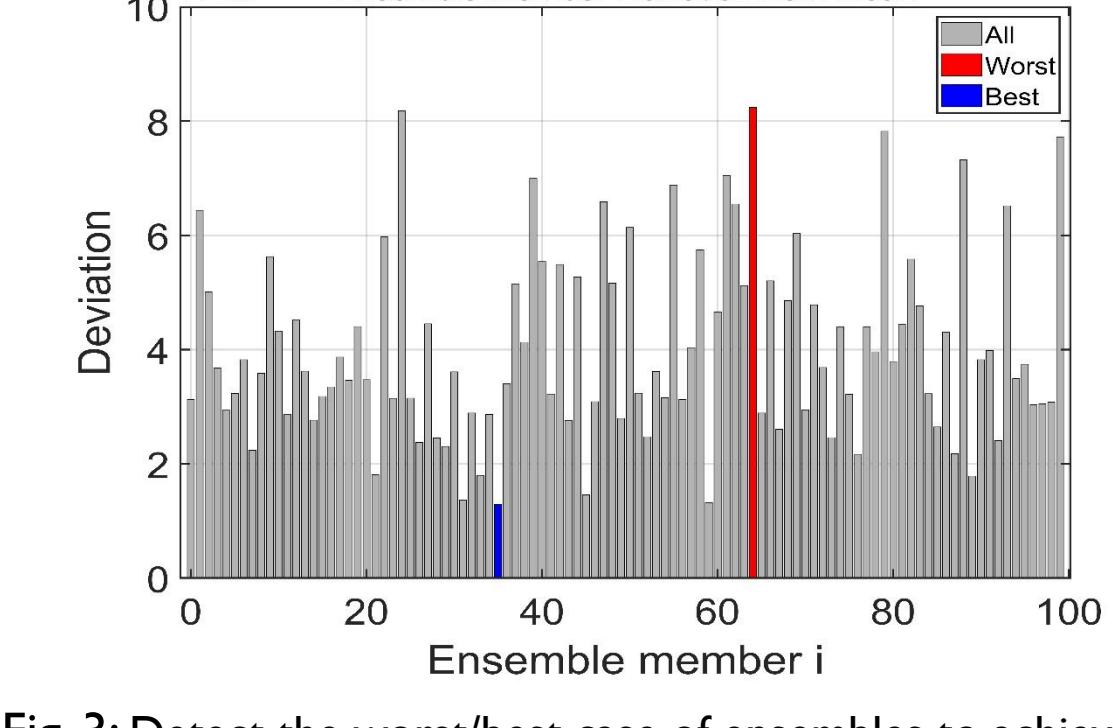


Fig. 3: Detect the worst/best case of ensembles to achieve Goal (2)

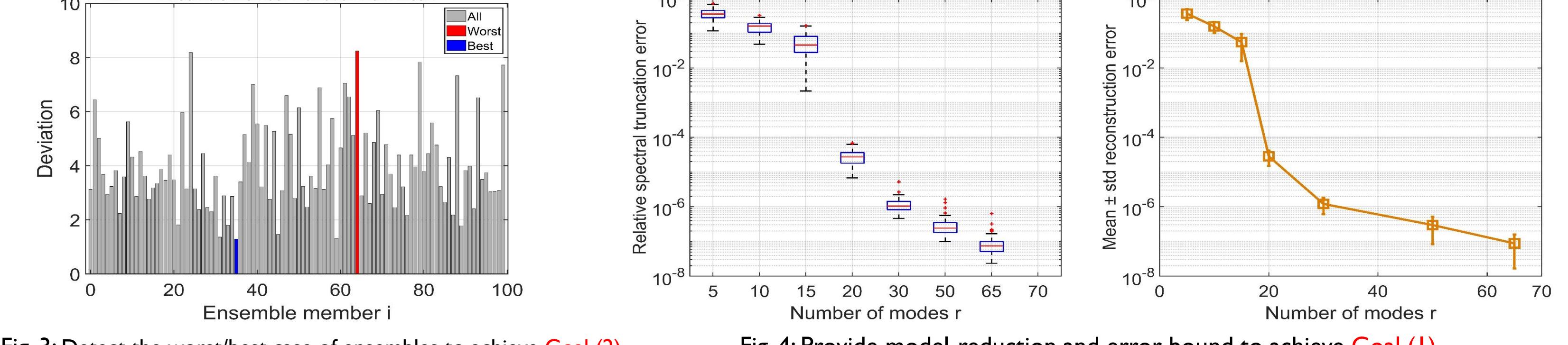
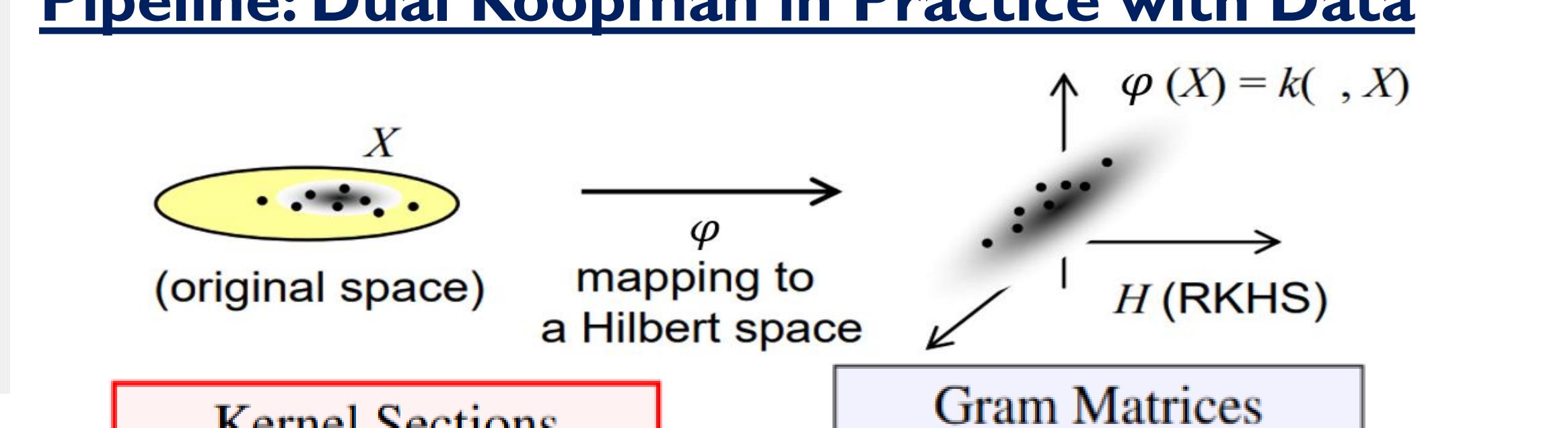
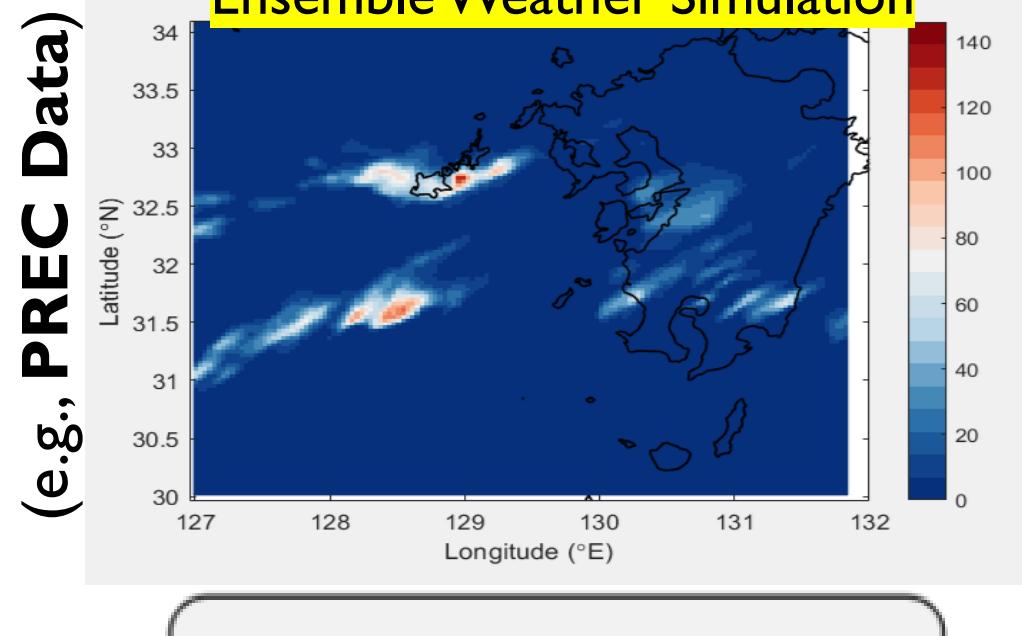


Fig. 4: Provide model-reduction and error bound to achieve Goal (1)



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