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SFB 1114

Scaling Cascades in Complex Systems

Nonlinear data assimilation via hybrid particle-Kalman filters and optimal coupling

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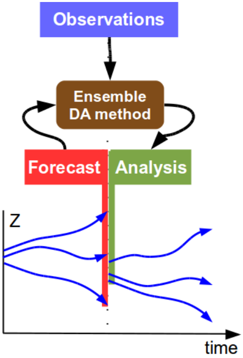


Traditional approaches

- Ensemble Kalman Filters
  - + Robust and moderately affordable
  - − Biased for non-Gaussian PDFs
- Traditional Particle Filters
  - + Non-Gaussianity properly handled
  - − Liable to the "Curse of Dimensionality"

Some recent developments

- Localized particle filters [Lei and Bickel, 2011][Poterjoy, 2015]
- Hybrid Kalman-particle filters [Frei and Künsch, 2013][Chustagulprom et al., 2016]
- Optimal transportation based particle filters [Reich, 2013]
- Intrinsic Dimension [Agapiou et al, arXiv:1511.06196]

Outline

Motivation

Linear Ensemble Transform Filters

Hybrid Ensemble Transform Filter

Single one-dimensional DA step

Non-spatially extended dynamical systems

Spatially extended systems

Conclusions and Prospect

- Forecast and Analysis ensembles:

$$z_i^{\mathrm{f}}, z_i^{\mathrm{a}}, \qquad i = 1, \ldots, M$$

- Update step via a General linear transformation [Reich and Cotter, 2015]

$$z_j^{\mathrm{a}} = \sum_{i=1}^{M} z_i^{\mathrm{f}} d_{ij}$$

- Transform coefficients satisfy

$$\sum_{i=1}^{M} d_{ij} = 1$$

$$\sum_{j=1}^{M} d_{ij} = M w_i$$

ESRF as a LETF:

$$z_j^{\mathrm{a}} = \sum_{i=1}^{M} z_i^{\mathrm{f}} \hat{w}_i + \sum_{i=1}^{M} (z_i^{\mathrm{f}} - \bar{z}^{\mathrm{f}}) s_{ij} = \sum_{i=1}^{M} z_i^{\mathrm{f}} d_{ij}^{\mathrm{KF}}$$

- Transform coefficients:

$$d_{ij}^{\mathrm{KF}} = d_{ij}^{\mathrm{KF}}(\{z_l^{\mathrm{f}}\}, y_{\mathrm{obs}}) := s_{ij} + \hat{w}_i - \frac{1}{M},$$

- Square root matrix: $S = \{s_{ij}\}$

$$S = \left\{ I + \frac{1}{M-1} (HA^{\mathrm{f}})^{\mathrm{T}} R^{-1} HA^{\mathrm{f}} \right\}^{-1/2},$$

- ESRF “Weights”:

$$\hat{w}_i = \frac{1}{M} - \frac{1}{M-1} e_i^T S^2 (HA^{\mathrm{f}})^{\mathrm{T}} R^{-1} (H\bar{z}^{\mathrm{f}} - y_{\mathrm{obs}}), \qquad \sum_{i=1}^{M} \hat{w}_i = 1$$

Analysis Mean

$$\bar{z}^{\mathrm{a}} = \sum_{i=1}^{M} w_i z_i^{\mathrm{f}}, \quad w_i \sim \exp\left(-\frac{1}{2}(Hz_i^{\mathrm{f}} - y_{\mathrm{obs}})^{\mathrm{T}} R^{-1} (Hz_i^{\mathrm{f}} - y_{\mathrm{obs}})\right)$$

ETPF transform update $DF : \{d_{ij}^{\mathrm{PF}}\}$

$$z_j^{\mathrm{a}} = \sum_{i=1}^{M} z_i^{\mathrm{f}} d_{ij}^{\mathrm{PF}}$$

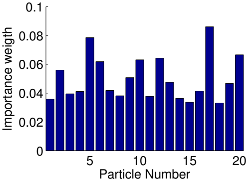
Transform constraints:

$$\sum_{i=1}^{M} d_{ij} = 1, \quad \sum_{j=1}^{M} d_{ij} = w_i M, \quad d_{ij} \geq 0,$$

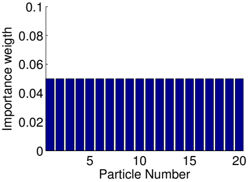
Minimal Transportation Cost:

$$D^{PF} = \arg\min\, J(D), \quad J(D) = \sum_{i,j=1}^{M} d_{ij} \|z_i^{\mathrm{f}} - z_j^{\mathrm{f}}\|^2$$

Optimal Transportation (OT) Problem



⇒ **Optimal Coupling** ⇒



Optimal transportation cost: min $J(D)$

- also known as Earth Mover distance
- takes into account shape of the PDFs

Optimal coupling: D^{PF}

- maximizes correlation between prior and posterior ensembles
- is deterministic, preserving the regularity of the state fields
- consistent with Bayes' formula [Reich 2013]
- convergence (regarding ensemble size) is faster than SIR-PFs at the cost of solving an optimal transportation problem

Exact solution

- Computational complexity $\mathcal{O}(M^3 \ln(M))$
- Efficient Earth Mover Distance algorithms available, e.g. FastEMD [Pele and Werman, 2009].

Entropic Regularized Approximation [Cuturi, 2013]

$$J(D) = \sum_{i,j=1}^{M} \left\{ d_{ij} \| z_i^{\mathrm{f}} - z_j^{\mathrm{f}} \|^2 + \frac{1}{\lambda} d_{ij} \ln d_{ij} \right\}$$

- Sinkhorn's fixed point iteration can be used.
- Computational complexity $\mathcal{O}(M^2 \cdot C(\lambda))$

1D Approximation(Each variable independently updated)

- OT problem reduces to reordering.
- Computational complexity $\mathcal{O}(M \ln(M))$
- No particle distance needed

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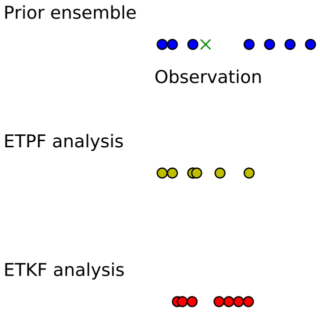
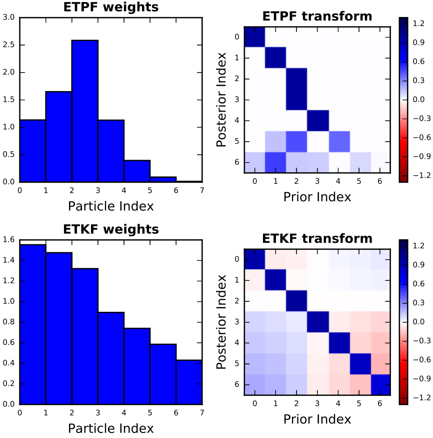
Observation within the convex hull





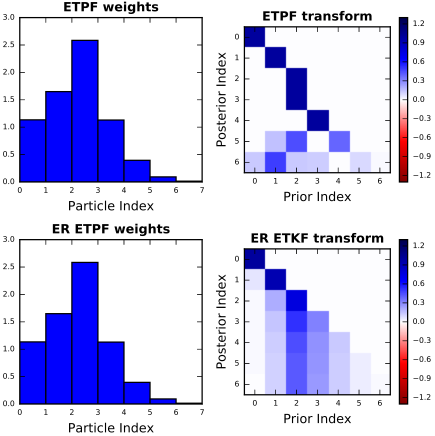
Observation within the convex hull

Prior ensemble

Observation

ETPF analysis

Entropic Reg. ETPF analysis



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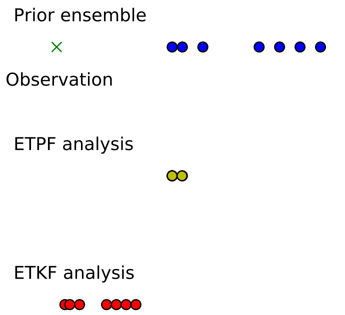
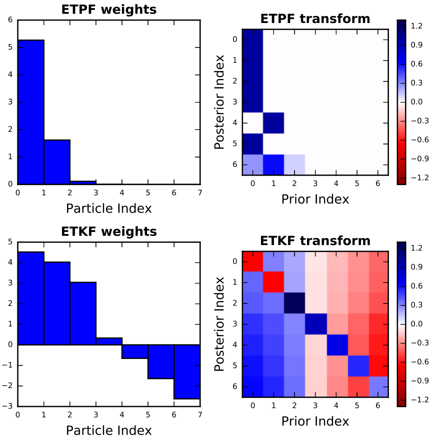
Observation outside the convex hull





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Likelihood splitting [Frei and Künsch, 2013]

$$\pi_Y(y_{\text{obs}}|z) \propto \exp\left(-\frac{1}{2}(\tilde{y}_z)^{\mathrm{T}}R^{-1}\tilde{y}_z\right), \quad \tilde{y}_z = Hz - y_{\text{obs}}$$

$$\propto \quad \exp\left(\alpha\left(-\frac{1}{2}(\tilde{y}_z)^{\mathrm{T}}R^{-1}\tilde{y}_z\right)\right) \quad \times \exp\left((1-\alpha)\left(-\frac{1}{2}(\tilde{y}_z)^{\mathrm{T}}R^{-1}\tilde{y}_z\right)\right)$$

$$\propto \quad \exp\left(-\frac{1}{2}(\tilde{y}_z)^{\mathrm{T}}\left(\frac{R}{\alpha}\right)^{-1}\tilde{y}_z\right) \quad \times \exp\left(-\frac{1}{2}(\tilde{y}_z)^{\mathrm{T}}\left(\frac{R}{1-\alpha}\right)^{-1}\tilde{y}_z\right)$$

$\Downarrow$ ETPF $\qquad$ $\Downarrow$ ESRF

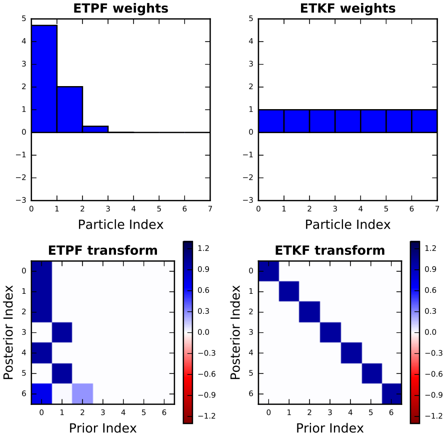
Bridging parameter extrems:

- $\alpha = 0 \Rightarrow$ Pure Kalman Filter
- $\alpha = 1 \Rightarrow$ Pure Particle Filter

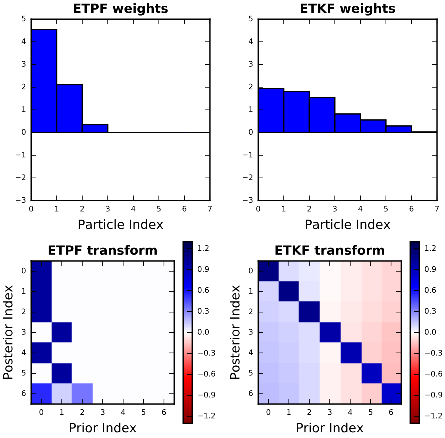
Models explored:

- Single DA step
- Lorenz 63
- Lorenz 96
- Lorenz 96 coupled to a wave equation
- Shallow water equations (2D)
- Modified shallow water equations (1D)

Bridging Parameter = 1

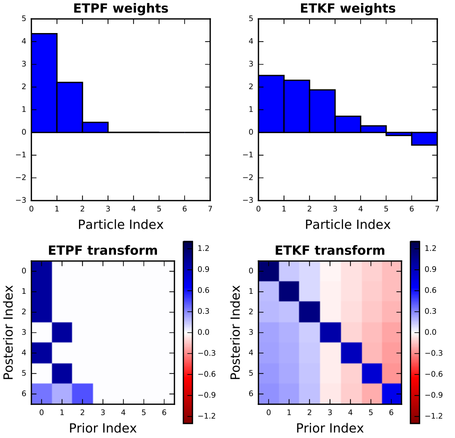


Bridging Parameter = 0.9



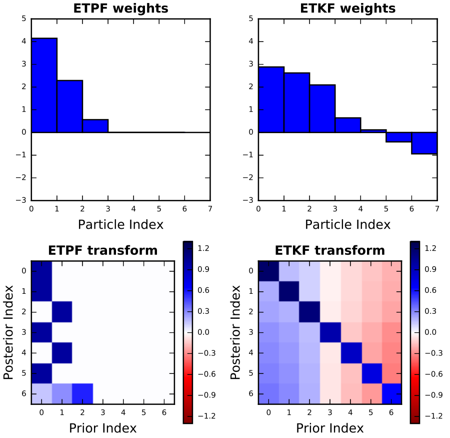
Single one-dimensional DA step

Bridging Parameter = 0.8

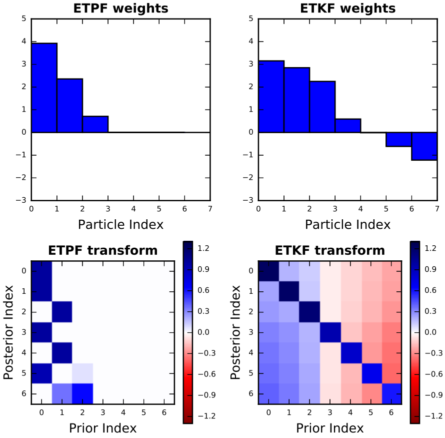


Single one-dimensional DA step

Bridging Parameter = 0.7

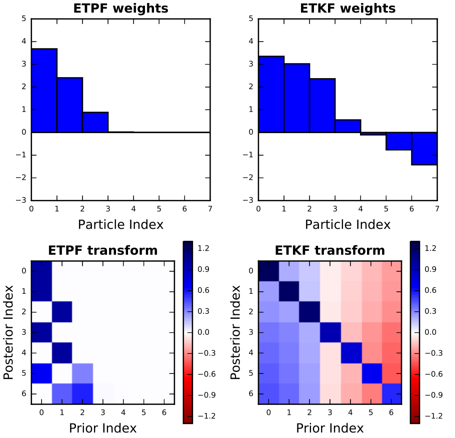


Bridging Parameter = 0.6

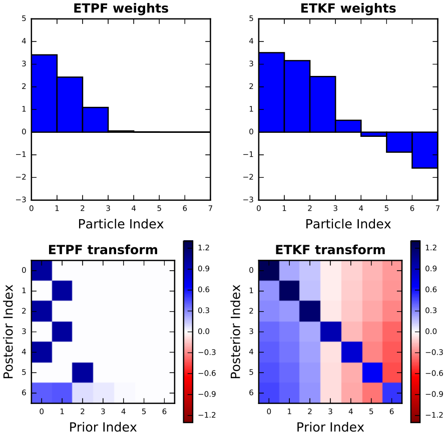


Single one-dimensional DA step

Bridging Parameter = 0.5

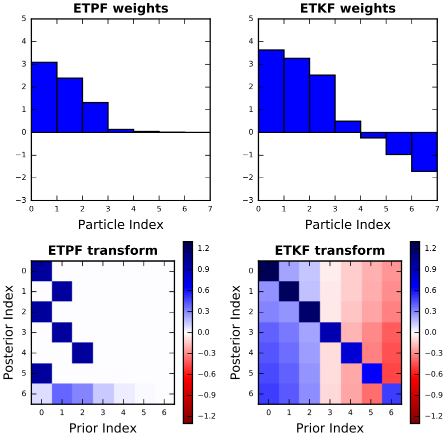


Bridging Parameter = 0.4

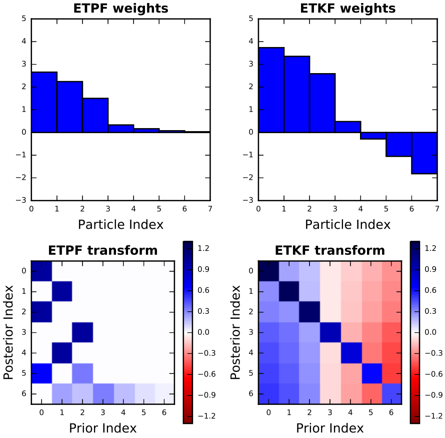


Single one-dimensional DA step

Bridging Parameter = 0.3

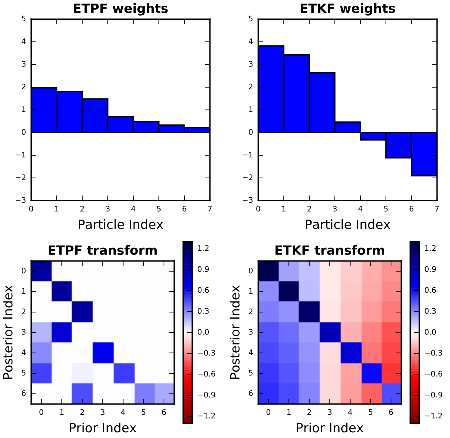


Bridging Parameter = 0.2

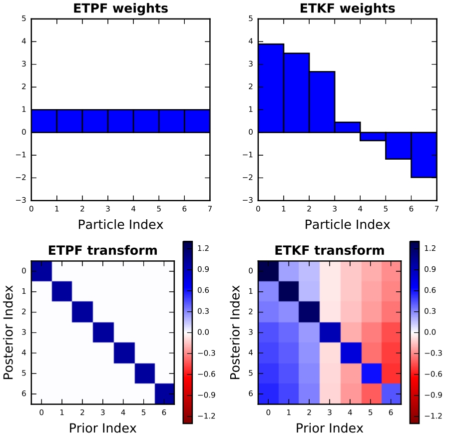


Single one-dimensional DA step

Bridging Parameter = 0.1



Bridging Parameter = 0



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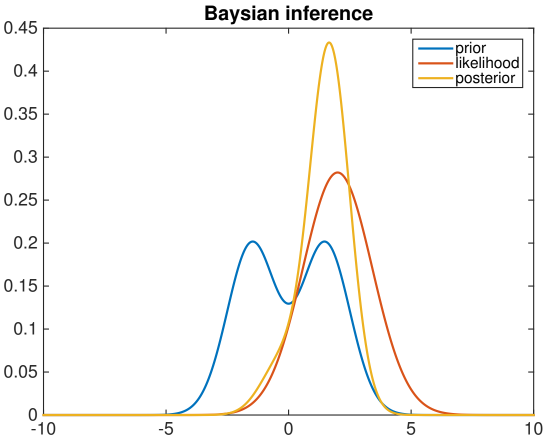
Bayesian Inference
for bimodal prior
and
Gaussian likelihood



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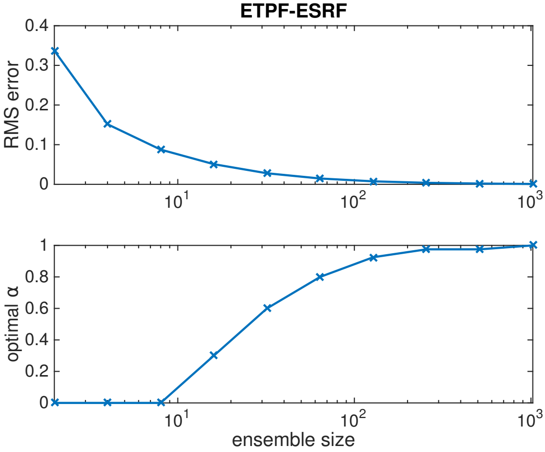
ETPF-ESRF

performance vs

ensemble size



Particle rejuvenation:

$$z_j^{\mathrm{a}} \to z_j^{\mathrm{a}} + \sum_{i=1}^{M} (z_i^{\mathrm{f}} - \bar{z}^{\mathrm{f}}) \frac{\beta \Xi_{ij}}{\sqrt{M-1}}$$

- β: Rejuvenation parameter
- $\{\Xi_{ij}\}$: i.i.d. Gaussian random variables with mean zero and variance one

Properties:

- Increase ensemble spread while preserving ensemble mean
- Ameliorates particle degeneracy
- Does not destroy spatial regularity

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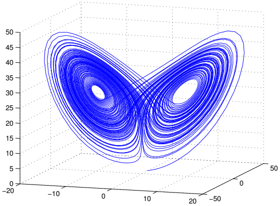
Dynamical system:

$$\dot{x}_1 = 10(x_2 - x_1)$$
$$\dot{x}_2 = x_1(28 - x_3) - x_2$$
$$\dot{x}_3 = x_1 x_2 - 8/3 x_3$$

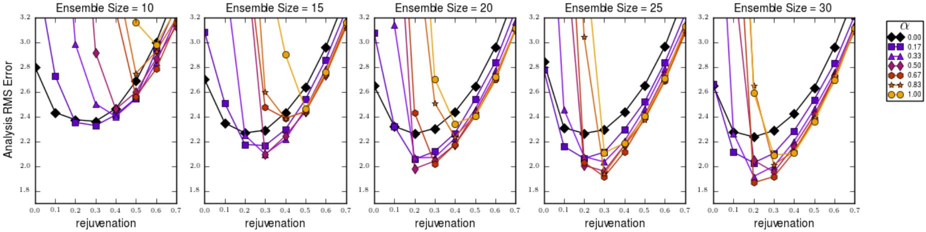


Perfect model DA experiments:

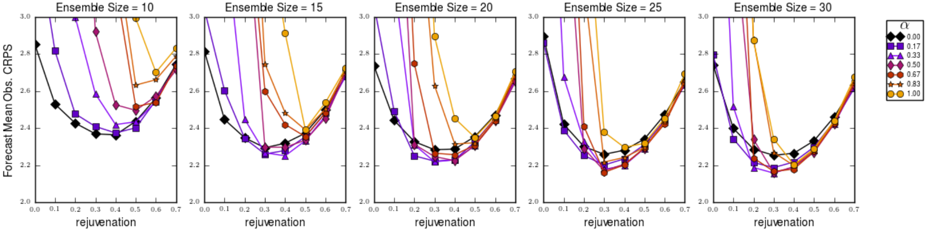
- x_1 observed every 12 time-steps
- Observation error variance $R = 8$

Example: Lorenz 63 model

PF-KF RMSE with exact OT solver



PF-KF CRPS with exact OT solver



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Possible updating sequences:

- ETPF-ESRF

$$z_j^{\mathrm{h}} = \sum_{i=1}^{M} z_i^{\mathrm{f}} d_{ij}^{\mathrm{PF}}, \qquad d_{ij}^{\mathrm{PF}} := d_{ij}^{\mathrm{PF}}(\alpha, \{z_l^{\mathrm{f}}\}, y_{\mathrm{obs}}),$$

$$z_j^{\mathrm{a}} = \sum_{i=1}^{M} z_i^{\mathrm{h}} d_{ij}^{\mathrm{KF}}, \qquad d_{ij}^{\mathrm{KF}} := d_{ij}^{\mathrm{KF}}(\alpha, \{z_l^{\mathrm{h}}\}, y_{\mathrm{obs}}).$$

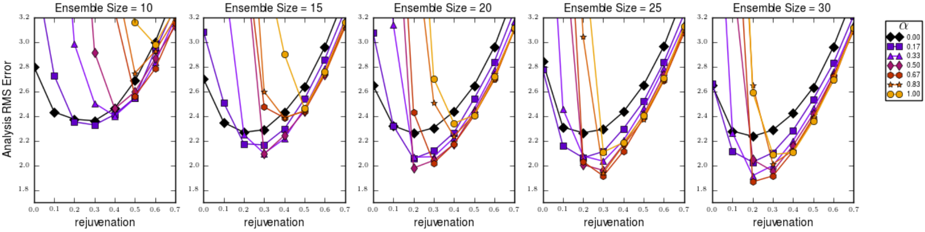
- ESRF-ETPF

$$z_j^{\mathrm{h}} = \sum_{i=1}^{M} z_i^{\mathrm{f}} d_{ij}^{\mathrm{KF}}, \qquad d_{ij}^{\mathrm{KF}} := d_{ij}^{\mathrm{KF}}(\alpha, \{z_l^{\mathrm{f}}\}, y_{\mathrm{obs}}),$$

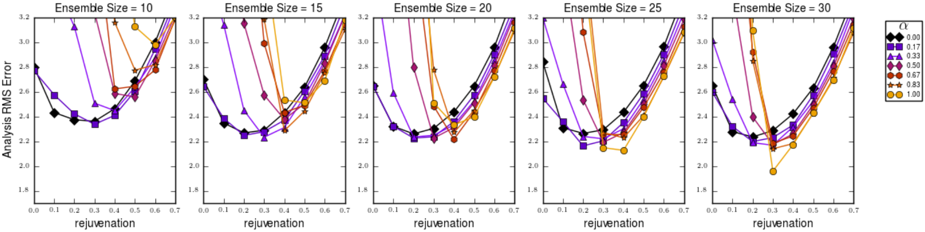
$$z_j^{\mathrm{a}} = \sum_{i=1}^{M} z_i^{\mathrm{h}} d_{ij}^{\mathrm{PF}}, \qquad d_{ij}^{\mathrm{PF}} := d_{ij}^{\mathrm{PF}}(\alpha, \{z_l^{\mathrm{h}}\}, y_{\mathrm{obs}}).$$

Updating order dependency

PF-KF RMSE with exact OT solver



KF-PF RMSE with exact OT solver



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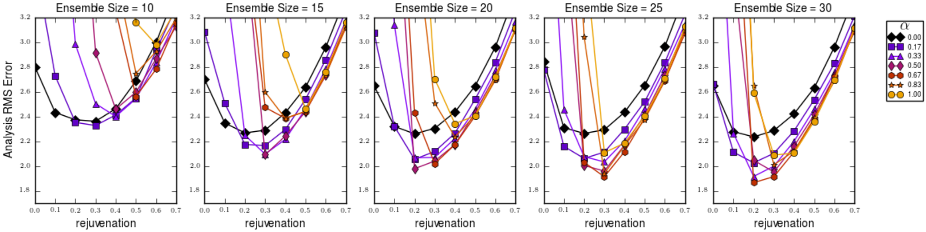
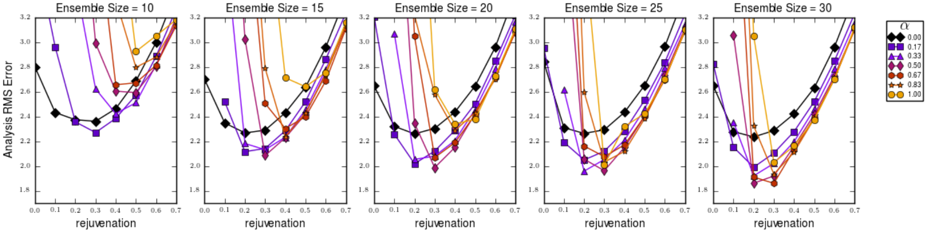
PF-KF RMSE with exact OT solver

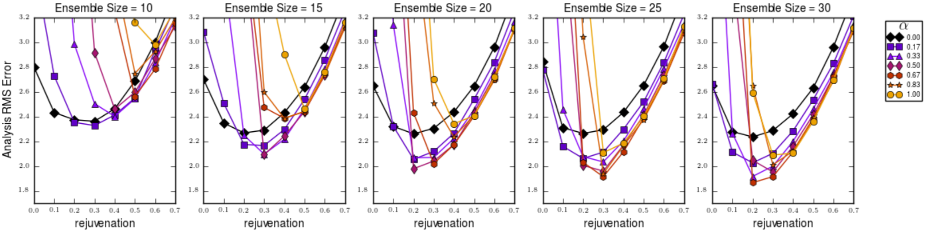


PF-KF RMSE solving entropic regularized OT problem

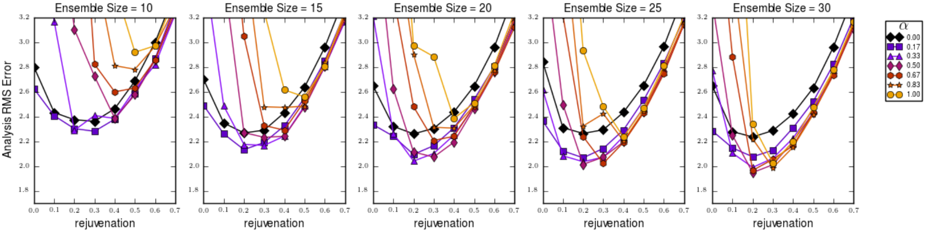


OT solver dependency

PF-KF RMSE with exact OT solver



PF-KF RMSE solving 1D OT problem



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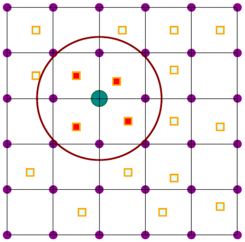
R-Localization

$$r_{qq}^{LOC}(x_k) = \frac{r_{qq}}{\rho\left(\frac{\|x_k - x_q\|}{R_{\text{loc}}}\right)},$$

with ρ a compactly supported tempering function.



- Directly applicable to Kalman Filters
- Directly applicable to importance weights

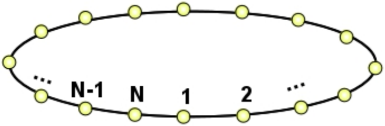
Particle distance Localization [Cheng and Reich, 2015]

$$c_{ij}(x) = \int_{\mathbb{R}} \rho\left(\frac{\|x_k - x_q\|}{C_{\text{loc}}}\right) \|z_i^{\text{f}}(x_q) - z_j^{\text{f}}(x_q)\|^2 dx_q$$

Dynamical system:

$$\dot{x}_j = (x_{j+1} - x_{j-2})x_{j-1} - x_j + F,$$
$$x_j = x_{j+N}$$

where $F = 8$ and $N = 40$.



Perfect model DA experiments:

- Odd variables observed every 22 time-steps
- Observation error variance $R = 8$
- Particle rejuvenation $\beta = 0.2$
- Localization radius is $R_{\text{loc}} = 4$
- OTP solved using FastEMD algorithm

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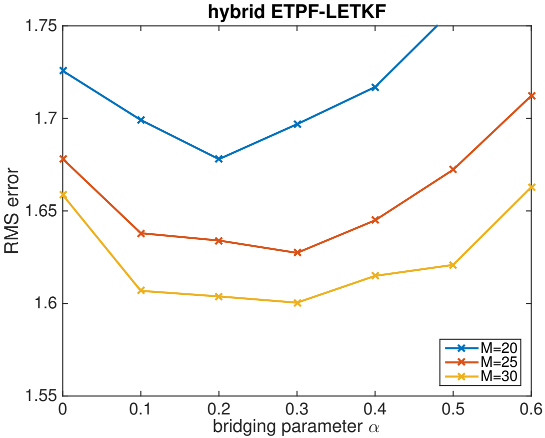
Skill dependence on bridging parameter for different ensemble sizes using fixed likelihood splitting



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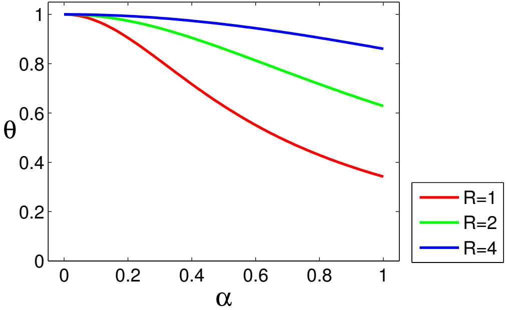
Normalized effective sample size: $\theta(\alpha) = \dfrac{1}{M\sum_{i=1}^{M} w_i(\alpha)^2}$

θ vs α for different obs. error levels



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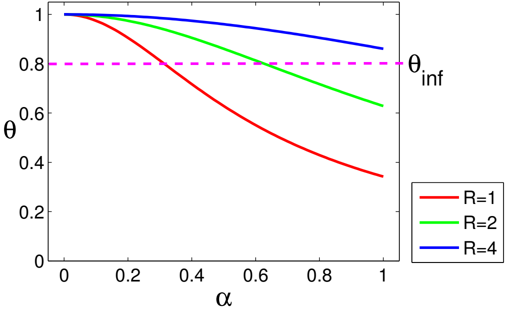
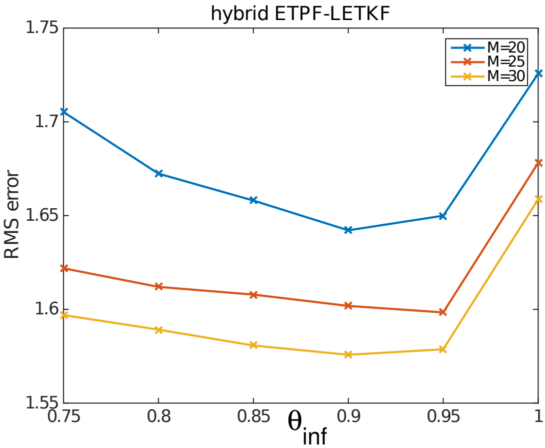
Normalized effective sample size: $\theta(\alpha) = \frac{1}{M\sum_{i=1}^{M} w_i(\alpha)^2}$

θ vs α for different obs. error levels



Adaptivity criterion: Set α to the maximal value for which $\theta \geq \theta_{inf}$.

Skill dependence on minimum effective sample size for different ensemble sizes using adaptive likelihood splitting



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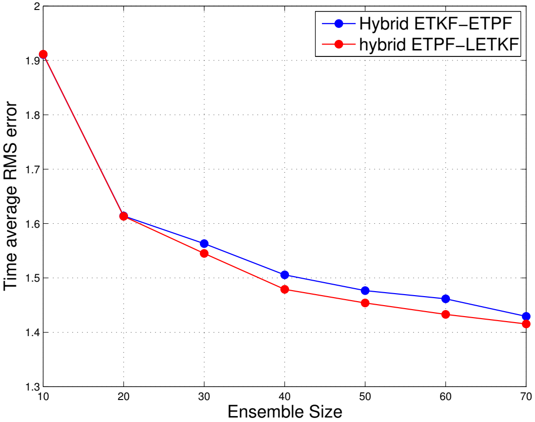
Skill dependence on ensemble size for both update orders using optimal fixed bridging parameter



- Proposed Hybrid scheme
  allows consistent localization for both filters,
  preserves model state regularity,
  outperforms both ETKF and ETPF for a suitable α
- Approximated OT solution approaches are promising cheaper options, in particular 1D approximation
- Update ordering sensitivity is model-dependent
- Adaptive likelihood splitting benefits spatially extended systems.

- ETPF and hybrid scheme being implemented for the German Weather Service (DWD)
- Second order accurate Ensemble Transform Particle Filter (under review)
- 1D OT approximation and then multivariate dependence recovery via Ensemble copula coupling [Schefzik et al., 2013]
- Generation of unbalanced fields through localization currently being addressed via mollification.

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Thanks!