Modeling and Analysis of Time Series Data
Chapter 11: Introduction to partially observed Markov process models

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Stochastic dynamic systems observed with noise

- Uncertainty and variability are common features of biological and social systems. Complex physical systems can also be unpredictable: we can only forecast weather reliably in the near future.
- Time series models of deterministic trend plus colored noise imply perfect predictability if the trend function enables extrapolation.
- To model variability and unpredictability in a dynamic system, we can specify a stochastic (i.e., random) model for the system.
- Often times, the full dynamic system is unobserved. We have only noisy or incomplete measurements.
- We model measurements as random variables conditional on the trajectory of the *latent process*. The latent process is also called a *state process* or *hidden process*.

The Markov property

- A model for a stochastic dynamic system has the *Markov property* if the future evolution of the system depends only on the current state, plus randomness introduced in future.
- A model with the Markov property may be called a *Markov chain* or a *Markov process*.
- We use the term Markov process since the term chain is often reserved for situations where either time or the latent state (or both) take discrete values.
- The Markov property is often used to model the latent process in a time series model.

Notation for discrete time Markov processes

- A time series model $X_{0:N}$ is a *Markov process* model if the conditional densities satisfy the *Markov property* [P1] that

$$\text{[P1]} \qquad f_{X_n|X_{0:n-1}}(x_n \,|\, x_{0:n-1}) = f_{X_n|X_{n-1}}(x_n \,|\, x_{n-1})$$

  for all $n \in 1:N$.

- We may suppose there is an underlying continuous time, t, such that X_n occurs at time t_n.

- We write $X(t)$ for the continuous time model, setting $X_n = X(t_n)$.

- $t_{1:N}$ are *measurement times*.

- t_0 is the *initialization time*.

Initial conditions

- We *initialize* the Markov process model at a time t_0, although data are collected only at times $t_{1:N}$.
- The initialization model could be deterministic (a fixed value) or a random variable.
- We model $X_0 = X(t_0)$ as a draw from a probability density function
$$f_{X_0}(x_0). \tag{1}$$
- A fixed initial value is a special case of a density corresponding to a point mass with probability one at the fixed value.
- A discrete probability mass function is a special case of a density corresponding to a collection of point masses.

The process model

- The probability density function $f_{X_n|X_{n-1}}(x_n \,|\, x_{n-1})$ is called the *one-step transition density* of the Markov process.
- The Markov property asserts that the next step taken by a Markov process follows the one-step transition density based on the current state, whatever the previous history of the process.
- For a Markov model, the full joint distribution of the latent process is entirely specified by the one-step transition densities, given the initial value.
- Therefore, we also call $f_{X_n|X_{n-1}}(x_n \,|\, x_{n-1})$ the *process model*.

The joint distribution in terms of one-step transition densities

Exercise. Use [P1] to derive an expression for the joint distribution of a Markov process as a product of the one-step transition densities. In other words, derive

$$\text{[P2]} \qquad f_{X_{0:N}}(x_{0:N}) = f_{X_0}(x_0) \prod_{n=1}^{N} f_{X_n|X_{n-1}}(x_n \mid x_{n-1}).$$

Hint: This involves elementary rules for manipulation of joint and conditional densities, together with application of the Markov property. It is a good exercise to work through by hand to build familiarity with the model class.

Question. Explain why a causal Gaussian AR(1) process is a Markov process.

Time-homogeneous transitions and stationarity

- The one-step transition density $f_{X_n|X_{n-1}}$ for a Markov process $X_{0:N}$ can depend on n.
- $X_{0:N}$ is *time-homogeneous* if $f_{X_n|X_{n-1}}$ does not depend on n, so there is a conditional density $f(\cdot\,|\,\cdot)$ such that, for all $n \in 1{:}N$,

$$f_{X_n|X_{n-1}}(x_n\,|\,x_{n-1}) = f(x_n\,|\,x_{n-1}). \tag{2}$$

Question. If $X_{0:N}$ is strictly stationary, it is time-homogeneous. Why?

Question. Time-homogeneity does not necessarily imply stationarity. Find a counter-example.

Partially observed Markov process (POMP) models

- *Partial observation* may mean either or both of (i) measurement noise; (ii) entirely unmeasured latent variables.
- These features are present in many systems.
- A *partially observed Markov process* (POMP) model is defined by putting together a Markov latent process model and a *measurement model*.
- POMP models are a general class, covering many models designed for specific applications.
- Statistical methods for this general class give us flexibility to develop specific POMP models appropriate to a range of applications.

The measurement model

- The *measurement process* is a collection of random variables $Y_{1:N}$ which models the data $y_{1:N}$.
- Y_n is assumed to depend on the latent process only through its value X_n at the time of the measurement. Formally, this assumption is:

$$\text{[P3]} \qquad f_{Y_n|X_{0:N},Y_{1:n-1},Y_{n+1:N}}(y_n \,|\, x_{0:N}, y_{1:n-1}, y_{n+1:N}) \\ = f_{Y_n|X_n}(y_n \,|\, x_n)$$

- We call $f_{Y_n|X_n}(y_n \,|\, x_n)$ the *measurement model*.

Time-homogeneous measurement models

- In general, the measurement model can depend on n or on any covariate time series.
- The measurement model is *time-homogeneous* if there is a conditional probability density function $g(\cdot \,|\, \cdot)$ such that, for all $n \in 1:N$,

$$f_{Y_n|X_n}(y_n \,|\, x_n) = g(y_n \,|\, x_n). \tag{3}$$

- Time-inhomogeneous process and measurement models are sufficiently common that we benefit from the extra generality of writing $f_{X_n|X_{n-1}}(x_n|x_{n-1})$ and $f_{Y_n|X_n}(y_n|x_n)$ versus $f(x_n|x_{n-1})$ and $g(y_n|x_n)$.

Prediction, filtering, smoothing and likelihood

Four basic calculations for working with POMP models

Many time series models in science, engineering and industry can be written as POMP models. A reason that POMP models form a useful tool for statistical work is that there are convenient recursive formulas to carry out four basic calculations:

1. Prediction
2. Filtering
3. Smoothing
4. Likelihood calculation

Prediction

- *One-step prediction* (also called forecasting) of the latent process at time t_{n+1} given data up to time t_n involves finding
$$f_{X_{n+1}|Y_{1:n}}(x_{n+1}\,|\,y_{1:n}). \tag{4}$$
- We may want to predict more than one time step ahead. However, one-step prediction turns out to be closely related to computing the likelihood function, and therefore central to statistical inference.
- Our prediction is a conditional probability density, not a point estimate. In the context of forecasting, this is called a *probabilistic forecast*. What are the advantages of a probabilistic forecast over a point forecast? Are there any disadvantages?

Filtering

- The *filtering* calculation at time t_n is to find the conditional distribution of the latent process X_n given data $y_{1:n}$ available at time t_n.
- Filtering involves calculating

$$f_{X_n|Y_{1:n}}(x_n \,|\, y_{1:n}). \tag{5}$$

- This can be evaluated numerically or algebraically. We will see that Monte Carlo methods can be a good tool.
- The name "filtering" comes from the history of signal processing. A noisy received signal was passed through capacitors and resistors to construct a band pass filter estimating the source signal, just like an optical filter removes unwanted frequencies of light.

Smoothing

- In the context of a POMP model, smoothing involves finding the conditional distribution of X_n given all the data, $y_{1:N}$.

- So, the smoothing calculation is to find

$$f_{X_n|Y_{1:N}}(x_n \,|\, y_{1:N}). \tag{6}$$

The likelihood

- The likelihood is the joint density of $Y_{1:N}$ evaluated at the data,
$$f_{Y_{1:N}}(y_{1:N}). \tag{7}$$
- The model may depend on a parameter vector θ. We can include θ in all the joint and conditional densities above. Then, the *likelihood function* is the likelihood viewed as a function of θ. We write
$$\mathcal{L}(\theta) = f_{Y_{1:N}}(y_{1:N};\, \theta) \tag{8}$$
- If we can compute $\mathcal{L}(\theta)$ then we can perform numerical optimization to get a maximum likelihood estimate.
- Likelihood evaluation and maximization lets us compute profile likelihood confidence intervals, carry out likelihood ratio tests, and make AIC model comparisons.

The prediction formula

- One-step prediction of the latent process at time t_n given data up to time t_{n-1} can be computed recursively in terms of the filtering problem at time t_{n-1}, via the *prediction formula* for $n \in 1:N$,

$$\text{[P4]} \quad f_{X_n|Y_{1:n-1}}(x_n \,|\, y_{1:n-1}) \;=\; \int f_{X_{n-1}|Y_{1:n-1}}(x_{n-1} \,|\, y_{1:n-1})\, f_{X_n|X_{n-1}}(x_n \,|\, x_{n-1})\, dx_{n-1}.$$

- For the case $n=1$, we let $1:k$ be the empty set when $k=0$, so that $f_{X_0|Y_{1:0}}(x_0 \,|\, y_{1:0})$ means $f_{X_0}(x_0)$. In other words, the filter distribution at time t_0 is the initial density for the latent process, since at time t_0 we have no data to condition on.

Exercise. Derive [P4] using the definition of a POMP model with elementary properties of joint and conditional densities.

Hints for deriving the recursion formulas

Any general identity holding for densities must also hold when we condition everything on a new variable.

Example 1. From

$$f_{XY}(x, y) = f_X(x)\, f_{Y|X}(y \,|\, x) \tag{9}$$

we can condition on Z to obtain

$$f_{XY|Z}(x, y \,|\, z) = f_{X|Z}(x \,|\, z)\, f_{Y|XZ}(y \,|\, x, z). \tag{10}$$

Example 2. The prediction formula is a special case of the identity

$$f_{X|Y}(x \,|\, y) = \int f_{XZ|Y}(x, z \,|\, y)\, dz. \tag{11}$$

Example 3. A conditional form of Bayes' identity is

$$f_{X|YZ}(x \,|\, y, z) = \frac{f_{Y|XZ}(y \,|\, x, z)\, f_{X|Z}(x \,|\, z)}{f_{Y|Z}(y \,|\, z)}. \tag{12}$$

The filtering formula

Filtering at time t_n can be computed by combining the new information in the datapoint y_n with the calculation of the one-step prediction of the latent process at time t_n given data up to time t_{n-1}.

- This is carried out via the *filtering formula* for $n \in 1:N$,

[P5] $$f_{X_n|Y_{1:n}}(x_n \,|\, y_{1:n}) = \frac{f_{X_n|Y_{1:n-1}}(x_n \,|\, y_{1:n-1})\, f_{Y_n|X_n}(y_n \,|\, x_n)}{f_{Y_n|Y_{1:n-1}}(y_n \,|\, y_{1:n-1})}.$$

Exercise. Derive [P5] using the definition of a POMP model with elementary properties of joint and conditional densities.

The prediction and filtering formulas are *recursive*. If they can be computed for time t_n then they enable the computation at time t_{n+1}.

The conditional likelihood formula

- The denominator in the filtering formula [P5] is the *conditional likelihood* of y_n given $y_{1:n-1}$.
- It can be computed in terms of the one-step prediction density, via the *conditional likelihood formula*,

$$\text{[P6]} \quad f_{Y_n|Y_{1:n-1}}(y_n \,|\, y_{1:n-1}) \;=\; \int f_{X_n|Y_{1:n-1}}(x_n \,|\, y_{1:n-1})\, f_{Y_n|X_n}(y_n \,|\, x_n)\, dx_n.$$

- To make this formula work for $n = 1$, we take advantage of the convention that $1:k$ is the empty set when $k = 0$.

Computation of the likelihood and log likelihood

- The likelihood of the entire dataset, $y_{1:N}$ can be found from [P6], using the identity

$$f_{Y_{1:N}}(y_{1:N}) = \prod_{n=1}^{N} f_{Y_n|Y_{1:n-1}}(y_n \,|\, y_{1:n-1}). \qquad (13)$$

- This equation uses the convention that $1:k$ is the empty set when $k=0$, so the first term in the product is

$$f_{Y_1|Y_{1:0}}(y_1 \,|\, y_{1:0}) = f_{Y_1}(y_1) \qquad (14)$$

- If our model has an unknown parameter θ then this gives the *log likelihood function* as a sum of conditional log likelihoods,

$$\ell(\theta) = \log \mathcal{L}(\theta) = \log f_{Y_{1:N}}(y_{1:N};\,\theta) = \sum_{n=1}^{N} \log f_{Y_n|Y_{1:n-1}}(y_n \,|\, y_{1:n-1};\,\theta).$$

The smoothing recursions

- Smoothing is less fundamental for likelihood-based inference than filtering and one-step prediction.
- Nevertheless, sometimes we want to compute the smoothing density, so we develop some necessary formulas.
- The filtering and prediction formulas are recursions forward in time: a solution at time t_{n-1} is used for the computation at t_n.
- For smoothing, we have *backwards smoothing recursion formulas*,

[P7] $f_{Y_{n:N}|X_n}(y_{n:N} \,|\, x_n) = f_{Y_n|X_n}(y_n \,|\, x_n) f_{Y_{n+1:N}|X_n}(y_{n+1:N} \,|\, x_n)$.

[P8] $$f_{Y_{n+1:N}|X_n}(y_{n+1:N} \,|\, x_n) = \int f_{Y_{n+1:N}|X_{n+1}}(y_{n+1:N} \,|\, x_{n+1})\, f_{X_{n+1}|X_n}(x_{n+1} \,|\, x_n)\, dx_{n+1}.$$

Combining recursions to find the smoothing distribution

The forwards and backwards recursion formulas together allow us to compute the *smoothing formula*,

$$\text{[P9]} \quad f_{X_n|Y_{1:N}}(x_n\,|\,y_{1:N}) = \frac{f_{X_n|Y_{1:n-1}}(x_n\,|\,y_{1:n-1})\, f_{Y_{n:N}|X_n}(y_{n:N}\,|\,x_n)}{f_{Y_{n:N}|Y_{1:n-1}}(y_{n:N}\,|\,y_{1:n-1})}.$$

Exercise. Show how [P7], [P8] and [P9] follow from the basic properties of conditional densities combined with the Markov property.

Hint: you can write the left hand side of [P9] as $f_{X|YZ}$ with $X = X_n$, $Y = Y_{1:n-1}$, $Z = Y_{n:N}$.

Linear Gaussian POMP (LG-POMP) models

Linear Gaussian partially observed Markov process (LG-POMP) models have many applications across science and engineering.

- Gaussian ARMA models are LG-POMP models. The POMP recursion formulas give a computationally efficient way to obtain the likelihood of a Gaussian ARMA model.
- Smoothing splines (including the Hodrick-Prescott filter, which is a smoothing spline) can be written as an LG-POMP model.
- The *Basic Structural Model* is an LG-POMP used for econometric forecasting. It models a stochastic trend, seasonality, and measurement error, in a framework with econometrically interpretable parameters. This is more interpretable than fitting SARIMA.

If an LG-POMP model is appropriate, you avoid Monte Carlo computations needed for inference in general nonlinear POMPs.

The general LG-POMP model

Suppose the latent process, $X_{0:N}$, and the observation process $\{Y_n\}$, take vector values with dimension d_X and d_Y. A general mean zero LG-POMP model is specified by

- A sequence of $d_X \times d_X$ matrices, $\mathbf{A}_{1:N}$,
- A sequence of $d_X \times d_X$ covariances, $\{\Sigma_{X,n}, n \in 0:N\}$,
- A sequence of $d_Y \times d_X$ matrices, $\mathbf{B}_{1:N}$,
- A sequence of $d_Y \times d_Y$ covariances, $\{\Sigma_{Y,n}, n \in 1:N\}$.

We initialize with $X_0 \sim \mathrm{N}[0, \Sigma_{X,0}]$ and then define the entire LG-POMP model by a recursion for $n \in 1:N$,

$$\begin{aligned} &\text{[LG1]} \qquad X_n &&= \mathbf{A}_n X_{n-1} + \epsilon_n, \qquad \epsilon_n \sim \mathrm{N}[0, \Sigma_{X,n}], \\ &\text{[LG2]} \qquad Y_n &&= \mathbf{B}_n X_n + \eta_n, \eta_n \sim \mathrm{N}[0, \Sigma_{Y,n}]. \end{aligned}$$

Often, but not always, we will have a *time-homogeneous* LG-POMP model, with $\mathbf{A}_n = \mathbf{A}$, $\mathbf{B}_n = \mathbf{B}$, $\Sigma_{X,n} = \Sigma_X$, and $\Sigma_{Y,n} = \Sigma_Y$ for $n \in 1:N$.

The LG-POMP representation of a Gaussian ARMA

- Let $\{Y_n\}$ be a Gaussian ARMA(p,q) model with noise process $\omega_n \sim \mathrm{N}[0,\sigma^2]$, defined by

$$Y_n = \sum_{j=1}^{p} \phi_j Y_{n-j} + \omega_n + \sum_{k=1}^{q} \theta_k \omega_{n-k}. \tag{15}$$

- We look for a time-homogeneous LG-POMP defined by [LG1] and [LG2] where Y_n is the first component of X_n with no measurement error.
- To do this, we define $d_X = r = \max(p, q+1)$ and

$$\mathbf{B} = (1, 0, 0, \dots, 0), \tag{16}$$

$$\Sigma_Y = 0. \tag{17}$$

- We require $\mathbf{A}$ and Σ_X such that Y_n satisfies the ARMA equation.

We state a solution and see if it works out. Consider

$$X_n = \left(\begin{array}{l} Y_n \\ \phi_2 Y_{n-1} + \dots + \phi_r Y_{n-r+1} + \theta_1 \omega_n + \dots + \theta_{r-1}\omega_{n-r+2} \\ \phi_3 Y_{n-1} + \dots + \phi_r Y_{n-r+1} + \theta_2 \omega_n + \dots + \theta_{r-1}\omega_{n-r+3} \\ \vdots \\ \phi_r Y_{n-1} + \theta_{r-1}\omega_n \end{array} \right)$$

We check that the ARMA equation matches the matrix equation

$$X_n = \mathbf{A} X_{n-1} + \left(\begin{array}{l} 1 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_{r-1} \end{array} \right) \omega_n, \text{ for } \mathbf{A} = \left(\begin{array}{ccccc} \phi_1 & 1 & 0 & \dots & 0 \\ \phi_2 & 0 & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \phi_{r-1} & 0 & \dots & 0 & 1 \\ \phi_r & 0 & \dots & 0 & 0 \end{array} \right)$$

This is a time-homogeneous LG-POMP, with $\mathbf{A}$, $\mathbf{B}$ and Σ_Y as above and

$$\Sigma_X = \sigma^2 (1, \theta_1, \theta_2, \dots, \theta_{r-1})^T (1, \theta_1, \theta_2, \dots, \theta_{r-1}). \qquad (18)$$

Different POMPs can give the same model for $Y_{1:N}$

- There are other LG-POMP representations giving rise to the same ARMA model.
- When only one component of a latent process is observed, any model giving rise to the same observed component is indistinguishable from the data.
- Here, the LG-POMP model has order $d_X^2 = r^2 = \max(p, q+1)^2$ parameters. The ARMA model has order r parameters, so we expect many ways to parameterize the ARMA model as a special case of the much larger LG-POMP model.
- This unidentifiability can also arise for non-Gaussian POMPs, but it is easier to see in the Gaussian case.

The basic structural model

- The *basic structural model* was developed for econometric analysis.
- It decomposes an observable process $Y_{1:N}$ as the sum of a *level* (L_n), a *trend* (T_n) describing the rate of change of the level, and a monthly *seasonal component* (S_n).
- The model supposes that the level, trend and seasonality are perturbed with Gaussian white noise at each time point,

$$\begin{array}{ll}
\text{[BSM1]} & Y_n = L_n + S_n + \epsilon_n \\
\text{[BSM2]} & L_n = L_{n-1} + T_{n-1} + \xi_n \\
\text{[BSM3]} & T_n = T_{n-1} + \zeta_n \\
\text{[BSM4]} & S_n = -\displaystyle\sum_{k=1}^{11} S_{n-k} + \eta_n
\end{array}$$

where $\epsilon_n \sim \mathrm{N}[0,\sigma^2_\epsilon]$, $\xi_n \sim \mathrm{N}[0,\sigma^2_\xi]$, $\zeta_n \sim \mathrm{N}[0,\sigma^2_\zeta]$, and $\eta_n \sim \mathrm{N}[0,\sigma^2_\eta]$.

Two common special cases of the basic structural model

- The *local linear trend* model is the basic structural model without the seasonal component, $\{S_n\}$.

- The *local level model* is the basic structural model without either the seasonal component, $\{S_n\}$, or the trend component, $\{T_n\}$. The local level model is therefore a random walk observed with measurement error.

Initial values for the basic structural model

- To complete the model, we need to specify initial values.
- We have an example of the common problem of failing to specify initial values: these are not explained in the documentation of the R implementation of the basic structural model, `StructTS`. We could go through the source code to find out what it does.
- Incidentally, `?StructTS` does give some advice which resonates with our experience earlier in the course that optimization for ARMA models is often imperfect.

"Optimization of structural models is a lot harder than many of the references admit. For example, the 'AirPassengers' data are considered in Brockwell & Davis (1996): their solution appears to be a local maximum, but nowhere near as good a fit as that produced by 'StructTS'. It is quite common to find fits with one or more variances zero, and this can include σ_ϵ^2."

The basic structural model is an LG-POMP model

[BSM1–4] can be put in matrix form. Set

$$X_n = (L_n, T_n, S_n, S_{n-1}, S_{n-2}, \dots, S_{n-10})^T, \tag{19}$$

$$Y_n = (1, 0, 1, 0, 0, \dots, 0) X_n + \epsilon_n. \tag{20}$$

We can identify matrices $\mathbf{A}$, $\mathbf{B}$, Σ_X and Σ_Y giving a time-homogeneous LG-POMP representation [LG1, LG2] for the basic structural model.

The transition matrix $\mathbf{A}$ combines the dynamics of level, trend, and seasonal components appropriately.

Spline smoothing and its LG-POMP representation

- Spline smoothing is a standard method to smooth scatter plots and time plots. For example, `smooth.spline` and `hpfilter` in R.
- A *smoothing spline* for an equally spaced time series $y_{1:N}$ collected at times $t_{1:N}$ is the sequence $x_{1:N}$ minimizing the *penalized sum of squares (PSS)*, defined as

[SS1] $$\mathrm{PSS}(x_{1:N};\lambda) = \sum_{n=1}^{N}(y_n - x_n)^2 + \lambda\sum_{n=3}^{N}(\Delta^2 x_n)^2.$$

- The spline is defined for all times, but here we are only concerned with its value at the times $t_{1:N}$.
- Here, $\Delta x_n = (1-B)x_n = x_n - x_{n-1}$.

- The *smoothing parameter*, λ, penalizes $x_{1:N}$ to prevent the spline from interpolating the data.
- If $\lambda = 0$, the spline will go through each data point, i.e, $x_{1:N}$ will interpolate $y_{1:N}$.
- If $\lambda = \infty$, the spline will be the ordinary least squares regression fit,
$$x_n = \alpha + \beta n, \tag{21}$$
since $\Delta^2(\alpha + \beta n) = 0$.
- Now consider the linear Gaussian model,

$$\begin{array}{lll} \text{[SS2]} & X_n & = 2X_{n-1} - X_{n-2} + \epsilon_n, \epsilon_n \sim \text{iid N}[0, \sigma^2/\lambda] \\ \text{[SS3]} & Y_n & = X_n + \eta_n, \eta_n \sim \text{iid N}[0, \sigma^2] \end{array}$$

- Note that $\Delta^2 X_n = \epsilon_n$.
- We will show that [SS1] is equivalent to [SS2,SS3].

Constructing a linear Gaussian POMP (LG-POMP) model matching [SS2] and [SS3]

Question. $\{X_n, Y_n\}$ defined in [SS2] and [SS3] is not quite an LG-POMP model. However, we can use $\{X_n\}$ and $\{Y_n\}$ to build an LG-POMP model. How?

Deriving the penalized spline from the LG-POMP

The joint density of $X_{1:N}$ and $Y_{1:N}$ in [SS2,SS3] is

$$f_{X_{1:N}Y_{1:N}}(x_{1:N}, y_{1:N}) = f_{X_{1:N}}(x_{1:N})\, f_{Y_{1:N}|X_{1:N}}(y_{1:N}\,|\,x_{1:N}).$$

Taking logs we get

$$\log f_{X_{1:N}Y_{1:N}}(x_{1:N}, y_{1:N}) = \log f_{X_{1:N}}(x_{1:N}) + \log f_{Y_{1:N}|X_{1:N}}(y_{1:N}\,|\,x_{1:N}).$$

[SS2,SS3] tell us that $\{\Delta^2 X_n, n \in 1:N\}$ and $\{Y_n - X_n, n \in 1:N\}$ are independent $\mathrm{N}[0, \sigma^2/\lambda]$ and $\mathrm{N}[0, \sigma^2]$. Thus,

$$\log f_{X_{1:N}Y_{1:N}}(x_{1:N}, y_{1:N};\, \sigma, \lambda) = \frac{-1}{2\sigma^2}\left[\sum_{n=1}^{N}(y_n - x_n)^2 - \lambda\sum_{n=3}^{N}(\Delta^2 x_n)^2\right] + C.$$

Here, C depends on σ and λ but not on $y_{1:N}$. C depends on the initial terms x_0 and x_{-1}, but we suppose these can be ignored, for example by modeling them with an improper uniform density.

- Comparing this with [SS1], we see that maximizing the density $f_{X_{1:N}Y_{1:N}}(x_{1:N}, y_{1:N};\, \sigma, \lambda)$ as a function of $x_{1:N}$ is the same problem as finding the smoothing spline by minimizing the penalized sum of squares.
- For a Gaussian density, the mode (i.e., the maximum of the density) is equal to the expected value. Therefore, we have

$$
\begin{aligned}
\operatorname*{argmin}_{x_{1:N}} \mathrm{PSS}(x_{1:N};\, \lambda) &= \operatorname*{argmax}_{x_{1:N}} f_{X_{1:N}Y_{1:N}}(x_{1:N}, y_{1:N};\, \sigma, \lambda) \\
&= \operatorname*{argmax}_{x_{1:N}} \frac{f_{X_{1:N}Y_{1:N}}(x_{1:N}, y_{1:N};\, \sigma, \lambda)}{f_{Y_{1:N}}(y_{1:N};\, \sigma, \lambda)} \\
&= \operatorname*{argmax}_{x_{1:N}} f_{X_{1:N}|Y_{1:N}}(x_{1:N} \,|\, y_{1:N};\, \sigma, \lambda) \\
&= \mathbb{E}\big[X_{1:N} \,|\, Y_{1:N} = y_{1:N};\, \sigma, \lambda\big].
\end{aligned}
$$

- Because a (conditional) normal distribution is characterized by its (conditional) mean and variance, the smoothing calculation for an LG-POMP model involves finding the conditional mean and variance of X_n given $Y_{1:N} = y_{1:N}$.
- We conclude that the smoothing problem for this LG-POMP model is the same as the spline smoothing problem defined by [SS1].
- If you have experience using smoothing splines, this connection may help you transfer that experience to POMP models.
- Once you have experience with POMP models, this connection helps you understand spline smoothers that are commonly used in many applications.
- For example, the smoothing parameter λ could be selected by maximum likelihood for the POMP model.

Why do we penalize by $\sum_n \left(\Delta^2 X_n\right)^2$ when smoothing?

Question. We found that the smoothing spline corresponds to a particular choice of LG-POMP model given by [SS2, SS3]. Why do we choose that penalty, rather than the equivalent penalty from some other LG-POMP model?

Note: This LG-POMP model is sometimes reasonable, but presumably there are other occasions when a different LG-POMP model would lead to superior performance.

The Kalman filter

- The *Kalman filter* is the name given to the prediction, filtering and smoothing formulas [P4–P9] for the linear Gaussian partially observed Markov process (LG-POMP) model.
- Linear Gaussian models have Gaussian conditional distributions.
- The integrals in the general POMP formulas can be found exactly for the Gaussian distribution, leading to linear algebra calculations of conditional means and variances.
- The R function `arima()` uses a Kalman filter to evaluate the likelihood of an ARMA model (or ARIMA, SARMA, SARIMA).

Review of the multivariate normal distribution

- A random variable X taking values in $\mathbb{R}^{d_X}$ is *multivariate normal* with mean μ_X and variance Σ_X if we can write
$$X = \mathbf{H}Z + \mu_X, \tag{22}$$
where Z is a vector of d_X independent identically distributed $\mathrm{N}[0,1]$ random variables and $\mathbf{H}$ is a $d_X \times d_X$ matrix square root of Σ_X, i.e.,
$$\mathbf{H}\mathbf{H}^T = \Sigma_X. \tag{23}$$
- A matrix square root of this type exists for any covariance matrix, though the choice of $\mathbf{H}$ is not unique.
- We write $X \sim \mathrm{N}[\mu_X, \Sigma_X]$. If Σ_X is invertible, X has a probability density function,
$$f_X(x) = \frac{1}{(2\pi)^{d_X/2}|\Sigma_X|^{1/2}} \exp\left\{-\frac{(x-\mu_X)\,[\Sigma_X]^{-1}\,(x-\mu_X)^T}{2}\right\}.$$

Joint multivariate normal vectors

X and Y are *joint multivariate normal* if the combined vector

$$Z = \begin{pmatrix} X \\ Y \end{pmatrix} \tag{24}$$

is multivariate normal. In this case, we write

$$\mu_Z = \begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix}, \quad \Sigma_Z = \begin{pmatrix} \Sigma_X & \Sigma_{XY} \\ \Sigma_{YX} & \Sigma_Y \end{pmatrix}, \tag{25}$$

where

$$\Sigma_{XY} = \mathrm{Cov}(X, Y) = \mathbb{E}\big[(X - \mu_X)\,(Y - \mu_Y)^T\big]. \tag{26}$$

- For joint multivariate normal random variables X and Y, we have the useful property that the conditional distribution of X given $Y = y$ is multivariate normal, with conditional mean and variance

$$
\begin{aligned}
&\text{[KF1]} \qquad \mu_{X|Y}(y) &&= \mu_X + \Sigma_{XY}\,\Sigma_Y^{-1}(y - \mu_Y),\\
&\text{[KF2]} \qquad \Sigma_{X|Y} &&= \Sigma_X - \Sigma_{XY}\,\Sigma_Y^{-1}\,\Sigma_{YX}.
\end{aligned}
$$

- We write this as

$$X \,|\, Y = y \sim \mathrm{N}\big[\,\mu_{X|Y}(y)\,,\,\Sigma_{X|Y}\big]. \tag{27}$$

- The joint multivariate normal has a special property that the conditional variance of X given $Y = y$ does not depend on the value of y. In non-Gaussian situations, it will usually depend on y.
- If Σ_Y is not invertible, we can interpret Σ_Y^{-1} as a generalized inverse.

Notation for the Kalman filter recursions

We define the conditional means and variances for the filtering, prediction and smoothing distributions:

$$
\begin{array}{lll}
\text{[KF3]} & X_n \,|\, Y_{1:n-1} & = y_{1:n-1} \sim \mathrm{N}\big[\, \mu_n^P(y_{1:n-1}),\, \Sigma_n^P \,\big], \\
\text{[KF4]} & X_n \,|\, Y_{1:n} & = y_{1:n} \sim \mathrm{N}\big[\, \mu_n^F(y_{1:n}),\, \Sigma_n^F \,\big], \\
\text{[KF5]} & X_n \,|\, Y_{1:N} & = y_{1:N} \sim \mathrm{N}\big[\, \mu_n^S(y_{1:N}),\, \Sigma_n^S \,\big].
\end{array}
$$

- For data $y_{1:N}$, we call $\mu_n^P = \mu_n^P(y_{1:n-1}) = \mathbb{E}\big[X_n \,|\, Y_{1:n-1} = y_{1:n-1}\big]$ the *prediction mean*, and Σ_n^P the *prediction variance*.
- $\mu_n^F = \mu_n^F(y_{1:n}) = \mathbb{E}\big[X_n \,|\, Y_{1:n} = y_{1:n}\big]$ is the *filter mean* and Σ_n^F the *filter variance*.
- $\mu_n^S = \mu_n^S(y_{1:N}) = \mathbb{E}\big[X_n \,|\, Y_{1:N} = y_{1:N}\big]$ is the *smoothed mean* and Σ_n^S the *smoothed variance*.

The Kalman matrix recursions

- Applying the properties of linear combinations of Normal random variables, we get the Kalman filter and prediction recursions:

$$
\begin{aligned}
&\text{[KF6]} \quad & \mu^P_{n+1}(y_{1:n}) &= \mathbf{A}_{n+1}\mu^F_n(y_{1:n}) \\
&\text{[KF7]} \quad & \Sigma^P_{n+1} &= \mathbf{A}_{n+1}\Sigma^F_n\mathbf{A}^T_{n+1} + \Sigma_{X,n+1}, \\
&\text{[KF8]} \quad & \Sigma^F_n &= \big([\Sigma^P_n]^{-1} + \mathbf{B}^T_n\Sigma^{-1}_{Y,n}\mathbf{B}_n\big)^{-1}, \\
&\text{[KF9]} \quad & \mu^F_n(y_{1:n}) &= \mu^P_n(y_{1:n-1}) + \Sigma^F_n\mathbf{B}^T_n\Sigma^{-1}_{Y,n}\{y_n - \mathbf{B}_n\mu^P_n(y_{1:n-1})
\end{aligned}
$$

Outline of a derivation of the Kalman matrix recursions

- The prediction recursions [KF6] and [KF7] follow from the property that if X is a d-dimensional multivariate normal, $X \sim \mathrm{N}(\mu, \Sigma)$, then $\mathbf{A}X + b \sim \mathrm{N}\big(\mathbf{A}\mu + b, \mathbf{A}\Sigma\mathbf{A}^T\big)$.
- Note that the multivariate normal identities [KF1,KF2] also hold when all variables are conditioned on some additional joint Gaussian variable, in this case $Y_{1:n-1}$.
- [KF8] and [KF9] can be deduced by writing out the joint density,
$$f_{X_n Y_n | Y_{1:n-1}}(x_n, y_n \,|\, y_{1:n-1}) \tag{28}$$
and completing the square in the exponent. The conditional density of X_n given $Y_{1:n}$ is proportional to this joint density, with proportionality constant allowing integration to one.

Exercise. The derivation of the Kalman filter is not central to this course. However, working through the algebra to your own satisfaction is a good exercise.

- The Kalman filter matrix equations are easy to code, and quick to compute unless the dimension of the latent space is very large.
- In numerical weather forecasting, with careful programming, they are solved with latent variables having dimension $d_X \approx 10^7$.
- A similar computation gives backward Kalman recursions. Putting the forward and backward Kalman recursions together, as in [P9], is called *Kalman smoothing*.

Further reading

- The approach in this chapter is aligned with King, Nguyen, and Ionides [1].
- Chapter 6 of Shumway and Stoffer [2] gives an approach emphasizing linear Gaussian state space models.

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References I

[1] Aaron A. King, Dao Nguyen, and Edward L. Ionides. "Statistical Inference for Partially Observed Markov Processes via the R Package pomp". In: *Journal of Statistical Software* 69.12 (Mar. 2016), pp. 1–43. DOI: 10.18637/jss.v069.i12.

[2] Robert H Shumway and David S Stoffer. *Time Series Analysis and its Applications: With R Examples*. 4th. Springer, 2017.