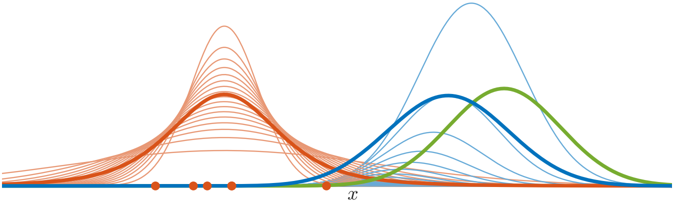
Adaptive covariance inflation in the EnKF by Gaussian scale mixtures



Patrick N. Raanes, Marc Bocquet, Alberto Carrassi

patrick.n.raanes@gmail.com

EnKF Workshop, Bergen, May 2018

Questions ∼answered in paper

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  - Why and how?
  - Can it be dissociated from **non-Gaussianity**?
- Does the **inherent bias** $\left(\mathbb{E}[\mathrm{tr}(\bar{\mathbf{P}}^a)] < \mathrm{tr}(\mathbf{P}^a)\right)$ cause
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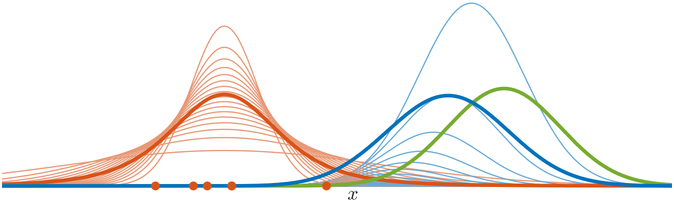

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Outline

- Idealistic contexts (with sampling error)
  - Revisiting the EnKF assumptions
    $\implies$ Gaussian scale mixture (EnKF-$\mathcal{N}$)
- With model error
  - Survey inflation estimation
    - ETKF-adaptive
    - EAKF-adaptive
  - EnKF-$\mathcal{N}$ hybrid
  - Benchmarks

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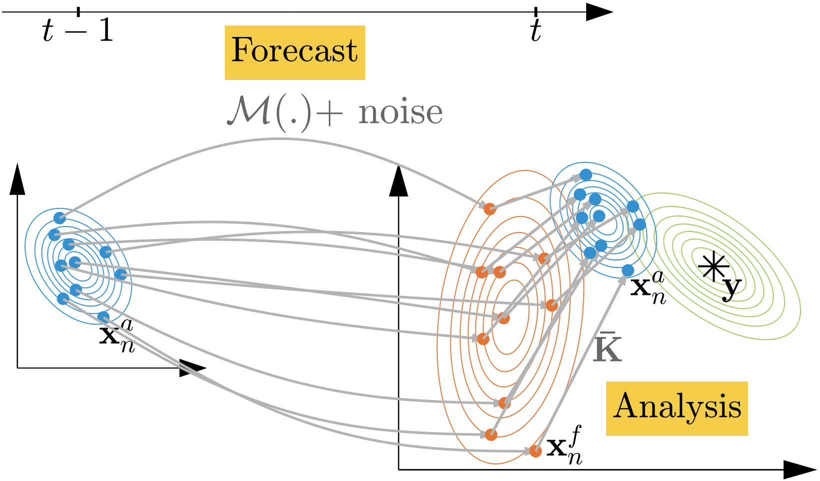
Idealistic contexts (EnKF-N)

Assume $\mathcal{M}, \mathcal{H}, \mathbf{Q}, \mathbf{R}$ are perfectly known,
and $p(\boldsymbol{x})$ and $p(\boldsymbol{y}|\boldsymbol{x})$ are always Gaussian.

EnKF



$t-1$
t
Forecast
$\mathcal{M}(.)+$ noise
$\mathbf{x}_n^a$
$\mathbf{x}_n^a$
$\mathbf{y}$
$\bar{\mathbf{K}}$
Analysis
$\mathbf{x}_n^f$

Revisiting EnKF assumptions

Denote $\boldsymbol{y}_{\text{prior}}$ all prior information on the "true" state, $\boldsymbol{x} \in \mathbb{R}^M$, and suppose that, with known mean ($\boldsymbol{b}$) and cov ($\mathbf{B}$),

$$p(\boldsymbol{x}|\boldsymbol{y}_{\text{prior}}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{b},\mathbf{B}) \,. \tag{1}$$

Computational costs induce:

$$\approx p(\boldsymbol{x}|\mathbf{E}) = \mathcal{N}(\boldsymbol{x}|\boldsymbol{b},\mathbf{B})$$

$\Longrightarrow$ "true" moments, $\boldsymbol{b}$ and $\mathbf{B}$, are unknowns,
to be estimated from $\mathbf{E}$.

Ensemble $\mathbf{E} = \begin{bmatrix} \boldsymbol{x}_1, & \ldots & \boldsymbol{x}_n, & \ldots & \boldsymbol{x}_N \end{bmatrix}$ *also* from (1) and iid.

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$$\approx p(x|\mathbf{E}) = \mathcal{N}(x|b, \mathbf{B})$$

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EnKF prior

But

$$p(\boldsymbol{x}|\mathbf{E}) = \int_{\mathcal{B}} \int_{\mathbb{R}^M} \mathcal{N}(\boldsymbol{x}|\boldsymbol{b}, \mathbf{B})\, p(\boldsymbol{b}, \mathbf{B}|\mathbf{E})\, \mathrm{d}\boldsymbol{b}\, \mathrm{d}\mathbf{B} \tag{2}$$

Recover standard EnKF by assuming $N=\infty$ so that

$$p(\boldsymbol{b}, \mathbf{B}|\mathbf{E}) = \delta(\boldsymbol{b} - \bar{\boldsymbol{x}})\delta(\mathbf{B} - \bar{\mathbf{B}}) \,,$$

where

$$\bar{\boldsymbol{x}} = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}_n \,, \qquad \bar{\mathbf{B}} = \frac{1}{N-1}\sum_{n=1}^{N} (\boldsymbol{x}_n - \bar{\boldsymbol{x}})(\boldsymbol{x}_n - \bar{\boldsymbol{x}})^{\mathsf{T}} \,. \tag{3}$$

The EnKF-N does not make this approximation.

EnKF prior

But

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EnKF-N via scale mixture

$$\text{Prior:} \quad p(\boldsymbol{x}|\mathbf{E}) = \iint \mathcal{N}(\boldsymbol{x}|\boldsymbol{b}, \mathbf{B})\, p(\boldsymbol{b}, \mathbf{B}|\mathbf{E})\, \mathrm{d}\boldsymbol{b}\, \mathrm{d}\mathbf{B} \tag{4}$$

(5)

(6)

(8)

EnKF-N via scale mixture

$$\text{Prior:} \quad p(\boldsymbol{x}|\mathbf{E}) = \iint \mathcal{N}(\boldsymbol{x}|\boldsymbol{b}, \mathbf{B})\, p(\boldsymbol{b}, \mathbf{B}|\mathbf{E})\, \mathrm{d}\boldsymbol{b}\, \mathrm{d}\mathbf{B} \tag{4}$$

$$\vdots$$

$$\vdots$$

$$\tag{5}$$

$$\vdots$$

$$\vdots \tag{6}$$

$$\vdots$$

$$\propto \left(1 + \tfrac{1}{N-1} \|\boldsymbol{x} - \bar{\boldsymbol{x}}\|^2_{\varepsilon_N \bar{\mathbf{B}}}\right)^{-N/2} \tag{7}$$

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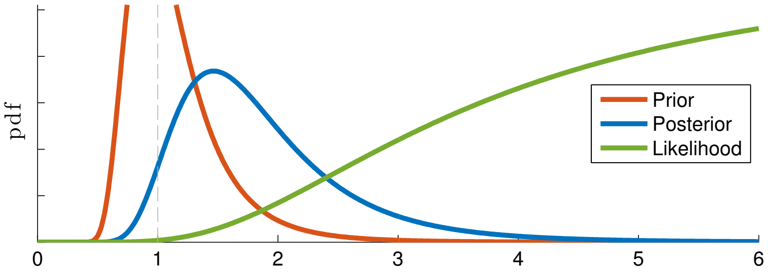
Mixing distributions – $p(\alpha|\ldots)$



Prior: $$p(\alpha|\mathbf{E}) = \chi^{-2}(\alpha|1, N-1)$$

Likelihood: $$p(\boldsymbol{x}_\star, \boldsymbol{y}|\alpha, \mathbf{E}) \propto \exp\left(-\frac{1}{2}\|\boldsymbol{y}-\mathbf{H}\bar{\boldsymbol{x}}\|^2_{\alpha\varepsilon_N \mathbf{H}\bar{\mathbf{B}}\mathbf{H}^\mathsf{T}+\mathbf{R}}\right)$$

$\Longrightarrow$ Posterior: $$p(\boldsymbol{x}_\star, \alpha|\boldsymbol{y}, \mathbf{E}) \propto \exp\left(-\frac{1}{2}\, D(\alpha)\right)$$

Summary – Perfect model scenario

- Even with a perfect model, Gaussian forecasts, and a deterministic EnKF, "sampling error" arises for $N < \infty$ due to nonlinearity, and inflation is necessary.
- Not assuming $\bar{\mathbf{B}} = \mathbf{B}$ as in the EnKF leads to a Gaussian scale mixture.
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With model error

Because all models are wrong.

Fundamentals

- Suppose $\boldsymbol{x}_n \sim \mathcal{N}(\boldsymbol{b}, \mathbf{B}/\beta)$, and $N = \infty$.
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$$\begin{aligned} p(\boldsymbol{y}|\beta) &= \mathcal{N}\left(\boldsymbol{y} \,|\, \mathbf{H}\bar{\boldsymbol{x}}, \bar{\mathbf{C}}(\beta)\right) , \\ \text{where} \quad \bar{\mathbf{C}}(\beta) &= \beta\mathbf{H}\bar{\mathbf{B}}\mathbf{H}^{\mathsf{T}} + \mathbf{R} , \end{aligned} \tag{10}$$

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ETKF adaptive inflation

- Again,

$$p(y|\beta) = \mathcal{N}\left(\bar{\delta} \,\middle|\, 0, \bar{\mathbf{C}}(\beta)\right), \tag{11}$$

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Renouncing Gaussianity

- Assume $\mathbf{H}\bar{\mathbf{B}}\mathbf{H}^\mathsf{T} \propto \mathbf{R}$.
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- Likelihood (14) conjugate to $p(\beta) = \chi^{-2}(\beta|\beta^{\mathsf{f}}, \nu^{\mathsf{f}})$, yielding

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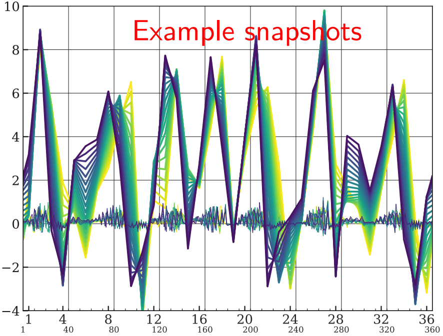
Two-layer Lorenz-96

Evolution

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \psi_i^+(\boldsymbol{x}) + F - h\frac{c}{b}\sum_{j=1}^{10} z_{j+10(i-1)}\,, \qquad i = 1, \ldots, 36,$$

$$\frac{\mathrm{d}z_j}{\mathrm{d}t} = \frac{c}{b}\psi_j^-(b\boldsymbol{z}) + 0 + h\frac{c}{b}x_{1+(j-1)//10}\,, \qquad j = 1, \ldots, 360,$$

where ψ_i is the single-layer Lorenz-96 dynamics.



$$\mathrm{RMSE} = \frac{1}{T}\sum_{t=1}^{T}\sqrt{\frac{1}{M}\|\bar{x}_t - x_t\|_2^2}\,.$$

$N = 20$, no localization.

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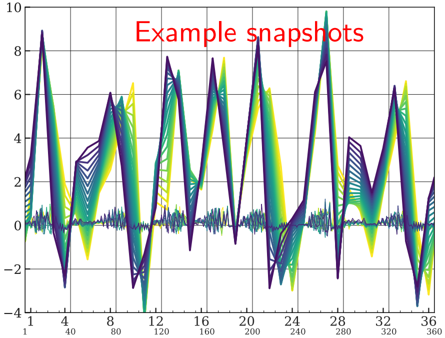

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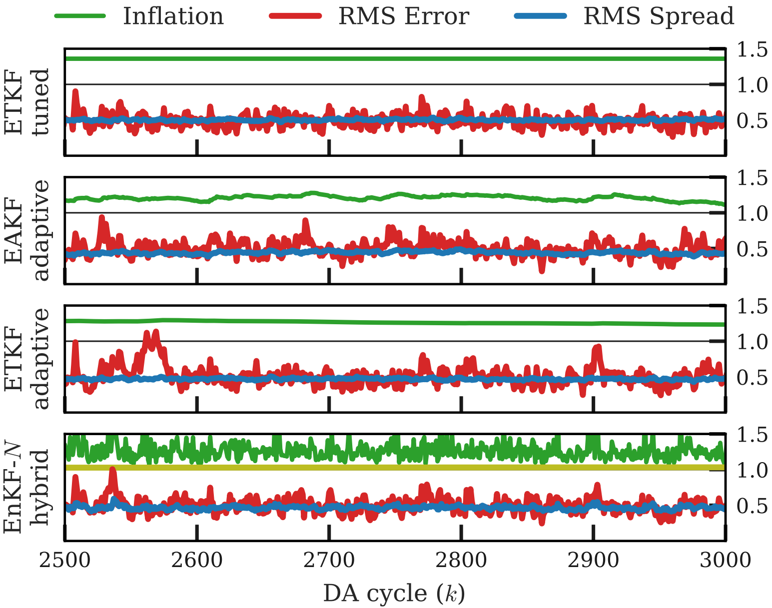
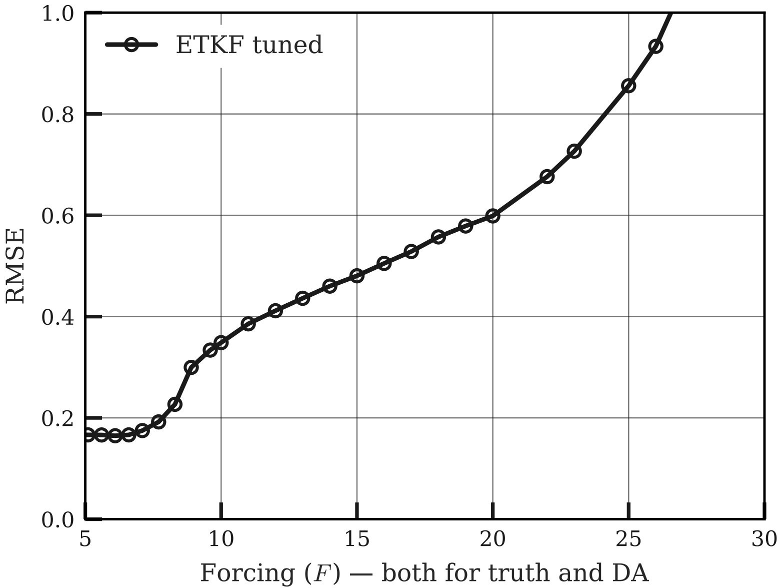
Illustration of time series



Benchmarks



ETKF tuned
RMSE
Forcing (F) — both for truth and DA
1.0
0.8
0.6
0.4
0.2
0.0
5
10
15
20
25
30

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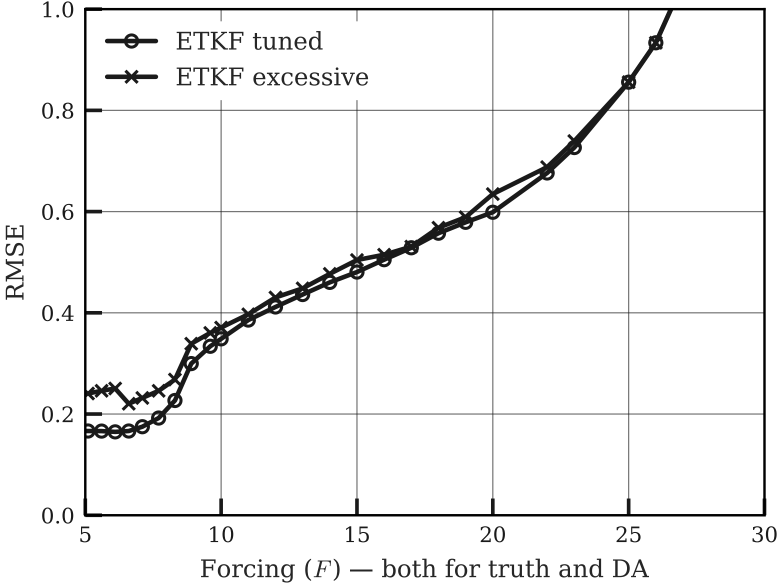

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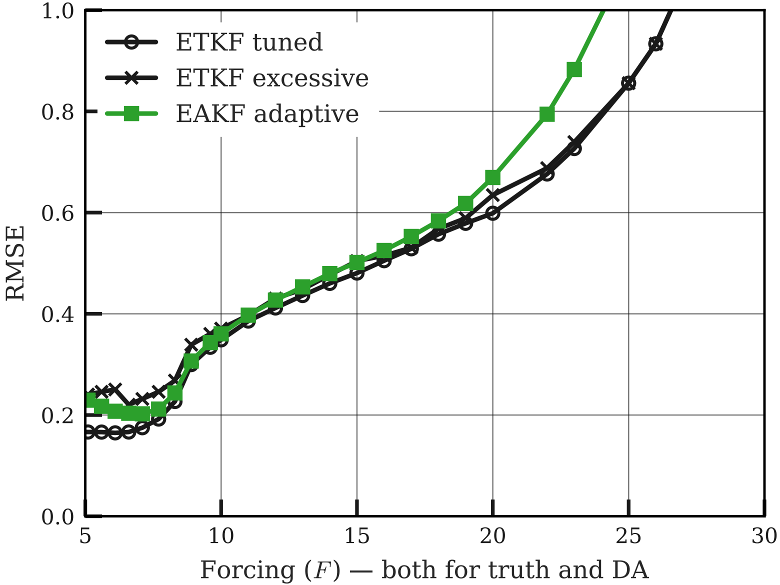

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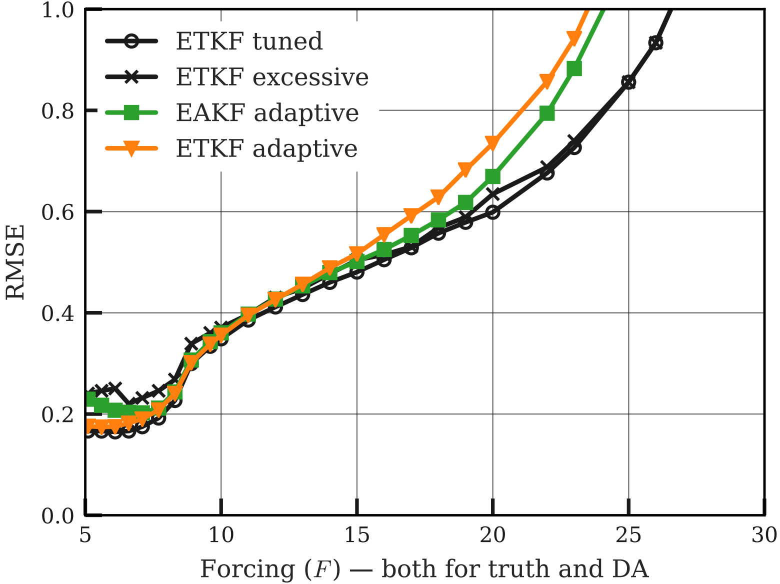
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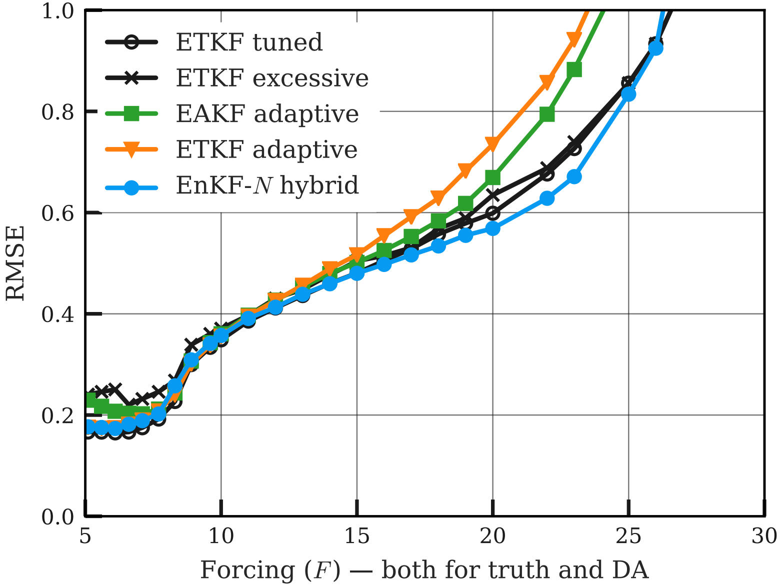

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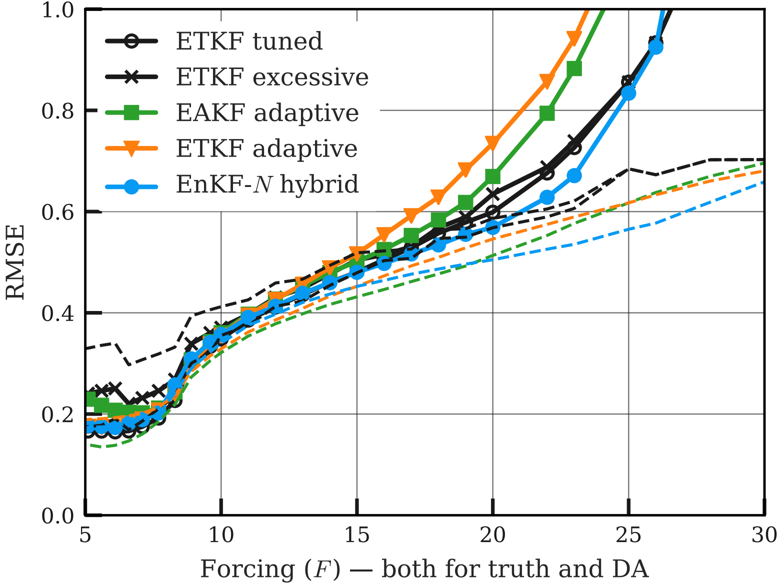

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Paper highlights:

- Cataloguing of **reasons to inflate**.
- **Inflation-centric** re-derivation of the dual **EnKF-N**.
- Formal **survey of adaptive inflation** methods.
- A simple **hybrid of EnKF-N and $\hat{\beta}_{\mathrm{R}}$**, which is shown to systematically (but moderately) improve filter accuracy (no re-tuning!).

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References 1

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- 2012: **Marc Bocquet and Pavel Sakov.** *Combining inflation-free and iterative ensemble Kalman filters for strongly nonlinear systems*. Nonlinear Processes in Geophysics
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- 2018: **Patrick N. Raanes, Marc Bocquet, and Alberto Carrassi.** *Adaptive covariance inflation in the ensemble Kalman filter by Gaussian scale mixtures*. QJRMS (minor rev), `arxiv.org/abs/1801.08474`

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UKF reinventing localization

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Multiple Sigma-point Kalman Smoothers for High-dimensional State-Space Models

Jordi Vilà-Valls*, Pau Closas†, Ángel F. García-Fernández‡ and Carles Fernández-Prades*
*Centre Tecnològic de Telecomunicacions de Catalunya (CTTC/CERCA), 08860, Barcelona, Spain
†Dept. of Electrical and Computer Eng., Northeastern University, Boston, MA 02115, USA
‡ Department of Electrical Engineering and Electronics, University of Liverpool, Liverpool, UK.
E-mail: {jvila,cfernandez}@cttc.cat, closas@northeastern.edu, angel.garcia-fernandez@liverpool.ac.uk

***Abstract*—This article presents a new multiple state-partitioning solution to the Bayesian smoothing problem in nonlinear high-dimensional Gaussian systems. The key idea is to partition the original state into several low-dimensional subspaces, and apply an individual smoother to each of them. The main goal is to reduce the state dimension each filter has to explore, to reduce the curse of dimensionality and eventual loss of accuracy. We provide the theoretical multiple smoothing formulation and a new nested sigma-point approximation to the resulting smoothing solution. The performance of the new approach is shown for the 40-dimensional Lorenz model.**

I. Introduction

In general, we are interested in nonlinear Gaussian state-space models (SSM), which are expressed as

$$\mathbf{x}_k = \mathbf{f}_{k-1}(\mathbf{x}_{k-1}) + \mathbf{v}_{k-1} \,, \qquad \mathbf{v}_{k-1} \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}_{k-1}), \tag{1}$$

$$\mathbf{y}_k = \mathbf{h}_k(\mathbf{x}_k) + \mathbf{n}_k \,, \qquad \mathbf{n}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{R}_k), \tag{2}$$

where $\mathbf{x}_k \in \mathbb{R}^{n_x}$ are the hidden states of the system, $\mathbf{y}_k \in \mathbb{R}^{n_y}$ the measurements at time k, $\mathbf{f}_{k-1}(\cdot)$ and $\mathbf{h}_k(\cdot)$ are the nonlinear process and measurement functions, and both Gaussian noises are assumed to be independent. The Bayesian smoothing solution is given by the marginal distri-

with $\mathbf{x}_k = [\mathbf{x}_k^{(1)}, \ldots, \mathbf{x}_k^{(S)}]$. The subspace process functions $\mathbf{f}_{k-1}^{(s)}(\cdot)$ can be different and the independent s-th subspace Gaussian process noise is $\mathbf{v}_{k-1}^{(s)} \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}_{k-1}^{(s)})$. The main idea is to partition the original state in several subspaces, and apply a low dimensional individual filter to each subspace, directly reducing the dimension each filter must explore. In this approach, we are interested in the subspace marginal smoothed posterior, $p(\mathbf{x}_k^{(s)}|\mathbf{y}_{1:N})$. In the multiple state-partioning framework, we make the approximation that the different subspaces are independent, which is typically accurate in applications such as multiple target tracking. Mathematically, this implies that the joint smoothing posterior is $p(\mathbf{x}_k^{(s)}, \mathbf{x}_k^{(-s)}|\mathbf{y}_{1:N}) \approx p(\mathbf{x}_k^{(s)}|\mathbf{y}_{1:N})p(\mathbf{x}_k^{(-s)}|\mathbf{y}_{1:N})$. In this contribution we extend previous results on MQKF [11] to the smoothing problem, and propose a new nested sigma-point approximation to the smoothing marginal posterior integrals.

II. Multiple Gaussian Smoothing

A. Background on Multiple Gaussian Filtering

As done in standard Bayesian filtering, the s-th subspace posterior can be recursively computed in two steps: *prediction*

Appendix

Parametric distributions – Table

Table 2: Parametric probability distributions. As elsewhere in the paper, $\boldsymbol{b}, \boldsymbol{x} \in \mathbb{R}^M$, $\mathbf{B}, \mathbf{S} \in \mathcal{B}$, $s, \beta > 0$, and it is assumed that $\nu > M$. The constants are $c_\mathcal{N} = (2\pi)^{-M/2}$, $c_t = \frac{\Gamma(\frac{\nu+M}{2})}{(\pi\nu)^{M/2}\Gamma(\nu/2)}$, $c_\mathcal{W} = \frac{\nu^{\nu/2}}{2^{\nu M/2}\Gamma_M(\nu/2)}$, and $c_\chi = c_\mathcal{W}$ with $M = 1$. The (unlisted) variance of element (i,j) of $\mathbf{B}$ with the Wishart distribution is $(s_{ij}^2 + s_{ii}s_{jj})/\nu$, where s_{ij} is element (i,j) of $\mathbf{S}$. The variances of the inverse-Wishart distribution are asymptotically, for $\nu \to \infty$, the same.

Name	**Symbol**	**Probability density function**	**Mean**	**Mode**	**(Co)Var**
Gauss./Normal	$\mathcal{N}(\boldsymbol{x}\|\boldsymbol{b}, \mathbf{B})$	$= c_\mathcal{N} \|\mathbf{B}\|^{-1/2} \exp\left(-\frac{1}{2}\|\boldsymbol{x} - \boldsymbol{b}\|_\mathbf{B}^2\right)$	$\boldsymbol{b}$	$\boldsymbol{b}$	$\mathbf{B}$
t distribution	$\boldsymbol{t}(\boldsymbol{x}\|\nu; \boldsymbol{b}, \mathbf{B})$	$= c_t \|\mathbf{B}\|^{-1/2}\left(1 + \frac{1}{\nu}\|\boldsymbol{x} - \boldsymbol{b}\|_\mathbf{B}^2\right)^{-(\nu+M)/2}$	$\boldsymbol{b}$	$\boldsymbol{b}$	$\frac{\nu}{\nu-2}\mathbf{B}$
Wishart	$\mathcal{W}^{+1}(\mathbf{B}\|\mathbf{S}, \nu)$	$= c_\mathcal{W} \|\mathbf{S}\|^{-\nu/2} \|\mathbf{B}\|^{(\nu-M-1)/2} e^{-\operatorname{tr}(\nu\mathbf{B}\mathbf{S}^{-1})/2}$	$\mathbf{S}$	$\frac{\nu-M-1}{\nu}\mathbf{S}$	
Inv-Wishart	$\mathcal{W}^{-1}(\mathbf{B}\|\mathbf{S}, \nu)$	$= c_\mathcal{W} \|\mathbf{S}\|^{\nu/2} \|\mathbf{B}\|^{-(\nu+M+1)/2} e^{-\operatorname{tr}(\nu\mathbf{S}\mathbf{B}^{-1})/2}$	$\frac{\nu}{\nu-M-1}\mathbf{S}$	$\frac{\nu}{\nu+M+1}\mathbf{S}$	
Chi-square	$\chi^{+2}(\beta\|s, \nu)$	$= c_\chi\, s^{-\nu/2} \beta^{\nu/2-1} e^{-\nu\beta/2s}$	s	$\frac{\nu-2}{\nu}s$	$2s^2/\nu$
Inv-chi-sq.	$\chi^{-2}(\beta\|s, \nu)$	$= c_\chi\, s^{\nu/2} \beta^{-\nu/2-1} e^{-\nu s/2\beta}$	$\frac{\nu}{\nu-2}s$	$\frac{\nu}{\nu+2}s$	$\frac{2(\nu s)^2}{(\nu-2)^2(\nu-4)}$

Parametric distributions – Properties

Property 1 The ("scaled") chi-square distribution is equivalent to the Gamma distribution:

$$\chi^{\pm 2}(\beta|s,\nu) = \mathrm{Gamma}^{\pm 1}(\beta|\nu/2, \nu s^{\mp 1}/2)\,, \tag{70}$$

where the switch sign $\pm$ has been used to represent both the regular and inverse distributions. The χ parameterization has been preferred for the notational simplicity of the relations of Properties 2 to 4.

Property 2 Asymptotic normality. If $\beta \sim \chi^{\pm 2}(s,\nu)$, then the distribution of $\sqrt{\nu}(\beta - s)$ converges to $\mathcal{N}(0, 2s^2)$ as $\nu \to \infty$. This shows that s is a location parameter, while $2s^2/\nu$ plays the role of variance, which is why this paper prefers referring to ν as "certainty" instead of "degree of freedom". The asymptotic result for χ^{+2} is a well known consequence of the central limit theorem, since β may then be written as an average of random variables. The result for χ^{-2} is less known, but can be shown by through the pointwise convergence of the pdf of $\sqrt{\nu}(\beta - s)$, normalized by its value at 0.

Property 3 In the univariate case ($M = 1$),

$$\mathcal{W}^{\pm 1}(\beta|s,\nu) = \chi^{\pm 2}(\beta|s,\nu)\,. \tag{71}$$

Property 4 Reciprocity. If $t = 1/\beta$:

$$\begin{aligned} p(\beta) &= \chi^{-2}(\beta|s,\nu) \\ \iff p(t) &= \chi^{+2}(t|1/s,\nu)\,. \end{aligned} \tag{72}$$

Property 5 Reciprocity. If $\mathbf{T} = \mathbf{B}^{-1}$:

$$\begin{aligned} p(\mathbf{B}) &= \mathcal{W}^{-1}(\mathbf{B}|\mathbf{S},\nu) \\ \iff p(\mathbf{T}) &= \mathcal{W}^{+1}(\mathbf{T}|\mathbf{S}^{-1},\nu)\,, \end{aligned} \tag{73}$$

as follows by the change of variables and the Jacobian $|\mathbf{T}|^{-(M+1)}$ [Muirhead, 1982, §. 2.1].

Property 6 Let $\boldsymbol{u} \neq \mathbf{0}$ be any m-dimensional vector, or an (almost never zero) random vector. If $\mathbf{T} \sim \mathcal{W}^{+1}(\mathbf{S},\nu)$ is independent of $\boldsymbol{u}$, then

$$\frac{\boldsymbol{u}^\mathsf{T}\mathbf{T}\boldsymbol{u}}{\boldsymbol{u}^\mathsf{T}\mathbf{S}\boldsymbol{u}} \sim \chi^{+2}(1,\nu)\,. \tag{74}$$

Moreover, this statistic is also independent of $\boldsymbol{u}$. Proof: Theorem 3.2.8 of Muirhead [1982].

EnKF-N mixing distribution

Instead, we assign the Jeffreys (hyper)prior:

$$p(\boldsymbol{b}, \mathbf{B}) \propto p(\mathbf{B}) \propto |\mathbf{B}|^{-(M+1)/2} \,, \tag{19}$$

and recall the likelihood:

$$p(\mathbf{E}|\boldsymbol{b}, \mathbf{B}) \propto \prod_{n=1}^{N} \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{b}, \mathbf{B}) \,, \tag{20}$$

yielding

$$p(\boldsymbol{b}, \mathbf{B}|\mathbf{E}) = \underbrace{\mathcal{N}(\boldsymbol{b}|\bar{\boldsymbol{x}}, \mathbf{B}/N)}_{p(\boldsymbol{b}|\mathbf{B},\mathbf{E})} \underbrace{\mathcal{W}^{-1}(\mathbf{B}|\bar{\mathbf{B}}, N-1)}_{p(\mathbf{B}|\mathbf{E})} \,, \tag{21}$$

where $\mathcal{W}^{-1}$ is the inverse-Wishart distribution (c.f. Table 2).

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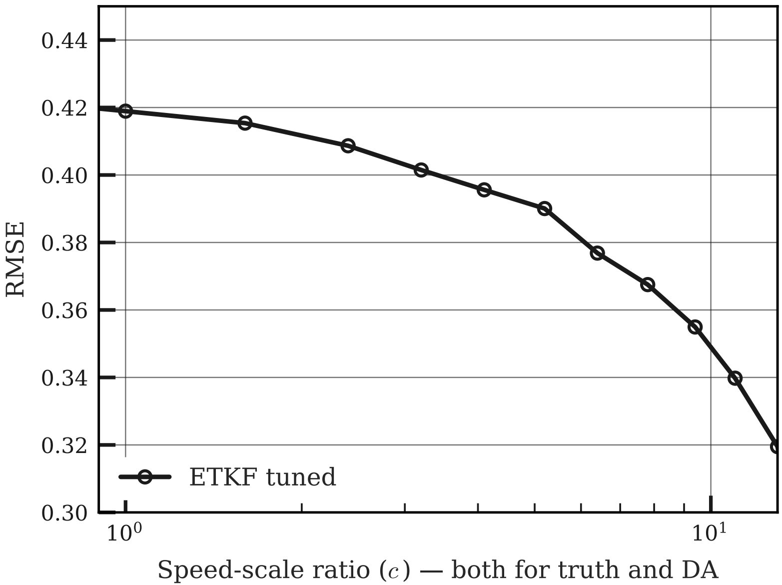
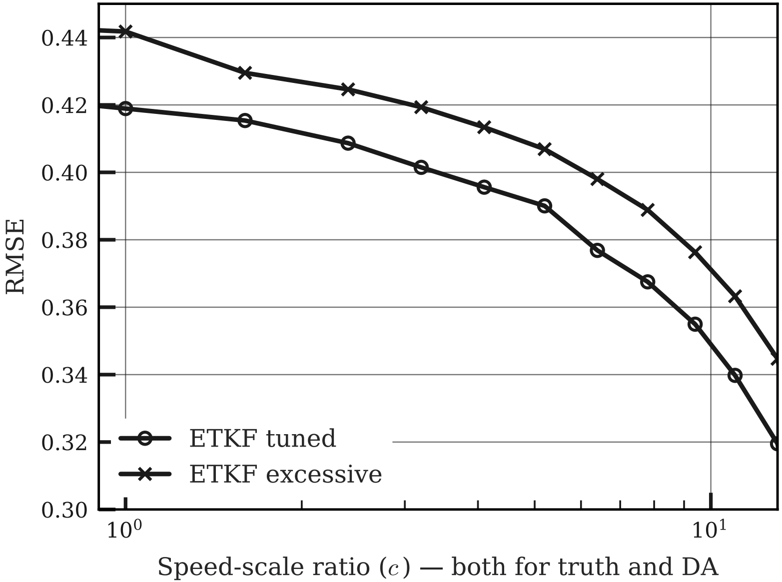
Benchmarks



RMSE
0.44
0.42
0.40
0.38
0.36
0.34
0.32
0.30
10^0
10^1
ETKF tuned
Speed-scale ratio (c) — both for truth and DA

Benchmarks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0.32
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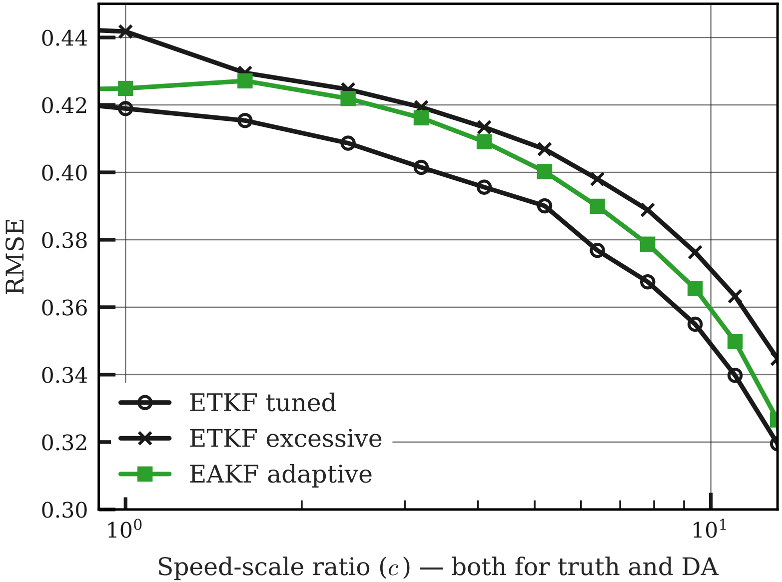
RMSE
ETKF tuned
ETKF excessive
10^0
10^1
Speed-scale ratio (c) — both for truth and DA

Benchmarks



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RMSE
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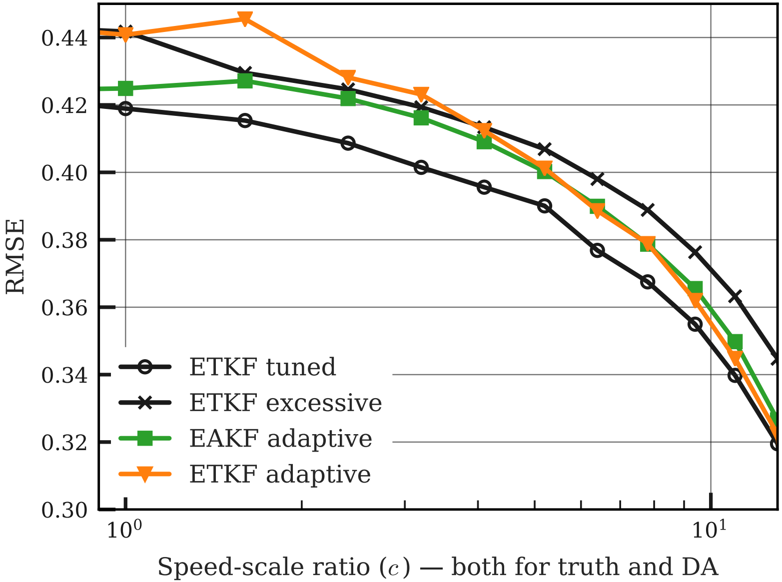
ETKF tuned
ETKF excessive
EAKF adaptive

Benchmarks



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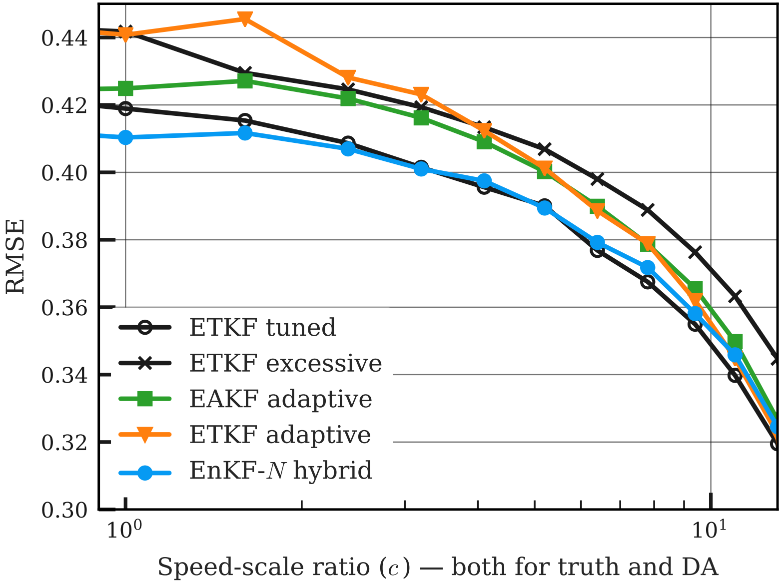
Benchmarks



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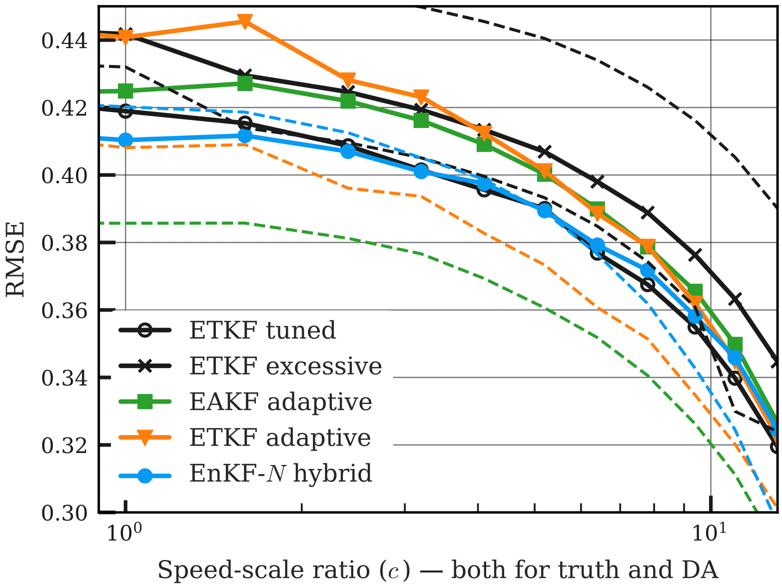
EnKF-N hybrid

Benchmarks



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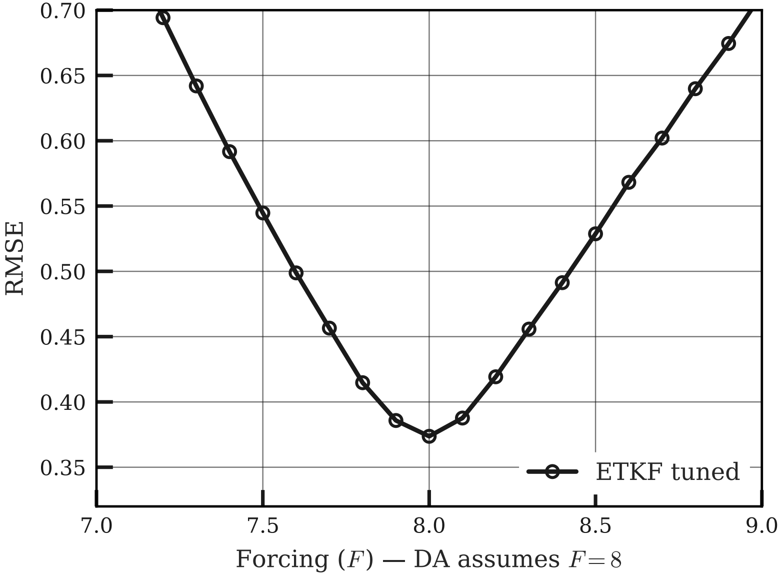
Benchmarks (single-layer)



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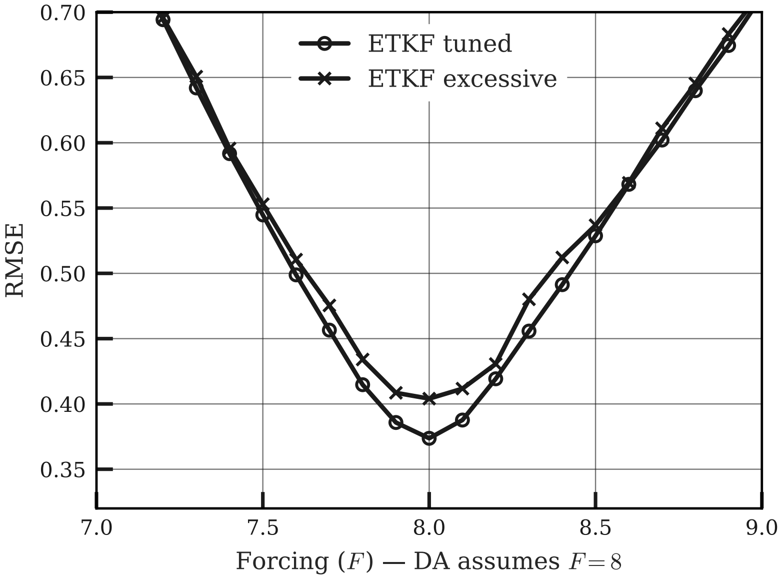

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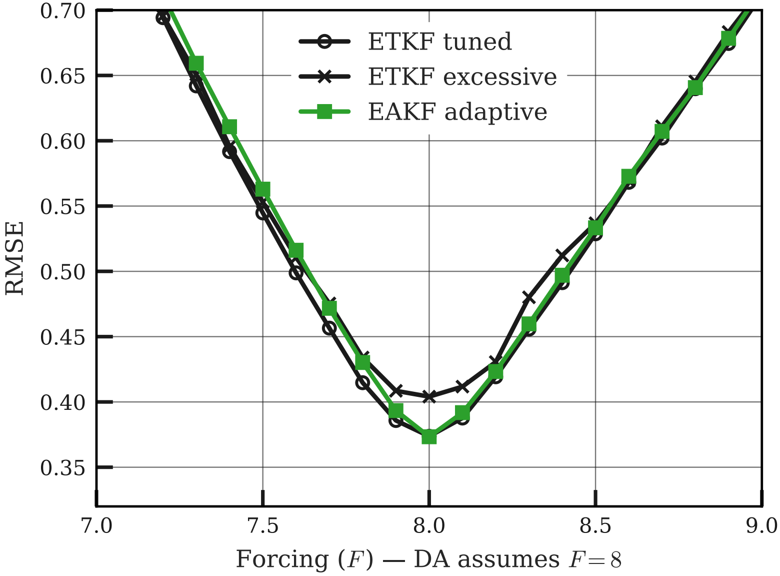

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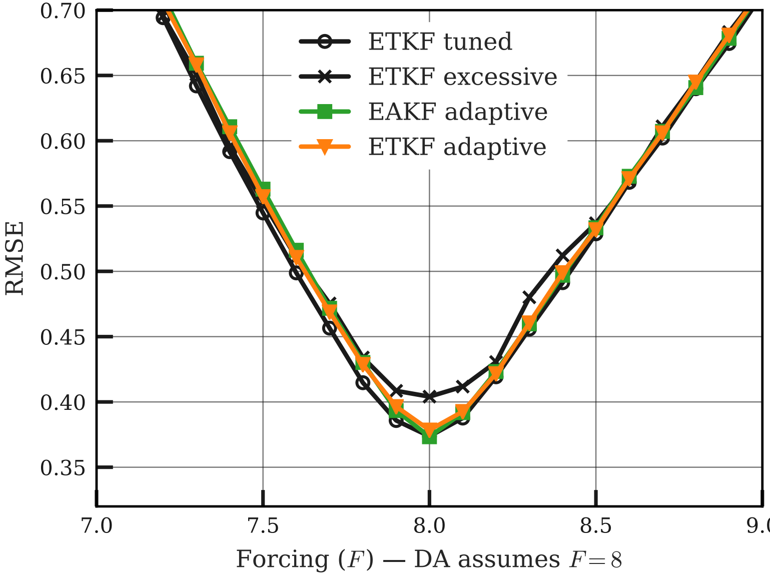

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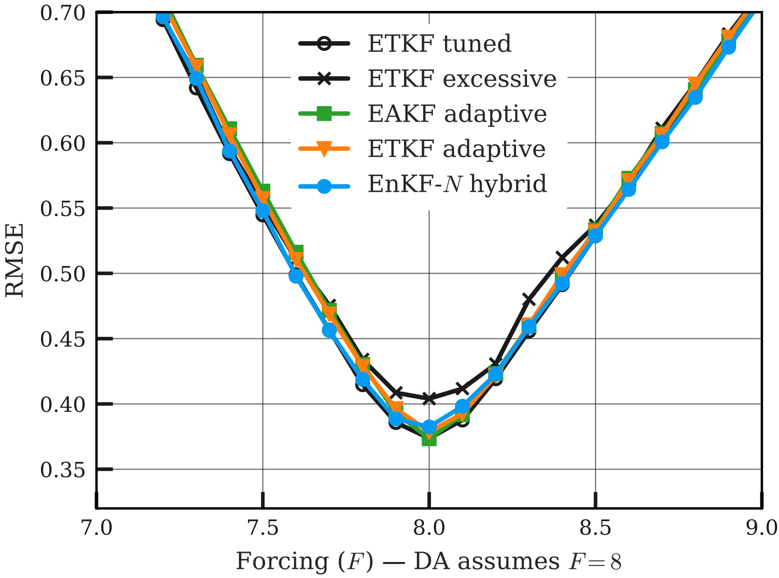

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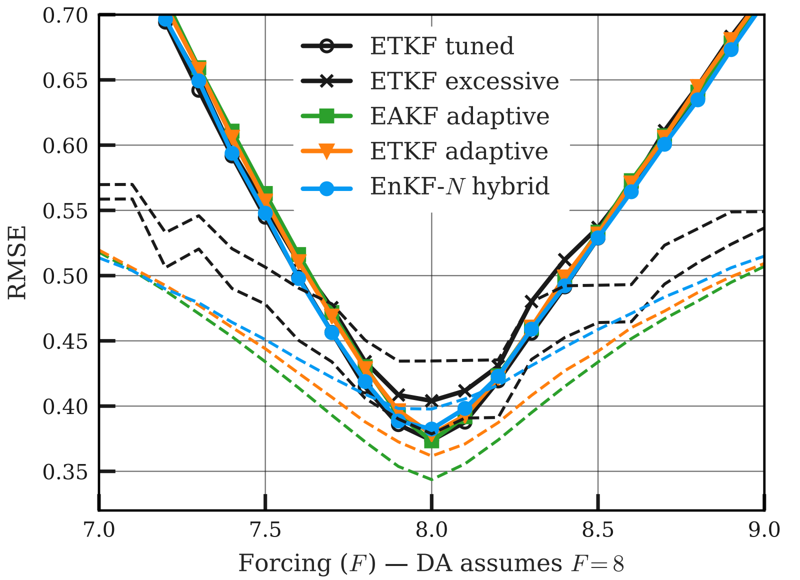
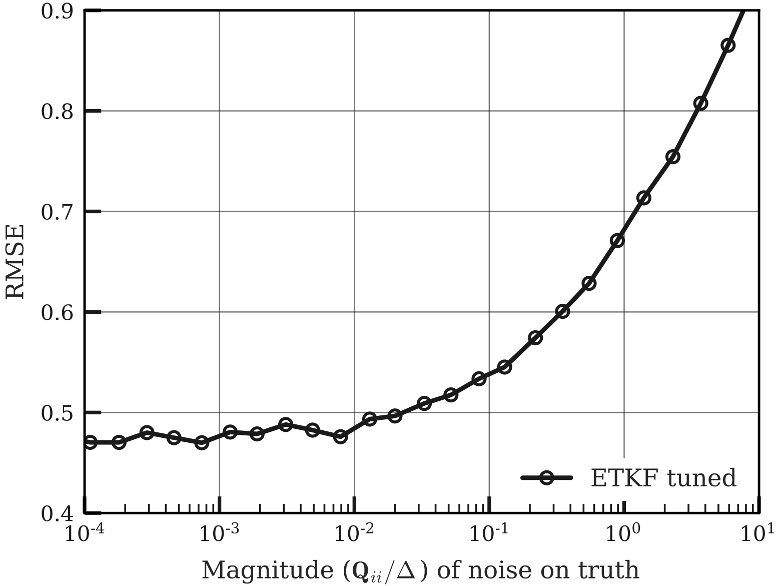


Benchmarks (Lorenz-63) – $N = 3$



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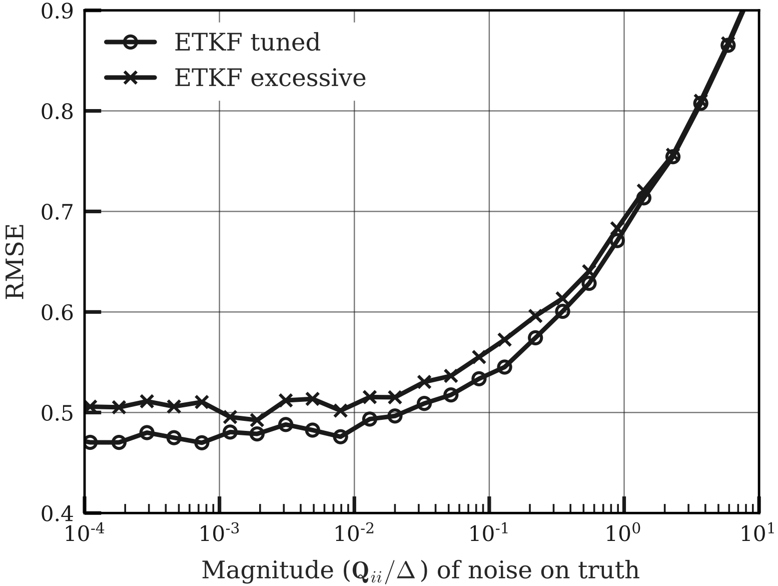

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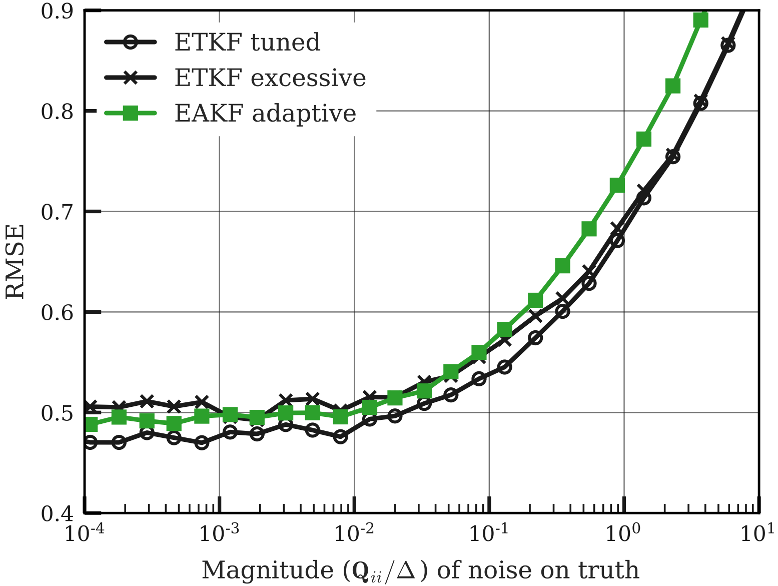

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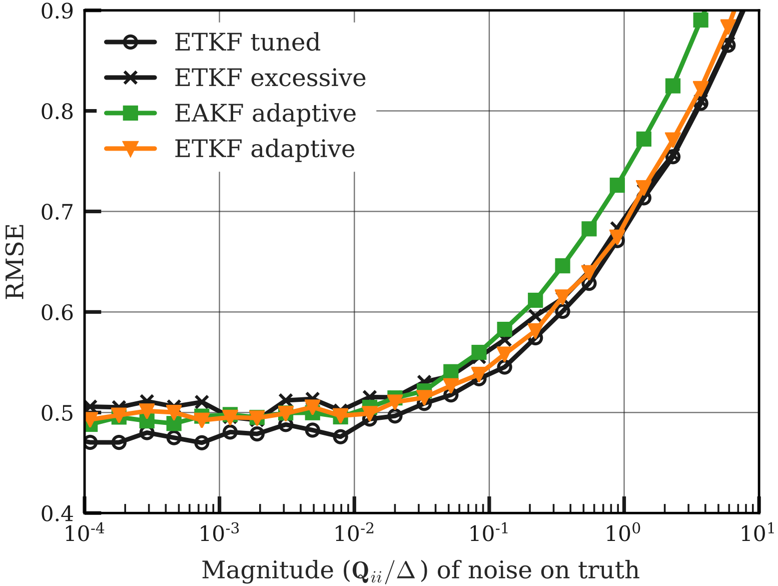

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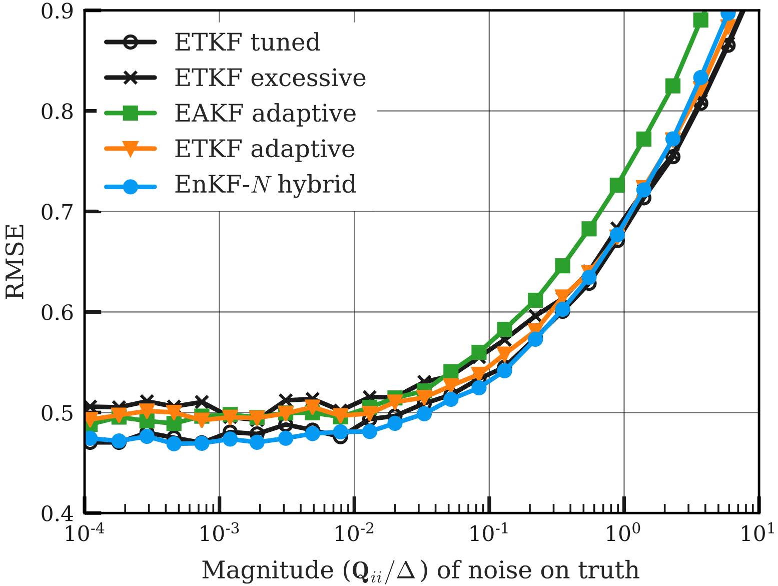

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