

# 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”

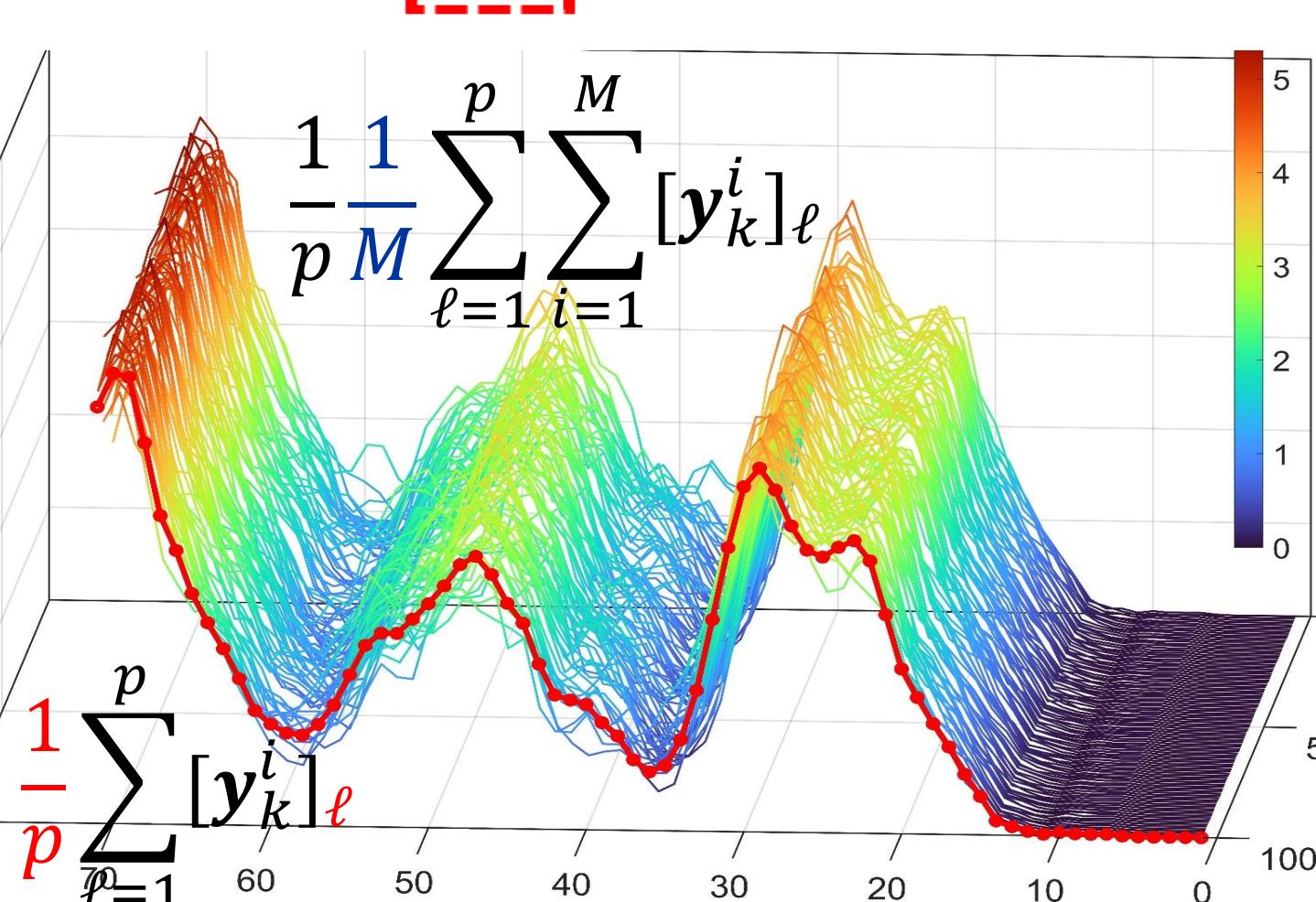
between an ensemble and their **ensemble mean**.

**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:

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

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

**Relationship:**  $\langle \phi_i, \psi_j \rangle = \delta_{ij}$

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

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

**Reproducing Kernel Hilbert Space**

$\langle \kappa_x, f \rangle = f(x)$

$\langle \kappa_x, \kappa_y \rangle = \delta_{xy}$

**Dual Koopman:**  $U^* \phi_j = \bar{\lambda}_j \phi_j$

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

**Roadmap of Dual Koopman:**

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

## 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**:

$$y_k^i - \langle y_k \rangle := C_f \mathcal{E}_k^i = \langle (U^k)^* (\kappa_{x_0^i} - \bar{\kappa}_{x_0}), f \rangle = \sum_{j=1}^{\infty} \bar{\lambda}_j^k \langle \psi_j, \kappa_{x_0^i} - \bar{\kappa}_{x_0} \rangle \frac{\langle \phi_j, f \rangle}{c_j}$$

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

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)**

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

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

Distinguishable? VS.

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

**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:**

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

$$y_k^i - \langle y_k \rangle \approx \sum_{j=1}^r \bar{\lambda}_j^k \frac{\langle \kappa_{x_0^i} - \bar{\kappa}_{x_0}, \phi_j \rangle \langle \phi_j, f \rangle}{\Delta \phi_j(0)} + R_k^i$$

**Ensemble Precipitation Weather data:**

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

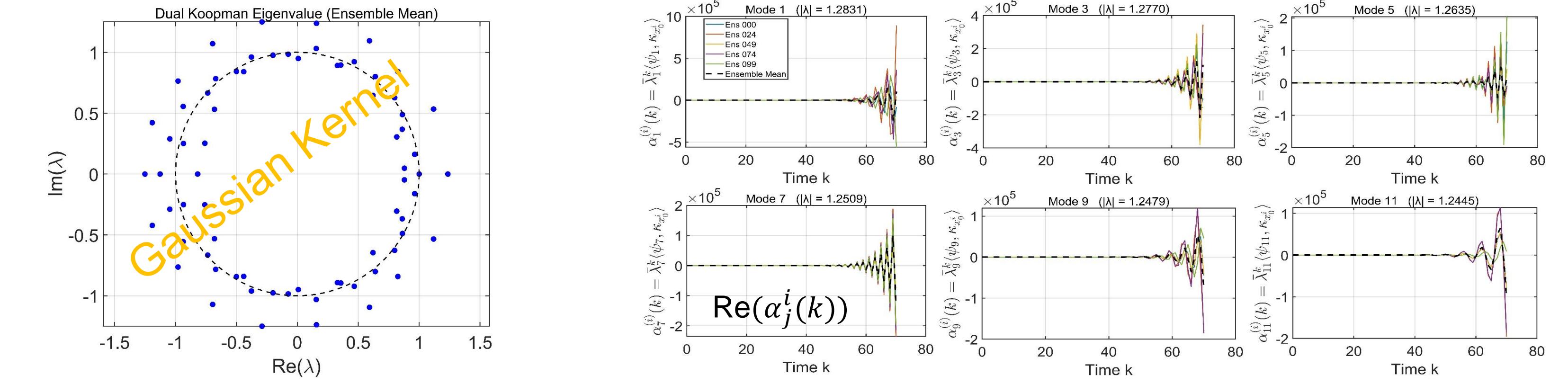


Fig. 1: Dual Koopman Eigenvalues and its absolute values

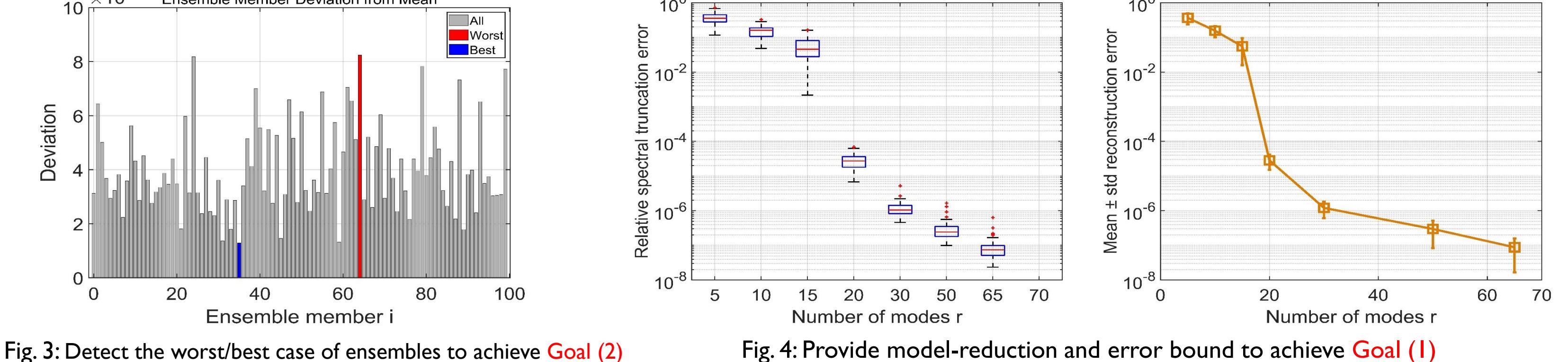


Fig. 2: Time-evolved dual Koopman amplitudes act on kernel sections (Gaussian)

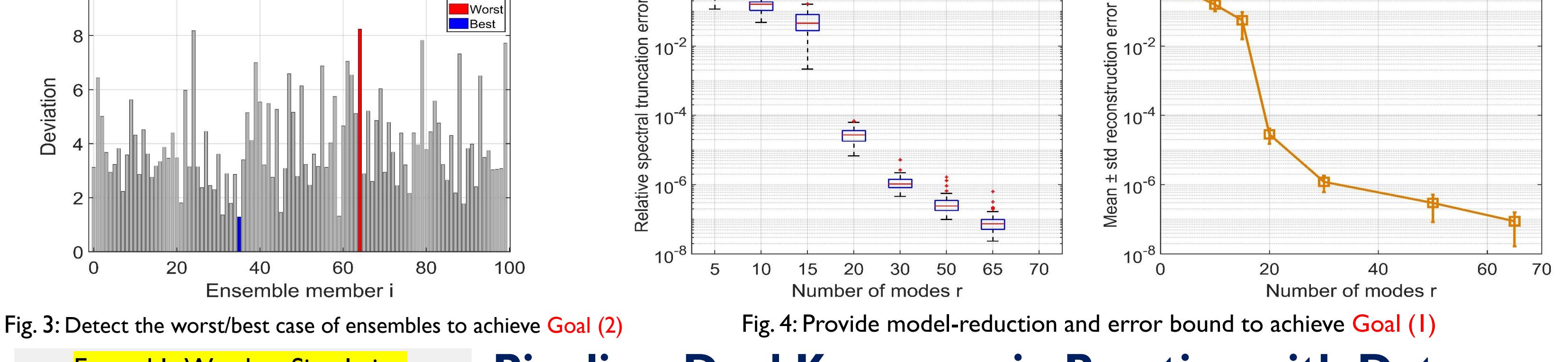
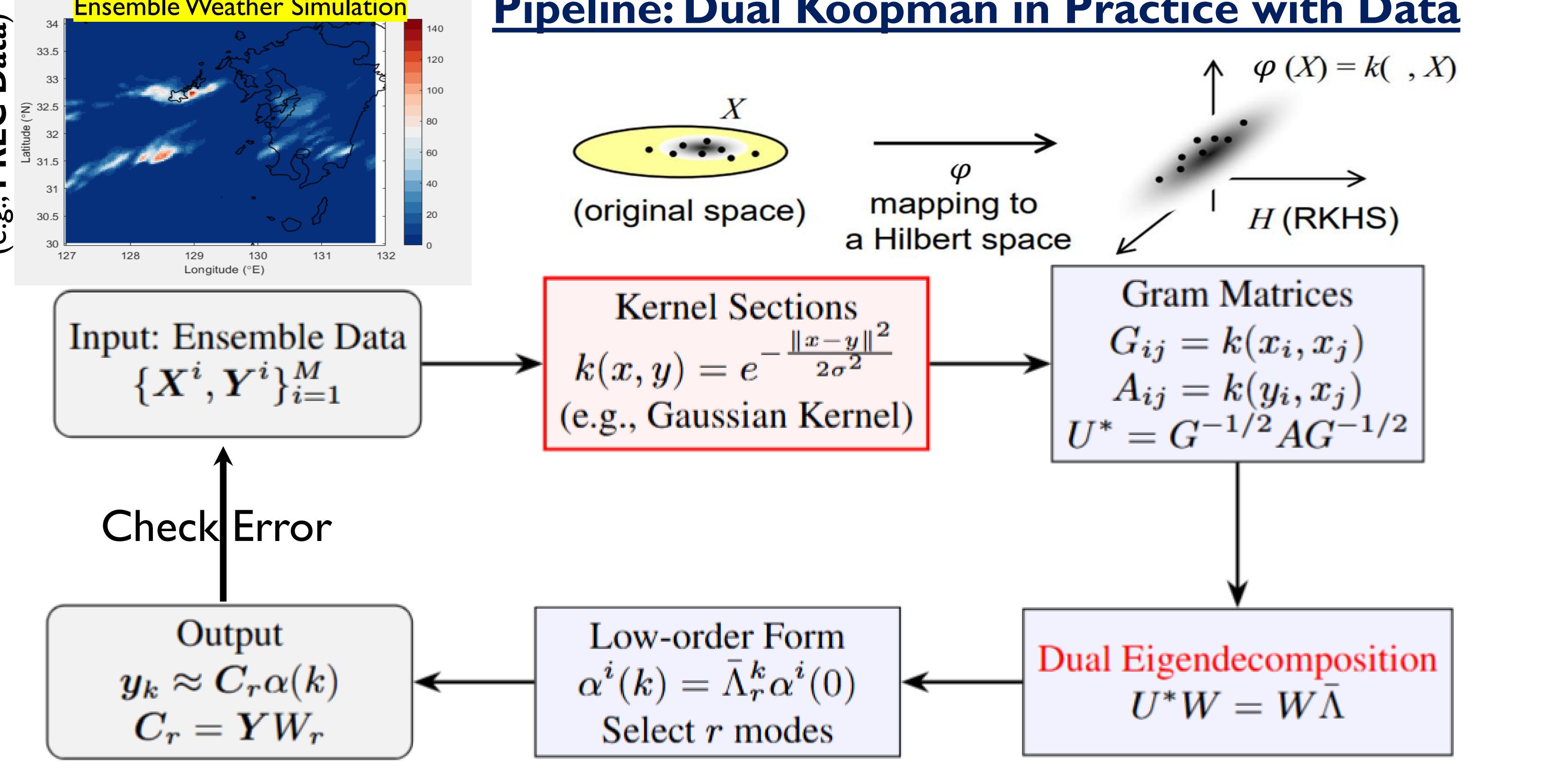


Fig. 3: Detect the worst/best case of ensembles to achieve Goal (2)



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



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## Acknowledgements:

This work was partly supported by JST Moonshot R&D, Grant No. JPMJMS2284.

We are grateful to Prof. Atsushi Okazaki (Chiba Univ.) for his valuable suggestions.