A review of Data Assimilation methods

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Managing Uncertainty in Complex Models

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Outline

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The basics of data assimilation

AIM: Keep track of the evolution of the state of some physical system (the atmosphere, the ocean, a moving object...) in order to estimate and predict.

Ingredients

- The state of the system: $\mathbf{x}_t$
- A forward (observation) model: $\mathbf{x}_t = m_t(\mathbf{x}_{t-1})$
- Observations of the true process: $\mathbf{y}_t = h(\mathbf{x}_t)$

- The state of the system is a vector of all variables necessary to fully describe the system
- Example: $\mathbf{x} = \{Temperature, Salinity, \ldots\}$

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- The system model allows us to propagate the state forward in time $\Rightarrow$ prediction / propagation step
- Most of the time, m_t is non-linear

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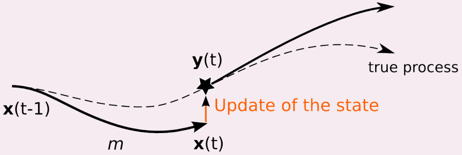
- The model is not a perfect representation of the process and will eventually diverge



- Use observations to correct the propagated state $\Rightarrow$ update step

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Ingredients

- The state of the system: $\mathbf{x}_t$
- A forward (observation) model: $\mathbf{x}_t = m_t(\mathbf{x}_{t-1}) + \eta_t$
- Observations of the true process: $\mathbf{y}_t = h(\mathbf{x}_t) + \varepsilon_t$

- Both the model and the observations are inaccurate
- Use a probabilistic framework to account for uncertainties: $p(\mathbf{x}_t|\mathbf{y}_{1:t})$

The basics of data assimilation

- Bayes' rule allows us to update the state's posterior distribution given the observation and the prior:

$$p(\mathbf{x}_t|\mathbf{y}_{1:t}) = \frac{p(\mathbf{y}_t|\mathbf{x}_t)\, p(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{y}_{1:t-1})}{p(\mathbf{y}_t)}$$

This is a filtering update.

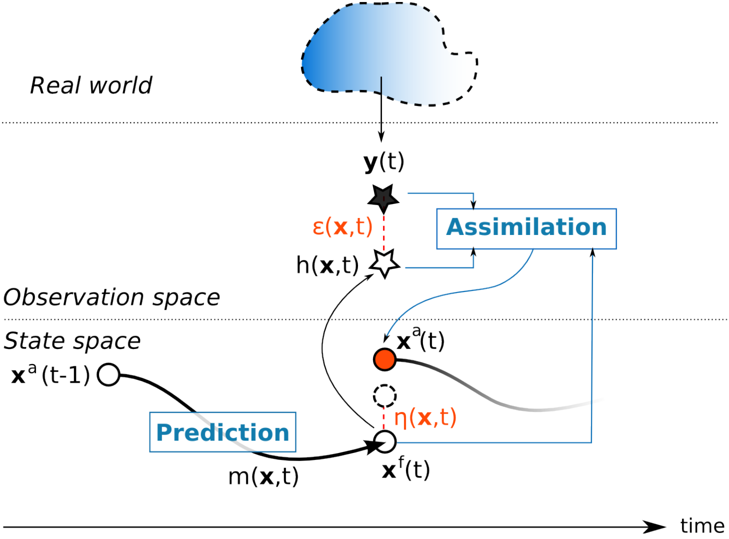
Data assimilation methods

Data assimilation methods can be categorised into:

	Filtering	Smoothing
Probabilistic	Kalman filter (KF)	Kalman smoother (KS)
	Extended KF	Extended KS
	Ensemble KF	Ensemble KS
	Particle filter	Particle smoother
Variational	3D VAR	4D VAR (strong/weak constraint)

Outline

The filtering problem



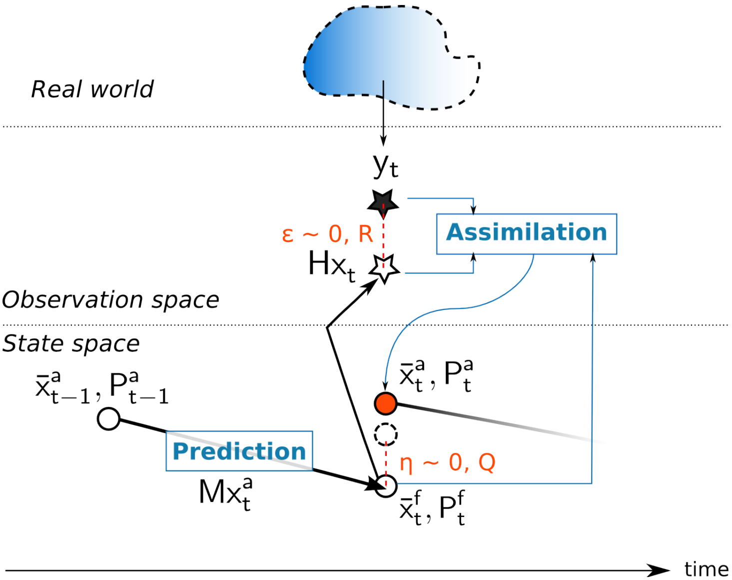
The Kalman Filter

Introduced by R. Kalman (and others) in the early 60's

Assumptions

- The state has a Gaussian distribution: $p(\mathbf{x}_{t-1}|\mathbf{y}_{1:t-1}) = \mathcal{N}(\bar{\mathbf{x}}_{t-1}, \mathbf{P}_{t-1})$
- The system model is linear: $m = \mathbf{M}$
- The model error is Gaussian white noise: $\eta \sim \mathcal{N}(0, \mathbf{Q})$
- The observation operator is linear: $h = \mathbf{H}$
- The observation has a Gaussian likelihood: $p(\mathbf{y}_t|\mathbf{x}_t^f) = \mathcal{N}(\mathbf{H}\mathbf{x}_t^f, \mathbf{R})$

The Kalman Filter



The Kalman Filter

Prediction step

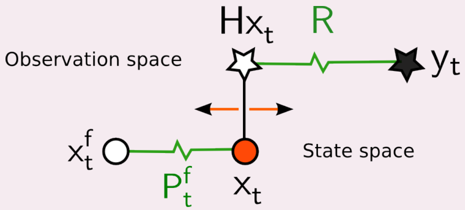
The predicted state $\mathbf{x}_t^f$ has a Gaussian distribution $\mathcal{N}(\bar{\mathbf{x}}_t^f, \mathbf{P}_t^f)$:

$$\bar{\mathbf{x}}_t^f = \mathbf{M}\bar{\mathbf{x}}_{t-1}$$

$$\mathbf{P}_t^f = \mathbf{M}\mathbf{P}_{t-1}\mathbf{M}^T + \mathbf{Q}$$

Update step

- A Best Linear Unbiased Estimated (BLUE) is sought



The Kalman Filter

Prediction step

The predicted state $\mathbf{x}_t^f$ has a Gaussian distribution $\mathcal{N}(\bar{\mathbf{x}}_t^f, \mathbf{P}_t^f)$:

$$\bar{\mathbf{x}}_t^f = \mathbf{M}\bar{\mathbf{x}}_{t-1}$$
$$\mathbf{P}_t^f = \mathbf{M}\mathbf{P}_{t-1}\mathbf{M}^T + \mathbf{Q}$$

Update step

- The updated state $\mathbf{x}_t^a$ has a Gaussian distribution $\mathcal{N}(\bar{\mathbf{x}}_t, \mathbf{P}_t^a)$:

$$\bar{\mathbf{x}}_t^a = \bar{\mathbf{x}}_t^f + \mathbf{K}(\mathbf{y}_t - \mathbf{H}\bar{\mathbf{x}}_t^f)$$
$$\mathbf{P}_t^a = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}_t^f$$
$$\mathbf{K} = \mathbf{P}_t^f\mathbf{H}^T(\mathbf{H}\mathbf{P}_t^f\mathbf{H}^T + \mathbf{R})^{-1}$$

Extensions to non-Linear/non-Gaussian case

The Kalman Filter's assumptions are very restrictive:

- What if the model m is non-linear?
- What if the observation operator h is non-linear?
- What if the various distributions (especially the errors) are non-Gaussian?

Several approximations can be introduced:

- Linearise the system and observation operator $\Rightarrow$ Extended KF
- Use a discrete approximation to the state's Gaussian distribution $\Rightarrow$ Ensemble KF, Unscented KF
- Use a Monte-Carlo approximation to the (non-Gaussian) state's distribution $\Rightarrow$ Particle Filter

The Extended Kalman Filter

Assumptions

- Same as the original Kalman Filter, but
- Use the tangent linear model $\hat{\mathbf{M}} = \frac{\partial m}{\partial \mathbf{x}_t}(\mathbf{x}^a_{t-1})$ in the propagation of the covariance

Prediction step

$$\bar{\mathbf{x}}^f_t = m(\bar{\mathbf{x}}^a_{t-1})$$
$$\mathbf{P}^f_t = \hat{\mathbf{M}}\mathbf{P}^a_{t-1}\mathbf{M}^T + \mathbf{Q}$$

The Extended Kalman Filter

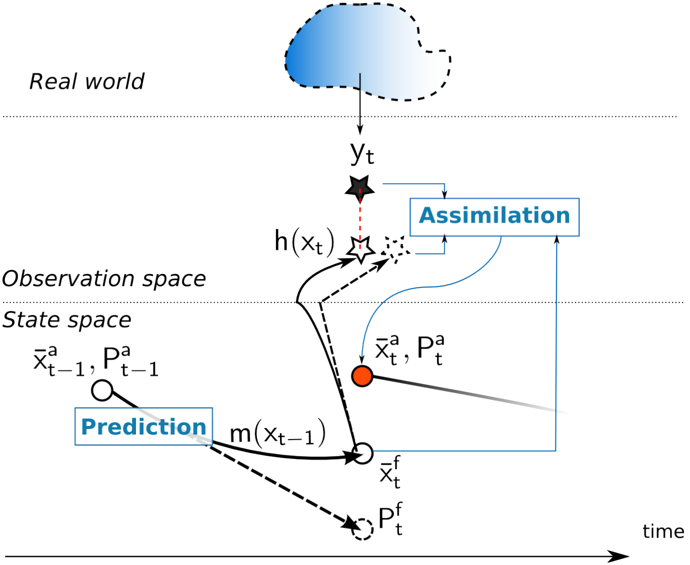
Assumptions

- Same as the original Kalman Filter, but
- Use the tangent linear observation operator $\hat{\mathbf{H}} = \frac{\partial h}{\partial \mathbf{x}_t}(\mathbf{x}_t^f)$ in the update equations

Update step

$$\bar{\mathbf{x}}_t^a = \bar{\mathbf{x}}_t^f + \mathbf{K}(\mathbf{y}_t - h(\bar{\mathbf{x}}_t^f))$$
$$\mathbf{P}_t^a = (\mathbf{I} - \mathbf{K}\hat{\mathbf{H}})\mathbf{P}_t^f$$
$$\mathbf{K} = \mathbf{P}_t^f\hat{\mathbf{H}}^{\mathrm{T}}(\hat{\mathbf{H}}\mathbf{P}_t^f\hat{\mathbf{H}}^{\mathrm{T}} + \mathbf{R})^{-1}$$

The Extended Kalman Filter



The Extended Kalman Filter

- The EKF is a straightforward adaptation of the KF for non-linear models
- However, EKF will fail if the model is strongly non-linear
- Still limited by the Gaussian assumption on all distributions

The Ensemble Kalman Filter

- Rather than linearise the model, approximate the state's distribution
- Use a sample of realisations from which the mean and covariance can be estimated

$$\{\mathbf{x}_i\}_{i=1:N} \sim \mathcal{N}(\bar{\mathbf{x}}, \mathbf{P})$$

$$\bar{\mathbf{x}} \approx \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_i$$

$$\mathbf{P} \approx \frac{1}{N-1}\sum_{i=1}^{N}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^{\mathsf{T}}$$

- Other assumptions are the same as in KF

The Ensemble Kalman Filter

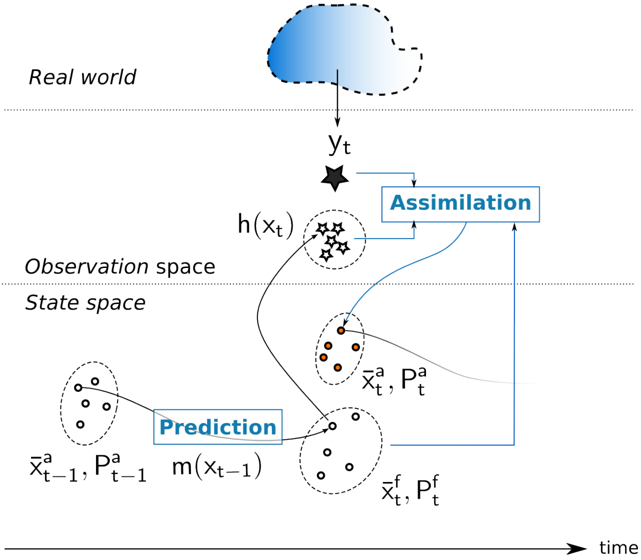
Prediction step

- Each ensemble member is propagated using the full non-linear model
- Mean and covariance are estimated from the propagated ensemble

Update step

- An ensemble of observed realisations is generated by perturbing the observation
- Each ensemble member is updated as in the KF
- This method is known to underestimate the updated covariance
  $\Rightarrow$ Square-root formulations of the filter address this issue

The Ensemble Kalman Filter



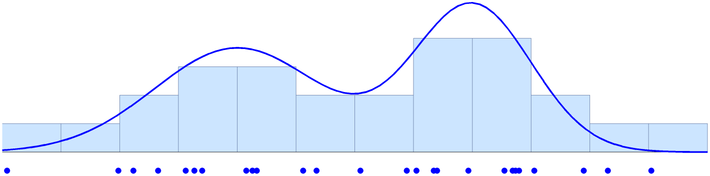
The Ensemble Kalman Filter

- The EnKF provides a robust approach to non-linear filtering
- It is used operationally in weather centres (Canada)
- Still relies on the assumption that all distributions are Gaussian
- Note in operational formulations the covariance matrices are never explicitly computed

The Particle Filter

- Discards the Gaussian assumption Kalman filters are based on
- Instead, represents $\mathrm{p}(\mathbf{x}|\mathbf{y})$ using a Monte-Carlo approximation:
  - a set of particles $\{\mathbf{x}^i\}_{i=1:N}$
  - a set of associated weights $\{w^i\}_{i=1:N}$
- Then

$$\mathrm{p}(\mathbf{x}|\mathbf{y}) \approx \sum_{i=1}^{N} w^i \, \delta(\mathbf{x}^i \in \mathrm{d}\mathbf{x})$$



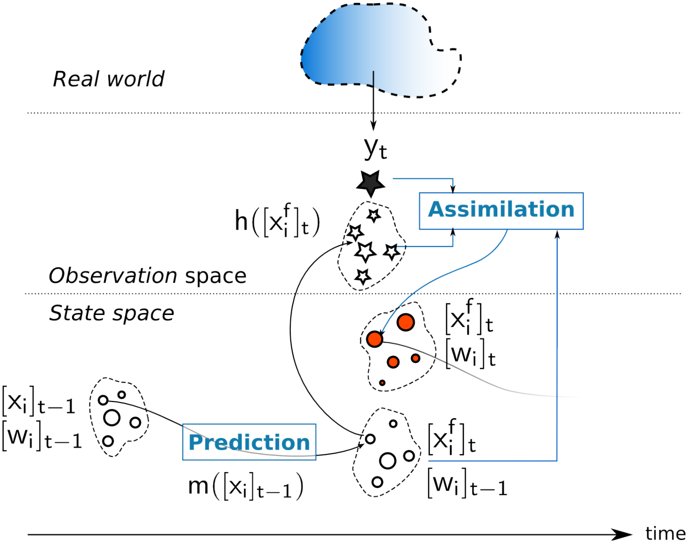
The Particle Filter

- Initialisation:
  - Sample N particles $\mathbf{x}_0^i$ from $p(\mathbf{x}_0)$
  - Set all weights w_0^i to $1/N$
- Prediction:
  - Propagate each particle through the full non-linear model
  - Leave weights unchanged
- Update:
  - Reweight (and normalise) particles according to the observation's likelihood:

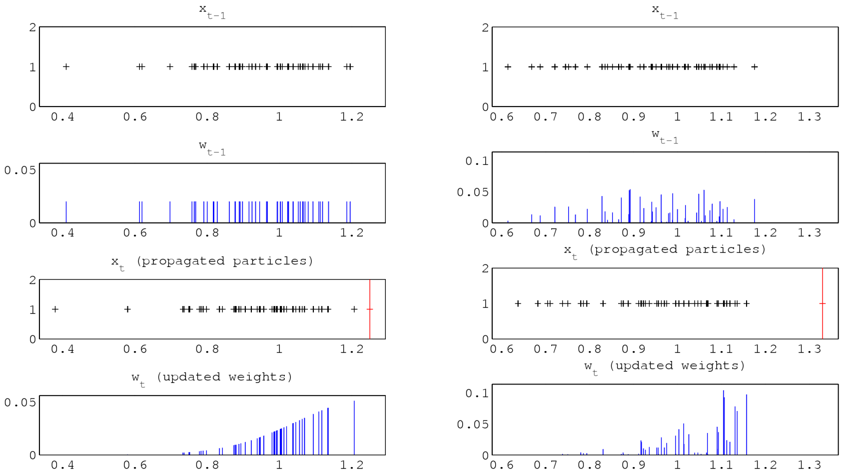
$$w_{\mathrm{t}+1}^i \propto w_{\mathrm{t}}^i \times \mathrm{p}(\mathbf{y}_{\mathrm{t}+1} | \mathbf{x}_{\mathrm{t}+1}^i)$$

  - Leave particles unchanged

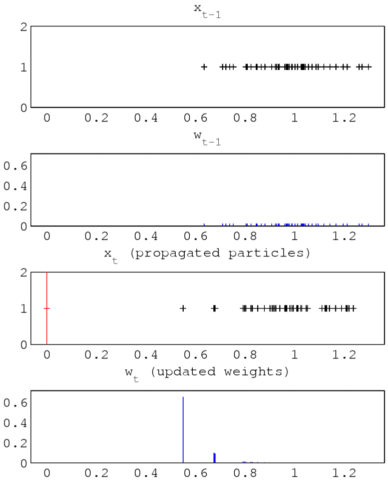
The Particle Filter



The Particle Filter



The Particle Filter



The Particle Filter

- The PF suffers from a degeneracy problem
  $\Rightarrow$ all but a few particles see their weight collapse to zero

- **Solution:** Introduce a resampling step after the update, whereby:
  - particles with high weights are duplicated,
  - particles with no weight are discarded,
  - all weights are reset to $1/N$

- Each particle is replicated M times, where $M \approx w^i \times N$

- Several resampling algorithms available: systematic importance resampling, multinomial resampling, stratified resampling ...

The Particle Filter

- Non-Gaussian, non-linear $\Rightarrow$ ideal in theory!
- However, the number of particles needed grows exponentially with the dimension of the state vector...
  $\Rightarrow$ Totally impractical in high-dimension

Outline

3D VAR

- Variational methods replace the update step with an optimisation problem
- Typically non-probabilistic (i.e. provide a single “best” estimate of the state)

Update step

- Given a first guess of the state (background) $\mathbf{x}^b$ with covariance matrix $\mathbf{B}$ (prior),
- And an observation likelihood with mean $h(\mathbf{x})$ and covariance matrix $\mathbf{R}$,
- The updated state minimises the departure to both the background and the observation:

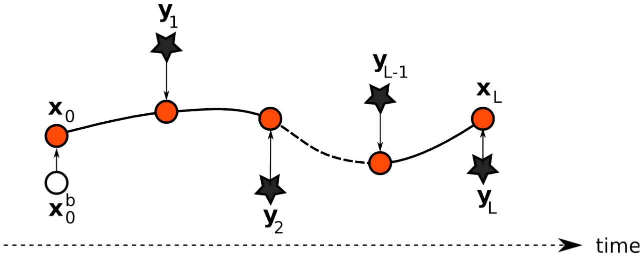
$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x}_\mathrm{t} - \mathbf{x}_\mathrm{t}^b)^\mathsf{T}\mathbf{B}^{-1}(\mathbf{x}_\mathrm{t} - \mathbf{x}_\mathrm{t}^b) + \frac{1}{2}(\mathbf{y}_\mathrm{t} - h(\mathbf{x}_\mathrm{t}))\mathbf{R}^{-1}(\mathbf{y}_\mathrm{t} - h(\mathbf{x}_\mathrm{t}))$$

4D VAR - Strong constraint

- 4D VAR adds in the temporal dimension
- The optimal trajectory minimises the departure to both the background and a series of observations:

$$J(\mathbf{x}_{0:L}) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^\top \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\sum_{t=1}^{L}(\mathbf{y}_\mathrm{t} - h(\mathbf{x}_\mathrm{t}))\mathbf{R}^{-1}(\mathbf{y}_\mathrm{t} - h(\mathbf{x}_\mathrm{t}))$$

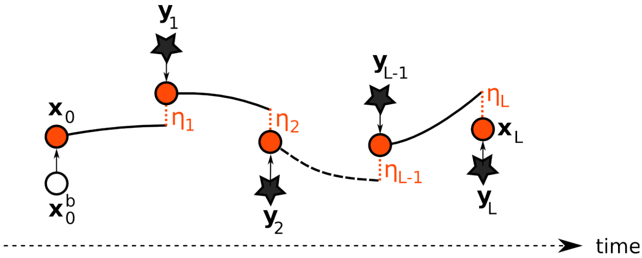
- There is no model error: the model acts as a strong constraint



4D VAR - Weak constraint

- Same as 4D VAR strong constraint, but allows for model error
- The cost function becomes:

$$J(\mathbf{x}_{0:L}) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}\sum_{t=1}^{L}(\mathbf{y}_{\mathrm{t}} - h(\mathbf{x}_{\mathrm{t}}))\mathbf{R}^{-1}(\mathbf{y}_{\mathrm{t}} - h(\mathbf{x}_{\mathrm{t}}))$$
$$+ \frac{1}{2}\sum_{t=1}^{L}\eta_{\mathrm{t}}^{\mathrm{T}}\mathbf{Q}^{-1}\eta_{\mathrm{t}}$$



Variational methods

- 3D VAR and 4D VAR are used operationally in several weather centres (UK, USA, Australia)
- Minimisation of the 4D VAR cost function relies on linearisation of the forward model
- Weak constraint 4D VAR is still very much at development stage

Summary

- Filtering methods provide a probabilistic means to estimate the state in real-time
- Most variational methods are non-probabilistic and replace the update step with an optimisation problem
- Smoothing methods extend filtering to the problem of estimating the trajectory of the state rather than its last value (similar to 4D VAR vs. 3D VAR)