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Ensemble smoothing under the influence of nonlinearity

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Outline

- Ensemble smoothers
- Influence of nonlinearity
- Influence of localization
- Smoothing in a real model

Ensemble Smoothers

Smoothers

Filters (e.g. Ensemble Kalman filter)

- Estimate using observations until analysis time

Smoothers perform retrospective analysis

- Use future observations for estimation in the past

- Example applications:

- Reanalysis
- Parameter estimation

Ensemble smoothing

- Smoothing is very simple (ensemble matrix $\mathbf{X}_{k|k-1}^f$)
(see e.g. Evensen, 2003)

$$\text{Filter: } \mathbf{X}_{k|k}^a = \mathbf{X}_{k|k-1}^f \mathbf{C}_k$$

$$\text{Smoother: } \mathbf{X}_{k-1|k}^a = \mathbf{X}_{k-1|k-1}^a \mathbf{C}_k$$

- Ensemble smoothing is cheap
 - e.g. E. Kalnay: “no-cost smoother”
 - weight matrix already computed in filter
 - just recombine previous ensemble states
(actually the most costly part of the filter)
 - but: smoothing is recursive – application of each \mathbf{C}_k
for all previous times within lag

Smoother with linear model

Smoother is optimal for linear systems:

→ Forecast of smoothed state = filter analysis at later time

$$\mathbf{X}_{i|k}^a = \mathbf{X}_{i,i}^a \prod_{j=i+1}^k \mathbf{C}_j \quad \mathbf{X}_{k|k}^a = \mathbf{M}_{k,i} \mathbf{X}_{i,i}^a \prod_{j=i+1}^k \mathbf{C}_j$$

→ Based on ensemble cross-correlation between two time instances

$$\overline{\mathbf{x}_{i|k}^a} = \overline{\mathbf{x}_{i|k-1}^a} + \mathbf{X}_{i|k-1}^{\prime a} \left(\mathbf{X}_{k|k}^{\prime a} \right)^T \mathbf{E}$$

→ Each additional lag reduces error
(if covariances are correctly estimated, Cohn et al. 1994)

(Ensemble perturbation matrix $\mathbf{X}' = \mathbf{X} - \bar{\mathbf{X}}$)

Smother and Nonlinearity

Smother and nonlinearity

- Optimality doesn't hold with nonlinear systems!

$$\overline{\mathbf{x}_{i|i+1}^a} = \overline{\mathbf{x}_{i|i}^a} + \underbrace{\mathbf{X}_{i|i}^{\prime a} \left(\mathbf{X}_{i+1|i+1}^{\prime a} \right)^T}_{\text{influenced by nonlinear model}} \tilde{\mathbf{E}}$$

influenced by nonlinear model

- ➔ What is the effect of the nonlinearity?
- ➔ Do ensembles just decorrelate?
(mentioned e.g. by Cosme et al. 2010)
- ➔ Consider smoother performance relative to filter
(Smoother reduces estimation error from the filter)

Numerical study with Lorenz-96

- Cheap and small model (state dimension 40)
- Local and global filters possible
- Nonlinearity controlled by forcing parameter F
 - Up to $F=4$: periodic waves; perturbations damped
 - $F>4$: non-periodic
- Nonlinearity of assimilation also influenced by forecast length

- Experiments over 20,000 time steps
- Use smoother with ESTKF (Nerger et al., 2012)
- Tune covariance inflation for minimal RMS errors
- Implemented in open source assimilation software PDAF
(<http://pdaf.awi.de>)

The ESTKF: First compare ETKF and SEIK

Square root of covariance matrix (ensemble size N , state dim n)

$$\mathbf{Z} = \mathbf{X}^f \mathbf{T} \quad \mathbf{P}^f = \mathbf{Z}\mathbf{Z}^T$$

Transformation matrix in ensemble space (small matrix)

$$\mathbf{A} = \left(\mathbf{G} + (\mathbf{HZ})^T \mathbf{R}^{-1} \mathbf{HZ} \right)^{-1}$$

Analysis state covariance matrix

$$\mathbf{P}^a = \mathbf{Z}\mathbf{A}\mathbf{Z}^T$$

Ensemble transformation based on square root of \mathbf{A}

$$\mathbf{X}^a \sim \mathbf{Z}\mathbf{L} \quad \mathbf{L}\mathbf{L}^T = \mathbf{A}$$

Very efficient:

Transformation matrix computed in space of dim. N or $N-1$

The T matrix

Matrix \mathbf{T} projects onto the error space spanned by ensemble

SEIK and ETKF use different projections \mathbf{T}

$$\mathbf{Z} = \mathbf{X}^f \mathbf{T}$$

For identical forecast ensembles both filters

- yield identical analysis state
- perform slightly different ensemble transformations
- also: SEIK is slightly faster than ETKF

- ETKF provides minimum transformation
 - desirable for least disturbing ensemble states

- How to get minimum transformation into SEIK?

Error Subspace Transform Kalman Filter (ESTKF)

Combine advantages of SEIK and ETKF

Redefine **T**:

1. Remove ensemble mean from all columns
2. Subtract fraction of last column from all others
3. Drop last column

Features of the ESTKF:

- Same ensemble transformation as ETKF
- Slightly cheaper computations
- Direct access to ensemble-spanned error space

T-matrix in SEIK and ESTKF

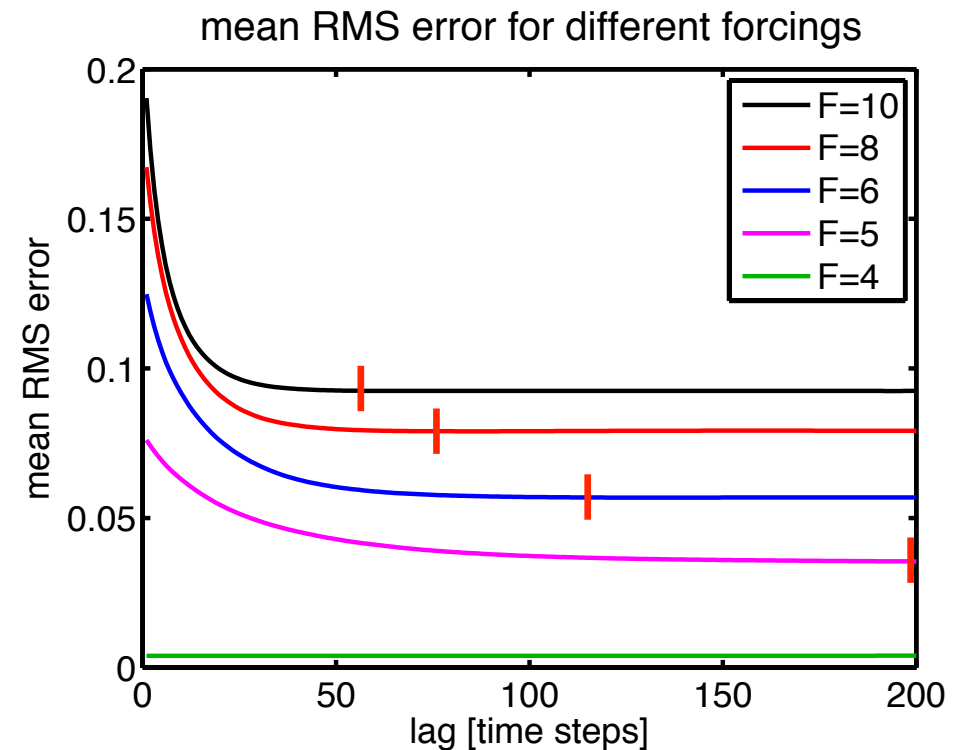
$$\text{SEIK:} \quad \mathbf{T}_{i,j} = \begin{cases} 1 - \frac{1}{N} & \text{for } i = j, i < N \\ -\frac{1}{N} & \text{for } i \neq j, i < N \\ -\frac{1}{N} & \text{for } i = N \end{cases}$$

$$\text{ESTKF:} \quad \hat{\mathbf{T}}_{i,j} = \begin{cases} 1 - \frac{1}{N} \frac{1}{\frac{1}{\sqrt{N}} + 1} & \text{for } i = j, i < N \\ -\frac{1}{N} \frac{1}{\frac{1}{\sqrt{N}} + 1} & \text{for } i \neq j, i < N \\ -\frac{1}{\sqrt{N}} & \text{for } i = N \end{cases}$$

- Efficient implementation as subtraction of means & last column
- ETKF: improve compute performance using a matrix \mathbf{T}

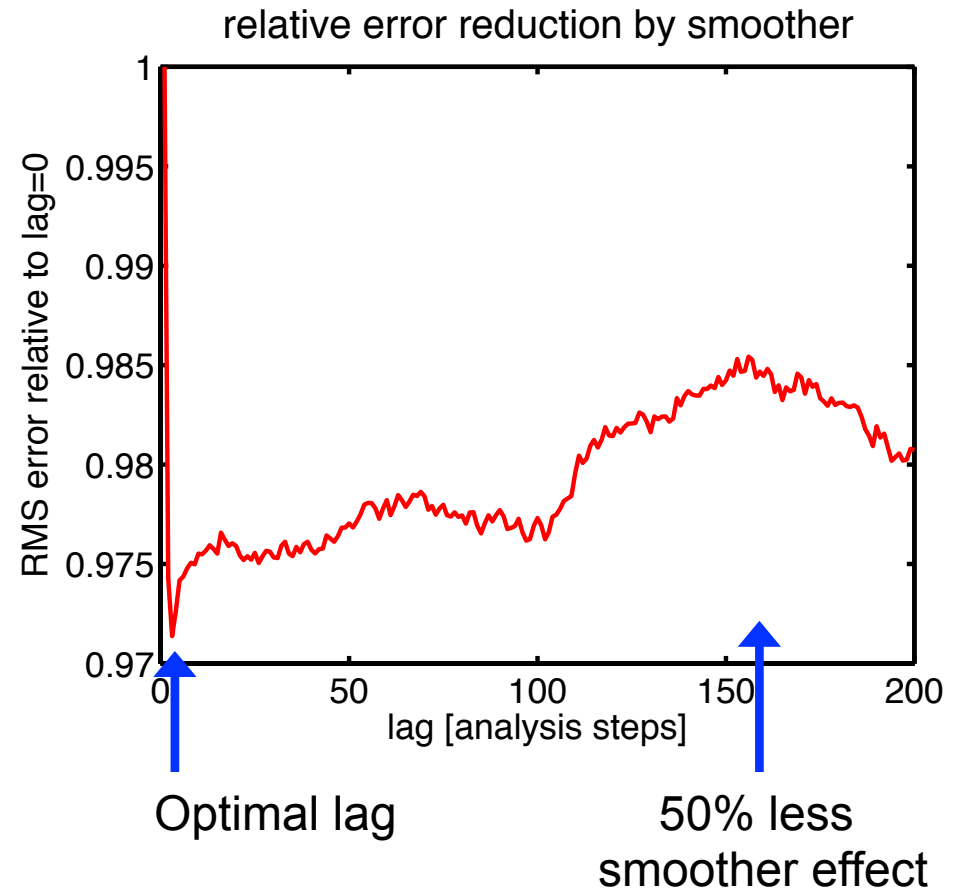
Effect of forcing on the smoother – optimal lag

- Assimilate at each time step
- Ensemble size $N=34$
- Global ESTKF
- Inflation tuned for minimal RMS errors (account for inflation in smoother)
- Up to $F=4$
 - very small RMS errors
- $F>4$
 - Strong growth in RMS
 - Clear impact of smoother
 - Optimal lag:
minimal RMS error (red lines)

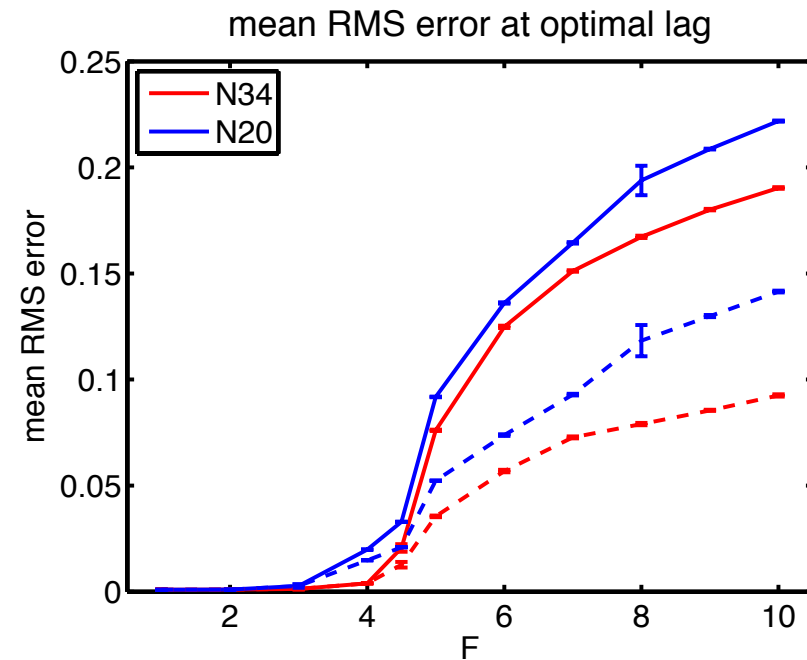
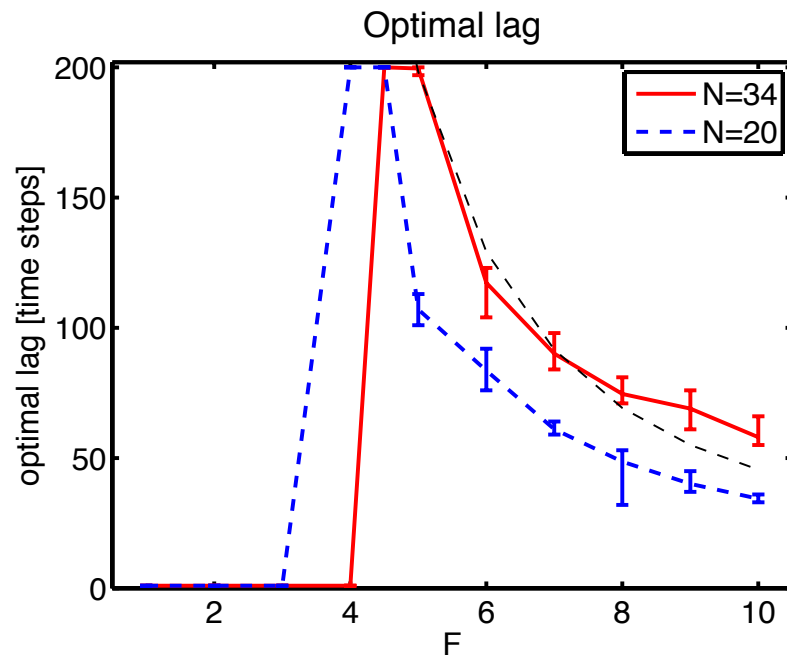


Stronger nonlinearity

- $F=7$
- Forecast length: 9 steps
- Clear error minimum at lag=2 analysis steps
 - ➔ the optimal lag
- Error increase beyond optimal lag (here 50%!)
 - ➔ spurious correlations

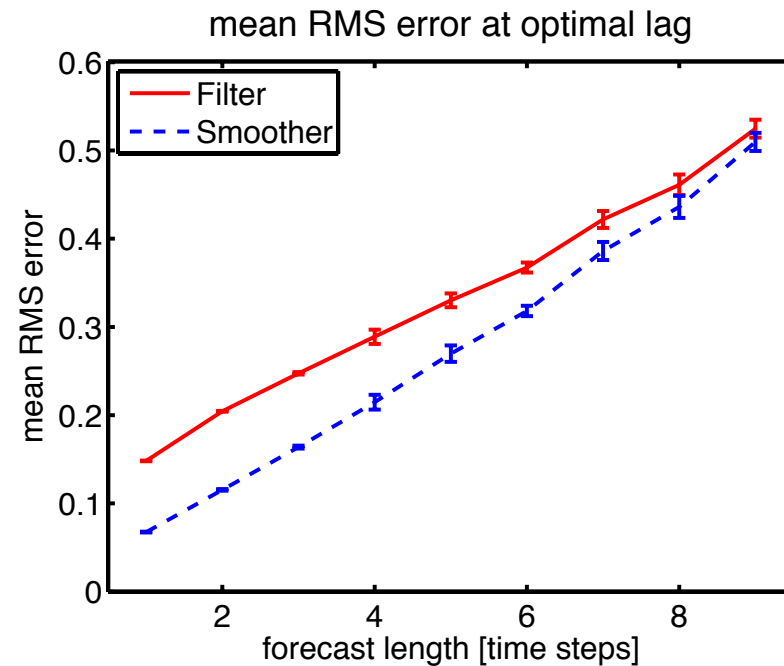
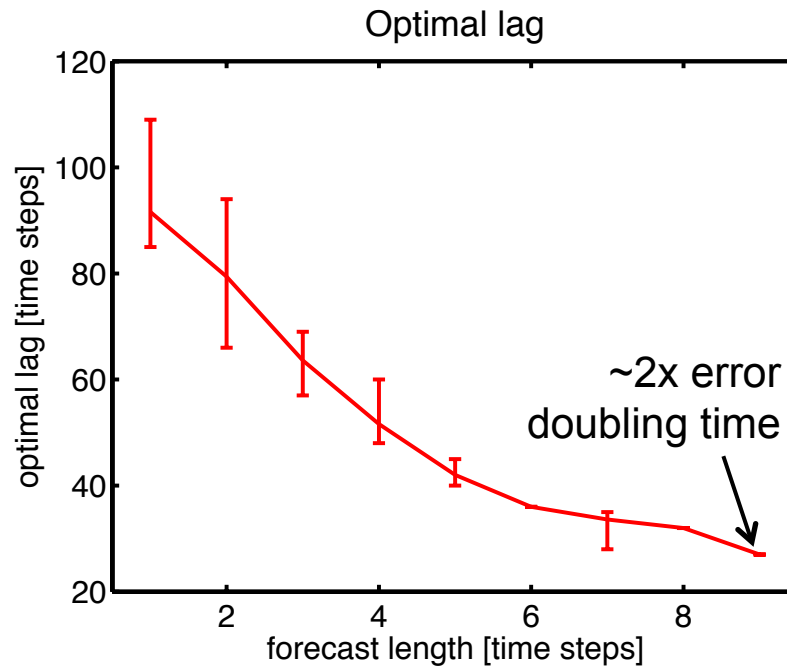


Impact of smoothing



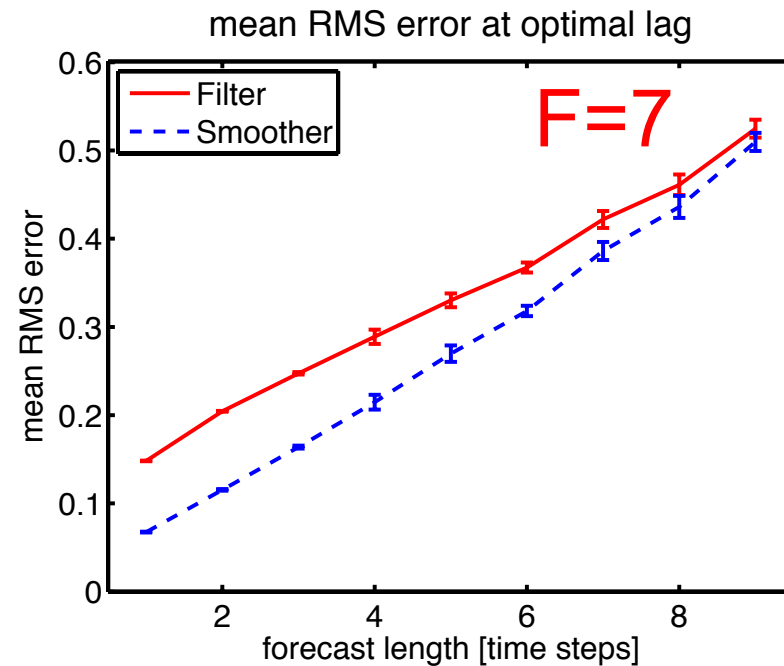
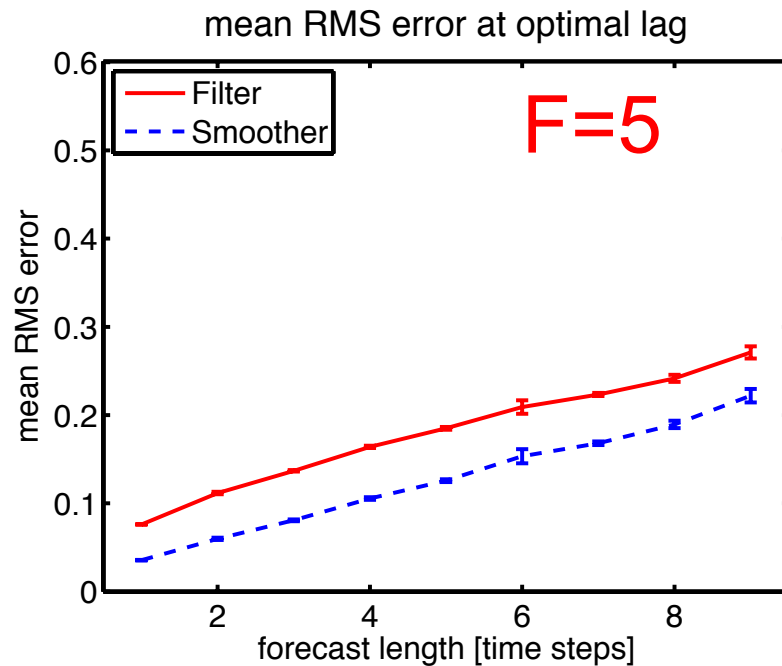
- Optimal lag (minimal RMS error)
 - Behavior similar to error-doubling time
- RMS error at optimal lag
 - Smoother reduces error by 50% for all $F > 4$
- Effect of sampling errors visible with smaller ensemble

Vary forecast length (F=7)



- Forecast length = time steps over which nonlinearity acts on ensemble
- Longer forecasts:
 - ➔ Optimal lag shrinks
 - ➔ RMS errors grow for filter and smoother
 - ➔ Improvement by smoother shrinks (depends on forcing strength)

Vary forecast length – different forcing strength



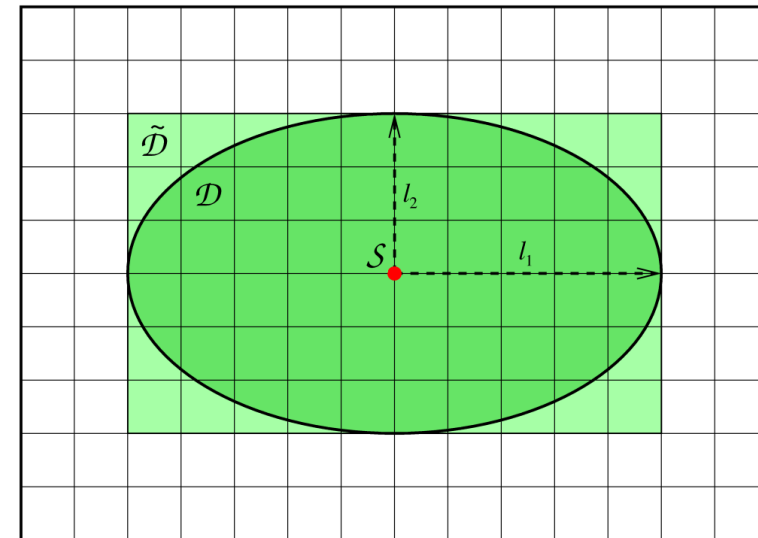
- Improvement by smoother depends on forcing strength
- Small forcing (F=5)
 - ➔ Approx. constant improvement by smoother
- Larger forcing (F=7)
 - ➔ Decreasing smoother effect

Impact of Localization

Domain & observation localization

Local Analysis:

- Update small regions (like single vertical columns)
- Observation localizations: Observations weighted according to distance
- Consider only observations with weight >0
- State update and ensemble transformation fully local

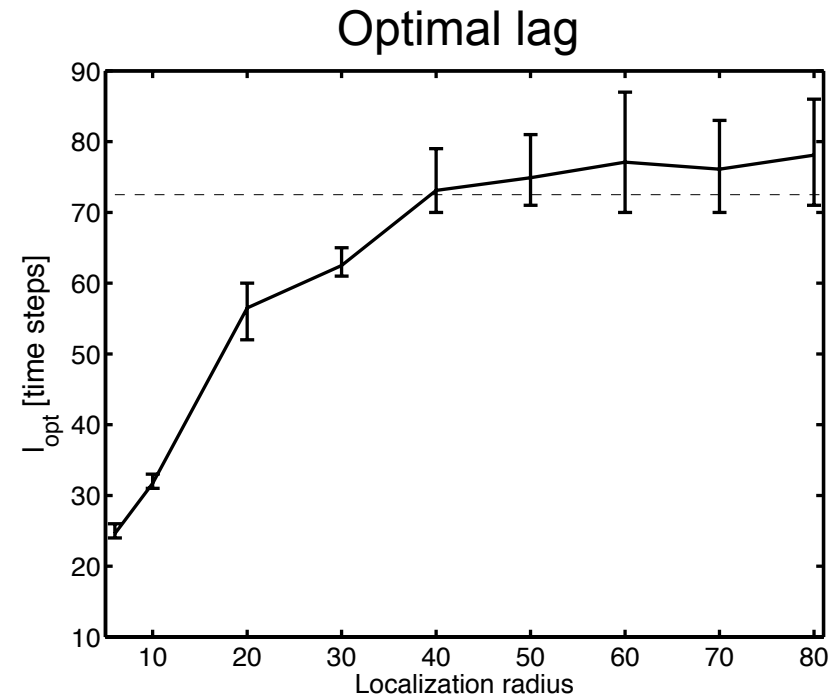
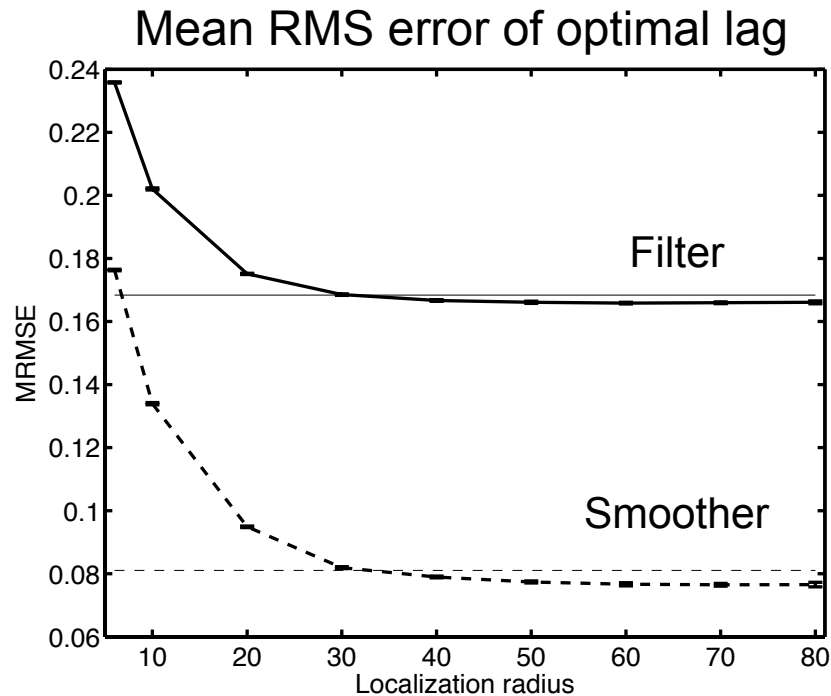


S: Analysis region

D: Corresponding data region

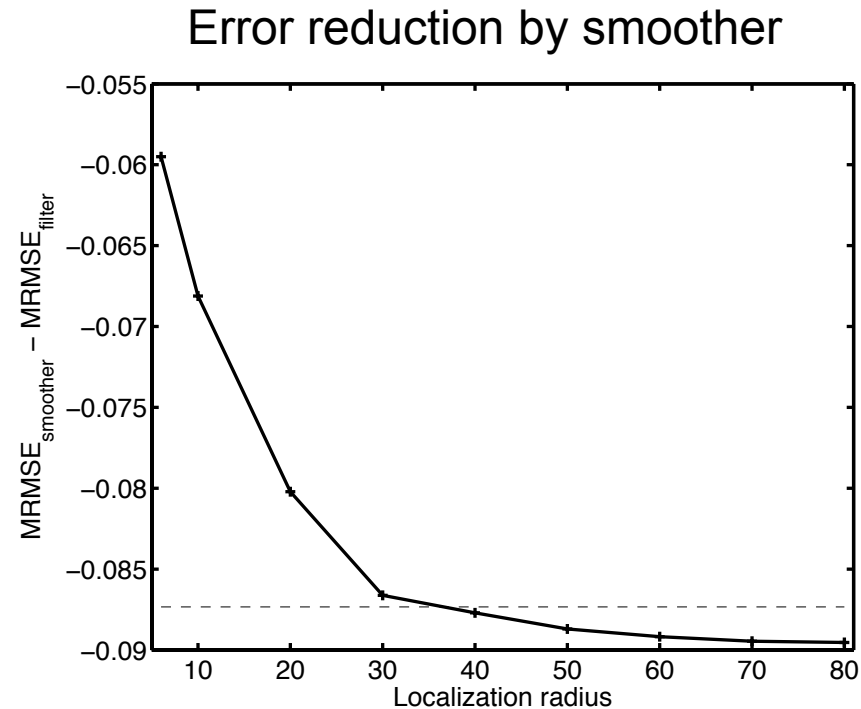
Similar to localization in LETKF (e.g. Hunt et al, 2007)

Influence of Localization on Smoothing



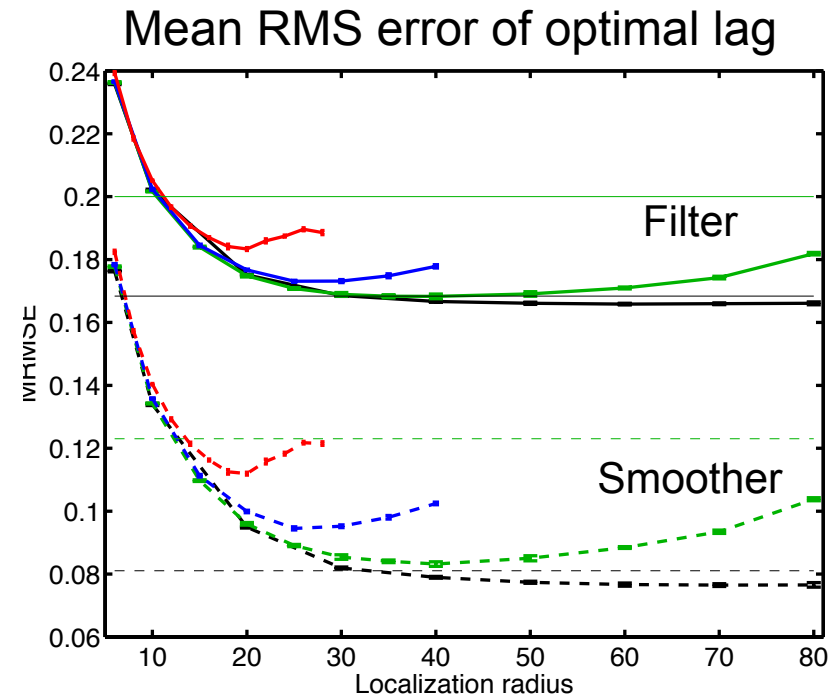
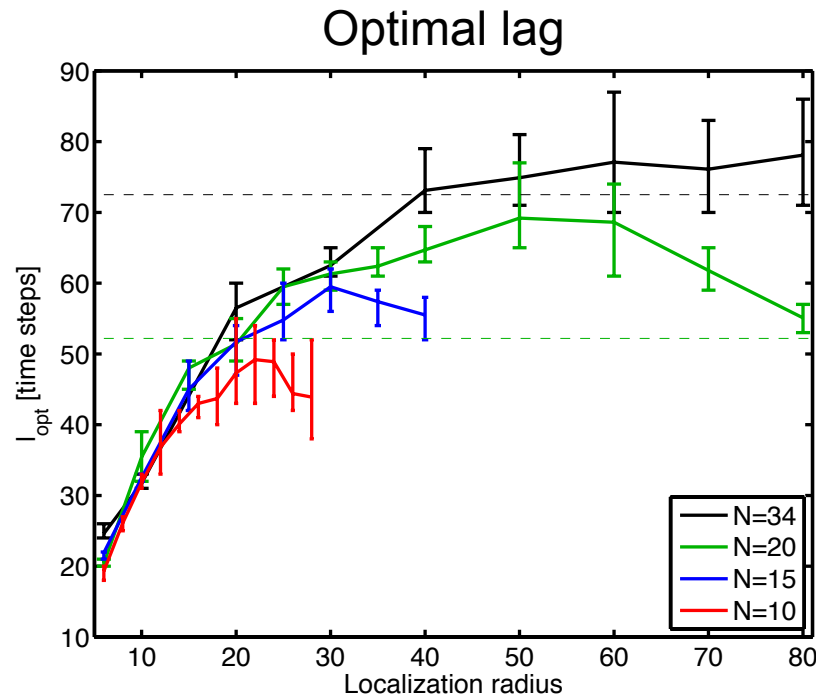
- Reduced RMS errors from filter and smoother by localization
 - localization is useful even for $N=34$
- Localization increases optimal lag
 - more observational information useable

Influence of Localization on Smoothing (2)



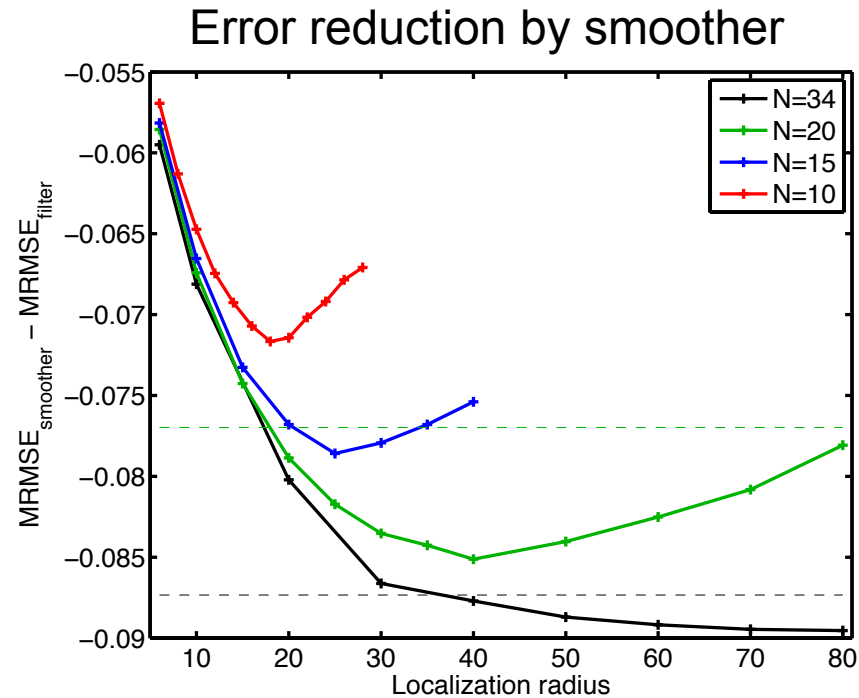
- Use filter error as baseline
- Smoother results in additional reduction
- Smoother is more efficient with localization than for global filter

Smoothing with localization – smaller ensembles



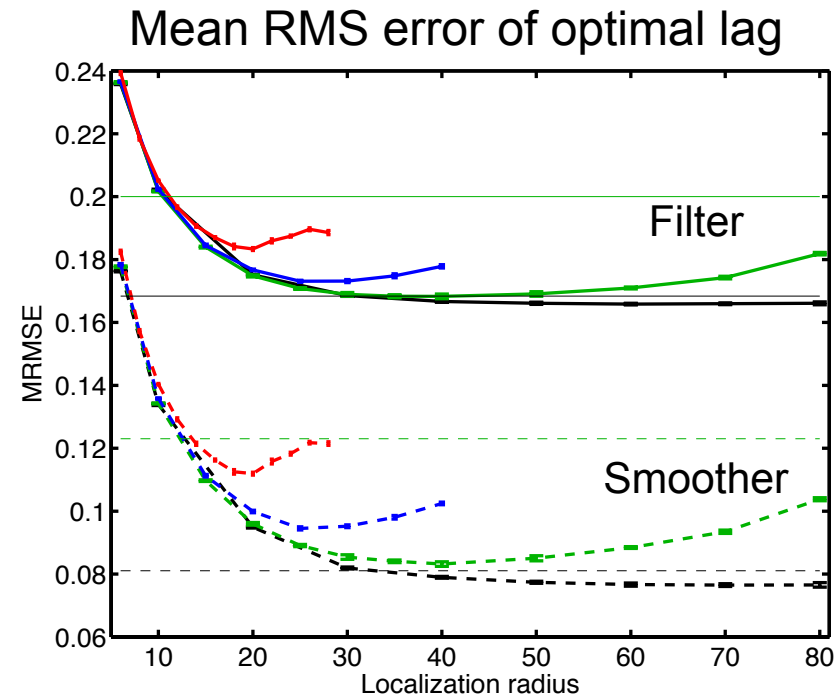
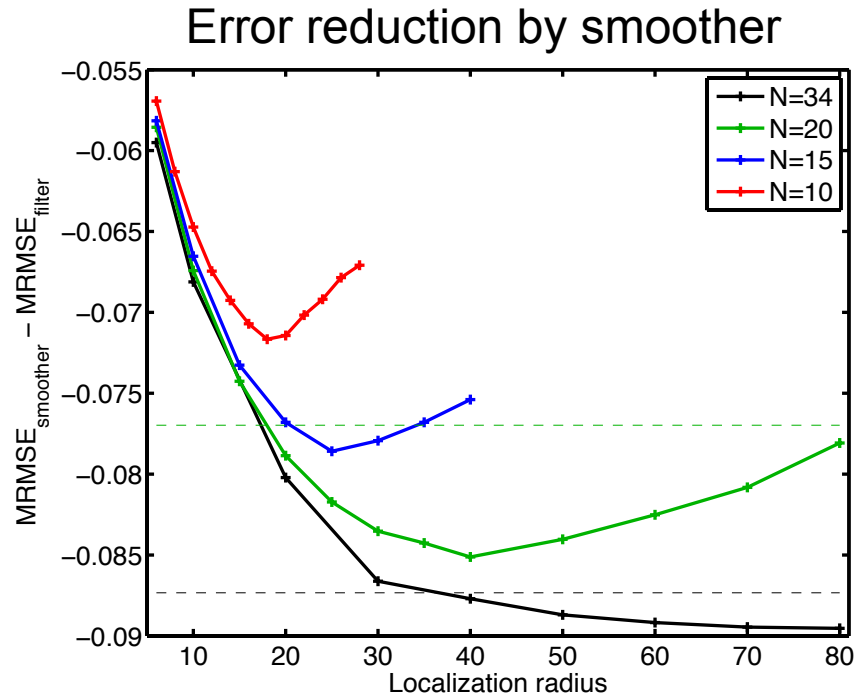
- Larger effect of localization with smaller ensembles
- Optimal lag shrinks (impact of sampling errors)
- Localization radius for maximum optimal lag slightly larger than for minimum RMS error

Smother error reduction – smaller ensembles



- Smoother impact grows with ensemble size
 - Effect of sampling errors
- RMS error from smoother decreases faster than from filter
 - Amplification effect (multiple use of matrix **C**)

Optimal localization radius



Same localization radius for

- minimum filter RMS error
- largest smoother impact
- ➔ No re-tuning of localization radius for optimal smoothing!

Smoothing in a Real Model

Global ocean model

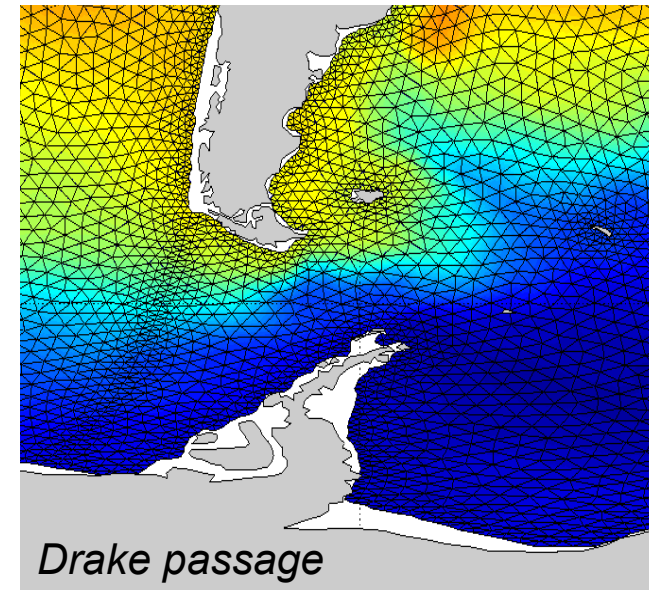
FESOM (Finite Element Sea-ice Ocean model, Danilov et al. 2004)

Global configuration

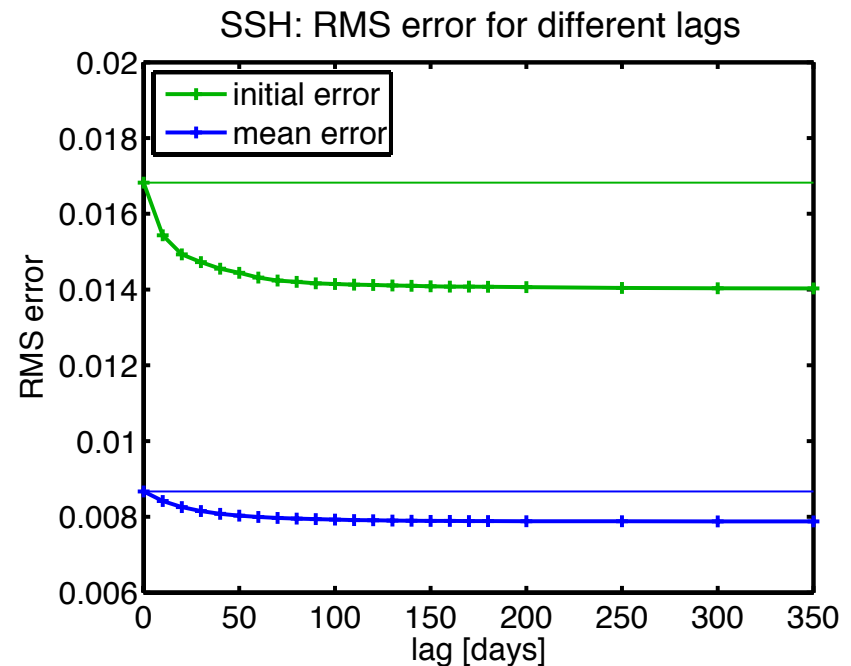
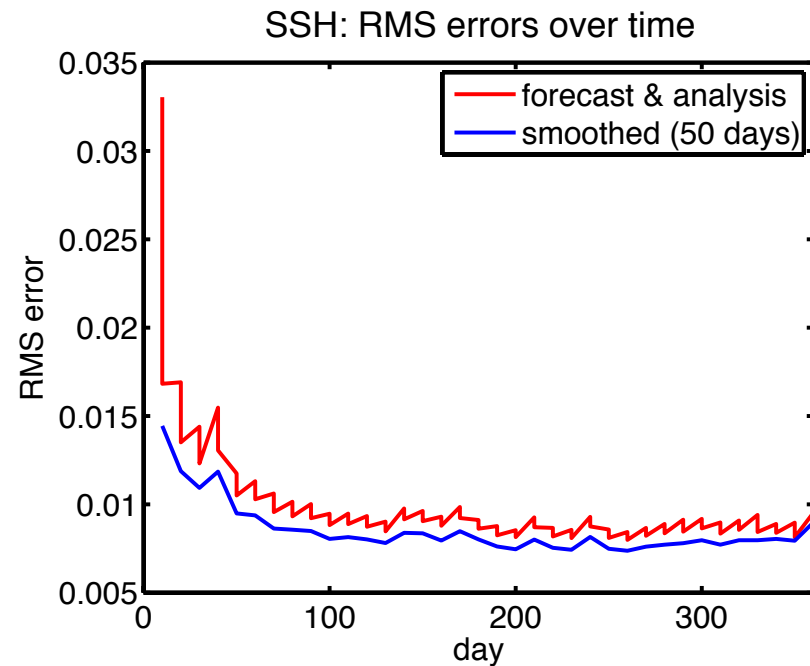
- 1.3° resolution, 40 levels
- horizontal refinement at equator
- state vector size 10^7
- weak nonlinearity (not easy to change)

Twin experiments with sea surface height data

- ensemble size 32
- assimilate each 10th day over 1 year
- ESTKF with smoother extension and localization (using PDAF environment as single program)
- inflation tuned for optimal performance ($\rho=0.9$)
- run using 2048 processor cores
(Timings: forecasts 8800s, filter+smoother 200s)



Effect of smoothing on global model



Typical behavior

- RMSE reduced by smoother

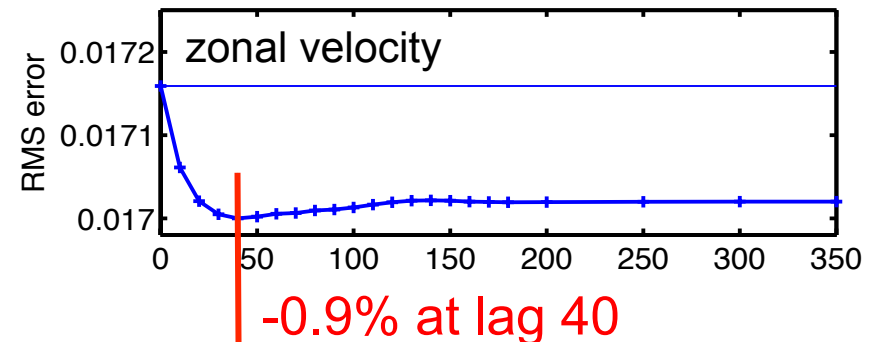
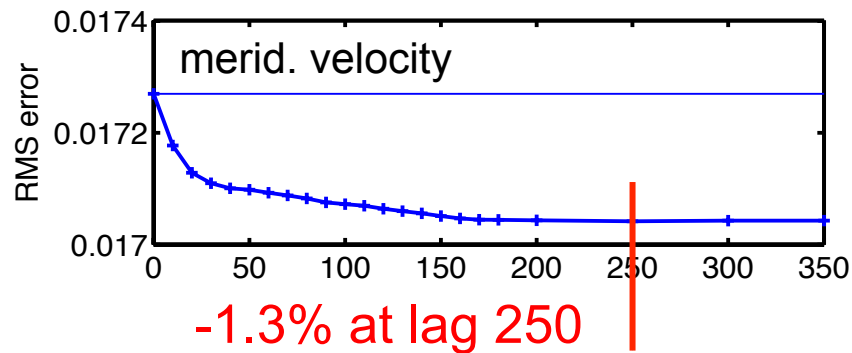
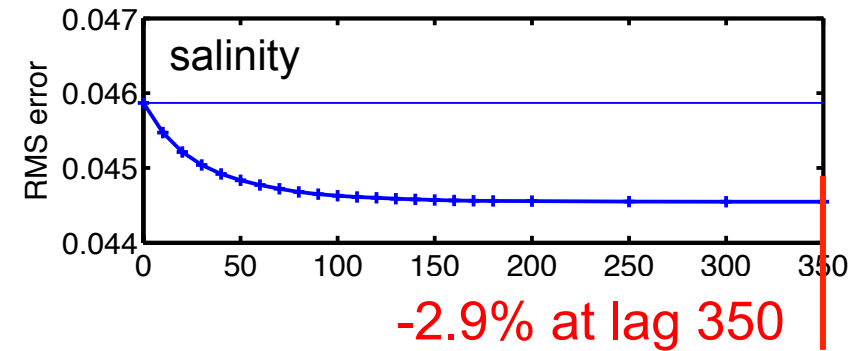
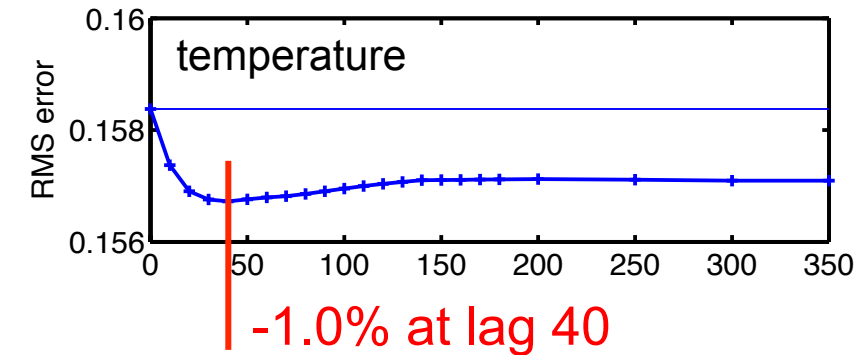
Error reductions:

~15% at initial time

~8% over the year

- Large impact of each lag up to 60 days
- Further reduction over full experiment (optimal lag = 350 days)

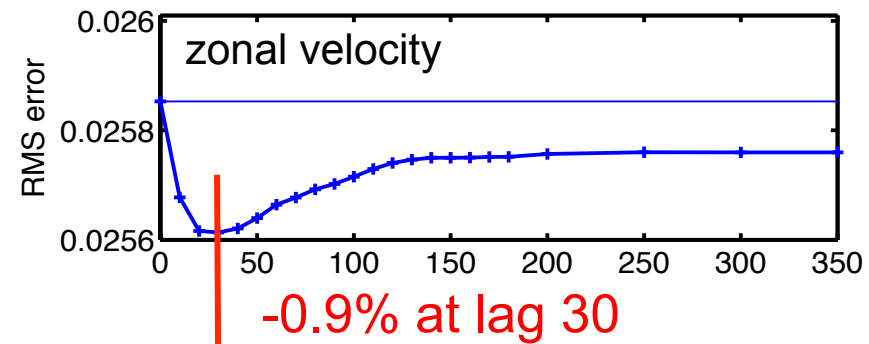
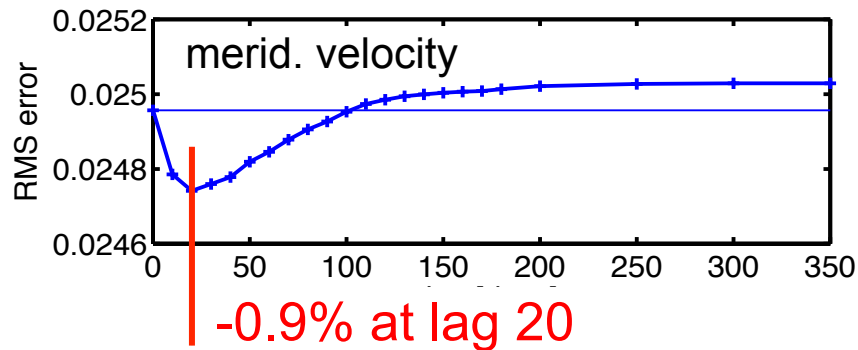
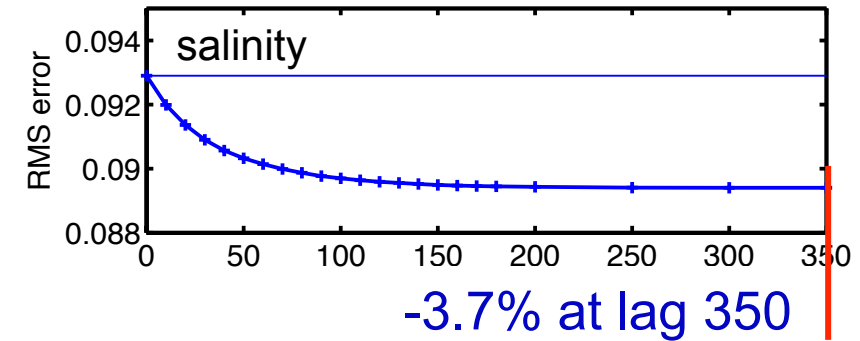
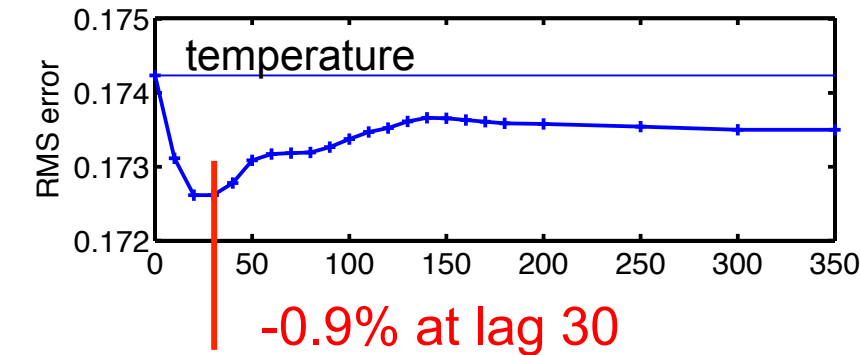
Multivariate effect of smoothing – 3D fields



3D fields:

- Multivariate impact smaller & specific for each field
- Optimal lag specific for field
- Optimal lag smaller than for SSH (e.g. temperature directly influenced by atmospheric forcing, Brusdal et al. 2003)

Multivariate effect of smoothing – surface fields



Ocean surface:

- Relative smoother impact not larger than for full 3D
- Deterioration for meridional velocity at long lags
- ➔ What is the optimal lag for multivariate assimilation?

Conclusion

- Multivariate assimilation:
 - Lag specific for field
 - Choose overall optimal lag or separate lags
 - Best filter configuration also good for smoother
- Nonlinearity:
 - Introduces spurious correlations in smoother
 - Error increase beyond optimal lag
 - Optimal lag: few times error doubling time
- Localization:
 - Increases smoother impact
 - Increases optimal lag

Thank you!

Web-Resources



www.data-assimilation.net



pdaf.awi.de