UNBC UNIVERSITY OF NORTHERN BRITISH COLUMBIA

Advanced Data Assimilation

in strongly nonlinear systems

via Sigma-point Kalman Filters

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Introduction

Data assimilation: A dynamical state-space estimation problem

$$\boldsymbol{\theta}_k = \boldsymbol{f}\left(\boldsymbol{\theta}_{k-1}, \boldsymbol{q}_{k-1}\right)$$

$$\psi_k = \boldsymbol{h}\left(\boldsymbol{\theta}_k, \boldsymbol{r}_k\right)$$

where $\boldsymbol{\theta}_k$ represents the system state vector at time k, $\boldsymbol{f}(\cdot)$ is the nonlinear function of the state, $\boldsymbol{q}_k$ is the random (white) model errors, ψ_k is the measured state, $\boldsymbol{h}(\cdot)$ is the measurement function, and $\boldsymbol{r}_k$ is the zero-mean random measurement noise.

Sigma-point Kalman filter

- **The SPKF algorithm has been successfully implemented in many areas like robotics, artificial intelligence, natural language processing, and global positioning systems navigation.**

- **The SPKF makes use of a reformulated Kalman gain K and "chooses" the ensemble deterministically in such a way that it can estimate the statistical moments of the nonlinear model accurately; in other words, the forecast error covariance equation is computed using deterministically chosen samples, called "sigma-points".**

Ref: (Nørgad Magnus et al. 2000; Ito and Xiong 2000; Lefebvre et al. 2002;Wan and Van Der Merve 2000; Haykin 2001; Van der Merwe 2004, Julier et al. 1995; Van der Merwe and Wan4 April 2001,M;).

Kalman gain & Covariance update equations

Standard equations:

$$K_k = P_{\theta_k}^{-} H^{\mathrm{T}} \left[H P_{\theta_k}^{-} H^{\mathrm{T}} + R \right]^{-1}$$

$$P_{\theta_k} = \left(I - K_k H \right) P_{\theta_k}^{-}$$

Alternative forms:

$$K_k = P_{\theta_k \tilde{\psi}_k} P_{\tilde{\psi}_k}^{-1}$$

$$P_{\theta_k} = P_{\theta_k}^{-} - K_k P_{\tilde{\psi}_k} K_k^{\mathrm{T}}$$

$P_{\theta_k \tilde{\psi}_k}$ ➔ cross-covariance between the state and observation errors

$P_{\tilde{\psi}_k}$ ➔ error covariance of the difference between model and observations

No linear assumption for measurement function.

Ref: (Simon, D. 2006, Gelb, A. 1974)

SP-Unscented Kalman filter

Unscented transformation (Julier et al. 1995; Julier 1998; Wan and Van Der Merve 2000; Julier 2002).

$$\mathcal{X}_{k,0} = \theta_k \qquad w_0^{(m)} = \frac{\lambda}{(L+\lambda)} \tag{2.42}$$

$$\mathcal{X}_{k,i}^{+} = \theta_k + \left(\sqrt{(L+\lambda)\,\boldsymbol{P}_{\boldsymbol{\theta}_k}}\right)_i \quad i=1,\ldots,L \qquad w_0^{(c)} = \frac{\lambda}{(L+\lambda)} + \left(1-\alpha^2+\beta\right) \tag{2.43}$$

$$\mathcal{X}_{k,i}^{-} = \theta_k - \left(\sqrt{(L+\lambda)\,\boldsymbol{P}_{\boldsymbol{\theta}_k}}\right)_i \quad i=(L+1),\ldots,2L \qquad w_i^{(m)} = w_i^{(c)} = \frac{1}{2\,(L+\lambda)} \quad i=1,\ldots,2L \tag{2.44}$$

$\lambda = \alpha^2\,(L+\kappa) - L$ is a scaling parameter.

The sigma-point vector is then propagated through the nonlinear model

SP-Central Difference KF

- **In SP-CDKF the analytical derivatives in EKF are replaced by numerically evaluated central divided differences, based on Sterling's polynomial interpolation.**

$$\mathcal{X}_{k,0} = \bar{\boldsymbol{\theta}}_k \qquad w_0^{(m)} = \frac{\delta^2 - L}{\delta^2}$$

$$\mathcal{X}_{k,i}^{+} = \bar{\boldsymbol{\theta}}_k + \left(\sqrt{\delta^2 \boldsymbol{P}_{\theta_k}}\right)_i \quad i = 1, \ldots, L \qquad w_i^{(m)} = \frac{1}{2\delta^2} \quad i = 1, \ldots, 2L$$

$$\mathcal{X}_{k,i}^{-} = \bar{\boldsymbol{\theta}}_k - \left(\sqrt{\delta^2 \boldsymbol{P}_{\theta_k}}\right)_i \quad i = (L+1), \ldots, 2L \qquad w_i^{(c_1)} = \frac{1}{4\delta^2} \quad i = 1, \ldots, 2L$$

$$w_i^{(c_2)} = \frac{\delta^2 - 1}{4\delta^4} \quad i = 1, \ldots, 2L$$

where δ is the central difference step size

Ref: (**Ito and Xiong 2000; Nørga°d Magnus et al. 2000; Lefebvre et al. 2002).**

SPKF and EnKF

- We can extend the sigma-point approach to ensemble Kalman filter and formulate the ensemble Kalman filter as a **"general sigma-point Kalman filter"** without a specific selection scheme.

we can consider each perturbed initial state as a EnKF *sigma-point.*

$$\mathcal{X}_{k,m} = \boldsymbol{\theta}_{k,m} + \epsilon_{k,m} \qquad w = \frac{1}{(M-1)}$$

Now the ensemble forecast error covariance given by

$$\boldsymbol{P}^f = \boldsymbol{P}^-_{\theta_k} \approx \frac{1}{M-1}\sum_{m=1}^{M}\left(\mathcal{X}^f_{k,m} - \overline{\mathcal{X}^f_k}\right)\left(\mathcal{X}^f_{k,m} - \overline{\mathcal{X}^f_k}\right)^{\mathrm{T}}$$

$$= w\sum_{m=1}^{M}\left(\mathcal{X}^f_{k,m} - \hat{\boldsymbol{\theta}}^-_k\right)\left(\mathcal{X}^f_{k,m} - \hat{\boldsymbol{\theta}}^-_k\right)^{\mathrm{T}}$$

where

$$\hat{\boldsymbol{\theta}}^-_k \approx \overline{\mathcal{X}^f_k} = w\sum_{m=1}^{M}\mathcal{X}^f_{k,m}$$

- In other words the forecast sigma-points in SP-UKF and SP-CDKF and other Sigma-point Kalman filter algorithms are actually specific ensembles conditioned on the specific selection schemes

Lorenz '63 model

$$\frac{dx}{dt} = \sigma\left(y - x\right) + q^x$$

$$\frac{dy}{dt} = \rho x - y - xz + q^y$$

$$\frac{dz}{dt} = xy - \beta z + q^z$$

True value: integrate the model over 4000 time steps using prescribed parameters and initial conditions.

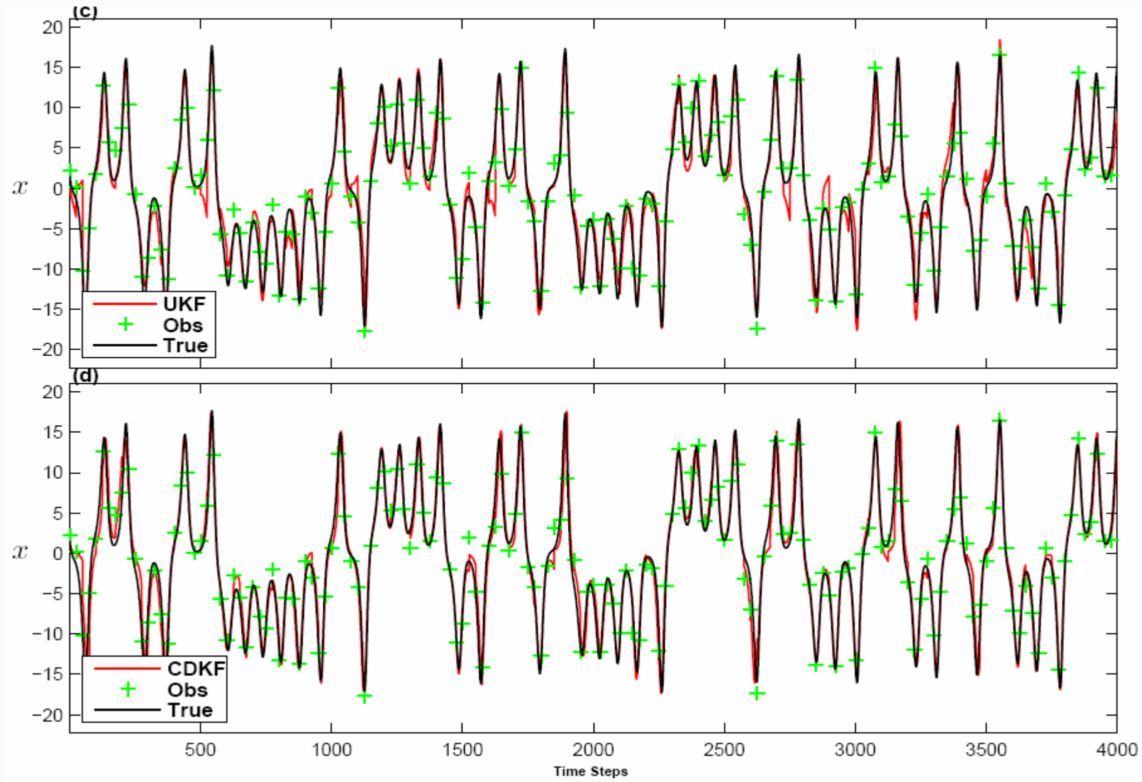
Observation: true value plus normal distribute noise;

Experimental conditions are the same as those used by Miller (Miller, 1994) and Evensen (Evensen 1997)

Lorenz model: state estimation

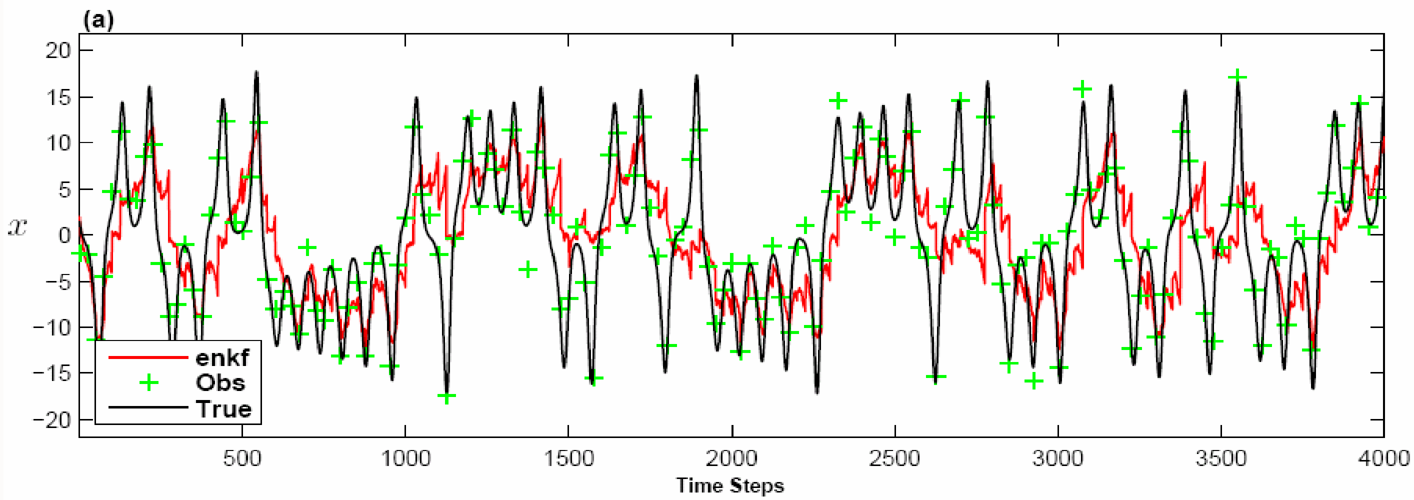
Observation and initial conditions: True values plus normal distributed noise. The assimilation interval is 25 time steps.

$N(0,\sqrt{2})$



An “unfair” comparison!

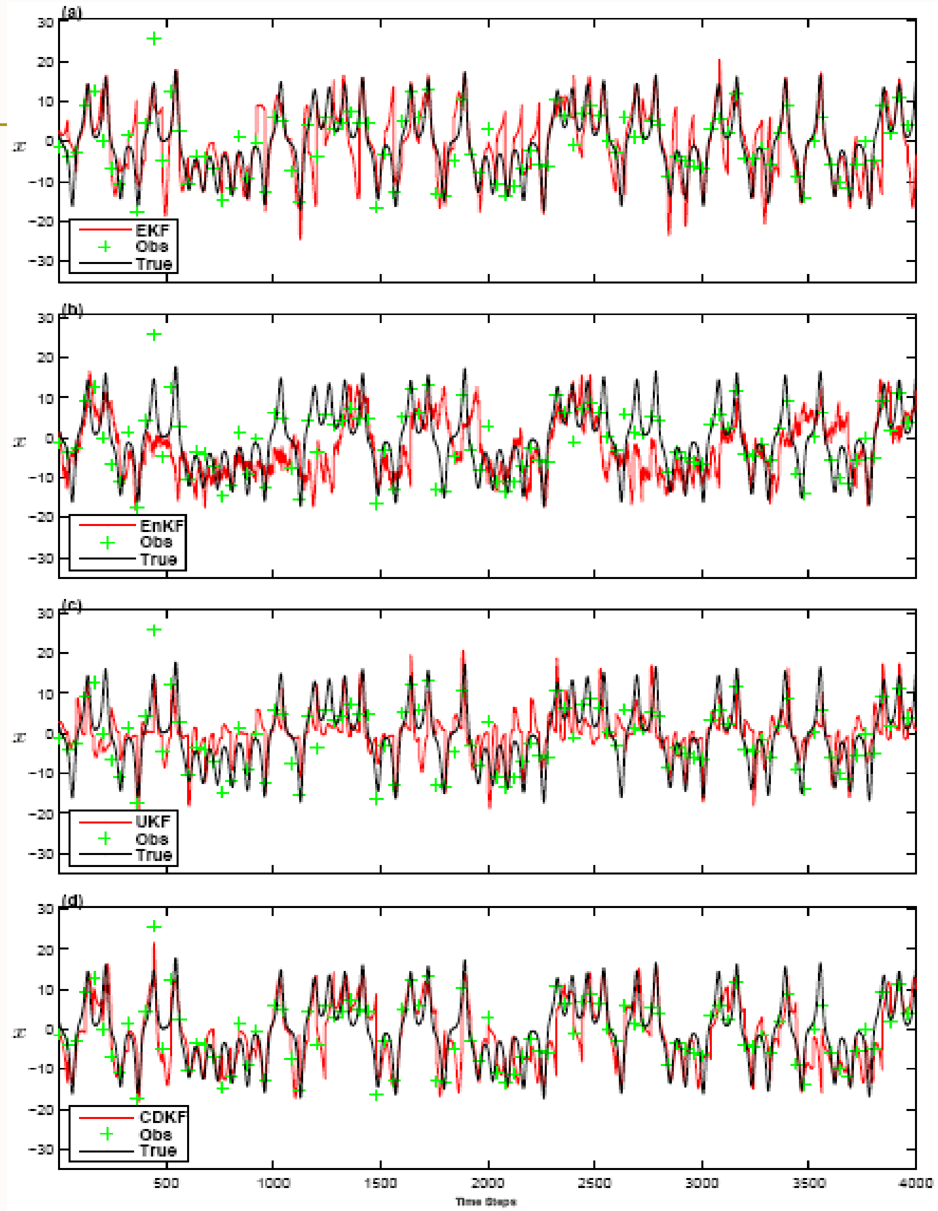
EnKF with 19 members



Assimilation Method	Computation Time (in Seconds)	RMSE
EKF	37.04	1.812
EnKF (with 1000 ensembles)	7143.57	1.987
EnKF (with 19 ensembles)	132.77	6.123
SP-UKF	133.91	1.640
SP-CDKF	90.42	1.592

noise $N(0, \sqrt{20})$.

Assimilation interval is 40 time steps.



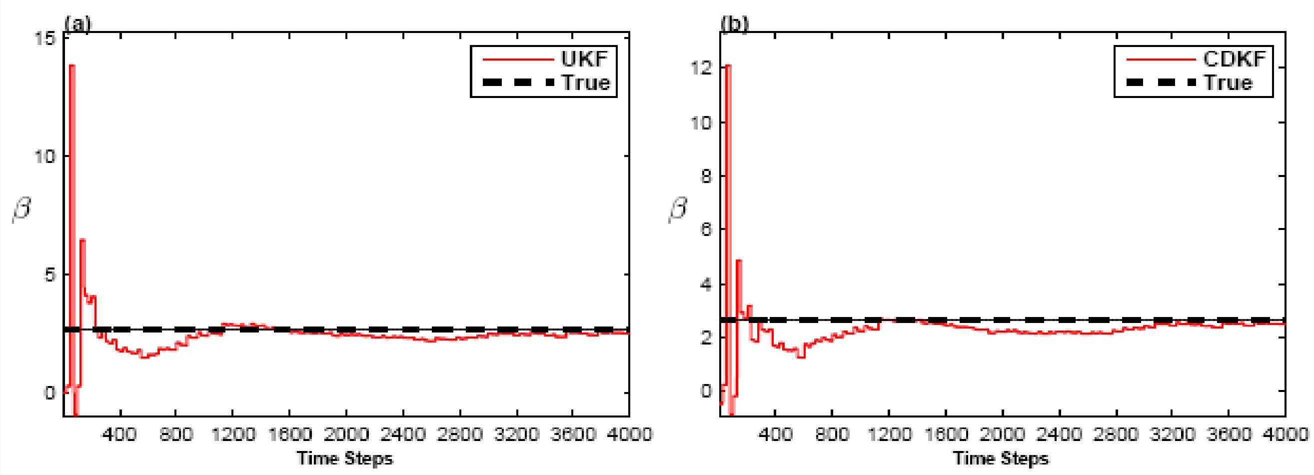
Parameter estimation

$$\boldsymbol{\Lambda}_k = \boldsymbol{\Lambda}_{k-1} + \boldsymbol{q}_{k-1}^{\Lambda}$$

$$\psi_k = \boldsymbol{f}\left(\boldsymbol{\theta}_k, \boldsymbol{\Lambda}_k\right) + \boldsymbol{r}_k^{\Lambda}$$

where $\boldsymbol{f}(\cdot)$ is the nonlinear measurement model given by the Lorenz equations

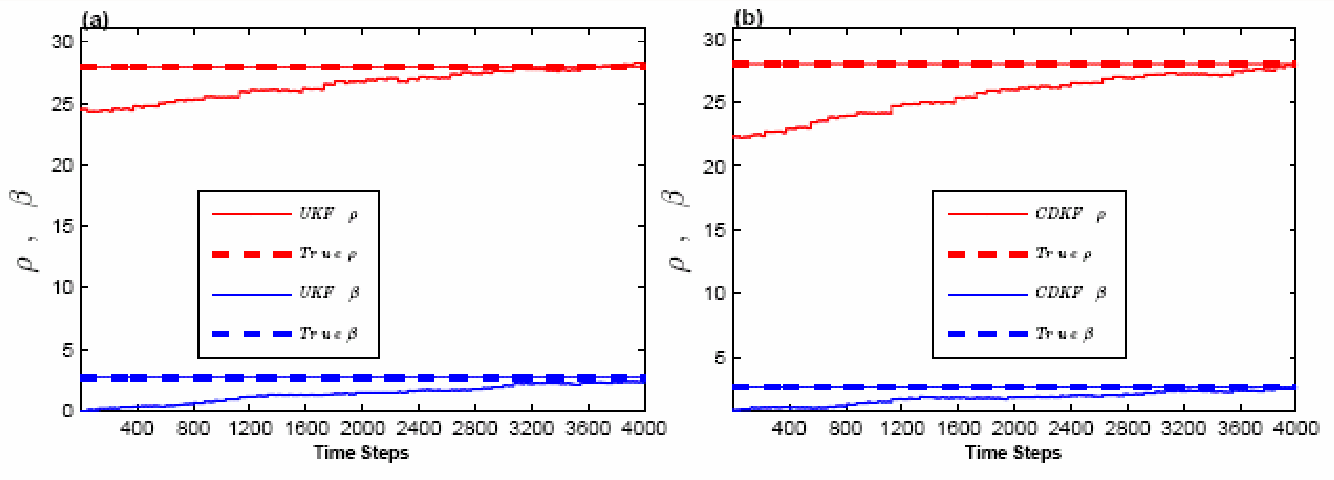
$\boldsymbol{\Lambda}$ is the parameter vector which constitutes the dynamical parameters

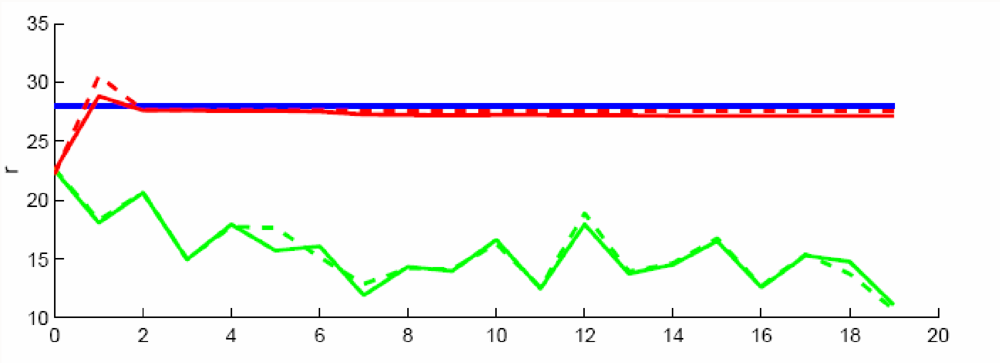


Parameter estimation

Simultaneous estimation of two parameters:

Initial parameters = true parameter plus normal distributed noise of covariance 100.





Kivman, G.A. 2003: Sequential parameter estimation for stochastic system, Nonlinear. Process. in Geophysics, 10, 253-259.

A “big” drawback of SPKF

- For an L-dimensional system, the number of sigma-points required to estimate the true statistics is 2L+1
- 2L+1 sigma-point integration is impossible, when the dimension system is of the order of millions as happens often in GCMs

A Possible solution – reducing sigma-points

$$\mathcal{X}_{k,0} = \theta_k \qquad w_0^{(m)} = \frac{\lambda}{(L+\lambda)} \qquad (2.42)$$

$$\mathcal{X}_{k,i}^{+} = \theta_k + \left(\sqrt{(L+\lambda)\,\boldsymbol{P}_{\boldsymbol{\theta}_k}}\right)_i \quad i=1,\ldots,L \qquad w_0^{(c)} = \frac{\lambda}{(L+\lambda)} + \left(1-\alpha^2+\beta\right) \qquad (2.43)$$

$$\mathcal{X}_{k,i}^{-} = \theta_k - \left(\sqrt{(L+\lambda)\,\boldsymbol{P}_{\boldsymbol{\theta}_k}}\right)_i \quad i=(L+1),\ldots,2L \qquad w_i^{(m)} = w_i^{(c)} = \frac{1}{2(L+\lambda)} \quad i=1,\ldots,2L \qquad (2.44)$$

A subspace approach with sigma-points:

Lermusiaux et. al. [Lermusiaux, 1997; Lermusiaux and Robinson, 1999] proposed a method to reduce error space, called the Error Subspace Statistical Estimation (ESSE).

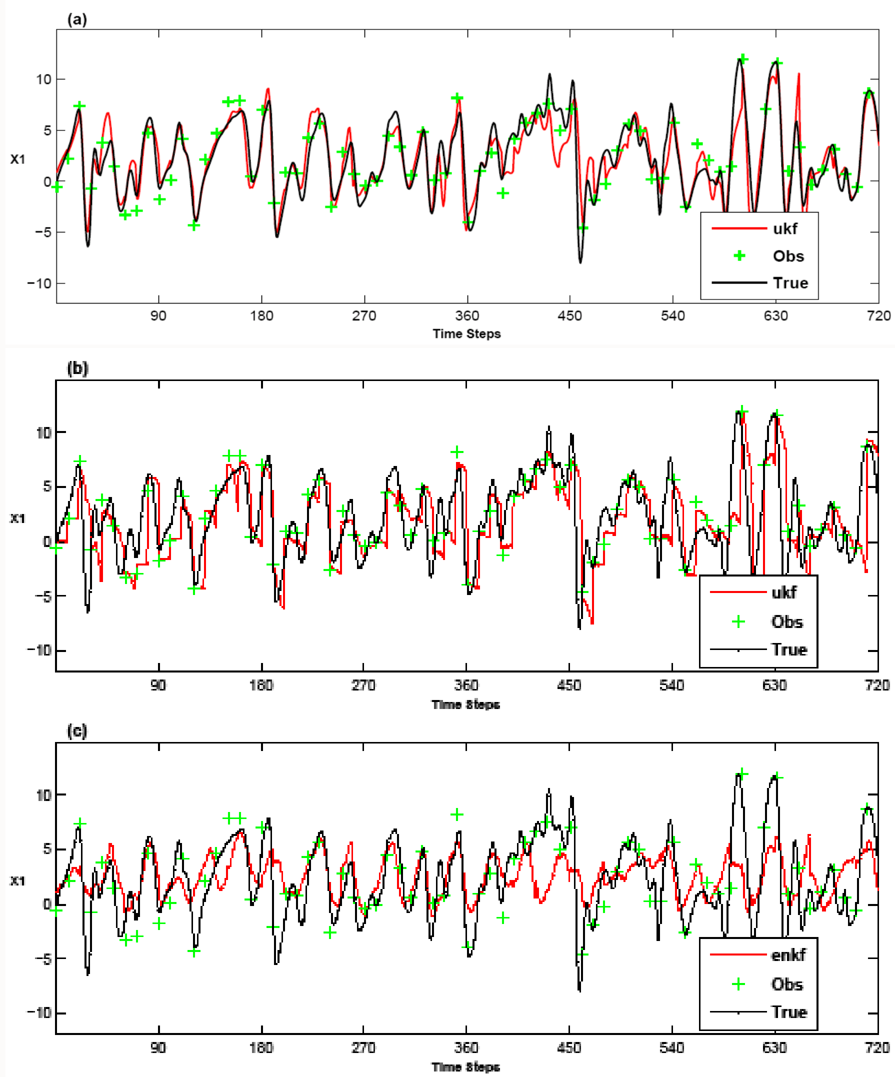
Theoretically the most important sigma-points should be chosen based on reduced rank approximation. We have used principal component analysis (PCA) to identify the most important sigma-points.

A Reduced SPKF - (Lorenz ’96 model: 36 variables)

with Full Sigma-points (241)

with reduced Sigma-points (20)

with EnKF of 20 members



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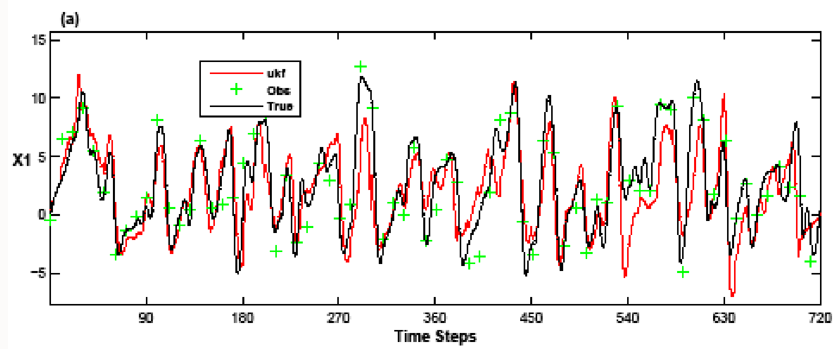
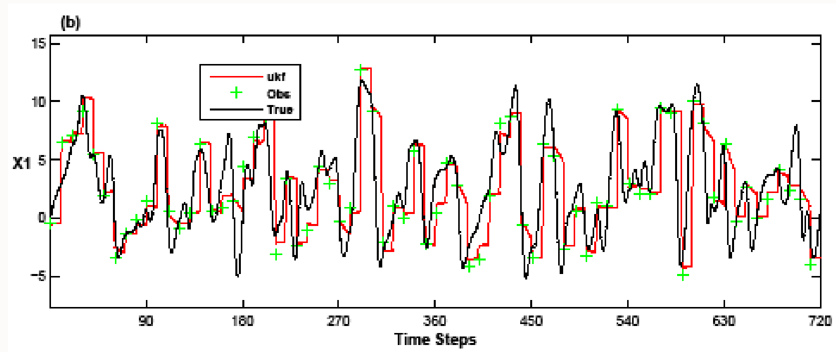
A Reduced SPKF - (Lorenz ’96 model: 960 variables)

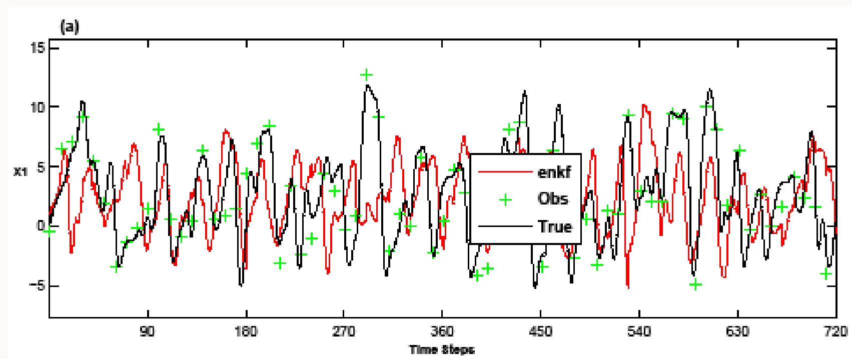
with full Sigma-points (5761)



with reduced Sigma-points (200)



with EnKF of 200 members



Conclusion

- The SPKF is a technique for a derivative-less optimal estimation using a deterministic sampling approach that ensures accurate estimation of error statistics.
- The SPKF is capable of estimating model state and parameters with better accuracy than EKF and EnKF for strong nonlinear systems.
- The SPKF is practically difficult for high dimensional systems. A possible solution is to reduce the number of sigma-points by "selecting a particular set of sigma-points".

Thank You.

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NSERC CRSNG

GOAPP Global Ocean-Atmosphere Prediction and Predictability