Dynamically constrained uncertainty for the Kalman filter covariance in the presence of model error

Colin Grudzien[1]
Alberto Carrassi[2], Marc Bocquet[3]

1) Nansen Environmental and Remote Sensing Center, Colin.Grudzien@nersc.no
2) Nansen Environmental and Remote Sensing Center, Alberto.Carrassi@nersc.no
3) École des Ponts ParisTech, Marc.Bocquet@enpc.fr

Assimilation in the unstable subspace (AUS)

- Numerical results demonstrate that the skill of ensemble DA methods in chaotic systems is related to dynamic instabilities [Ng et al. 2011].
- Asymptotic properties of ensemble-based covariances relate to the multiplicity and strength of unstable Lyapunov exponents [Sakov & Oke 2008; Carrassi et al. 2009].
- Trevisan et al. proposed filtering methodology for dimensional reduction to exploit this property called **Assimilation in the Unstable Subspace**.
- The goal of AUS is to **dynamically** target
  - **corrections** [Trevisan et al. 2010; Trevisan & Palatella 2011; Palatella & Trevisan 2015] **and**
  - **observations** [Trevisan & Uboldi 2004; Carrassi et. al. 2007]

  in data assimilation design to minimize the forecast uncertainty while reducing the computational burden of DA.

A mathematical framework for AUS

- A mathematical framework for AUS is established for **perfect, linear models.**
- Asymptotically, the support of the KF forecast uncertainty is confined to the span of the **unstable-neutral BLVS** [Gurumoorthy et al. 2017; Bocquet et al. 2017].
- This is likewise demonstrated for the smoothing problem [Bocquet & Carrassi 2017].
- **This work extends the mathematical framework for AUS to linear, imperfect models.**
- We bound the forecast uncertainty in terms of the **dynamic expansion** of errors relative to the **constraints due to observations,** the precision therein.
- We produce **necessary** and **sufficient** conditions for the boundedness of forecast errors.
- This work extends the central hypotheses of AUS, to **model error**.

The square root Kalman filter

- Linear model and observation processes are given by

$$\mathbf{x}_{k+1} = \mathbf{M}_{k+1}\mathbf{x}_k + \mathbf{w}_{k+1} \qquad \mathbf{w}_k \sim N(0, \mathbf{Q}_k)$$
$$\mathbf{y}_{k+1} = \mathbf{H}_{k+1}\mathbf{x}_k + \mathbf{v}_{k+1} \qquad \mathbf{v}_k \sim N(0, \mathbf{R}_k)$$

- The square root forecast error Ricatti equation is given [Bocquet et al. 2017]

$$\mathbf{P}_{k+1} = \mathbf{M}_{k+1}\mathbf{X}_k \left(\mathbf{I}_r + \mathbf{X}_k^{\mathrm{T}}\mathbf{H}_k^{\mathrm{T}}\mathbf{R}_k^{-1}\mathbf{H}_k\mathbf{X}_k\right)^{-1}\mathbf{X}_k^{\mathrm{T}}\mathbf{M}_{k+1}^{\mathrm{T}} + \mathbf{Q}_{k+1}$$

where $\mathbf{P}_k = \mathbf{X}_k\mathbf{X}_k^{\mathrm{T}}$ and $\mathbf{X}_k \in \mathbb{R}^{n\times r}$ is a rank r square root [Tippet et al. 2008].

Stabilizing errors with observations

- We represent the **minimal observational constraint** by

$$\alpha_k \triangleq \sigma_r\left(\mathbf{R}_k^{-\frac{1}{2}}\mathbf{H}_k\mathbf{X}_k\right)^2 \qquad \alpha \triangleq \inf_k\{\alpha_k\}$$

- We will recursively apply the inequality

$$\left(\mathbf{I}_r + \mathbf{X}_k^{\mathrm{T}}\mathbf{H}_k^{\mathrm{T}}\mathbf{R}_k^{-1}\mathbf{H}_k\mathbf{X}_k\right)^{-1} \leq (1+\alpha)^{-1}\,\mathbf{I}_r$$

Geometrically bounding the square root

- We denote

$$\mathbf{P}_0 \triangleq \mathbf{Q}_0$$

and bound the forecast covariance at time k :

$$\mathbf{P}_k \leq \sum_{l=0}^{k} \left(\frac{1}{1+\alpha} \right)^{k-l} \mathbf{M}_{k:l} \mathbf{Q}_l \mathbf{M}_{k:l}^{\mathrm{T}}$$

Bounding forecast errors

- The projection of the forecast error is bounded in the i^{th} backwards Lyapunov vector whenever we have

$$\frac{e^{2\lambda_i}}{1+\alpha} < 1$$

- The inequality is trivially true for any **stable mode**, even when $\alpha = 0$ and there are no observations:

$$\mathbf{H}_k \triangleq \mathbf{0}$$

Sufficient conditions for bounded forecast error

- If the anomaly dimension is greater than the observational dimension, then $\alpha = 0$.
- Let anomaly dimension $\leq$ observational dimension, **and**

  $$\alpha > e^{2\lambda_1} - 1$$

  then the forecast error is bounded [Grudzien et al. 2017].
- It was noted previously under **ideal** assumptions [Carrassi et al. 2008], we now prove this a **generic** condition for all **perfect models**:

  if observations are confined to the unstable-neutral subspace, with the above **minimal precision**, the forecast error of the (reduced rank) Kalman filter [Bocquet et al. 2017] is uniformly bounded [Grudzien et al. 2017].

Necessary conditions for bounded forecast error

- The **maximal observational constraint** is described by

$$\beta_k \triangleq \sigma_1 \left(\mathbf{R}_k^{-\frac{1}{2}} \mathbf{H}_k \mathbf{X}_k \right)^2 \qquad \beta \triangleq \sup_k \{\beta_k\}$$

- Assume the forecast error is uniformly bounded, then

$$\sum_{l=0}^{k} \left(\frac{1}{1+\beta} \right)^{k-l} \mathbf{M}_{k:l} \mathbf{Q}_l \mathbf{M}_{k:l}^{\mathrm{T}} \leq \mathbf{P}_k < \infty$$

from which we recover a **necessary** condition:

the maximal observational constraint is stronger than the maximal instability which forces the model error [Grudzien et al. 2017].

Dynamics of uncertainty in the stable subspace

- The uncertainty in the stable BLVs is **bounded independently of filtering** [Grudzien et al. 2017]**.**
- Still, the uniform bound may be **impractically large**. In a **reduced rank square root approximation**, the error in the stable subspace may cause the filter to diverge.
- This was previously noted, due to the non-linear interactions of uncertainty in **perfect models** [Ng et al. 2011].
- This was corrected as a second order term in EKF-AUS for nonlinear perfect models [Palatella & Trevisan 2015].
- **We demonstrate this is an irreducible, first order effect in the presence of model error.**

The model invariant evolution of uncertainty

- Suppose model error is time invariant and spatially uncorrelated in a basis of backwards Lyapunov vectors.
- The evolution of the freely forecasted uncertainty in the i^{th} BLV is given by

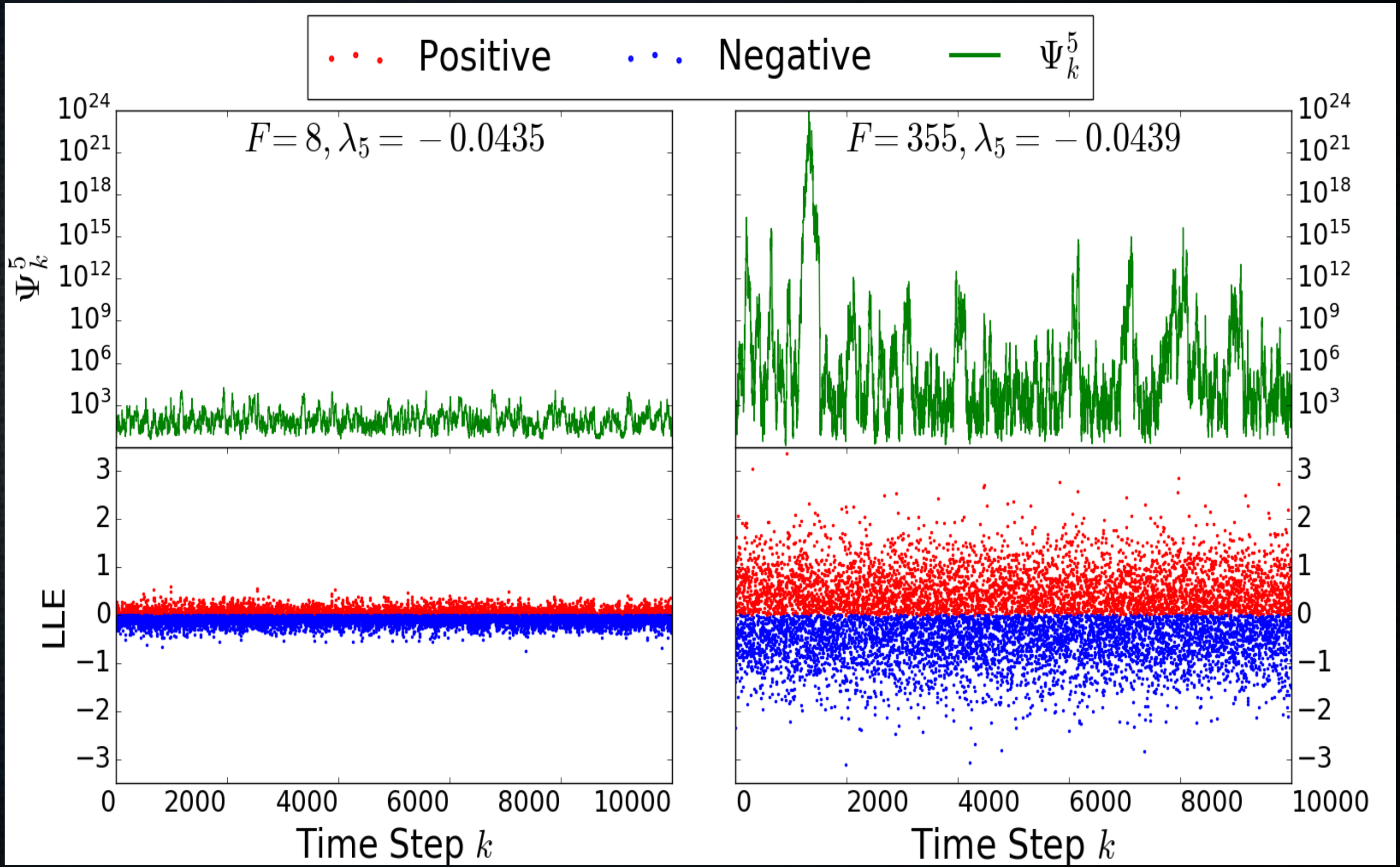
$$\Psi_k^i \triangleq \sum_{l=0}^{k} \parallel \left(\mathbf{T}_{k:l}^{\mathrm{T}}\right)^i \parallel^2$$

[Grudzien et al. 2017].

- For any stable BLV, the free uncertainty can be stably computed recursively by QR factorizations [Grudzien et al. 2017].

Transient instability in the stable subspace

- We study discrete, linearized Lorenz '96 with 10 dimensions and 6 stable modes.
- We vary the forcing parameter F.
- Variability in the local Lyapunov exoponents of the stable modes forces transient instabilities.



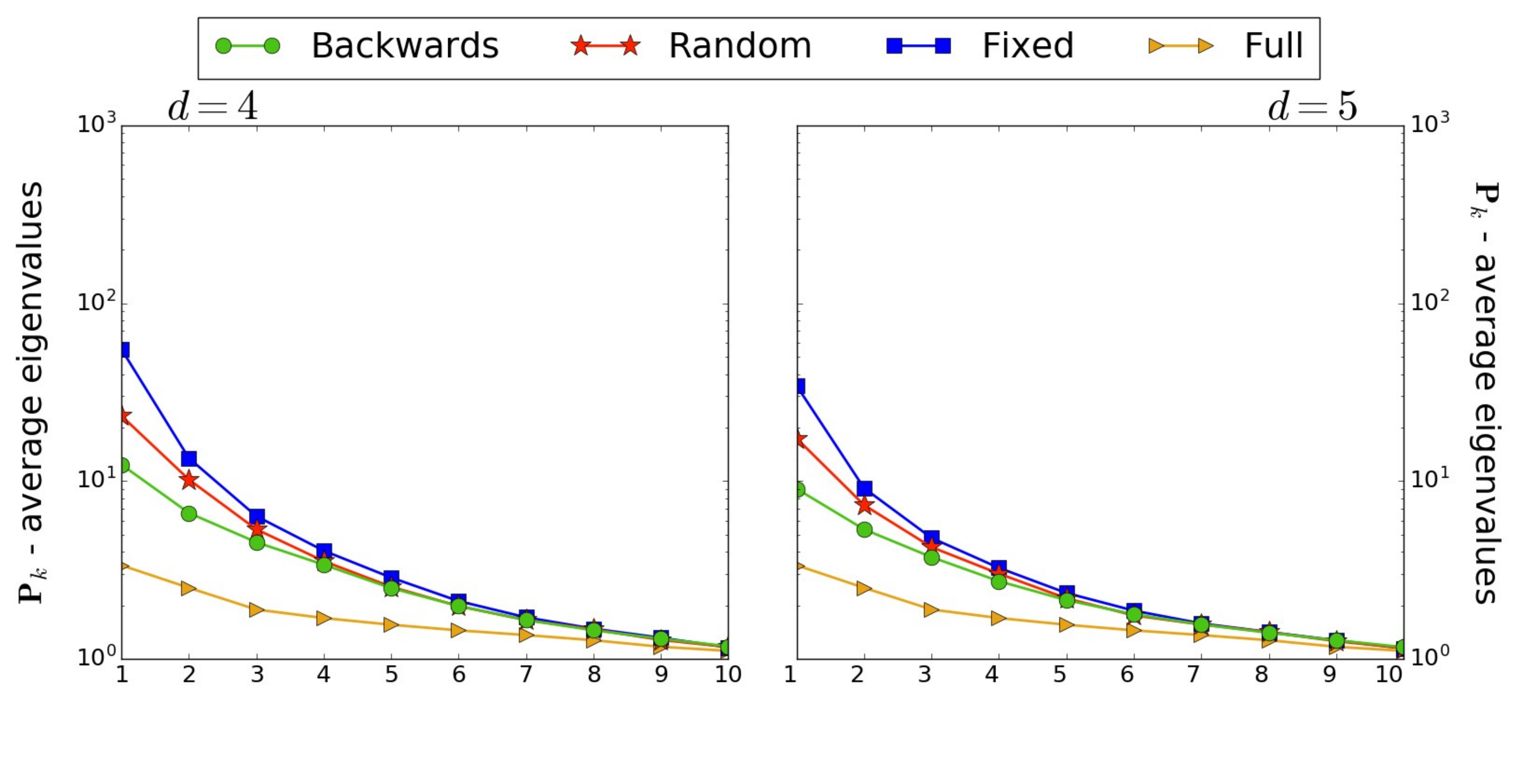
Dynamically selected observations

- Observations should minimize the forecast uncertainty given a fixed dimension of the observational space $d \ll n$.
- For an **arbitrary, linear observation operator** we take the QR factorization of the transpose

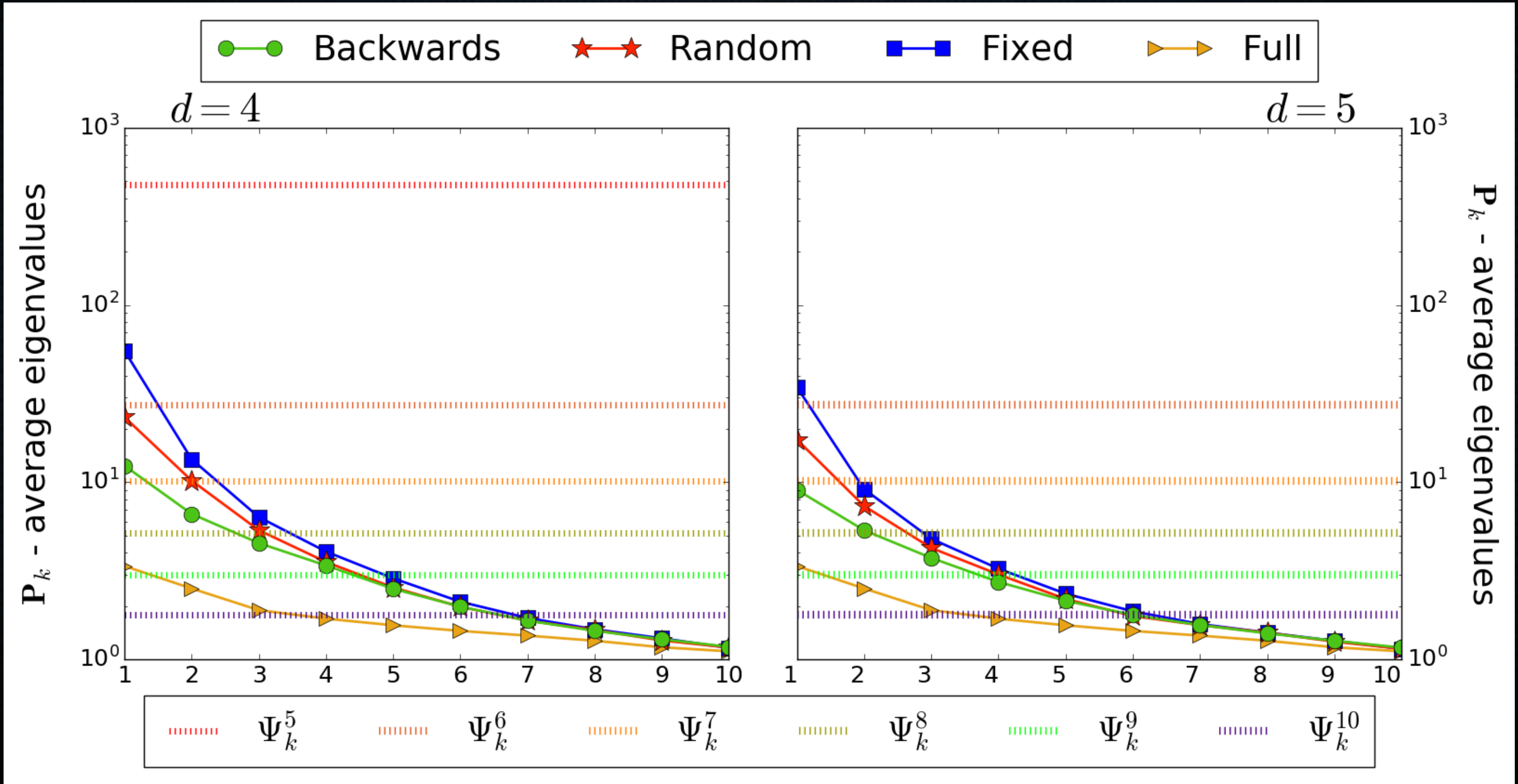
$$\mathbf{H}_k^{\mathrm{T}} = \mathbf{U}_k \mathbf{G}_k \quad \Rightarrow \quad \mathbf{H}_k = \mathbf{G}_k^{\mathrm{T}} \mathbf{U}_k^{\mathrm{T}}$$

- This is the choice of an **optimal subspace** representation of the uncertainty, given by the span of the columns of $\mathbf{U}_k$.
- In **perfect models**, we know this is the span of the **unstable and neutral backwards** Lyapunov vectors [Bocquet et al. 2017]. Our work verifies the dynamic observation paradigm utilizing bred vectors in AUS [Carrassi et al. 2008].

Dynamic observations and the forecast covariance



The unconstrained stable forecast



Conclusion

- AUS methodology can be used for reduced rank square root filters in the presence of model error, following this framework:
  - Dynamically observe the **unstable, neutral and weakly stable** modes.
  - Corrections to the state estimate should account for the growth of error in all of the above directions.
  - Observations in this space should should satisfy a minimum precision:

$$\alpha > e^{2\lambda_1} - 1$$

  - Unfiltered error in stable modes is bounded by the freely evolved uncertainty, and can be estimated offline.
- Implementing the above framework is ongoing work.

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