Study of the Algorithmic Complexity of the Ensemble Kalman Filter and its Efficient Implementations

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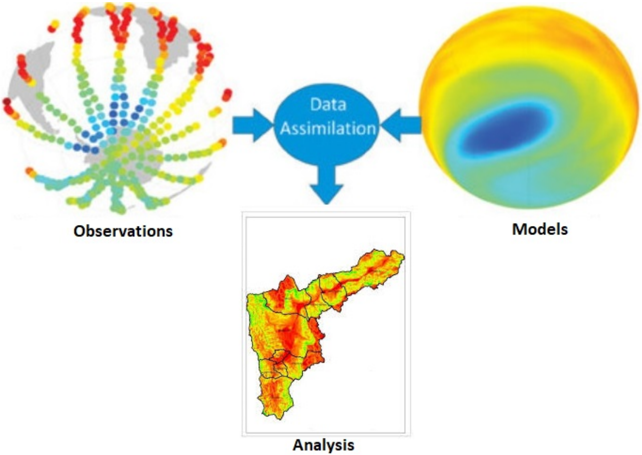
Outline

Introduction



Introduction

Linear and Non-Linear Data Assimilation

Gaussian

Ensemble Kalman Filter-EnKF

Variational Data Assimilation

Non-Gaussian

Particle Filters

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Introduction

Linear and Non-Linear Data Assimilation

Gaussian

- Ensemble Kalman Filter-EnKF
- Variational Data Assimilation

Non-Gaussian

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Current Work

- REnKF
- En 4DVar
- PF 4DVar

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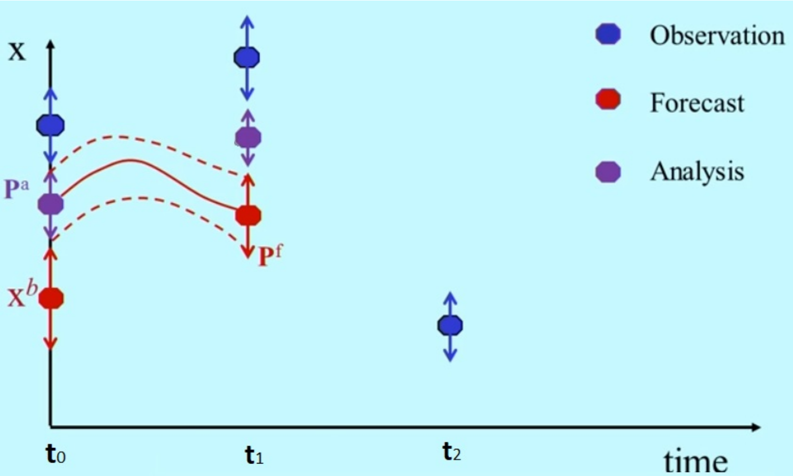
Foundation of the Problem

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x}) \cdot p(\mathbf{x})}{p(\mathbf{y})}$$

Kalman Filter



Kalman Filter

Assume we seek to estimate the state $\mathbf{x} \in \mathbb{R}^n$

$$\mathbf{x}_{k+1} = \mathbf{M}\left(\mathbf{x}_k, t_k\right) + \mathbf{w}_k,$$

using the measurements $\mathbf{y} \in \mathbb{R}^m$

$$\mathbf{y}_k = \mathbf{H}_k \mathbf{x}_k + \mathbf{v}_k,$$

with

$$\mathbf{w}_k \sim \mathbf{N}(\mathbf{0}, \mathbf{Q}_k),$$
$$\mathbf{v}_k \sim \mathbf{N}(\mathbf{0}, \mathbf{R}_k),$$

$\mathbf{Q}_k \in \mathbb{R}^{n\times n}$, $\mathbf{R}_k \in \mathbb{R}^{m\times m}$.
$\mathbf{M} : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $\mathbf{H} : \mathbb{R}^m \rightarrow \mathbb{R}^n$.

Kalman Filter

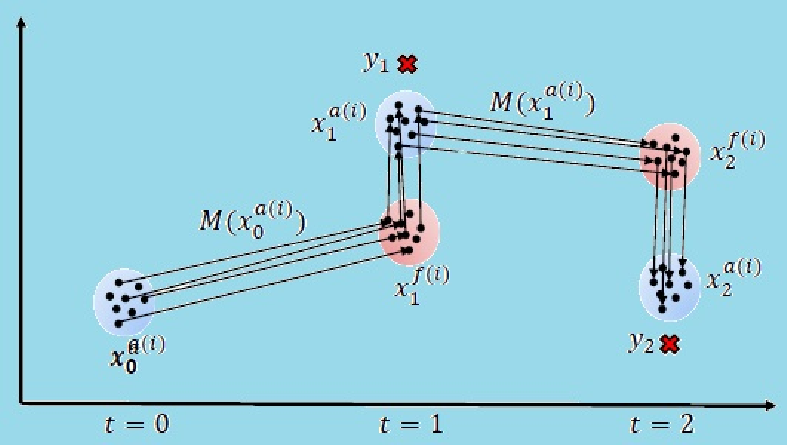
1. Forecast Step:

$$\mathbf{x}^f_{k+1} = \mathbf{M}_{k+1}\mathbf{x}^a_k,$$
$$\mathbf{P}^f_{k+1} = \mathbf{M}_{k+1}\mathbf{P}^a_k\mathbf{M}^T_{k+1} + \mathbf{Q}_{k+1}.$$

2. Analysis Step:

$$\mathbf{K}_{k+1} = \mathbf{P}^f_{k+1}\mathbf{H}^T\left(\mathbf{H}\mathbf{P}^f_{k+1}\mathbf{H}^T + \mathbf{R}_{k+1}\right)^{-1},$$
$$\mathbf{x}^a_{k+1} = \mathbf{x}^f_{k+1} + \mathbf{K}_{k+1}\left(\mathbf{y}_{k+1} - \mathbf{H}\mathbf{x}^f_{k+1}\right),$$
$$\mathbf{P}^a_{k+1} = \left(\mathbf{I} - \mathbf{K}_{k+1}\mathbf{H}\right)\mathbf{P}^f_{k+1}.$$

Ensemble Kalman Filter EnKF



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Ensemble Kalman Filter EnKF

1. Forecast Step:

$$\mathbf{x}_{k+1}^{f} = \mathbf{M}_{k+1}\left(\mathbf{x}_{k}^{a}\right),$$
$$\mathbf{P}_{k+1}^{f} = \frac{1}{N-1}\sum_{i=1}^{N}\left(\mathbf{x}_{i}^{f} - \overline{\mathbf{x}}^{f}\right)\left(\mathbf{x}_{i}^{f} - \overline{\mathbf{x}}^{f}\right)^{T},$$

with N, number of ensemble members and

$$\overline{\mathbf{x}}^{f} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_{i}^{f}.$$

2. Analysis Step:

$$\mathbf{K}_{k+1} = \mathbf{P}_{k+1}^{f}\mathbf{H}^{T}\left(\mathbf{H}\mathbf{P}_{k+1}^{f}\mathbf{H}^{T} + \mathbf{R}_{k+1}\right)^{-1},$$
$$\mathbf{x}_{k+1}^{a} = \mathbf{x}_{k+1}^{f} + \mathbf{K}_{k+1}\left(\mathbf{y}_{k+1} - \mathbf{H}\mathbf{x}_{k+1}^{f}\right).$$

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Efficient Implementation

- **Advantage**
  1. To reduce the computational cost, in terms of the number of operations, of assimilating large data sets.
  2. The resulting algorithms scale linearly with respect to the number of observations.

Efficient Implementation

- **Advantage**
  1. To reduce the computational cost, in terms of the number of operations, of assimilating large data sets.
  2. The resulting algorithms scale linearly with respect to the number of observations.
- **Issues**
  1. The computational cost of the subsequent matrix operations can become expensive.
  2. The additional operations may contribute significantly to the total computational cost of the implementation.

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SVD Implementation

procedure (SVD-EnKF)$\left(\mathbf{X}, \mathbf{X}', \mathbf{HX}', \mathbf{D}, \mathbf{E}\right)$

  $[\Sigma,\ \mathbf{U},\ \mathbf{V}] \leftarrow \text{SVD}(\mathbf{HX}' + \mathbf{E})\ (mN^2)$

  $\Lambda \leftarrow \Sigma\Sigma^T\ (m)$

  $s \leftarrow \sum_i \lambda_{i,i}\ (m)$

  $p \leftarrow max\left\{k \mid \sum_k \lambda_{k,k|s<0.99}\right\}$

  $\mathbf{X}_1 \leftarrow \Lambda^{-1}\mathbf{U}^T\ (mp)$

  $\mathbf{X}_2 \leftarrow \mathbf{X}_1\mathbf{D}\ (mnp)$

  $\mathbf{X}_3 \leftarrow \mathbf{U}\mathbf{X}_2\ (mNp)$

  $\mathbf{X}_4 \leftarrow \left(\mathbf{HX}'\right)^T\mathbf{X}_3\ (mN^2)$

  $\mathbf{X}^a \leftarrow \mathbf{X} + \mathbf{X}'\mathbf{X}_4\ (nN^2)$

  return $\mathbf{X}^a$

end procedure

Computational cost: $O\left(nN^2 + mN^2 + mNp + mN + m\right)$

Cholesky Decomposition Implementation

procedure (CHOL-EnKF)$\left(\mathbf{X}, \mathbf{X}', \mathbf{HX}', \mathbf{D}, \mathbf{E}\right)$

$\mathbf{R} \leftarrow \frac{1}{N-1}\text{diag}\left(\mathbf{E}\mathbf{E}^T\right)$

$\mathbf{Q} \leftarrow (N-1)\,\mathbf{I} + \left(HX'\right)^T \mathbf{R}^{-1}\left(\mathbf{HX}'\right)\ \left(mN^2\right)$

$\mathbf{L}\mathbf{L}^T \leftarrow \textbf{CHOLESKYM}\left(\mathbf{Q}\right)\ \left(N^3\right)$

$\mathbf{Z} \leftarrow \left(\mathbf{HX}'\right)^T \mathbf{R}^{-1}\mathbf{D}\ \left(mN^2\right)$

$\mathbf{W} \leftarrow \mathbf{Q}^{-1}\mathbf{Z}\ \left(N^3\right)$

$\mathbf{M} \leftarrow \mathbf{R}^{-1}\left[\mathbf{I} - \left(\mathbf{HX}'\mathbf{W}\right)\right]\ \left(mN^2\right)$

$\mathbf{Z} \leftarrow \left(\mathbf{HX}'\right)^T \mathbf{M}\ \left(mN^2\right)$

$\mathbf{X}^a \leftarrow \mathbf{X} + \frac{1}{N-1}\mathbf{X}'\mathbf{Z}\ \left(nN^2\right)$

return $\mathbf{X}^a$

end procedure

Computational cost: $O\left(N^3 + nN^2 + mN^2\right)$

Sherman Morrison Implementation

procedure (MF-EnKF)$\left(\mathbf{X}, \mathbf{X}', \mathbf{HX}', \mathbf{D}, \mathbf{E}\right)$
    $\mathbf{R} \leftarrow \text{diag}\left(\mathbf{E}\mathbf{E}^T\right)$
    call **SM** $\left(\mathbf{R}, \mathbf{HX}', \mathbf{HX}', \mathbf{d}_1, \mathbf{z}_1\right)$ $\left(mN^2\right)$
    $\mathbf{w} \leftarrow \mathbb{X}' \left(\mathbf{HX}'\right)^T \mathbf{z}_1$ $\left(nN\right)$
    $\mathbf{x}_1^a \leftarrow \mathbf{x}_1 + \mathbf{w}$ $\left(n\right)$
    for do $i \leftarrow 2, \ldots N$ do
        call **SIMPLIFIED** $\left(\mathbf{R}, \mathbf{HX}', \mathbf{d}_i, \mathbf{z}_i\right)$ $\left(mN\right)$
        $\mathbf{w} \leftarrow \mathbf{X}' \left(\mathbf{HX}'\right)^T \mathbf{z}_i$ $\left(nN\right)$
        $\mathbf{x}_1^a \leftarrow \mathbf{x}_i + \mathbf{w}$ $\left(n\right)$
    end for
    return $\mathbf{X}^a$
end procedure

Computational cost: $O\left(mN^2 + nN + mN + n\right)$

Thanks!

References

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Sherman-Morrison Solver

Sherman-Morrison solver as described in Evensen 1994 y Maponi 2007.

procedure (SM)$(\mathbf{A}_0, \mathbf{U}, \mathbf{V}, \mathbf{b}, \mathbf{x})$
    Solve $\mathbf{A}_0\mathbf{x}_0 \leftarrow \mathbf{b}$
    Solve $\mathbf{A}_0\mathbf{y}_{0,k} \leftarrow \mathbf{u}_k$ for $k \leftarrow 1, \ldots, N$
    for do $i \leftarrow 1 \ldots, N-1$
        $$\mathbf{x}_i \leftarrow \mathbf{x}_{i-1} - \frac{\mathbf{v}_i^T \mathbf{x}_{i-1}}{1+\mathbf{v}_i^T \mathbf{y}_{i-1,i}} \mathbf{y}_{i-1,i}$$
        for do $k \leftarrow i+1, \ldots, N$
            $$y_{i,k} \leftarrow y_{i-1,k} - \frac{\mathbf{v}_i^T \mathbf{y}_{i-1,k}}{1+\mathbf{v}_i^T \mathbf{y}_{i-1,i}} \mathbf{y}_{i-1,i}$$
        end for
    end for
    $$\mathbf{x}_N \leftarrow \mathbf{x}_{N-1} - \frac{\mathbf{v}_N^T \mathbf{x}_{N-1}}{1+\mathbf{v}_N^T \mathbf{y}_{N-1,N}} \mathbf{y}_{i-1,i}$$
    return $\mathbf{x}$
end procedure

Simplified Sherman-Morrison Solver Subsequent Right-hand Sides

procedure (SIMPLIFIED)($\mathbf{A}_0$,$\mathbf{V}$,$\mathbf{b}$,$\mathbf{x}$)
    Solve $\mathbf{A}_0\mathbf{x}_0 \leftarrow \mathbf{b}$
    for **do** $i \leftarrow 1, \ldots, N$
        $\mathbf{x}_i \leftarrow \mathbf{x}_{i-1} - \frac{\mathbf{v}_i^T \mathbf{x}_{i-1}}{1+\mathbf{v}_i^T \mathbf{y}_{i-1,i}} \mathbf{y}_{i-1,i}$
    end for
    return $\mathbf{x}$
end procedure