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

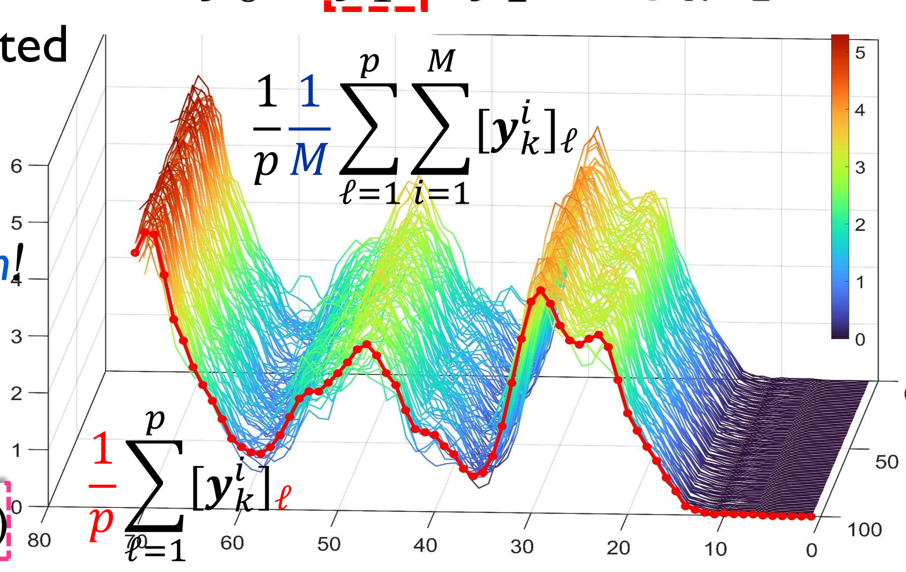
Given: *Ensemble (a collection of trajectories from M initial conditions* $x_0^1, x_0^2, \dots, x_0^M$)

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).*

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

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)



Preliminaries and Problem Formulation

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

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

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

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

Distinguishable? VS.

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

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

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

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.*

Koopman and its Dual Koopman Approach

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

Standard Koopman on RKHS:

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

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

Dual Koopman on RKHS:

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

Relationship

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

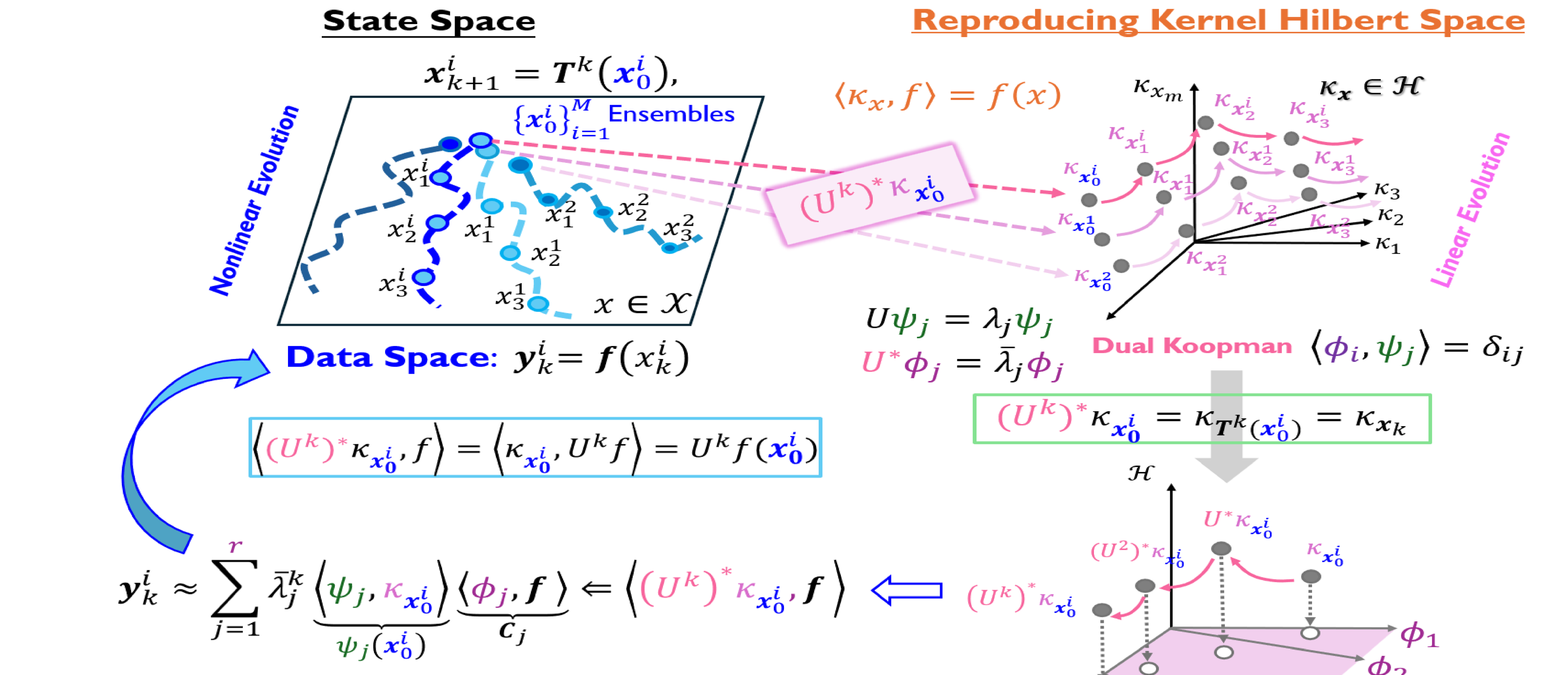
Koopman & its Dual:

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

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

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

Dual Koopman (✓): Distinguish the ensemble member between any x_0^i using the ***kernel sections*** $\kappa_{x_0^i}$.



Sketch of Dual Koopman

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* $\mathcal{H}_r = \mathrm{span}\{\phi_1,\dots,\phi_r\}$.

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:*

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

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

$$\|R_k^i\| \le \sum_{j\ge r+1}|\bar{\lambda}_j|^k\left|\left\langle \psi_j, \kappa_{x_0^i} - \bar{\kappa}_{x_0}\right\rangle\right||c_j|$$

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

Numerical Experiment: PREC Deviation Analysis

Return to Ensemble Data Space:

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

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

Ensemble Precipitation Weather data:

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

- Dual Koopman amplitudes with time evolution:

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

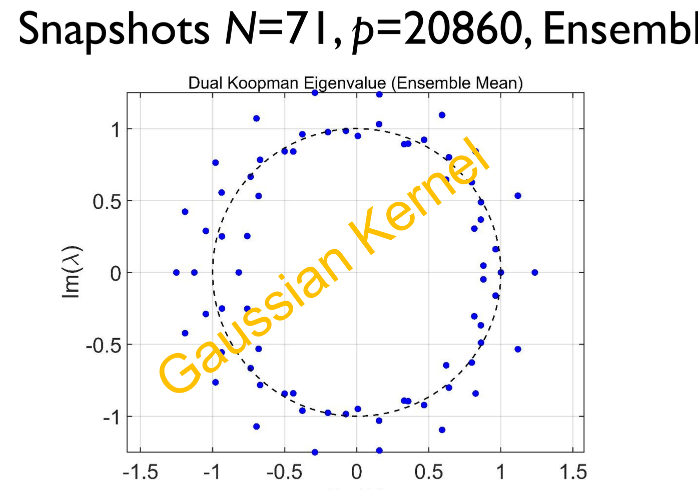


Fig. 1: Dual Koopman Eigenvalues and its absolute values

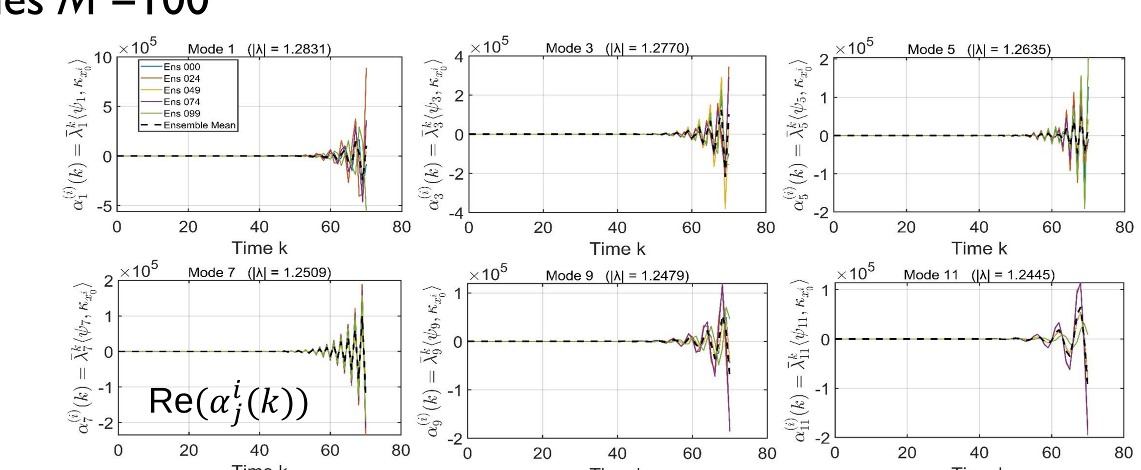


Fig. 2: Time-evolved *dual Koopman amplitudes act on* kernel sections (Gaussian)

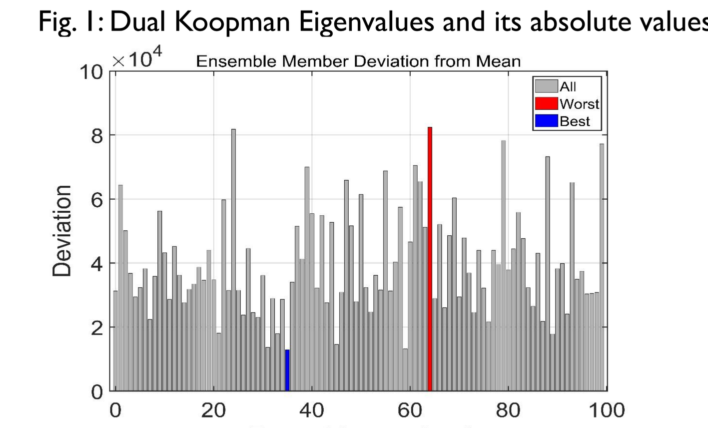


Fig. 3: Detect the worst/best case of ensembles to achieve Goal (2)

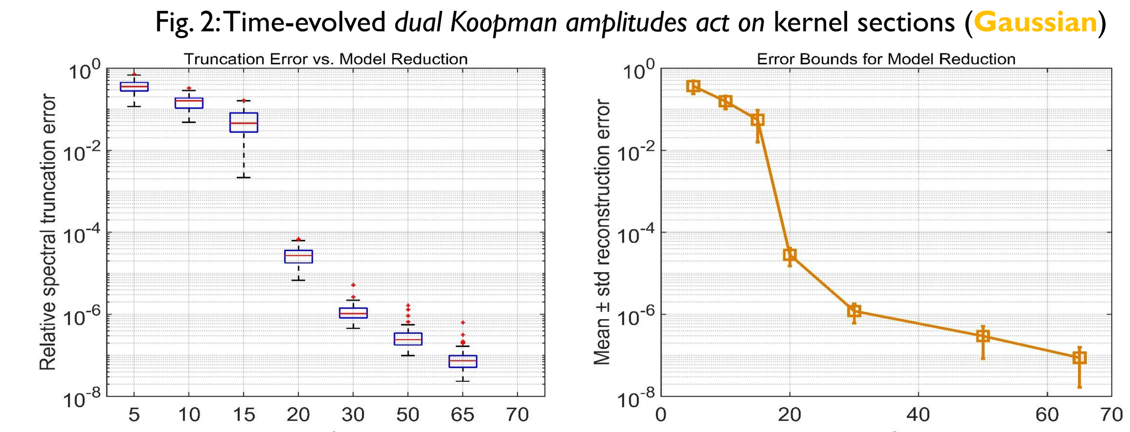
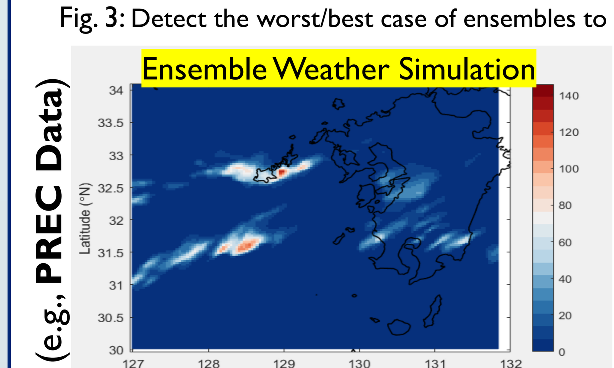
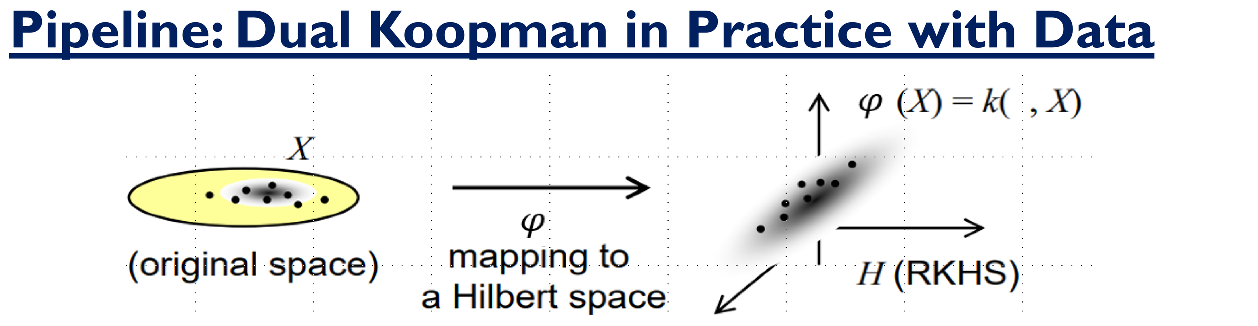
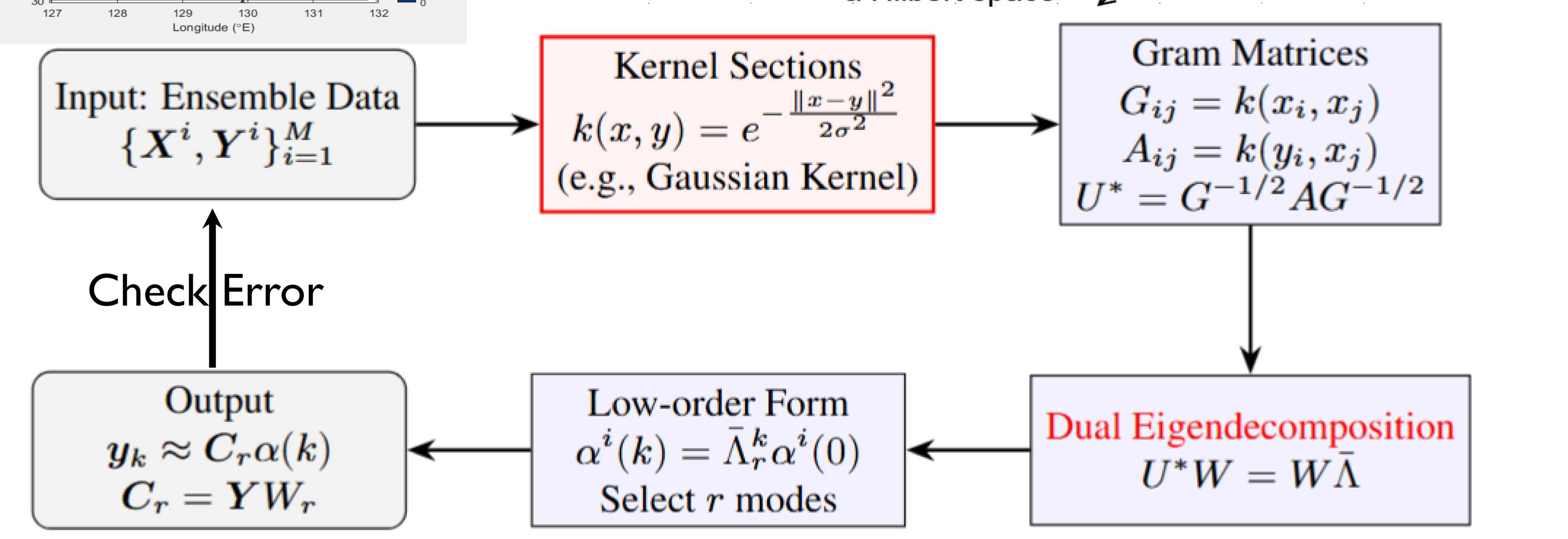


Fig. 4: Provide model-reduction and error bound to achieve Goal (1)



Pipeline: Dual Koopman in Practice with Data





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