Data Assimilation tutorial on the Kalman filter

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1   Introduction

In this tutorial we shall look at the assimilation of observations distributed in time using two techniques based on the Kalman filter. These are the 'extended Kalman filter' and the 'ensemble Kalman filter'.

Both techniques assimilate the observations sequentially in time. Their algorithms, detailed below, involve a *forecast step*, in which a previous estimate of the state is evolved forward to the time of the observation, and an *update step*, where the evolved estimate of the state is updated using information from the observations.

In this practical these two schemes will be applied to the highly non-linear Lorenz 1963 model equations.

2   The Extended Kalman Filter

The extended Kalman filter (EKF) uses an explicit formula for the evolution of the prior estimate and its' error covariance. The EKF is optimal for linear models and Gaussian errors.

2.1   Algorithm

INPUTS:

- Prior guess of initial state, $\mathbf{x}^b$,

- a description of how the state evolves in time, $\mathbf{x}^{new} = \mathcal{M}(\mathbf{x}^{old})$,

- observations throughout the assimilation window, $\mathbf{y}$,

- a description of how the observations relate to the state, $\mathbf{y} = \mathcal{H}(\mathbf{x})$.

We also need the error covariance matrices of

- the prior guess, $\mathbf{B}$,

- the observations, $\mathbf{R}$, and

- the computer model, $\mathbf{Q}$.

—

1. Set $\mathbf{x}^f(1) = \mathbf{x}^b$ and $\mathbf{P}^f(1) = \mathbf{B}$.

2. **Prediction step**:

    (a) Propagate the prior guess forward in time:

    $$\mathbf{x}^f(t + \Delta t) = \mathcal{M}(\mathbf{x}^f(t))$$

    Δt is the model time step.

    (b) Propagate the prior guess error covariance matrix forward in time:

    $$\mathbf{P}^f(t + \Delta t) = \mathbf{M}\mathbf{P}^f(t)\mathbf{M}^T + \mathbf{Q}$$

    $\mathbf{M}$ is the tangent linear of $\mathcal{M}(\mathbf{x})$ evaluated at $\mathbf{x} = \mathbf{x}^f(t)$.

3. **Update step**, at time of the ith observation, τ_i:

(a) Calculate the Kalman gain matrix:

$$\mathbf{K} = \mathbf{P}^{\mathrm{f}}(\tau_i)\mathbf{H}^{\mathrm{T}}(\mathbf{R} + \mathbf{H}\mathbf{P}^{\mathrm{f}}(\tau_i)\mathbf{H}^{\mathrm{T}})^{-1}$$

$\mathbf{H}$ is the tangent linear of $\mathcal{H}(\mathbf{x})$ evaluated at $\mathbf{x} = \mathbf{x}^{\mathrm{f}}(\tau_i)$.

(b) Update the estimate of the state using the observations, this is the analysis at time τ_i:

$$\mathbf{x}^{\mathrm{a}}(i) = \mathbf{x}^{\mathrm{f}}(\tau_i) + \mathbf{K}(\mathbf{y} - \mathcal{H}(\mathbf{x}^{\mathrm{f}}(\tau_i)))$$

(c) Calculate the analysis error covariance matrix:

$$\mathbf{P}^{\mathrm{a}}(i) = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}^{\mathrm{f}}(\tau_i)$$

4. Set $\mathbf{x}^{\mathrm{f}}(\tau_i) = \mathbf{x}^{\mathrm{a}}(i)$ and $\mathbf{P}^{\mathrm{f}}(\tau_i) = \mathbf{P}^{\mathrm{a}}(i)$.

5. Repeat steps 2 and 3 until all observations have been assimilated.

3   The Ensemble Kalman Filter

For large systems, the EKF is infeasible due to the need to calculate and store $\mathbf{P}^{\mathrm{f}}$ and $\mathbf{P}^{\mathrm{a}}$. The ensemble Kalman filter (EnKF) [Evensen, 1994, Houtekamer and Mitchell, 1998] gives a statistical approximation to the EKF by sampling the errors of the forecast and analysis.

There are many different types of Ensemble Kalman filter. Here we shall look one of the most simple types: the perturbed observation ensemble Kalman filter.

3.1   Algorithm

INPUTS: $\mathbf{x}^{\mathrm{b}}$, $\mathbf{y}$, $\mathbf{B}$, $\mathbf{R}$, $\mathbf{Q}$, $\mathcal{M}(\mathbf{x})$, $\mathcal{H}(\mathbf{x})$ (see §2.1).

1. Generate ensemble of size N at initial time given $\mathbf{x}^{\mathrm{b}}$, and $\mathbf{B}$.

$$\mathbf{x}_j(0) = \mathbf{x}^{\mathrm{b}} + \boldsymbol{\eta}, \text{ for } j = 1, N.$$

$\boldsymbol{\eta}$ has been randomly drawn from a normal distribution with zero mean and covariance $\mathbf{B}$.

2. **Prediction step**:

(a) Propagate each ensemble member forward using a stochastic model.

$$\mathbf{x}_j(t + \Delta t) = \mathcal{M}(\mathbf{x}_j(t)) + \sqrt{\Delta t}\boldsymbol{\zeta}, \text{ for } j = 1, N.$$

$\boldsymbol{\zeta}$ has been randomly drawn from a normal distribution with zero mean and covariance $\mathbf{Q}$.

3. **Update step**, at time of the ith observation, τ_i:

(a) Calculate the Kalman gain matrix.

$$\mathbf{K} = \mathbf{P}^{\mathrm{f}}\mathbf{H}(\mathbf{H}\mathbf{P}^{\mathrm{f}}\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}.$$

$\mathbf{P}^{\mathrm{f}}$ is the evolved $\mathbf{B}$ matrix, represented by the spread in the evolved ensemble at time τ_i.

$$\mathbf{P}^{\mathrm{f}} = \frac{1}{N-1}\sum(\mathbf{x}_j(\tau_i) - \bar{\mathbf{x}})(\mathbf{x}_j(\tau_i) - \bar{\mathbf{x}})^{\mathrm{T}},$$

where $\bar{\mathbf{x}}$ is the mean of the ensemble.

(b) Update each ensemble member using the perturbed observations

$$\mathbf{x}_j(\tau_i) = \mathbf{x}_j(\tau_i) + \mathbf{K}\left(\mathbf{y}(\tau_i) + \boldsymbol{\epsilon} - \mathcal{H}(\mathbf{x}_j(\tau_i))\right)$$

$\boldsymbol{\epsilon}$ has been randomly drawn from a normal distribution with zero mean and covariance $\mathbf{R}$. The analysis can be calculated as the mean of this updated ensemble, $\mathbf{x}^{\mathrm{a}}(\tau_i) = \frac{1}{N-1}\sum \mathbf{x}_j(\tau_i)$

(c) Calculate the analysis error covariance matrix:

$$\mathbf{P}^{\mathrm{a}} = \frac{1}{N-1}\sum(\mathbf{x}_j(\tau_i) - \mathbf{x}^{\mathrm{a}})(\mathbf{x}_j(\tau_i) - \mathbf{x}^{\mathrm{a}})^{\mathrm{T}}.$$

As can be seen, this step is not necessary but provides a useful diagnostic in toy experiments.

4. Repeat steps 2 and 3 until all observations have been assimilated.

4 The Lorenz 63 model

To test these data assimilation schemes we will use the low-dimensional Lorenz 1963 model [Lorenz, 1963], given by

$$\begin{aligned}\frac{dx}{dt} &= \sigma(y - x)\\ \frac{dy}{dt} &= -xz + \rho x - y \qquad\qquad (1)\\ \frac{dz}{dt} &= xy - \beta z.\end{aligned}$$

Using the following parameters, $\sigma=10$, $\rho = 28$ and $\beta = 8/3$, (1) gives rise to a chaotic system with a strange attractor. The solution is seen to orbit around two equilibrium points giving two 'regimes'.

The model is discretised using a modified Euler scheme, as follows:

$$\begin{aligned}kx(1) &= \Delta t\sigma(y^{t-1} - x^{t-1})\\ ky(1) &= \Delta t(-x^{t-1}zt - 1 + \rho x^{t-1} - y^{t-1})\\ kz(1) &= \Delta t(x^{t-1}y^{t-1} - \beta z^{t-1})\end{aligned}$$

$$\begin{aligned}kx(2) &= \Delta t\sigma(y^{t-1} + ky(1) - x^{t-1} - kx(1))\\ ky(2) &= \Delta t(-(x^{t-1} + kx(1))(zt - 1 + kz(1)) + \rho(x^{t-1} + kx(1)) - (y^{t-1} + ky(1)))\\ kz(2) &= \Delta t((x^{t-1} + kx(1))(y^{t-1} + ky(1)) - \beta(z^{t-1}) + kz(1))\end{aligned}$$

$$\begin{aligned}x^t &= x^{t-1} + 0.5(kx(1) + kx(2))\\ y^t &= y^{t-1} + 0.5(ky(1) + ky(2))\\ z^t &= z^{t-1} + 0.5(kz(1) + kz(2))\end{aligned}$$

5 Running the code

The code can be run by open MATLAB, navigating to the KF directory and typing KF_menu. You will then be asked to choose between the Extended Kalman filter or Ensemble Kalman filter. You must then give the necessary inputs when prompted. To use the suggested values simply press 'OK'.

This is a 'twin' experiment, in which the truth is known and used to generate the observations and background.

6 Suggested exercises

1. First compare EKF and EnKF using the suggested inputs. Look at the true error in the analysis given by $\mathbf{x}_a - \mathbf{x}_t$ and the analysis error variances approximated by the chosen DA method.

2. For both the extended and ensemble Kalman filter look at:

(a) the sensitivity of the solution to the errors in the background.

(b) the sensitivity of the solution to the accuracy and frequency of observations: is it better to have frequent but inaccurate observations or infrequent but accurate ones?

(c) the sensitivity of the solution to the model error. This involves finding where $\mathbf{Q}$ is defined in the respective code. What is the impact of excluding the model error correlations? What is the impact of increasing the magnitude of model error variances?

3. For just the ensemble Kalman filter, what is the effect of changing:

    (a) the size of the ensemble?

   (b) the size of the observation perturbation? This involves finding the update step in the code, *EnKF.m*.

7 Extended exercises

It is interesting to see how robust these methods are to the validity of assumptions made. For example have a look at what happens when:

1. the observation error is correlated in time or simply biased.

2. the model of the evolution of the state is biased compared to the true evolution of state.

References

G. Evensen. Sequential data assimilation with a nonlinear quasi-geostrophic model using monte carlo methods to forecast error statistics. *J. Geophysic. Res.*, 99 (C5):10143–10162, 1994.

P. L. Houtekamer and H. L. Mitchell. Data assimilation using an ensemble kalman filter technique. *Mon. Wea. Rev.*, 126:798–811, 1998.

E. N. Lorenz. Deterministic nonperiodic flow. *J. Atmos. Sci.*, 20:130–141, 1963.
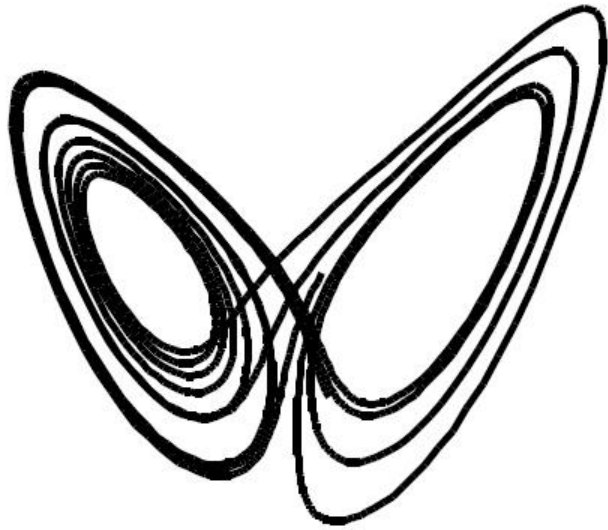
The Kalman Filter

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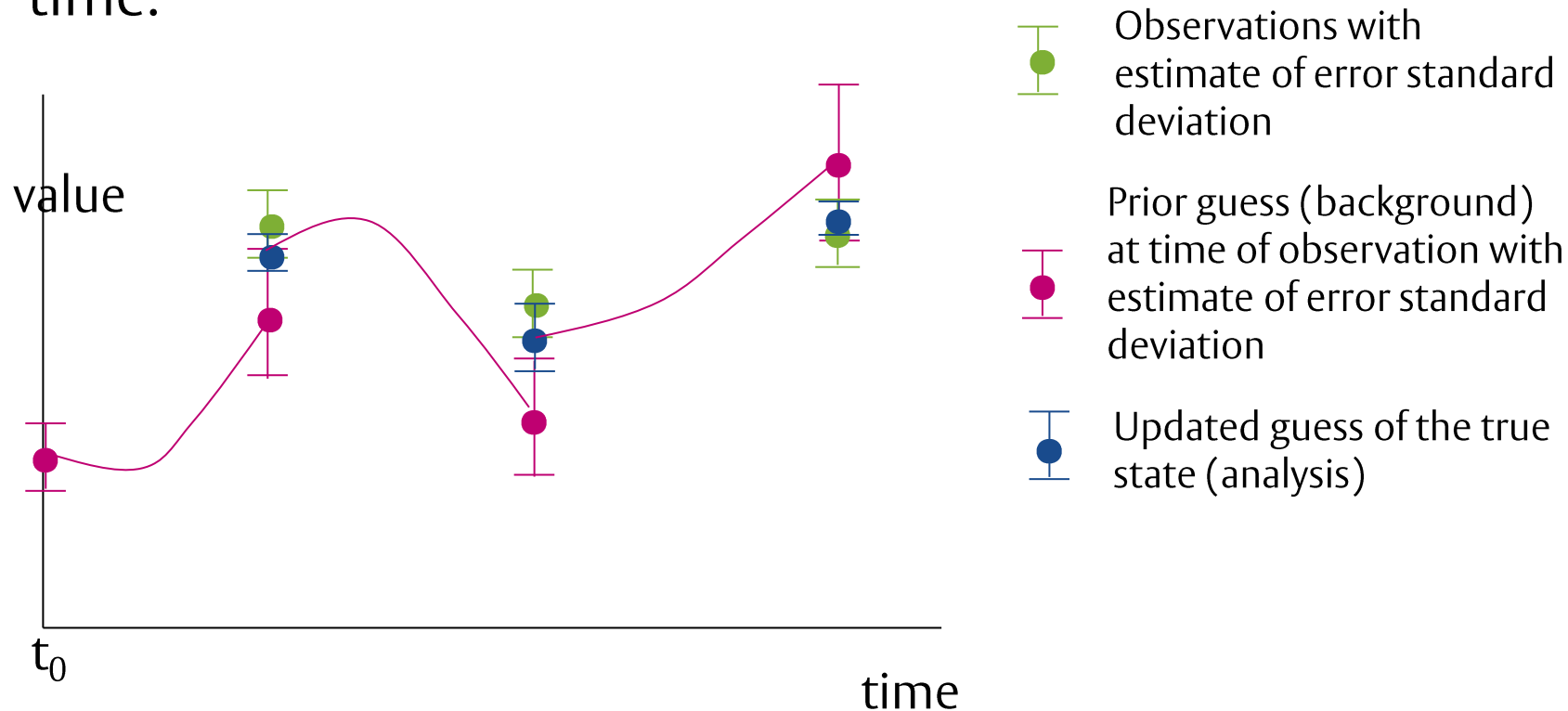
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Dynamical data assimilation

- In today and tomorrow's practical we will be looking at methods for assimilating observations made at different times.

- To do this we need to introduce a dynamical model so that we can compare the background, which is valid at an initial time, to the observations.

The Kalman filter
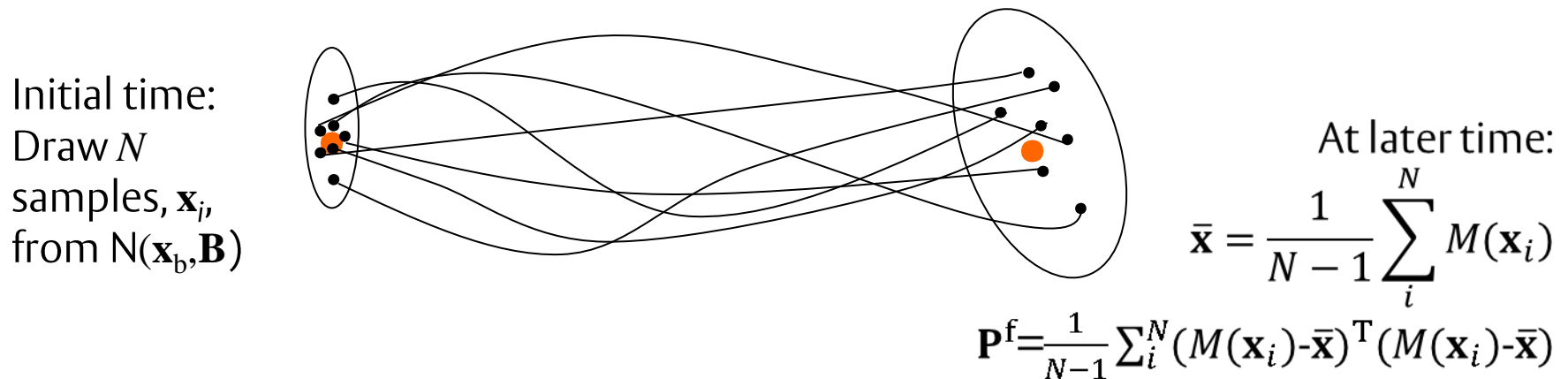
- The Kalman filter assimilates observations sequentially in time.

value

Observations with estimate of error standard deviation

Prior guess (background) at time of observation with estimate of error standard deviation

Updated guess of the true state (analysis)

t_0

time

Schematic of a1D example

The Kalman Filter

- To assimilate the observations at different times we need to understand how our prior guess of the state (the background) and it's error covariances evolve in time.

- One way is to explicitly evolve them using the dynamical model.

- $\mathbf{x}^f(t) = M(\mathbf{x}^f(t\text{-}1))$
  - M is our dynamical model

- $\mathbf{P}^f(t) = \mathbf{M}\mathbf{P}^f(t\text{-}1)\mathbf{M}^T + \mathbf{Q}$
  - $\mathbf{M} = \mathrm{d}M(\mathbf{x})/\mathrm{d}\mathbf{x}$ is the tangent linear approximation of M, and $\mathbf{Q}$ is the model error covariance matrix

- This is the Extended Kalman filter method

The Kalman Filter

- Another way of measuring how the error covariances evolve in time is to sample from the initial error distribution and then apply the model to each sample. From this evolved sample we can estimate the error covariances and the mean at the later time.

Initial time: Draw N samples, $\mathbf{x}_i$, from $N(\mathbf{x}_b, \mathbf{B})$

At later time:

$$\bar{\mathbf{x}} = \frac{1}{N-1} \sum_i^N M(\mathbf{x}_i)$$

$$\mathbf{P}^f = \frac{1}{N-1} \sum_i^N (M(\mathbf{x}_i) - \bar{\mathbf{x}})^T (M(\mathbf{x}_i) - \bar{\mathbf{x}})$$

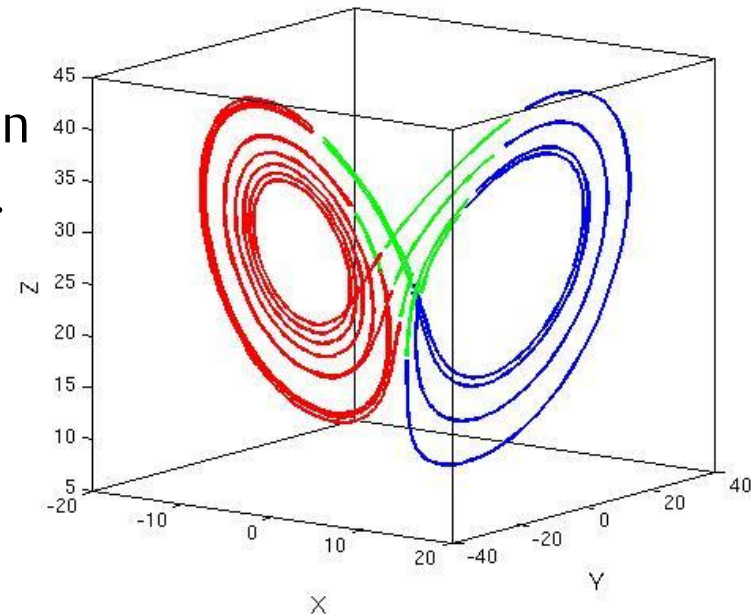- This is the Ensemble Kalman filter method

The update step

- At the time of the observations we now have the evolved prior mean and error covariance.

- The calculation of the analysis is similar to the optimal interpolation method introduced in yesterdays practical. See separate hand out for more details.

- At this stage the analysis error covariance is also calculated.

- The analysis and analysis error covariances are then evolved to the next observation time to become our prior estimate.

- And the process is repeated

The Dynamical model

- In this practical we will be using the Lorenz model because
    - It is a toy model with three dimensions allowing us to perform a series of experiments and analyse all aspects of the output
    - It is chaotic, meaning a small error in the initial conditions quickly grows.
    - It orbits around two stable points, giving two 'regimes'. Accurately forecasting the switch from one regime to another is particularly difficult.
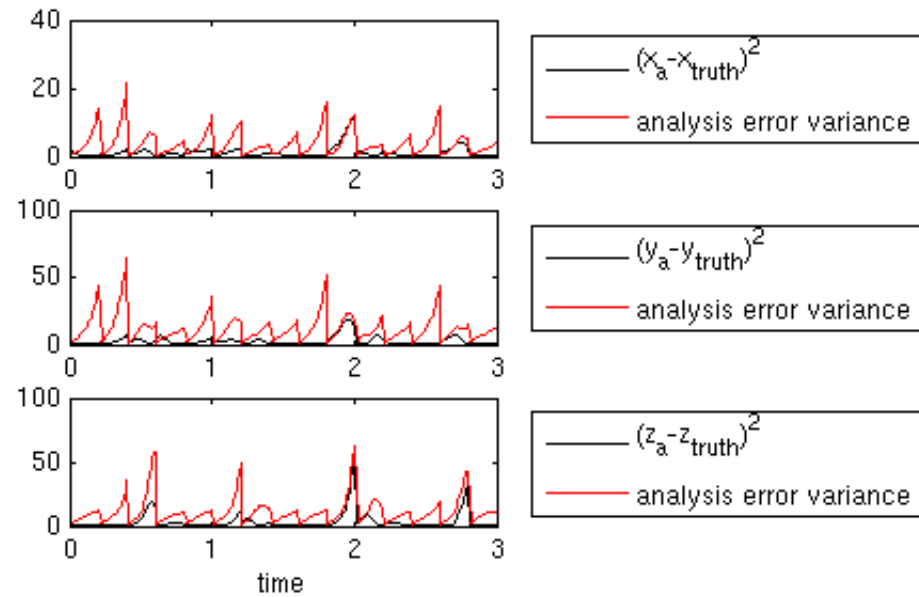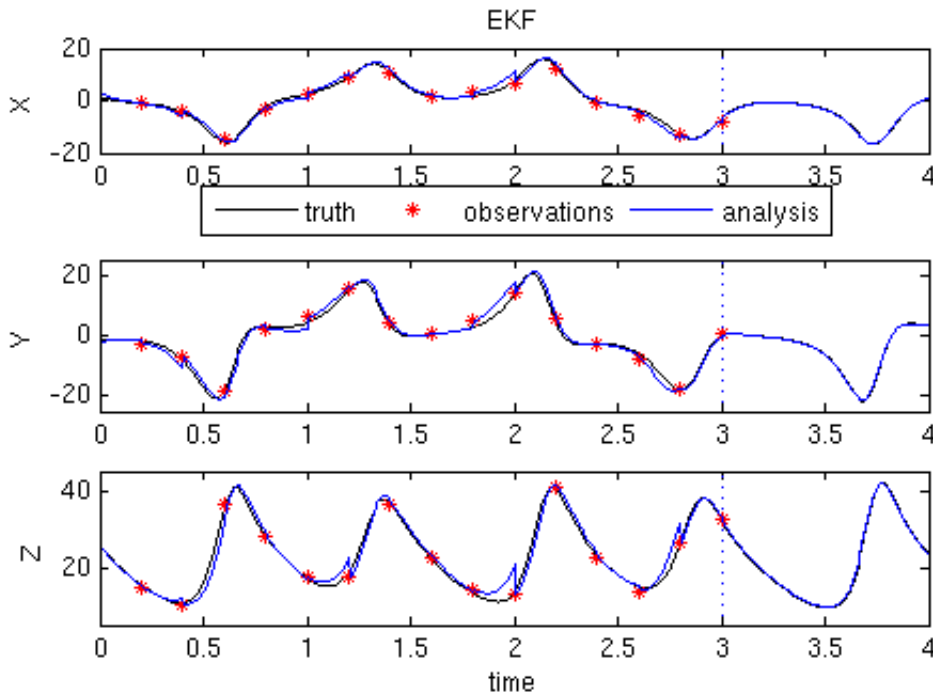
Running the code

- Follow the instructions for running the code.

- You will be given a choice to use the Extended Kalman filter or the Ensemble Kalman filter.

- In each case you must choose the true initial conditions, from this the observations and background will be generated. The analysis trajectory may then be compared to the true trajectory.

Example output- Extended KF

EKF

truth   *   observations   —— analysis

The regime changes can be seen when the x and y values change sign.

$(x_a - x_{truth})^2$

analysis error variance

$(y_a - y_{truth})^2$

analysis error variance

$(z_a - z_{truth})^2$

analysis error variance

Example output- Ensemble KF

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