Filtering, data assimilation, SDE's

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Contents

Last week

Statistical methods to handle uncertainty in differential equation models:

- Least squares estimation of unknown parameters (finite dimensional).
- Bayesian estimation of unknown inputs (infinite dimensional).
- Recursive estimation of state of a system with incomplete and noisy data (filtering, data assimilation).
- Explicit inclusion of a bias term.
- Time-varying parameters.
- Stochastic differential equations (SDE's): Noise is included in the dynamics.

Today

Take up two topics in some more detail

- Filtering for state space models: Kalman, Ensemble Kalman and Particle Filters.
- SDE's: Ito formula, Simulation, Girsanov's theorem, Estimation of parameters.

General state space models

Consist of an unobserved state sequence (x_t) and an observation sequence (y_t) of the following form

$$\begin{aligned} x_t &= g(x_{t-1}) + U_t, \\ y_t &= h(x_t) + V_t \end{aligned}$$

where the system noises U_t and observation noises V_t are all mutually independent.

Graphical representation:

$$\begin{array}{ccccccccc} \cdots & \rightarrow & x_{t-1} & \rightarrow & x_t & \rightarrow & x_{t+1} & \rightarrow & \ldots \\ & & \downarrow & & \downarrow & & \downarrow & & \\ \cdots & & y_{t-1} & & y_t & & y_{t+1} & & \ldots \end{array}$$

Scope of the model

- (x_t) is Markovian, (y_t) is not.
- Usually x_t is high-dimensional.
- Often components of x_t associated with some spatial location.
- State evolution can be deterministic, i.e. $U_t = 0$.
- In a fluid model, x_t can be the velocity field on a fine grid, y_t velocity measured on a coarse grid.
- Noise need not be additive.
- g, h and noise distributions could depend on t.

Goals

Use observations $(y_1, \dots y_s)$ and knowledge about the dynamics to determine an unobserved state x_t

$s < t$	Prediction, Forecasting
$s = t$	Filtering, Nowcasting, Analysis
$s > t$	Smoothing, Backcasting, Reanalysis.

Both available information and unknown variable change with time.

Predictive and filter distributions: Recursions

Describe imperfect knowledge about x_t by probability distributions.

Predictive distribution μ_t = distribution of x_t given $y_1, \ldots y_{t-1}$.

Filter distribution ν_t = distribution of x_t given $y_1, \ldots y_t$.

ν_0 = initial distribution of x_0.

Propagation, Forecast

$$\mu_t(dx_t) = \int f_U(x_t - g(x_{t-1}))\nu_{t-1}(dx_{t-1})\, dx_t.$$

Update, Analysis

$$\nu_t(dx_t) = \frac{f_V(y_t - h(x_t))\mu_t(dx_t)}{\int f_V(y_t - h(x))\mu_t(dx)}.$$

Linear Gaussian model: Kalman filter

Exact solution is available if

$$g(x) = Gx, \; h(x) = Hx, \; U_t \sim \mathcal{N}(0, R), \quad V_t \sim \mathcal{N}(0, Q).$$

If $\nu_0 = \mathcal{N}(0, P_0^f)$, then for all t

$$\mu_t = \mathcal{N}(m_t^p, P_t^p), \quad \nu_t = \mathcal{N}(m_t^f, P_t^f).$$

Recursions for means and covariances:

$$m_t^p = G m_{t-1}^f, \quad P_t^p = G P_{t-1}^f G^T + R$$

and

$$m_t^f = m_t^p + K_t(y_t - H m_t^p), \quad P_t^f = (I - K_t H) P_t^p$$

where K_t is the gain matrix

$$K_t = P_t^p H^T (Q + H P_t^p H^T)^{-1}.$$

Monte Carlo propagation and update

Monte Carlo methods represent μ_t and ν_t by samples (ensembles) $(\tilde{x}_{t,j}; 1 \leq j \leq N)$ and $(x_{t,j}; 1 \leq j \leq N)$ which evolve in time.

Propagation: From $(x_{t-1,j})$ to $(\tilde{x}_{t,j})$.

$$\tilde{x}_{t,j} = g(x_{t-1,j}) + U_{t,j}$$

where $U_{t,j}$ are independent replicates of U_t.

Update: From $(\tilde{x}_{t,j})$ to $(x_{t,j})$. Two methods, particle and ensemble filters.

Particle filter update

If μ_t is discrete with values $(\tilde{x}_{t,j})$ and weights $1/N$, then by Bayes formula ν_t is also discrete with the same values, but weights

$$w_{t,j} = \frac{f_V(y_t - h(\tilde{x}_{t,j}))}{\sum_k f_V(y_t - h(\tilde{x}_{t,k}))}.$$

Could propagate a weighted discrete ν_t, but weights degenerate quickly during the iterations. To overcome this, use resampling: Choose $\tilde{x}_{t,j}$ approximately $Nw_{t,j}$ times. High weight particles are multiplied, low weight particles die out. See separate figure.

If the evolution of states is stochastic, ties are broken during the next propagation step. Otherwise, need to add a bit of noise.

Illustration

Consider

$$x_t = 0.5x_{t-1} + 25\frac{x_{t-1}}{1 + x_{t-1}^2} + \gamma\cos(1.2t) + U_t, \quad y_t = \frac{x_t^2}{20} + V_t.$$

which goes back to Andrade Netto et al., IEEE Trans. Autom. Control (1978). y_t carries no information about the sign of x_t.

In another window a simulation from the model and 10% and 90% filter quantiles are shown.

Improving the performance of particle filters

Particle filter is inefficient if weights before resampling vary widely. As in importance sampling, can use a wrong transition density $q(x_t \mid x_{t-1,j})$ in the propagation step and correct with the weights

$$w_{t,j} \propto \frac{f_V(y_t - h(\tilde{x}_{t,j}))f_U(\tilde{x}_{t,j} - g(x_{t-1,j}))}{q(\tilde{x}_{t,j} \mid x_{t-1,j})}.$$

Various ideas for constructing good $q's$ (that depend on y_t) exist.

Ensemble filter update

Assume a linear observation function with Gaussian noise:

$$h(x) = Hx, \quad V \sim \mathcal{N}(0, Q).$$

The Kalman filter update gives $\nu_t = \mathcal{N}(m_t^f, P_t^f)$ where

$$m_t^f = m_t^p + K_t(y_t - Hm_t^p), \; P_t^f = (I - K_t H)P_t^p.$$

Note: This is only correct if also μ_t is Gaussian.

The ensemble Kalman filter estimates m_t^p and P_t^p from $(\tilde{x}_{t,j})$, computes m_t^f and P_t^f and then samples $(x_{t,j})$ from $\mathcal{N}(m_t^f, P_t^f)$.

Implementing the ensemble filter

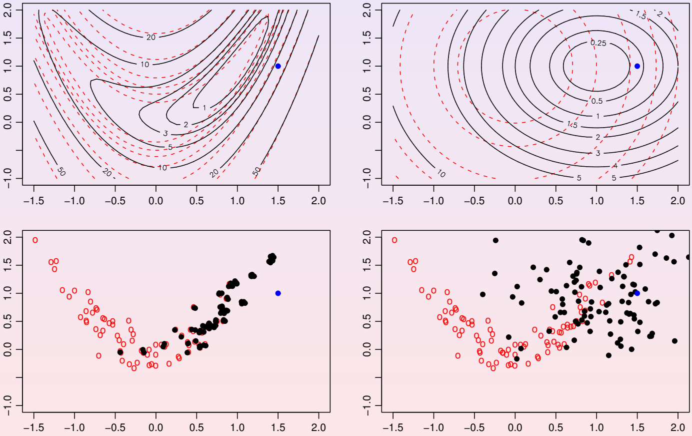
Sampling is possible without computing P_t^f or taking its square root. Can take $z_j \sim \mathcal{N}(m_t^p, P_t^p)$ and $V_j \sim \mathcal{N}(0, Q)$ and put

$$x_{t,j} = z_j + K_t(y_t - Hz_j + V_j).$$

To reduce the error due to the Gaussian assumption and to avoid taking the square root of P_t^p, take $z_j = \tilde{x}_{t,j}$. (Still need to estimate P_t^p to compute K_t).

Changing y_t results in an additive shift of the filter sample. Not correct if the shape of ν_t depends on y_t.

Illustration of particle and ensemble updates



Difficulties in high dimensions

Size of the sample N is typically much smaller than dimensions of the state vector x and observation vector y.

Ensemble filter can cope with this. Can reduce the error in estimating P_t^p by sparsity assumptions.

Particle filter typically degenerates: Updating puts all the weights on one value in the sample. Challenge: Modify the particle filter so that it also works in high dimensions.

The likelihood function

Let g, h, f_U and f_V depend on an unknown parameter θ.

Cannot compute the log likelihood function:

$$\begin{aligned}\log L(\theta) &= \sum_t \log p(y_t \mid y_1, \ldots y_{t-1}, \theta) \\ &= \sum_t \log \int f_V(y_t - h(x_t)) d\mu_t(x_t)\end{aligned}$$

(In the last expression both the integrand and μ_t depend on θ.)

Offline estimation

This means: All observations are available at the beginning.
Options

- Estimate θ and (x_t) by MCMC,
- Estimate θ by stochastic EM,
- Approximate the likelihood by filtering and maximize it.

Efficient implementations of all these options are challenging.

Online estimation

Observations become available sequentially.
Options

- Take θ as part of the state vector with deterministic evolution $\theta_t = \theta_{t-1}$.
- Approximate ν_t and its derivative w.r.t. to θ by Monte Carlo methods and use recursive optimization.

Again, this is not easy.

An SDE has the following form

$$dx_t = g(x_t)dt + \sigma(x_t)dB_t$$

where the increments $dB(t)$ of Brownian motion are jointly Gaussian with

$$E[dB_t] = 0, E[dB_t dB_s^T] = \delta_{ts}\ I\ dt$$

(I is the identity matrix, x_t and g are vectors, σ is a matrix).

Rigorously, an SDE is defined as an integral equation. I use the Ito version of the stochastic integral.

The solution of an SDE is a Markov process in continuous time.

Ito formula

ODE's and SDE's are different! E.g. the "intuitive" result

$$d(f(x_t)) = \frac{\partial f}{\partial x}(x_t)dx_t$$

is no longer correct. One has to expand f up to second order, using

$$dx_t dx_t^T = \sigma(x_t)\sigma(x_t)^T dt.$$

Example: If $z_t = \exp(\lambda t + \sigma B_t)$, then

$$dz_t = (\lambda + \sigma dB_t)z_t + \frac{1}{2}\sigma^2 z_t dt.$$

Simulating an SDE

To simulate the solution of an SDE, the easiest method is the Euler approximation

$$x_{t+h} = x_t + h\, g(x_t) + \mathcal{N}(0, h\, \sigma(x_t)\sigma(x_t)^T)).$$

There are better alternatives, but these are different from those used to solve ODE's.

Exact simulation

Gareth Roberts and coworkers found a way to simulate "exactly" the solution from an SDE of the following form

$$dx_t = g(x_t)dt + dB_t, \quad g = \frac{\partial G}{\partial x}.$$

Exactly means that we can generate values x_{t_i} on an arbitrary grid which can be refined later on.

This can be done by simulating Brownian motion and using importance sampling. The importance weights are given by the density of the distribution of x with respect to that of B. For this, we need Girsanov's formula.

Girsanov's formula

This density is equal to

$$\exp\left(\int_0^t g(B_s)dB_s - \frac{1}{2}\int_0^t g(B_s)^2 ds\right).$$

Ito's formula allows to get rid of the stochastic integral:

$$\int_0^t g(B_s)dB_s = G(B_t) - G(B_0) - \frac{1}{2}\int_0^t \Delta G(B_s)ds.$$

To compute this, we still need the whole path of B. But can generate random unbiased weights that need B only at a finite number of (random) time points.

Statistics for SDE's

A key quantity in statistical applications of SDE's are the transition densities for $p(x_t \mid x_s)$. Exact computation requires solving a PDE (Fokker-Planck). Aproximate computations

- Euler approximation

$$p(x_t|x_s) \approx \phi(x_t; x_s + (t-s)g(x_s), (t-s)\sigma(x_s)\sigma(x_s)^T).$$

- Importance sampling approximations with additional intermediate time points.
- Unbiased estimation as in the case of exact simulation.

The End

Thank you for your attention.