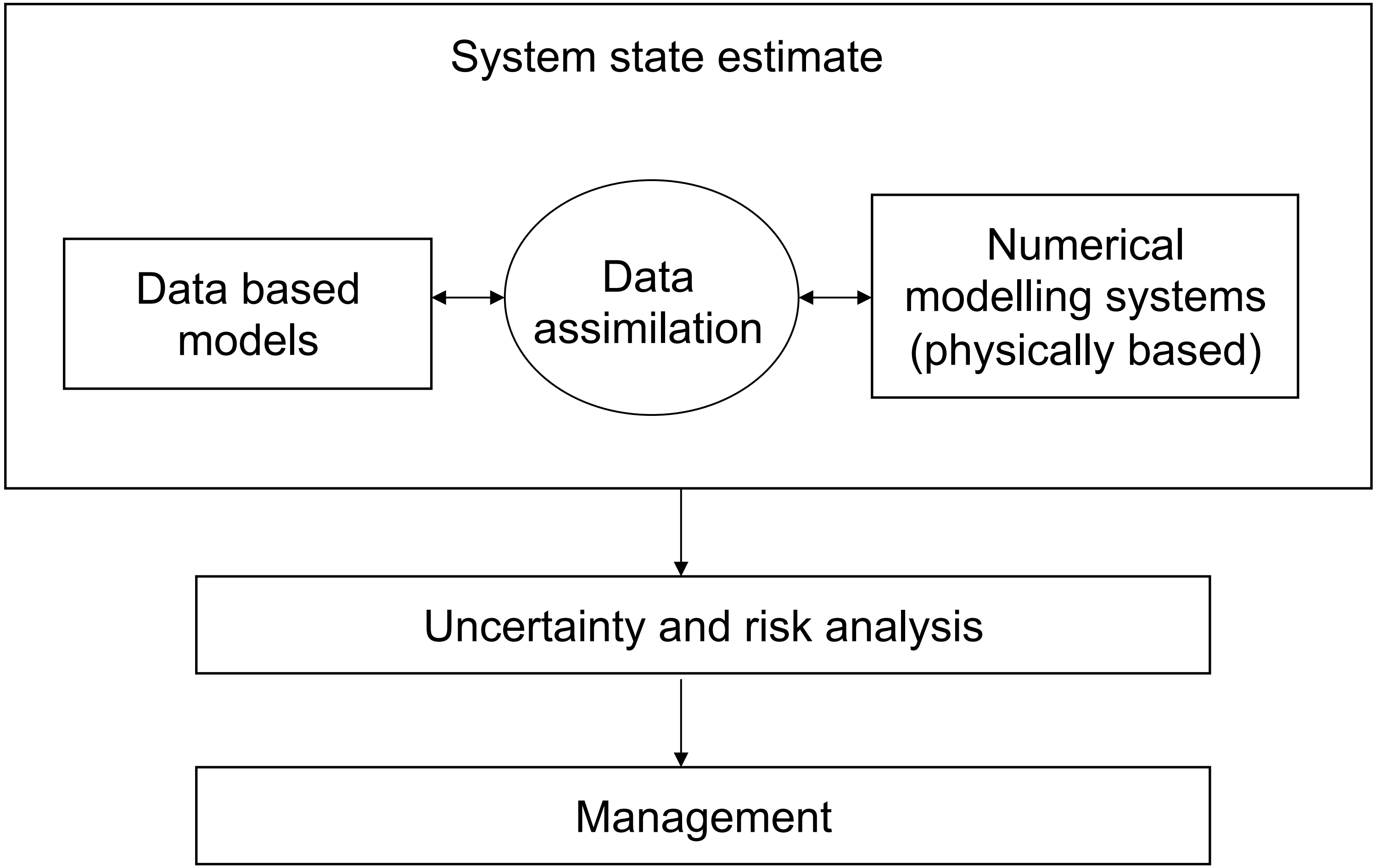
DATA ASSIMILATION

Data-Model Integration

(with focus on Kalman Filter)

Introduction

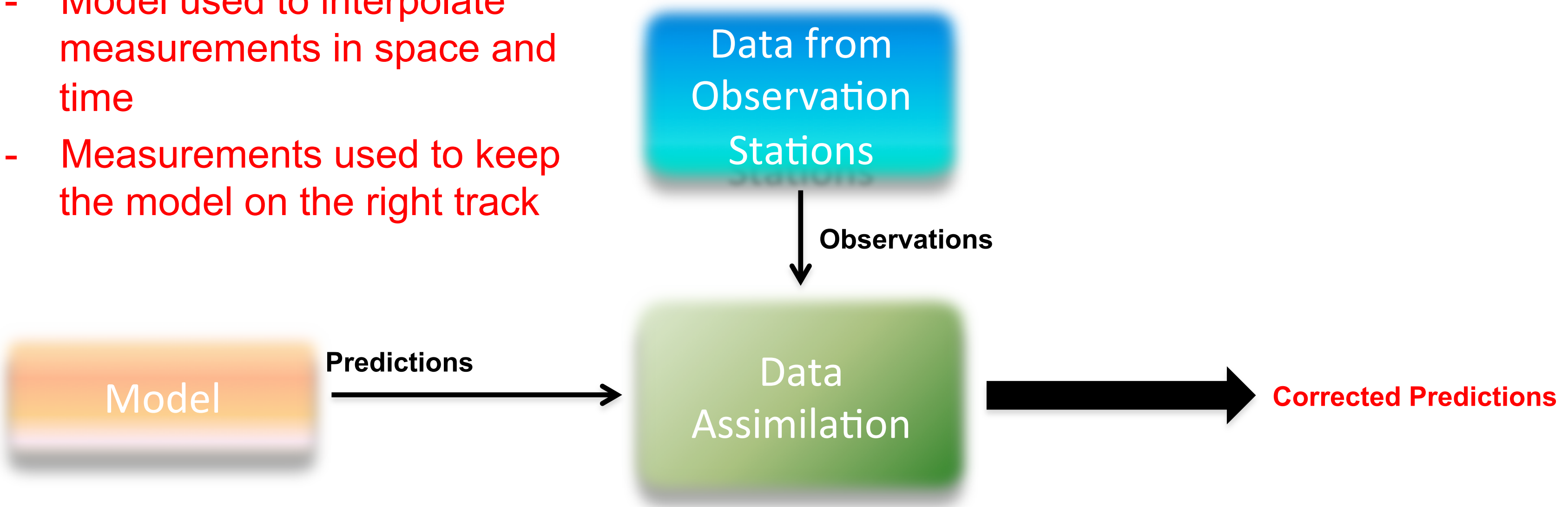


Data-Model Integration – Data Assimilation

- Monitoring network
  + Expensive
  + Sparse information in space and time
  + Precise

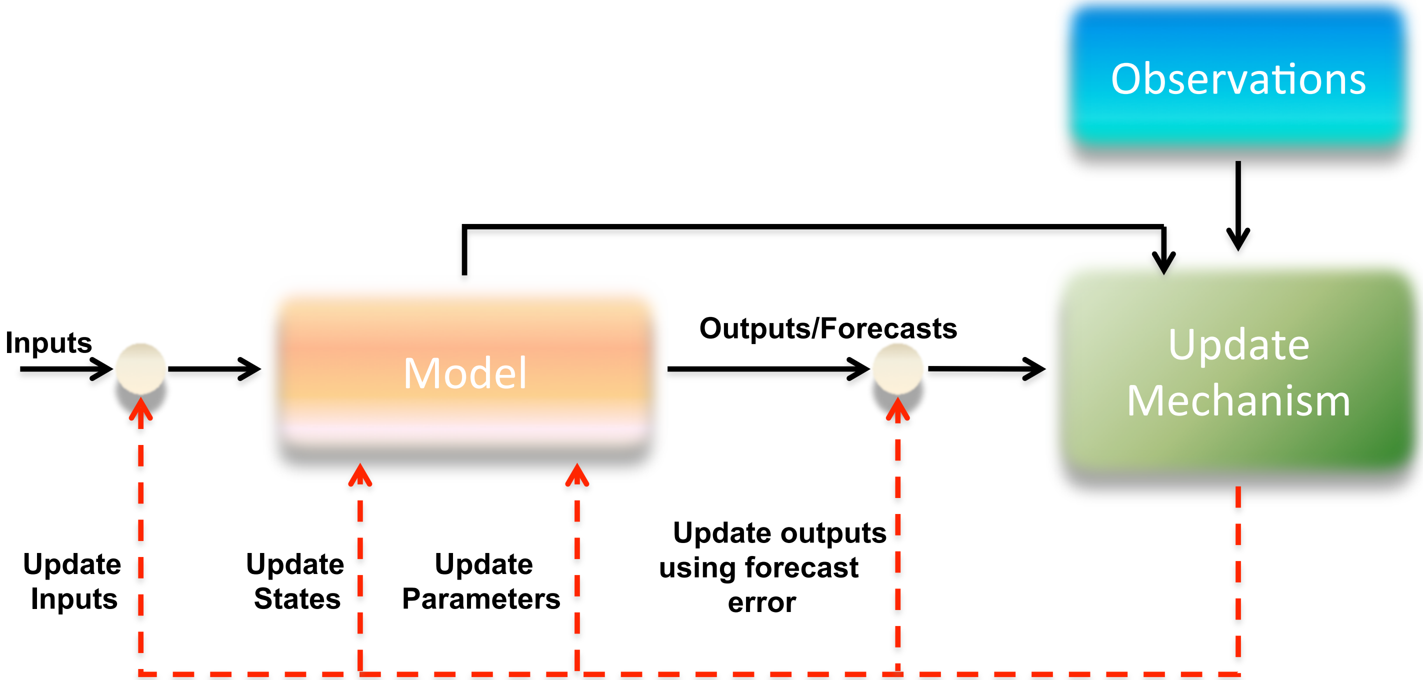
- Modelling system
  + Cheap
  + High resolution in space and time
  - Model uncertainties

- Data assimilation
  - Optimal blending of observations and models
  - Model used to interpolate measurements in space and time
  - Measurements used to keep the model on the right track



Data Assimilation Approaches

- Update model inputs (address input uncertainties)
- Update model state variables (Eg. Kalman filtering)
- Update model parameters
- Update output variables (Error forecasting)



Data Assimilation Methods

- Variational methods
  - Statistical minimisation of cost function that measure differences between simulations and observations conditioned on model dynamics
  - ➢ Optimisation algorithms
  - ➢ Adjoint method (strong/weak constraint)
- Sequential methods
  - Updating of system state during a forward model integration according to error correlation structure (on-line assimilation)
  - ➢ Fixed error correlation structure: e.g. optimal interpolation, nudging
  - ➢ Dynamical evolution of error correlation structure: Kalman filter
- Error correction
  - Correction of model simulation with a forecast of the model error in measurement locations
  - ➢ Time series analysis methods (e.g. ARMAX, local linear models, ANN, GP)

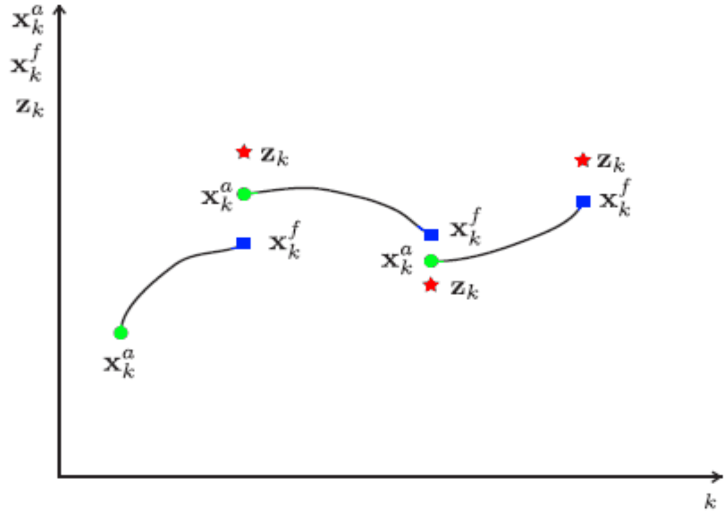
Data Assimilation using Kalman Filter (Contd..)

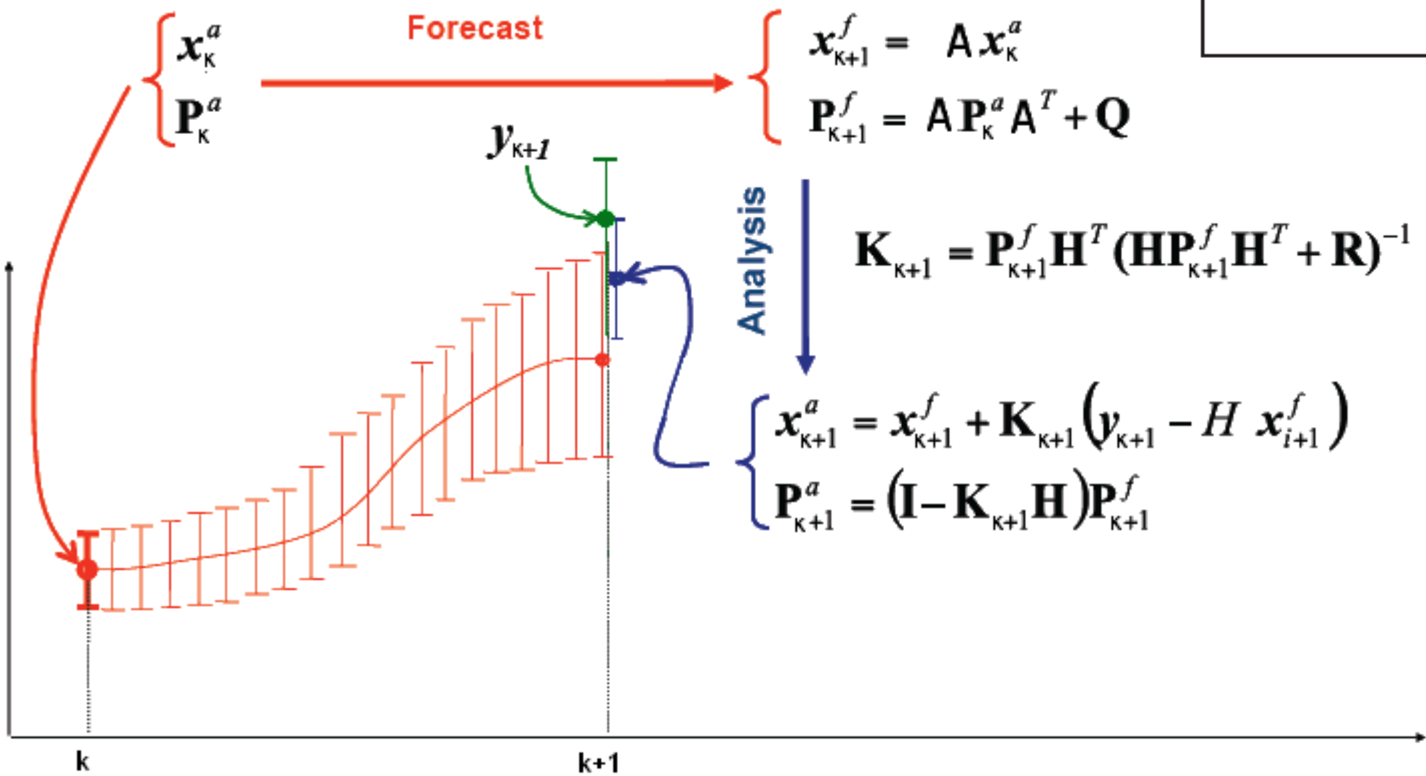
- Process model:

$$x_{k+1} = Ax_k + Bu_k + w_k$$

- Measurement model:

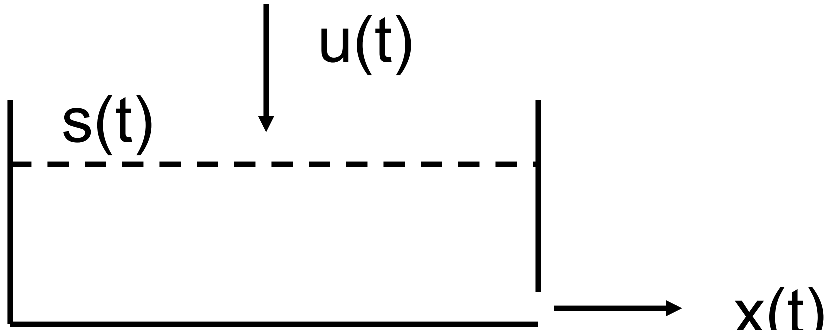
$$y_{k+1} = Hx_{k+1} + v_k$$





Kalman filter: Introductory example

- Linear reservoir model



- Governing equations

$$\frac{ds}{dt} = u - x \quad , \quad s = c_T x$$

Kalman filter: System equation

- System equation

$$x_{k+1} = Ax_k + Bu_{k+1} \quad , A = \exp\left(-\frac{\Delta t}{c_T}\right), \;\; B = (1 - A)$$

- Stochastic system equation

$$x_{k+1} = Ax_k + Bu_{k+1} + \varepsilon_k$$

$$E\{\varepsilon_k\} = 0 \quad , \quad Var\{\varepsilon_k\} = Q_k$$

Kalman filter: Model Propagation

- State propagation/forecast

$$x_1^f = Ax_0^f + Bu_1$$

- Error propagation

$$P_1^f = E\{(x_1 - x_1^f)^2\} = A^2 P_0^f + Q$$

Kalman filter: Measurement equation

- Measurement equation

$$z_k = x_k = Cx_k \quad , \quad C = 1$$

- Stochastic measurement equation

$$z_k = Cx_k + \eta_k$$

$$E\{\eta_k\} = 0 \quad , \quad Var\{\eta_k\} = R_k \quad , \quad Cov\{\varepsilon_k, \eta_k\} = 0$$

Kalman filter: Update procedure

- Updated estimate: linear combination

$$x_1^a = x_1^f + K(z_1 - Cx_1^f)$$

- Updated variance

$$P_1^a = E\{(x_1 - x_1^a)^2\} = (1 - CK)^2 P_1^f + CK^2$$

- What value of K should we use?

Kalman filter: Kalman gain (1)

- Kalman gain *K*

$$wrt K \ \min(P_1^a)$$

$$K = \frac{CP_1^f}{C^2 P_1^f + R}$$

- Best Linear Unbiased Estimator (BLUE)
  - Minimum prediction error variance
  - Normal distributed system and measurement noise: Maximum likelihood estimator

Kalman filter: Kalman gain (2)

- Measurement update equations

$$x_1^a = x_1^f + K(z_1 - Cx_1^f) = x_1^f + K(z_1 - x_1^f)$$

$$P_1^a = (1 - KC)P_1^f = (1 - K)P_1^f$$

$$K = \frac{MP_1^f}{M^2 P_1^f + R} = \frac{P_1^f}{P_1^f + R}$$

- ➢ $P_1^f > R$: More weight on model forecast
- ➢ $P_1^f < R$: More weight on measurement

Kalman filter: Numerical example (1)

- System parameters:

$$c_T = 10\Delta t$$

$$A = 0.905 \quad , \quad B = 0.095$$

$$Q = 1$$

- Initial values

$$x_0^f = 20$$

$$P_0^f = Var\{x_0^f\} = 10$$

Kalman filter: Numerical example (2)

- Model forecast (u_1 = 0)

$$x_1^f = Ax_0^f + Bu_1 = 0.905 \cdot 20 = 18.1$$

$$P_1^f = A^2 P_0^f + Q = 0.905^2 \cdot 10 + 1 = 9.19$$

- Measurement update

$$z_1 = 10 \quad , \quad R = 1$$

$$K = \frac{P_1^f}{P_1^f + R} = \frac{9.19}{9.19 + 1} = 0.90$$

$$x_1^a = x_1^f + K(z_1 - x_1^f) = 18.1 + 0.90 \cdot (10 - 18.1) = 10.8$$

$$P_1^a = (1 - K)P_1^f = (1 - 0.90) \cdot 9.19 = 0.92$$

Kalman filter: Numerical example (3)

- Model forecast ($u_2 = 0$)

$$x_2^f = Ax_1^a + Bu_2 = 0.905 \cdot 10.8 = 9.77$$

$$P_2^f = A^2 P_1^a + Q = 0.905^2 \cdot 0.92 + 1 = 1.75$$

- Measurement update

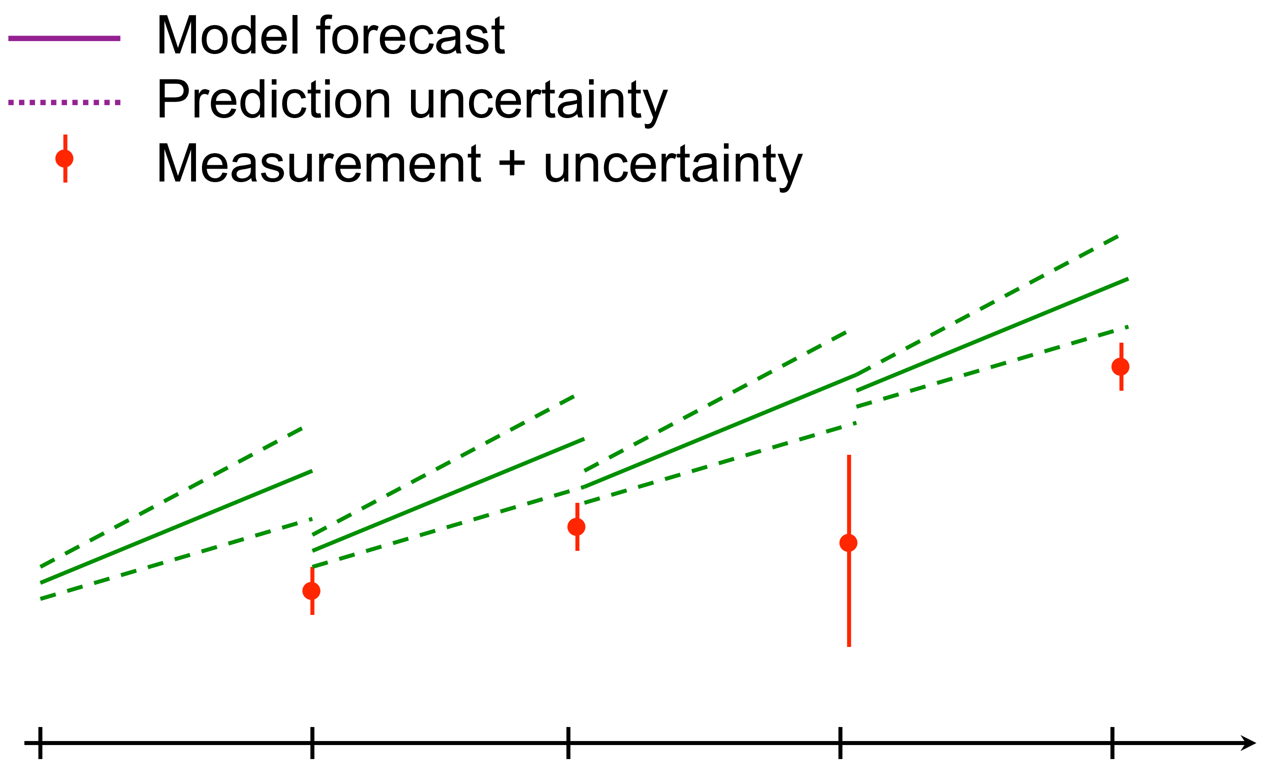
$$z_2 = 9 \quad , \quad R = 1$$

$$K = \frac{P_2^f}{P_2^f + R} = \frac{1.75}{1.75 + 1} = 0.64$$

$$x_2^a = x_2^f + K(z_2 - x_2^f) = 9.77 + 0.64 \cdot (9 - 9.77) = 9.28$$

$$P_2^a = (1 - K)P_2^f = (1 - 0.64) \cdot 1.75 = 0.63$$

Sequential model update



System and measurement equations

- System equation

$$x_{k+1} = Ax_k + Bu_{k+1} + \varepsilon_k$$

$$E\{\varepsilon_k\} = 0 \quad , \quad Var\{\varepsilon_k\} = Q_k$$

  - *x, ε* *n* x 1 vector
  - *u* *l* x 1 vector
  - *A, Q* *n* x *n* matrix
  - B *n* x *l* matrix

- Measurement equation

$$z_k = Cx_k + \eta_k$$

$$E\{\eta_k\} = 0 \quad , \quad Var\{\eta_k\} = R_k \quad , \quad Cov\{\varepsilon_k, \eta_k\} = 0$$

  - *z, η* *m* x 1 vector
  - *C* *m* x *n* matrix
  - R*m* x *m* matrix

Kalman filter equations

- Model forecast

$$x_k^f = Ax_{k-1}^a + Bu_k$$

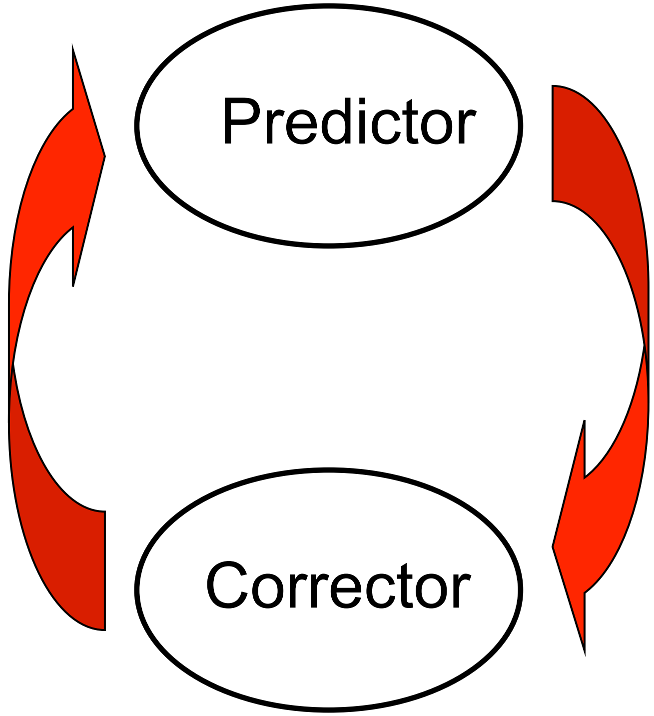
$$P_k^f = AP_{k-1}^a A^T + Q$$

- Measurement update

$$K_k = P_k^f C^T \left[CP_k^f C^T + R \right]^{-1}$$

$$x_k^a = x_k^f + K_k (z_k - Cx_k^f)$$

$$P_k^a = (I - K_k C) P_k^f$$



Application in numerical modelling

- High-dimensional systems
  - Propagation of error covariance matrix computationally infeasible
- Non-linear model dynamics
- Non-linear Measurement equation
- More complex error description
  - Non-additive noise
  - Non-Gausian
  - Coloured noise

High-dimensional systems

- Model propagation

$$x_k^f = Ax_{k-1}^a + Bu_k$$

Matrix-vector multiplication: O(n^2)

- Propagation of error covariance matrix

$$P_k^f = AP_{k-1}^a A^T + Q$$

Matrix-matrix multiplication: O(n^3)
Storage requirements: O(n^2)

- Infeasible for complex numerical models (state vector dimension $n > 10^4$)

Non-linear model dynamics: Extended Kalman filter

- System equation

$$x_k = \Phi(x_{k-1}, u_k, \varepsilon_k)$$

- Model propagation

$$x_k = \Phi(x_{k-1}, u_k, 0)$$

- Propagation of error covariance matrix: statistical linearisation

$$P_k^f = AP_{k-1}^a A^T + WQW^T$$

A: Jacobian matrix of partial derivatives of Φ with respect to x

W: Jacobian matrix of partial derivatives of Φ with respect to ε

More complex error description

- Coloured noise: augmented state vector formulation

$$\begin{pmatrix} x_k \\ \varepsilon_k \end{pmatrix} = \begin{pmatrix} A & I \\ 0 & H \end{pmatrix} \begin{pmatrix} x_{k-1} \\ \varepsilon_{k-1} \end{pmatrix} + Bu_k + \begin{pmatrix} 0 \\ I \end{pmatrix} \nu_k$$

  H: coulered noise model operator

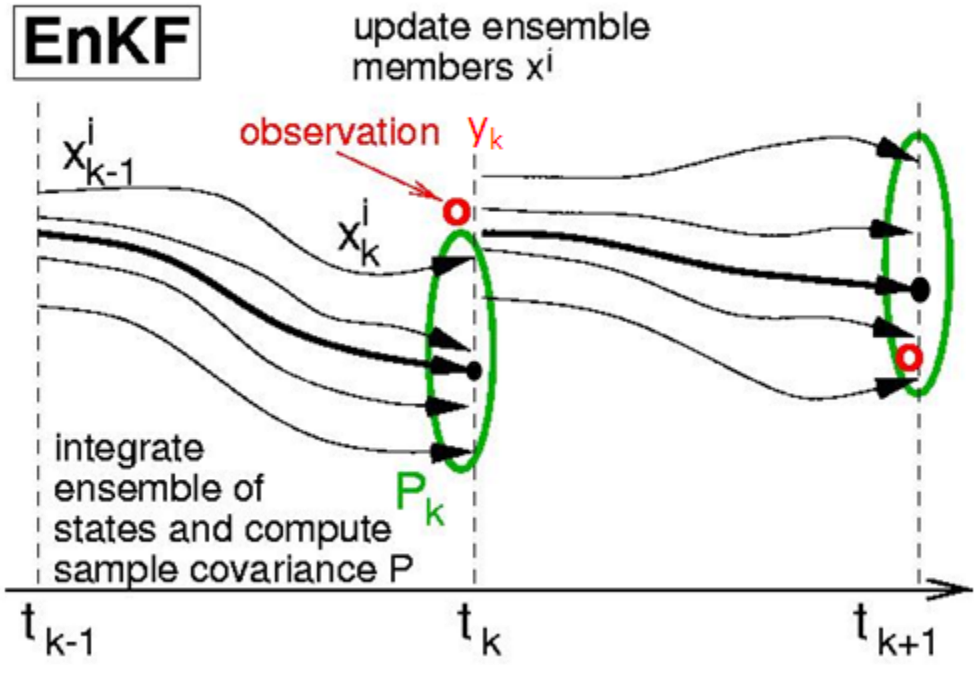
  ν: White noise process

- Non-Gausian error description: higher order filters

Approximate Kalman filter schemes

- Simplification of model dynamics for propagation of error covariance matrix
  - Coarse grid
  - Simplified physical description
- Approximation of error covariance modelling
  - Monte Carlo simulation: propagation of ensemble of model states
  - Reduced rank approximation
  - Steady state assumption (no error propagation)
- Hybrid methods
  - Combinations of above

Ensemble Kalman filter (EnKF)



$$X = [\mathbf{x}_1, \ldots, \mathbf{x}_N] = [\mathbf{x}_i] \,.$$

$$D = [\mathbf{d}_1, \ldots, \mathbf{d}_N] = [\mathbf{d}_i] \,, \quad \mathbf{d}_i = \mathbf{d} + \epsilon_i,$$

$$E(X) = \frac{1}{N} \sum_{k=1}^{N} \mathbf{x}_k, \quad C = \frac{AA^T}{N-1},$$

$$A = X - E(X) = X - \frac{1}{N} (X\mathbf{e}_{N\times 1})\, \mathbf{e}_{1\times N},$$

Propagation t_{k-1} to t_k:

$x_k^{i-} = f(x_{k-1}^{i+}) + e_k^i$

e = model error

Update at t_k:

$x_k^{i+} = x_k^{i-} + K_k(y_k^i - x_k^{i-})$

for each ensemble member i=1…N

$K_k = P_k (P_k + R_k)^{-1}$

with P_k computed from ensemble spread

Reduced rank square root filter (RRSQRT)

- Square root of error covariance matrix approximated by a matrix of lower rank q << dimension of state vector
- Propagation of covariance matrix: q model runs
- Combination of propagated error and new model error using eigenvalue decomposition
- Ensemble KF with error propagation in the directions of the most leading eigenvalues.

Other assimilation schemes

- State update

$$x_k^a = x_k^f + K_k(z_k - Cx_k^f)$$

- Determination of weighting matrix K?
- Optimal interpolation / statistical interpolation
  - Fixed error hypothesis (weighting matrix assigned and fixed)
  - Steady-state Kalman filter
- Nudging / direct relaxation
  - Observable state variables are relaxed to the observations (weighting matrix assigned and diagonal)
  - Other state variables are modified according to the model dynamics