NAVAL POSTGRADUATE SCHOOL

Data Assimilation for Models with a Sparse Error Covariance

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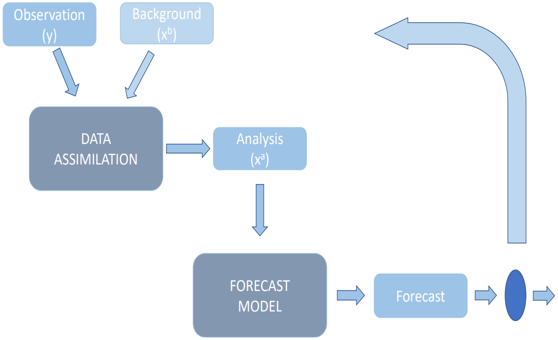
Numerical Weather Prediction



Data Assimilation

System Model

$$
\begin{aligned}
x_{k+1} &= \mathcal{M}(x_k) + \eta_k, \quad x_k \in \mathbb{R}^n, \quad \eta_k \sim \text{model uncertainty}, Q \\
y_k &= \mathcal{H}(x_k) + \delta_k, \quad y_k \in \mathbb{R}^m, \quad \delta_k \sim \text{sensor noise}, R
\end{aligned}
$$

Linearization

$$
\begin{aligned}
x_{k+1} &= M_k x_k + \cdots \\
y_k &= H_k x_k + \cdots
\end{aligned}
$$

Both n and m are very large. In daily operations, only a small part of sensor data is used.

Challenges

4D-Var

- It is an effective method to provide estimation results with an affordable computational load.
- The method does not provide information about error covariance.
- It requires tangent linear models and adjoint models.

EnKF

- EnKF does not require tangent linear model and adjoint model
- It contains partial information about error statistics
- Undersampling and rank deficiency
- Filter divergence, inbreeding, spurious correlations

Sparsity-based Filters

Sparsity-based filters: The goal is to avoid rank deficiency, provide more error covariance information, and achieve granularity control for optimal parallelism.

A variety of parallel computing architectures are available; and new technologies are being developed rapidly.

- Multi-core CPU
- General-purpose GPU
- Clusters or massively parallel computing
- Grid computing
- Application-specific integrated curcuits
- ......

Sparsity of error covariance

Ensemble	Sparse Covariance
X X X X X	X
X X X X X	X X
X X X X X	X X X
X X X X X	X X X X
X X X X X	0 X X X X
X X X X X	0 0 X X X X
X X X X X	0 0 0 X X X X
X X X X X	0 0 0 0 X X X X
X X X X X	0 0 0 0 0 X X X X
X X X X X	0 0 0 0 0 0 X X X X
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X X X X X	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 X X X X

Sparsity based methods

- Approximately sparse error covariance

$$N_{sp} = \text{maximum number of nonzero entries in columns}$$
$$\mathcal{I}_i(P) = \text{indices of nonzero entries in the } i\text{th-column}$$

- Component-based numerical model

$$\mathcal{M}(x_k^{sp}; \mathcal{I}) \text{ or } \mathcal{M}^{comp}$$
$$\mathcal{I} = \text{ indices of entries to be evaluated}$$

A progressive approach

Assume

$$M_k P_k M_k^T = P_k + \Delta P_{k+1}$$

To estimate ΔP_{k+1}, assume

$$M_{k+1} = I + \Delta M_k$$

$$x_{k+1} = \mathcal{M}(x_k) = x_k + \Delta(x_k)$$

Then

$$\begin{aligned} M_k P_k M_k^T &= (I + \Delta M_k) P_k (I + \Delta M_k^T) \\ &= P_k + \Delta M_k P_k + (\Delta M_k P_k)^T + \cdots \\ &\approx \left(\mathcal{M}(x_k + \delta P_k) - \mathcal{M}(x_k)\right)/\delta \\ &+ \left(\mathcal{M}(x_k + \delta P_k) - \mathcal{M}(x_k)\right)^T/\delta - P_k \end{aligned}$$

Progressive KF

Background $x_{k|k}$ and $P^{sp}_{k|k}$ (sparse covariance approximation)

Forecast

$$\begin{aligned}
x_{k+1|k} &= \mathcal{M}(x_{k|k}) \\
y_{k+1|k} &= \mathcal{H}(x_{k|k}) \\
P^{sp}_{k+1|k} &= \left(\mathcal{M}^{comp}(x^{sp}_{k|k} + \delta P^{sp}_{k|k}) - \mathcal{M}^{comp}(x^{sp}_{k|k})\right)/\delta \\
&\quad + \left(\mathcal{M}^{comp}(x^{sp}_{k|k} + \delta P^{sp}_{k|k}) - \mathcal{M}^{comp}(x^{sp}_{k|k})\right)^T/\delta \\
&\quad - P^{sp}_{k|k} + Q
\end{aligned}$$

Analysis

$$\begin{aligned}
K &= P^{sp}_{k+1|k} H^T_{k+1} (H_{k+1} P^{sp}_{k+1|k} H^T_{k+1} + R)^{-1} \\
P^{sp}_{k+1|k+1} &= (I - K H_{k+1}) P^{sp}_{k+1|k} \\
x_{k+1|k+1} &= x_{k+1|k} + K(y_{k+1} - y_{k+1|k})
\end{aligned}$$

Computational load

Progressive KF Full model	number of model components evaluation
$\mathcal{M}(x_k)$ $\mathcal{M}\left(x_k + \delta P_k(:, i)\right)$ $i = 1, 2, \cdots, n$	$(n+1)nN_p$ N_p- progressive steps
Progressive KF Component-based model	
$\mathcal{M}(x_k)$ $\mathcal{M}\left(x_k + \delta P_k(:, i), \mathcal{I}_i(P)\right)$ $i = 1, 2, \cdots, n$	$(N_{sp}+1)nN_p$
Ensemble KF	
$\mathcal{M}(x_k^i)$ $i = 1, 2, \cdots, N_{ens}$	$N_{ens}n$

Avoid rank deficiency and achieve granularity control

Ensemble

```
X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
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X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
X X X X X
```

Rank: N_{ens}

Size: n x N_{ens}

Sparse Covariance

```
X
XX
XXXX
XXXXX
0000XX
00000XX
000000XX
0000000XX
00000000XX
000000XXXXX
0000000XXXXX
00000000XXXXX
00000000000XXX
000000000000XXX
0000000000000XXX
00000000000000XXX
000000000000000XXX
0000000000000000XXX
00000000000000000XXX
000000000000000000XXX
```

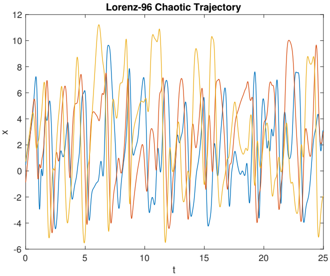
- **P has full rank**
- **N_{sp} is a variable**
- **Tasks can be grouped in different size:**
  Coarse-grained, medium-grained, fine-grained
- **P localization is straightforward**

Lorenz-96 model

$$\frac{dx_i}{dt} = (x_{i+1} - x_{i-2})x_{i-1} - x_i + F, \quad i = 1, 2, \cdots, m$$
$$x_{m+1} = x_1$$

Discretization - 4th-order RK

$$x_k = \mathcal{M}(x_{k-1})$$
$$\Delta t = 0.025$$
$$F = 8$$
$$m = 40$$



A comparison

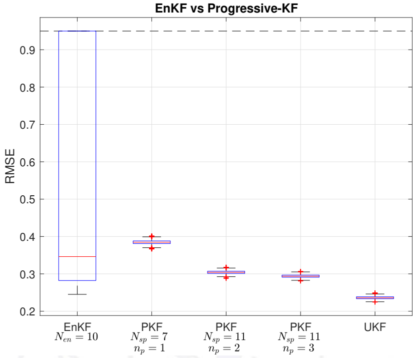
$N = 1000$ initial states in $[-1\ 1]$ - uniform distribution.

$N_{filter} = 4000$ filter steps

$m = 20$ measurement locations

$R = I$

Filter	Size	CMPT EVAL
EnKF	$N_{ens} = 10$	400
P-KF	$N_{sp} = 7$, $N_p = 1$	320
P-KF	$N_{sp} = 11$, $N_p = 2$	480x2
P-KF	$N_{sp} = 11$, $N_p = 3$	480x3



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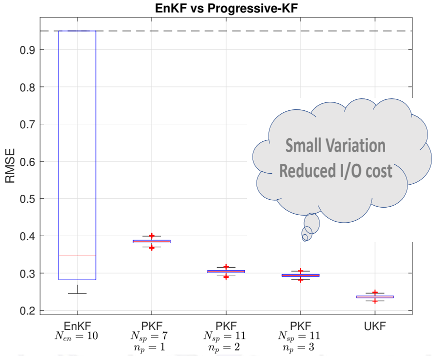

Unscented KF (UKF)

σ-points $x^i_{k|k}$, $0 \leq i \leq 2n$

$$x^0_{k|k} = x_{k|k}$$

Forecast $x^i_{k+1|k} = \mathcal{M}(x^i_{k|k}), \quad y^i_{k+1|k} = \mathcal{H}(x^i_{k|k}), \quad 0 \leq i \leq 2n$

$$\bar{x}_{k+1} = \sum_{i=0}^{2n} w_i x^i_{k+1|k}, \quad \bar{y}_{k+1} = \sum_{i=0}^{2n} w_i y^i_{k+1|k}$$

$$P_{k+1|k} = \sum_{i=0}^{2n} w_i \Delta x^i_{k+1} (\Delta x^i_{k+1})^T + Q$$

$$\Delta x^i_{k+1} = x^i_{k+1|k} - \bar{x}_{k+1}$$

$$w_0 = \frac{\kappa}{n+\kappa}, \; w_i = \frac{\kappa}{2(n+\kappa)}$$

UKF (Cont.)

Analysis

$$P^{yy} = \sum_{i=0}^{2n} w_i \Delta y^i_{k+1} (\Delta y^i_{k+1})^T + R, \quad \Delta y_{k+1} = y^i_{k+1|k} - \bar{y}_{k+1}$$

$$P^{xy} = \sum_{i=0}^{2n} w_i \Delta x^i_{k+1} (\Delta y^i_{k+1})^T$$

$$K P^{yy} = P^{xy}$$

$$x_{k+1|k+1} = \bar{x}_{k+1} + K(y_{k+1} - \bar{y}_{k+1})$$

Update

$$P_{k+1|k+1} = P_{k+1|k} - K(P^{xy})^T$$

$$x^i_{k+1|k+1} = x_{k+1|k+1} + \sqrt{(n+\kappa) P_{k+1|k+1}}, \quad i = 1, 2, \cdots, n$$

$$x^i_{k+1|k+1} = x_{k+1|k+1} - \sqrt{(n+\kappa) P_{k+1|k+1}}, \quad i = n+1, \cdots, 2n$$

Sparsity of square root matrix

Theorem (S. Toledo). If P is a symmetric positive definite matrix. The amount of storage for a Cholesky decomposition of P is $O(n + 2\eta(P))$, where $\eta(P)$ is the number of nonzero entries in P.

Assumption: The sparsity patterns of P and $(\sqrt{P})^f$ are known.

Sparse UKF

Sparse σ-points

$$x^0_{k|k} = x_{k|k}$$

$$\sigma^i,\ \mathcal{I}_i \text{ (sparsity index)} \qquad 1 \le i \le n$$

Forecast

$$x^0_{k+1|k} = \mathcal{M}(x^0_{k|k}),$$

$$x^i_{k+1|k} = \mathcal{M}^{comp}(x^0_{k|k} + \sigma^i), \qquad x^{i+n}_{k+1|k} = \mathcal{M}^{comp}(x^0_{k|k} - \sigma^i)$$

$$y^i_{k+1|k} = \mathcal{H}(x^i_{k+1|k} \triangleright_{\mathcal{I}_i} x^0_{k+1|k}), \qquad 1 \le i \le 2n$$

$$\bar{x}_{k+1} = \sum_{i=0}^{2n} w_i (x^i_{k+1|k} \triangleright_{\mathcal{I}_i} x^0_{k+1|k}), \quad \bar{y}_{k+1} = \sum_{i=0}^{2n} w_i y^i_{k+1|k}$$

$$P^{sp}_{k+1|k} = \sum_{i=0}^{2n} w_i \left(\Delta x^i_{k+1} (\Delta x^i_{k+1})^T \right)^{sp} + Q$$

$$w_0 = \frac{\kappa}{n+\kappa},\ w_i = \frac{\kappa}{2(n+\kappa)},\ \Delta x^i_{k+1} = x^i_{k+1|k} \triangleright_{\mathcal{I}_i} x^0_{k+1|k} - \bar{x}_{k+1}$$

$x^{sp}_1 \triangleright_{\mathcal{I}} x_2$ - merging operation.

Sparse UKF (Cont.)

Analysis

$$P^{yy} = \sum_{i=0}^{2n} w_i \Delta y^i_{k+1} (\Delta y^i_{k+1})^T, \quad \Delta y^i_{k+1} = y^i_{k+1|k} - \bar{y}_{k+1}$$

$$P^{xy} = \sum_{i=0}^{2n} w_i \Delta x^i_{k+1} (\Delta y^i_{k+1})^T$$

$$K P^{yy} = P^{xy}$$

$$x_{k+1|k+1} = \bar{x}_{k+1} + K(y_{k+1} - \bar{y}_{k+1})$$

Update

$$P^{sp}_{k+1|k+1} = P^{sp}_{k+1|k} - \left(K(P^{xy})^T\right)^{sp}$$

$$\sigma^i, \mathcal{I}_i \sim \sqrt{(n+\kappa) P^{sp}_{k+1|k+1}}, \qquad i = 1, 2, \cdots, n$$

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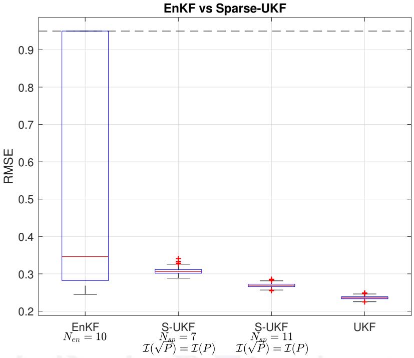
S-UKF	$N_{sp} = 7$	600
S-UKF	$N_{sp} = 11$	920



Sparsity-based Filters

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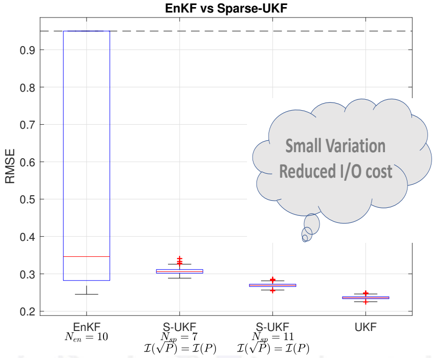

Summary

	Progressive KF	Sparse UKF
Full rank covariance	✓	✓
Small variation	✓	✓
Reduced I/O cost	✓	✓
$P_{k+1} \approx P_k + \Delta P_k$	✓	
Cholesky decomposition		✓

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Cholesky decomposition		✓

Thank you!