A new Hierarchical Bayes approach to ensemble-variational data assimilation

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Methodological problems in the existing data assimilation approaches we intend to alleviate with the new technique

1. All existing Var, EnKF, and EnVar analysis equations assume that the effective background-error covariance matrix B is exact. But this is never the case.
2. EnVar takes a *linear combination* of static and ensemble covariances to specify B. This is ad hoc.
3. EnKF and EnVar use an ad-hoc localization. This is not theoretically optimal.
4. In the Var, EnKF, and EnVar analysis equations, there is no intrinsic feedback from observations to background-error statistics. This requires external adaptation or manual tuning.

The proposed paradigm

In words: Acknowledge that B is uncertain and random and update it along with the state.

Observations for B: both the ensemble and the ordinary observations contain info on B.

Level	Gnrlzd bckg	Prior	Gnrlzd obs	Update
2	Static $\mathbf{B}_0$	$p(\mathbf{B}\mid\mathbf{B}_0)$	Ensm $\mathbf{X^e}$, $\mathbf{x^{obs}}$	$\mathbf{B}_0 \Rightarrow \boxed{\mathbf{B}} \Leftarrow \mathbf{X^e}, \mathbf{x^{obs}}$
1	$\mathbf{x^b} = \mathbf{x^f}$ or $\overline{\mathbf{x^e}}$	$\mu\mathbf{B}_0 + (1-\mu)\mathbf{X^e}\mathbf{X^{eT}} \circ \mathbf{C}$	$\mathbf{x^{obs}}$	$\mathbf{x^b} \Rightarrow \boxed{\mathbf{x}} \Leftarrow \mathbf{x^{obs}}$

Level 2: extension by the new approach.

Level 1: the existing EnVar technique.

Hierarchical Bayes EnVar (HB-EnVar): principle

$$p(\mathbf{x}, \mathbf{m}, \mathbf{B} | \mathbf{x^f}, \mathbf{X^e}, \mathbf{x^{obs}}) \propto p(\mathbf{m}|\mathbf{x^f}) p(\mathbf{B}|\mathbf{B}_0) p(\mathbf{x}|\mathbf{m}, \mathbf{B}) p(\mathbf{X^e}|\mathbf{m}, \mathbf{B}) p(\mathbf{x^{obs}}|\mathbf{x})$$

The goal is the *posterior distribution* of $\mathbf{x}$ and its mean $\hat{\mathbf{x}}$ in particular.

Ensemble likelihood

$$p(\mathbf{X^e}|\mathbf{m},\mathbf{B}) \propto |\mathbf{B}|^{-N/2} \mathrm{e}^{-\frac{1}{2}\sum_{\mathrm{k=1}}^{\mathrm{N}} (\mathbf{x_k^e}-\mathbf{m})^\top \mathbf{B^{-1}} (\mathbf{x_k^e}-\mathbf{m})},$$

– no need and no room for approximations.

The prior pdf for $\mathbf{B}$: square-root Gaussian

$$\mathbf{B} = \mathbf{W}\mathbf{W}^\top$$

$\mathbf{W}$ is a Gaussian random matrix.

1) Its pdf:

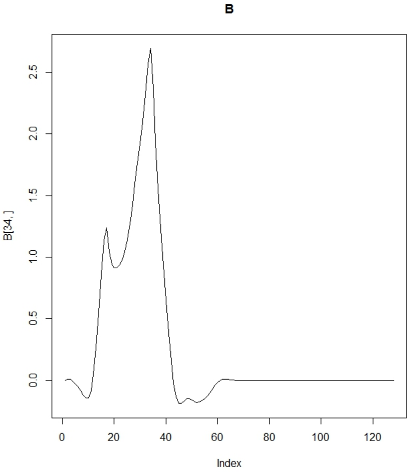
$$p(\mathbf{W}) \propto \mathrm{e}^{-\frac{1}{2}\,\mathrm{tr}[(\mathbf{W}-\mathbf{W_0})\mathbf{U^{-1}}(\mathbf{W}-\mathbf{W_0})^\top\mathbf{U^{-1}}]}$$

2) Sampling:

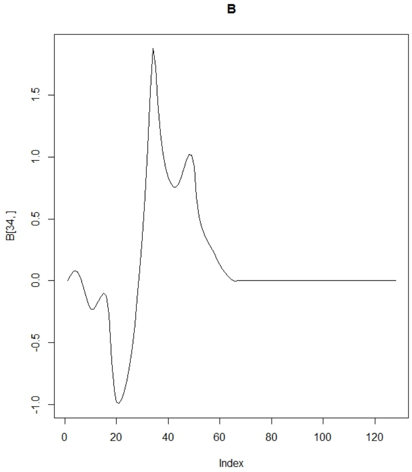
$$\mathbf{W} = \mathbf{W}_0 + \mathbf{\Phi}\mathbf{Y}\mathbf{\Phi}^\top,$$

where $\mathbf{Y}$ is the pure-noise matrix, with $\mathcal{N}(0,1)$ independent entries.

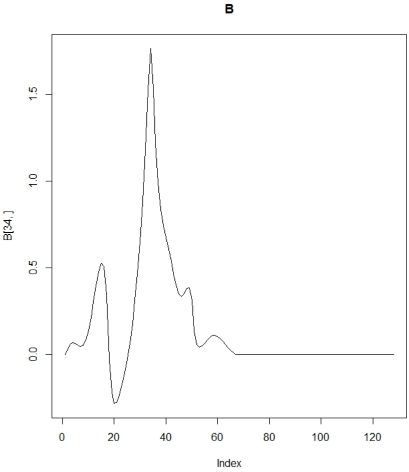
Random samples from $p(\mathbf{B})$



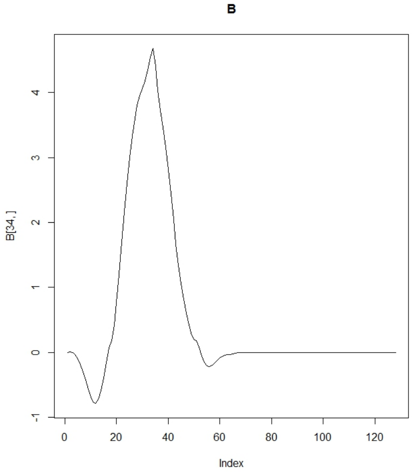
Random samples from $p(\mathbf{B})$



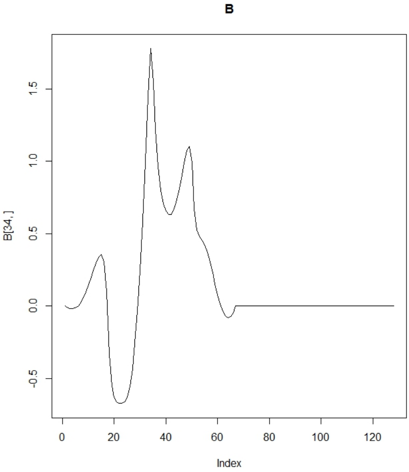
Random samples from $p(\mathbf{B})$



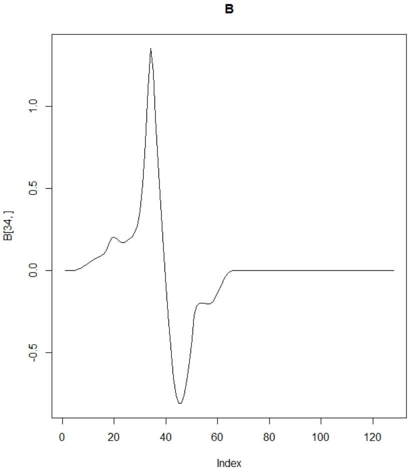
Random samples from $p(\mathbf{B})$



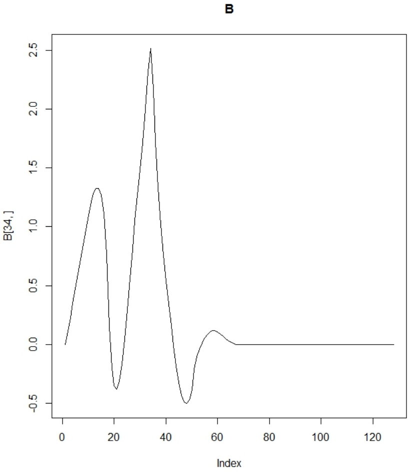
Random samples from $p(\mathbf{B})$



Random samples from $p(\mathbf{B})$



Random samples from $p(\mathbf{B})$



The posterior pdf

$$p_{post}(\mathbf{x}) = \int p_{post}(\mathbf{W}) \cdot p_{post}(\mathbf{x}|\mathbf{W})\, \mathrm{d}\mathbf{W}$$

$$p_{post}(\mathbf{x}|\mathbf{W}) \propto \mathcal{N}(\mathbf{x}^{\mathbf{a}}(\mathbf{m}, \mathbf{W}), \mathbf{B}^{\mathbf{a}}(\mathbf{W})),$$

$$p_{post}(\mathbf{W}) \propto p(\mathbf{W})\phi(\mathbf{W}),$$

$$\phi(\mathbf{W}) := |\mathbf{W}|^{-N} \cdot \mathrm{e}^{-\frac{1}{2}\sum \mathbf{f}_{\mathrm{k}}^{\top}\mathbf{f}_{\mathrm{k}}} \cdot \frac{1}{|\mathbf{G}|^{1/2}} \cdot \mathrm{e}^{\frac{1}{2}\mathbf{v}^{\top}\mathbf{R}^{-1}\mathbf{H}\mathbf{W}\mathbf{G}^{-1}\mathbf{W}^{\top}\mathbf{H}^{\top}\mathbf{R}^{-1}\mathbf{v}}$$

$$\mathbf{W} \cdot \mathbf{f}_k = \mathbf{x}_k^e - \mathbf{m}$$

$$\mathbf{G} := \mathbf{I} + \mathbf{W}^{\top}\mathbf{H}^{\top}\mathbf{R}^{-1}\mathbf{H}\mathbf{W}$$

Here **v** is the innovation vector, hence the adaptive effect.

Importance sampling

$$\hat{\mathbf{x}} = \int p_{post}(\mathbf{W}) \cdot \mathbf{x}^{\mathbf{a}}(\mathbf{m}, \mathbf{W})\, \mathrm{d}\mathbf{W}$$

$$\hat{\mathbf{x}} = \mathrm{E}\, \mathbf{x}^{\mathbf{a}}(\mathbf{m}, \mathbf{W}) = \mathrm{E}_{\,q(\mathbf{W})} \frac{p_{post}(\mathbf{W})}{q(\mathbf{W})} \mathbf{x}^{\mathbf{a}}(\mathbf{m}, \mathbf{W})$$

$$\hat{\mathbf{x}} \approx \overline{\mathbf{x}^{\mathbf{a}}} := \sum_{m=1}^{M} w_m \cdot \mathbf{x}^{\mathbf{a}}(\mathbf{m}, \mathbf{W}_m^{+})$$

=Selection of q: Gaussian pdf centered at the EnVar $\mathbf{W}_{EV}$.

=Localization is achieved by introducing *sparsity* within the *proposal distribution* q for $\mathbf{W}$.

=The ordinary analysis step is included in the importance sampling analysis.

=EnVar can be reproduced within HB-EnVar by nullifying the prior uncertainty in $\mathbf{B}$.

Analysis: Monte-Carlo sampling from the posterior

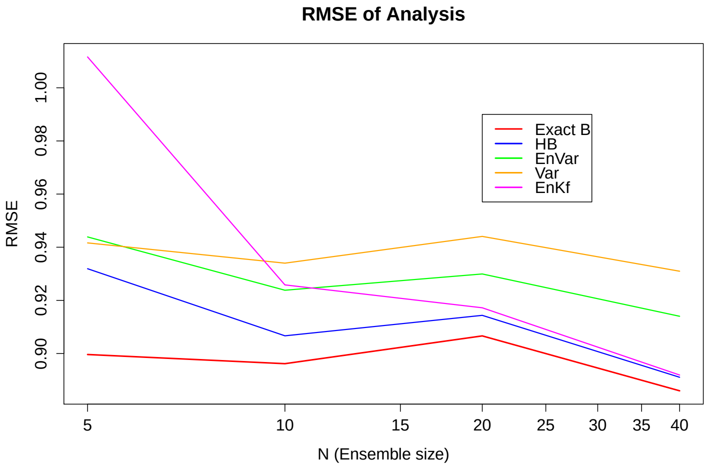
1. Draw M samples $\mathbf{W}_m^+$ from the proposal density of $\mathbf{W}$.
2. Compute their non-normalized importance weights:

$$\phi'(\mathbf{W}_m^+) := \frac{p_{post}(\mathbf{W}_m^+)}{q(\mathbf{W}_m^+)}$$

3. Normalize the importance weights, so that they sum up to one—getting w_m.
4. Perform m ordinary optimal analyses $\mathbf{x}_m^a$ with background-error covariance matrices $\mathbf{B}_m = \mathbf{W}_m^+ \cdot (\mathbf{W}_m^+)^\top$.
5. Average $\mathbf{x}_m^a$ with weights w_m:

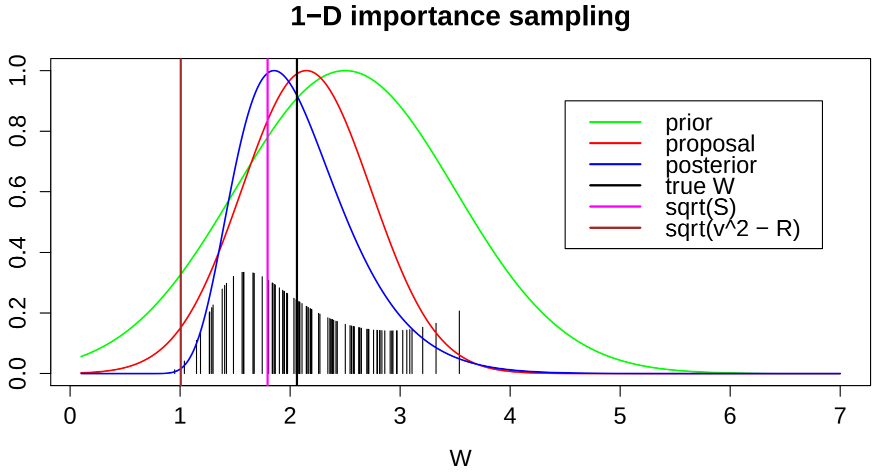
$$\overline{\mathbf{x}^\mathbf{a}} = \sum_{m=1}^{M} w_m \cdot \mathbf{x}^\mathbf{a}(\mathbf{B}_m)$$

1-D illustrative example: dependence on the ensemble size



In the toy problem, the deterministic HB-EnVar analysis outperforms Var, EnKF, and EnVar.

PDFs: prior, posterior, proposal, and importance weights



Conclusions

Main aspects HB-EnVar

- Background-error covariance matrix **B** is treated as a sparse *random matrix* and updated in the optimal scheme along with the state.
- The key element of the proposed technique is the *prior distribution* of **B**.
- Ensemble members are treated as *observations* on the background-error covariance matrix and *assimilated* along with ordinary observations.
- The technique is computationally expensive.

Potential benefits of HB-EnVar

- Optimized hybridization of static and ensemble covariances.
- Optimized combination of deterministic background and ensemble mean.
- Optimized localization.
- Optimized feedback from observations to background-error covariances.
- Uncertainty in **B** is explicitly accounted for in generation of the analysis ensemble, resulting in the *increased spread*.