Hybrid 4DVAR and nonlinear EnKS methods

Parallel 4DVAR without tangents and adjoints

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Summary

Motivation

- 4DVAR sets up a very large nonlinear least squares problem.
- Expensive: iterations, each evaluating the model, tangent and adjoing operators, and solving large linear least squares.
- Extra code for tangent and adjoint operators.
- Iterations may not converge, not even locally.
- Need to parallelize.

Method

- Solve the linear least squares from 4DVAR by EnKS, naturally parallel over the ensemble members.
- Linear algebra glue is cheap, or use parallel dense libraries.
- Finite differences $\Rightarrow$ no tangent and adjoint operators needed.
- Add Tikhonov regularization to the linear least squares $\Rightarrow$ Levelberg-Marquardt method, guaranteed convergence.
- Cheap and simple implementation of Tikhonov regularization within EnKS as an additional observation.

Weak Constraint 4DVAR

- We want to determine $x_0, \ldots, x_k$ (x_i = state at time i) approximately from model and observations (data)

$$
\begin{array}{rclll}
x_0 & \approx & x_{\mathrm{b}} & \text{state at time 0} \approx \text{the background} \\
x_i & \approx & \mathcal{M}_i\left(x_{i-1}\right) & \text{state evolution} \approx \text{by the model} \\
\mathcal{H}_i\left(x_i\right) & \approx & y_i & \text{value of observation operator} \approx \text{the data}
\end{array}
$$

- quantify "$\approx$" by covariances

$$
x_0 \approx x_{\mathrm{b}} \;\Leftrightarrow\; \left\|x_0 - x_{\mathrm{b}}\right\|^2_{\mathbf{B}^{-1}} = \left(x_0 - x_{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(x_0 - x_{\mathrm{b}}\right) \approx 0 \text{ etc.}
$$

- $\Rightarrow$ **nonlinear least squares problem**

$$
\left\|x_0 - x_{\mathrm{b}}\right\|^2_{\mathbf{B}^{-1}} + \sum_{i=1}^{k} \left\|x_i - \mathcal{M}_i\left(x_{i-1}\right)\right\|^2_{\mathbf{Q}_i^{-1}} + \sum_{i=1}^{k} \left\|y_i - \mathcal{H}_i\left(x_i\right)\right\|^2_{\mathbf{R}_i^{-1}} \to \min_{x_{0:k}}
$$

- Originally in 4DVAR, $x_i = \mathcal{M}_i\left(x_{i-1}\right)$. The weak constraint $x_i \approx \mathcal{M}_i\left(x_{i-1}\right)$ accounts for model error (Trémolet, 2007).

Incremental 4DVAR

- Incremental approach (Courtier et al., 1994): linearization

$$\mathcal{M}_i\left(x_{i-1}+\delta x_{i-1}\right) \approx \mathcal{M}_i\left(x_{i-1}\right)+\mathcal{M}_i'\left(x_{i-1}\right)\delta x_{i-1}$$
$$\mathcal{H}_i\left(x_i+\delta x_i\right) \approx \mathcal{H}_i\left(x_i\right)+\mathcal{H}_i'\left(\delta x_i\right)$$

- gives the **Gauss-Newton method** (Bell, 1994), iterations

$$x_{0:k} \leftarrow x_{0:k}+\delta x_{0:k}$$

with the **linear least squares** problem for the increments $\delta x_{0:k}$

$$\left\|x_0+\delta x_0-x_{\mathrm{b}}\right\|_{\mathbf{B}^{-1}}^2+\sum_{i=1}^k\left\|x_i+\delta x_i-\mathcal{M}_i\left(x_{i-1}\right)-\mathcal{M}_i'\left(x_{i-1}\right)\delta x_{i-1}\right\|_{\mathbf{Q}_i^{-1}}^2$$
$$+\sum_{i=1}^k\left\|y_i-\mathcal{H}_i\left(x_i\right)-\mathcal{H}_i'\left(x_i\right)\delta x_i\right\|_{\mathbf{R}_i^{-1}}^2 \rightarrow \min_{\delta x_{0:k}}$$

Linearized 4DVAR as Kalman smoother

Write the linear least squares problem for the increments $z_{0:k} = \delta x_{0:k}$ as

$$\|z_0 - z_\mathrm{b}\|^2_{\mathbf{B}^{-1}} + \sum_{i=1}^{k} \|z_i - \mathbf{M}_i z_{i-1} - m_i\|^2_{\mathbf{Q}_i^{-1}} + \sum_{i=1}^{k} \|d_i - \mathbf{H}_i z_i\|^2_{\mathbf{R}_i^{-1}} \to \min_{z_{0:k}}$$

$$z_\mathrm{b} = x_\mathrm{b} - x_0, \quad m_i = \mathcal{M}_i\left(x_{i-1}\right) - x_i, \quad d_i = y_i - \mathcal{H}_i\left(x_i\right),$$

$$\mathbf{M}_i = \mathcal{M}_i'\left(x_{i-1}\right), \quad \mathbf{H}_i = \mathcal{H}_i'\left(x_i\right)$$

- This is the same function as minimized in the Kalman smoother (Rauch et al., 1965; Bell, 1994)

$$\begin{aligned} Z_0 &= z_\mathrm{b} & +V_0, &\quad V_0 \sim N\left(0, \mathbf{B}\right) \\ Z_i &= \mathbf{M}_i Z_{i-1} + m_i & +V_i, &\quad V_i \sim N\left(0, \mathbf{Q}_i\right) \\ d_i &= \mathbf{H}_i Z_i & +W_i, &\quad W_i \sim N\left(0, \mathbf{R}_i\right) \end{aligned}$$

- The least squares solution is the mean conditioned on the data

$$z_{0:k} = E\left(Z_{0:k} | d_{1:k}\right).$$

Kalman smoother for 4DVAR increments

- The least squares solution is the maximum likelihood estimate

$$p\left(z_{0:k}|d_{1:k}\right) = p\left(z_0\right)\prod_{i=1}^{k} p\left(z_i|z_{i-1},d_i\right)$$

$$\propto p\left(z_0\right)\prod_{i=1}^{k} p\left(d_i|z_i\right)p\left(z_i|z_{i-1}\right)$$

$$\propto \underbrace{e^{-\frac{1}{2}\|z_0-z_\mathrm{b}\|^2_{\mathbf{B}^{-1}}}}_{\propto\ p(z_0)}\prod_{i=1}^{k}\underbrace{e^{-\frac{1}{2}\|\mathbf{H}_i z_i-d_i\|^2_{\mathbf{R}_i^{-1}}}}_{\propto\ p\left(d_i|z_i\right)}\underbrace{e^{-\frac{1}{2}\|z_i-\mathbf{M}_i z_{i-1}-m_i\|^2_{\mathbf{Q}_i^{-1}}}}_{\propto\ p(z_i|z_{i-1})}\to\max_{z_{0:k}}$$

  by the Bayes theorem and the independence of the errors.
- All distributions in the linearized problem for the increments δx_i are gaussian $\Rightarrow$

$$\textbf{least squares solution} = \textbf{max of the joint pdf}\ p\left(z_{0:k}|d_{1:k}\right)$$
$$= \textbf{mean of the joint pdf}\ p\left(z_{0:k}|d_{1:k}\right)$$

Kalman smoother

- Recall: $\delta x_{0:k}$ are the mean of the smoothing pdf $p\left(\delta x_{0:k} | d_{1:k}\right)$:

$$\underbrace{p\left(z_{0:k} | d_{1:k}\right)}_{\substack{\text{joint analysis at}\\ \text{times 0 to } k}} \propto p\left(z_0\right) \prod_{i=1}^{k} \underbrace{p\left(d_i | z_i\right)}_{\substack{\text{Bayesian}\\ \text{update at } i}} \underbrace{p\left(z_i | z_{i-1}\right)}_{\substack{\text{advance time}\\ i-1 \text{ to } i}}$$

- Rewrite as the recursion:

$$\underbrace{p\left(z_{0:k} | d_{1:k}\right)}_{\substack{\text{joint analysis at}\\ \text{times 0 to } k}} = \underbrace{p\left(d_k | z_k\right)}_{\substack{\text{Bayesian}\\ \text{update at } k}} \underbrace{p\left(z_k | z_{k-1}\right)}_{\substack{\text{advance time}\\ k-1 \text{ to } k}} \underbrace{p\left(z_{0:k-1} | d_{1:k-1}\right)}_{\substack{\text{joint analysis at}\\ \text{times 0 to } k-1}}$$

- Compare with the filter (sequential Bayesian estimation):

$$\underbrace{p\left(z_k | d_{1:k}\right)}_{\substack{\text{analysis at}\\ \text{time } k}} \propto \underbrace{p\left(d_k | z_k\right)}_{\substack{\text{Bayesian}\\ \text{update at } k}} \overbrace{\underbrace{p\left(z_k | z_{k-1}\right)}_{\substack{\text{advance time}\\ k-1 \text{ to } k}} \underbrace{p\left(z_{k-1} | d_{1:k-1}\right)}_{\substack{\text{analysis at}\\ \text{time } k-1}}}^{p(z_k | d_{1:k-1}) = \text{forecast at time } k}$$

  - **Smoother = filter + update the history exactly the same way.**

Ensemble Kalman smoother (EnKS)

Ensembles: $U^N = [u^1, \ldots, u^N]$. $V^N \sim N(m, \mathbf{A})$ is i.i.d. from $N(m, \mathbf{A})$, $Z^N_{i|k}$ is ensemble of states at time i, conditioned on all data up to time i.

Ensemble Kalman filter (EnKF): Initialize $Z^N_{0|0} \sim N(z_\mathrm{b}, \mathbf{B})$.

For $i = 1, \ldots, k$, advance in time

$$Z^N_{i|i-1} = \mathbf{M}_i Z^N_{i-1|i-1} + V_i, \quad V_i \sim N(m_i, \mathbf{Q}_i)$$

followed by the analysis step

$$Z^N_{i|i} = Z^N_{i|i-1} - \mathbf{P}^N_i \mathbf{H}^\mathrm{T}_i (\mathbf{H}_i \mathbf{P}^N_i \mathbf{H}^\mathrm{T}_i + \mathbf{R}_i)^{-1} (\mathbf{H}_i Z^N_{i|i-1} - D_i), \quad D_i \sim N(d_i, \mathbf{R}_i)$$

$$\mathbf{P}^N_i = \frac{1}{N-1} (Z^N_{i|i-1} - \overline{Z}^N_{i|i-1})(Z^N_{i|i-1} - \overline{Z}^N_{i|i-1})^\mathrm{T} \quad \text{(sample covariance)}$$

So the analysis step makes linear combinations (transformation by a $\mathbf{T}^N_i$):

$$Z^N_{i|i} = Z^N_{i|i-1} \mathbf{T}^N_i, \quad \mathbf{T}^N_i \in \mathbb{R}^{N \times N}.$$

EnKS = EnKF + transform the history exactly the same way:

$$Z^N_{0:i|i} = Z^N_{0:i|i-1} \mathbf{T}^N_i.$$

Derivative-free implementation of the EnKS - model

The linearized model $\mathbf{M}_i = \mathcal{M}_i' \left(x_{i-1} \right)$ occurs only in advancing the time as action on the ensemble $Z^N = [z^n] = [\delta x^n]$

$$\mathbf{M}_i \delta x_{i-1}^n + m_i = \mathcal{M}_i' \left(x_{i-1} \right) \delta x_{i-1}^n + \mathcal{M}_i \left(x_{i-1} \right) - x_i$$

Approximating by finite differences with a parameter $\tau > 0$:

$$\mathbf{M}_i \delta x_{i-1}^n + m_i \approx \frac{\mathcal{M}_i \left(x_{i-1} + \tau \delta x_{i-1}^n \right) - \mathcal{M}_i \left(x_{i-1} \right)}{\tau} + \mathcal{M}_i \left(x_{i-1} \right) - x_i$$

Needs $N + 1$ evaluations of $\mathcal{M}_i$, at x_{i-1} and $x_{i-1} + \tau \delta x_{i-1}^n$.

Accurate in the limit $\tau \to 0$.
For $\tau = 1$, recover the nonlinear model: $\mathcal{M}_i \left(x_{i-1} + \delta x_{i-1}^n \right) - x_i$

Derivative-free implementation of the EnKS - observation

The observation matrix occurs only in the action on the ensemble,

$$\mathbf{H}_i Z^N = \left[\mathbf{H}_i \delta x^1, \ldots, \mathbf{H}_i \delta x^N\right].$$

Approximating by finite differences with a parameter $\tau > 0$:

$$\mathbf{H}_i \delta x_i^n \approx \frac{\mathcal{H}_i\left(x_{i-1} + \tau \delta x_{i-1}^n\right) - \mathcal{H}_i\left(x_{i-1}\right)}{\tau}$$

Needs $N+1$ evaluations of $\mathcal{H}_i$, at x_{i-1} and $x_{i-1} + \tau \delta x_{i-1}^n$.

Accurate in the limit $\tau \to 0$.

$\tau = 1 \Rightarrow$ becomes exactly the EnKS run on the nonlinear problem
$\Rightarrow$ EnKS independent of the point of linearization
$\Rightarrow$ no convergence of the 4DVAR iterations.
In our tests, $\tau = 0.1$ seems to work well enough.

Tikhonov regularization and Levenberg-Marquardt method

- Gauss-Newton may not converge, even locally. Add a penalty (Tikhonov regularization) to control the size of the increments δx_i :

$$\|\delta x_0 - z_\mathrm{b}\|^2_{\mathbf{B}^{-1}} + \sum_{i=1}^{k} \|\delta x_i - \mathbf{M}_i \delta x_{i-1} - m_i\|^2_{\mathbf{Q}_i^{-1}} + \sum_{i=1}^{k} \|d_i - \mathbf{H}_i \delta x_i\|^2_{\mathbf{R}_i^{-1}}$$
$$+ \gamma \sum_{i=0}^{k} \|\delta x_i\|^2_{\mathbf{S}_i^{-1}} \to \min_{\delta x_{0:k}}$$

- Becomes the Levenberg-Marquardt method, which is guaranteed to converge for large enough γ.
- Implement the regularization as independent observations $\delta x_i \approx 0$ with error covariance $\mathbf{S}_i$: simply run the analysis step the second time (Johns and Mandel, 2008). Here, this is statistically exact because the distributions in the Kalman smoother are gaussian.

Convergence of the ensemble Kalman smoother

- Consider reference random vector $Z_{i|k}$, the state at time i conditioned exactly on all data up to time k.
- **Algorithm** (Kalman smoother on reference random vectors) Initialize $Z_{0|0} \sim N(z_\mathrm{b}, \mathbf{B})$.
  For $i = 1, \ldots, k$, advance in time

$$Z_{i|i-1} = \mathbf{M}_i Z^N_{i-1|i-1} + V_i, \quad V_i \sim N(m_i, \mathbf{Q}_i)$$

  followed by the analysis step with the exact covariance

$$Z_{0:|i} = Z_{0:i|i-1} - \mathbf{P}_{0:i,i}\mathbf{H}_i^\mathrm{T}(\mathbf{H}_i\mathbf{P}_i\mathbf{H}_i^\mathrm{T} + \mathbf{R}_i)^{-1}(\mathbf{H}_i Z^n_{i|i-1} - D_i),$$

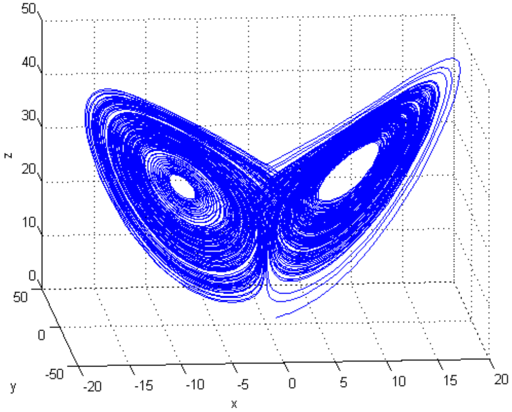
$$\text{where } \mathbf{P}_{0:i,i} = \mathrm{Cov}(Z_{0:i|i-1}, Z_{i|i-1}), \quad D_i \sim N(d_i, \mathbf{R}_i)$$

- **Theorem** $Z_{i|i}$ has the filtering distribution $p(z_i|d_{1:i})$.
- **Theorem** $Z_{0:i|i}$ has the smoothing distribution $p(z_{0:i}|d_{1:i})$.
- **Theorem** (Convergence of the ensemble Kalman smoother)

$$\mathbf{P}^N \to \mathbf{P}_i, \quad Z^j_{i|i} \to Z_{i|i} \text{ as } N \to \infty, \text{for all } i, \text{ in all } L^p, 1 \le p < \infty.$$

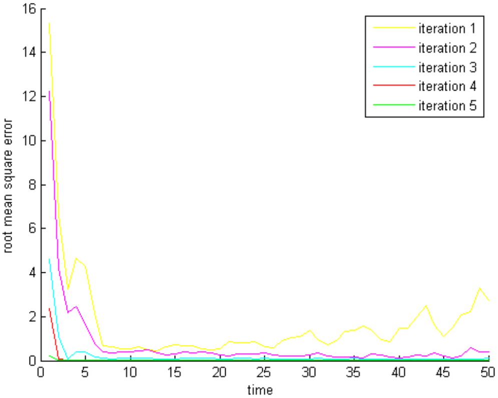
Computational results

Lorenz 63 model



$$\frac{dx}{dt} = -\sigma(x - y)$$
$$\frac{dy}{dt} = \rho x - y - xz$$
$$\frac{dz}{dt} = xy - \beta z$$

EnKS-4DVAR for Lorenz 63 model



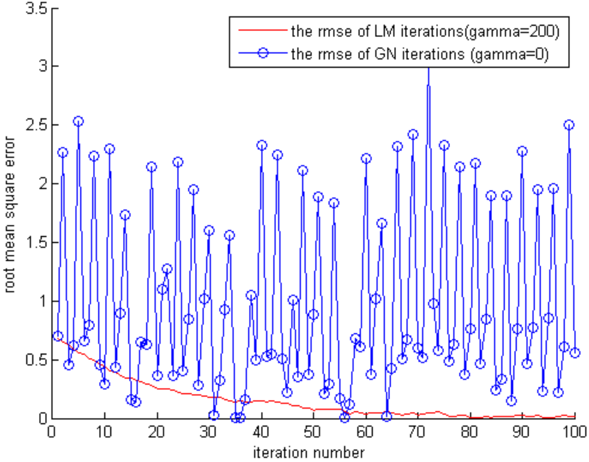
Root mean square error of EnKS-4DVAR iterations over 50 timesteps

Iteration	1	2	3	4	5	6
RMSE	20.16	15.37	3.73	2.53	0.09	0.09

An example where Gauss-Newton does not converge

$$(x_0 - 2)^2 + (3 + x_1^2)^2 + 10^6 (x_0 - x_1)^2 \to \min$$

4DVAR with $x_b = 2$, $\mathbf{B} = \mathbf{I}$, $M_1 = I$, $\mathcal{H}_1(x) = x^2$, $y_1 = 3$, $\mathbf{Q}_1 = 10^{-6}$



Related work

- The equivalence between weak constraint 4DVAR and Kalman smoothing is approximate for nonlinear problems, but still useful (Fisher et al., 2005).
- Hamill and Snyder (2000) estimated backgroud covariance from ensemble for 4DVAR.
- Gradient methods in the span of the ensemble for one analysis cycle (i.e., 3DVAR) include Zupanski (2005), Sakov et al. (2012) (with square root EnKF as a linear solver in Newton method), and Bocquet and Sakov (2012), who added regularization and use LETKF-like approach to minimize the nonlinear cost function over linear combinations of the ensemble.
- Liu et al. (2008, 2009) combine ensembles with (strong constraint) 4DVAR and minimize in the observation space.
- Zhang et al. (2009) use EnKF to obtain the covariance for 4DVAR, and 4DVAR to feed the mean analysis into EnKF.

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