

# Analysis of Time Series

## Chapter 10: Introduction to partially observed Markov process models

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### Contents

<b>1 Stochastic dynamic systems observed with noise</b>	<b>1</b>
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## 1 Stochastic dynamic systems observed with noise

### Partially observed Markov processes (POMP) models

- Uncertainty and variability are ubiquitous features of processes in the biological and social sciences. A physical system obeying Newton’s laws is fully predictable, but complex systems are in practice not perfectly predictable—we can only forecast weather reliably in the near future.
- Basic time series models of deterministic trend plus colored noise imply perfect predictability if the trend function enables extrapolation.
- To model variability and unpredictability in low frequency components, we may wish to specify a random process model for how the system evolves. We could call this a “stochastic trend” approach, though that is an oxymoron since we’ve defined trend to be expected value for the model.
- As in the deterministic signal plus noise model, we will model the observations as random variables conditional on the trajectory of a **latent process**. It can also be called a **state process** or a **hidden process**.

### The Markov property

- A standard class of latent process models is characterized by the requirement that the future evolution of the system depends only on the current state, plus randomness introduced in future.
- A model of this type is called a **Markov chain** for a discrete time model or a **Markov process** in continuous time.
- We use the term Markov process for both discrete and continuous time.
- **Partial observations** here mean either or both of (i) measurement noise; (ii) entirely unmeasured latent variables. Both these features are present in many systems.
- A **partially observed Markov process** (POMP) model is defined by putting together a latent process model and an observation model.

- Often, much of the scientific interest is in understanding what models for the behavior of this latent process are consistent with the data.
- A good model for the underlying, but imperfectly observed, dynamics of a system can also lead to a skillful forecast.
- We are going to introduce a general framework for specifying POMP models. This generality will give us the flexibility to develop models and methods appropriate to a range of applications.

### Discrete time Markov processes

A time series model  $X_{0:N}$  is a **Markov process** model if the conditional densities satisfy the **Markov property** that, for all  $n \in 1 : N$ .

$$[MP1] \quad f_{X_n|X_{1:n-1}}(x_n | x_{1:n-1}) = f_{X_n|X_{n-1}}(x_n | x_{n-1}),$$

We suppose that the random process  $X_n$  occurs at time  $t_n$  for  $n \in 0 : N$ , so the discrete time process corresponds to time points in continuous time.

### Initial conditions

- We have **initialized** the Markov process model at a time  $t_0$ , although we will suppose that data are collected only at times  $t_{1:N}$ .
- The initialization model could be deterministic (a fixed value) or a random variable.
- Formally, a fixed initial value is a special case of a discrete distribution having a point mass with probability one at the fixed value. Therefore, fixed initial values are covered in our framework since we use probability density functions to describe both discrete and continuous probability distributions.
- Mathematically, a probability mass function (for discrete distributions) is a probability density on a discrete space. We avoid getting sidetracked on to that topic, but it is worth noting that there is a proper mathematical justification for treating a probability mass function as a type of probability density function.
- It is not important whether to adopt the convention that the Markov process model is initialized at time  $t_1$  or at some previous time  $t_0$ . Here, we follow the choice to use  $t_0$ .

### The process model and one-step predictions

- 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.
- In words, the Markov property says 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 POMP model, the full joint distribution of the latent process is entirely specified by the one-step transition densities, given the initial value. We show this below.
- Therefore, we also call  $f_{X_n|X_{n-1}}(x_n | x_{n-1})$  the **process model**.

**Question 10.1.** Use [MP1] 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

$$[MP2] \quad f_{X_{0:N}}(x_{0:N}) = f_{X_0}(x_0) \prod_{n=1}^N f_{X_n|X_{n-1}}(x_n | x_{n-1}).$$

**Question 10.2.** Show that a causal Gaussian AR(1) process is a Markov process.

### Time homogeneous transitions and stationarity

In general, the one step transition probability density in a POMP model can depend on  $n$ . A latent process model  $X_{0:N}$  is **time-homogeneous** if the one step transition probability density does not depend on  $n$ , so there is a conditional density  $f(y|x)$  such that, for all  $n \in 1:N$ ,

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

**Question 10.3.** If  $X_{0:N}$  is stationary then it is time homogeneous. Why?

**Question 10.4.** Time homogeneity does not necessarily imply stationarity. Find a counter-example. What has to be added to time homogeneity to get stationarity?

## The measurement model

- We model the observation process random variables  $Y_{1:N}$ .
- For state space models, we will generally write the data as  $y_{1:N}^*$ .
- We model the measurement at time  $t_n$  to depend only on the value of the latent process at time  $t_n$ , conditionally independent of all other latent process and observation process variables. Formally, this assumption is,

$$[MP3] \quad f_{Y_n|X_{0:N}, Y_{1:n-1}, Y_{n+1:N}}(y_n | x_{0:N}, y_{1:n-1}, y_{n+1:N}) = f_{Y_n|X_n}(y_n | x_n).$$

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

## Time-inhomogeneous 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  $g(y | x)$  such that, for all  $n \in 1 : N$ ,

$$f_{Y_n|X_n}(y_n | x_n) = g(y_n | x_n). \quad (2)$$

## 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 of the latent process at time  $t_{n+1}$  given data up to time  $t_n$  involves finding

$$f_{X_{n+1}|Y_{1:n}}(x_{n+1} | y_{1:n}^*). \quad (3)$$

- We may want to carry out prediction (also called forecasting) more than one time step ahead. However, unless specified otherwise, the prediction calculation will be one-step prediction.
- One-step prediction turns out to be closely related to computing the likelihood function, and therefore central to statistical inference.
- We have required our prediction to be a conditional probability density, not a point estimate. In the context of forecasting, this is called a **probabilistic forecast**, and has advantages over a point estimate forecast. What are they? Are there any disadvantages to probabilistic forecasting?

## Filtering

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

$$f_{X_n|Y_{1:n}}(x_n | y_{1:n}^*). \quad (4)$$

- This can be calculated numerically or algebraically. We will also see that Monte Carlo methods can be a good tool.

## 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

$$f_{X_n|Y_{1:N}}(x_n | y_{1:N}^*). \quad (5)$$

## The likelihood

- The model may depend on a parameter vector  $\theta$ .
- Since we have not explicitly written this dependence above, the likelihood calculation is to evaluate the joint density of  $Y_{1:N}$  at the data,

$$f_{Y_{1:N}}(y_{1:N}^*). \quad (6)$$

- If we can compute this at any value of  $\theta$  we choose, 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 and filtering formulas

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

$$\begin{aligned} & [MP4] f_{X_n|Y_{1:n-1}}(x_n | y_{1:n-1}^*) \\ &= \int f_{X_{n-1}|Y_{1:n-1}}(x_{n-1} | y_{1:n-1}^*) f_{X_n|X_{n-1}}(x_n | x_{n-1}) dx_{n-1}. \end{aligned} \quad (7)$$

- To make this formula work for  $n = 1$ , we need the convention that  $1 : k$  is the empty set when  $k = 0$ . Conditioning on an empty collection of random variables is the same as not conditioning at all! In this case, we have by definition that

$$f_{X_0|Y_{1:0}}(x_0 | y_{1:0}^*) = f_{X_0}(x_0). \quad (8)$$

- In other words, the filtering calculation at time  $t_0$  is the initial density for the latent process. This makes sense, since at time  $t_0$  we have no data to condition on.

**Hints for homework: deriving the recursion formulae**

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

**Example 1.** From

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

we can condition on  $Z$  to obtain

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

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

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

**Question 10.5.** Why is the following identity true?

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

- 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  $n \in 1 : N$ ,

$$[MP5] f_{X_n|Y_{1:n}}(x_n | y_{1:n}^*) = \frac{f_{X_n|Y_{1:n-1}}(x_n | y_{1:n-1}^*) f_{Y_n|X_n}(y_n^* | x_n)}{f_{Y_n|Y_{1:n-1}}(y_n^* | y_{1:n-1}^*)}.$$

- The denominator in the filtering formula [MP5] 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**,

$$[MP6] f_{Y_n|Y_{1:n-1}}(y_n^* | y_{1:n-1}^*) = \int f_{X_n|Y_{1:n-1}}(x_n | y_{1:n-1}^*) f_{Y_n|X_n}(y_n^* | x_n) dx_n. \quad (13)$$

- To make this formula work for  $n = 1$ , we again take advantage of the convention that  $1 : k$  is the empty set when  $k = 0$ .
- The prediction and filtering formulas are **recursive**. If they can be computed for time  $t_n$  then they provide the foundation for the following computation at time  $t_{n+1}$ .

**Question 10.6.** Give a detailed derivation of [MP4], [MP5] and [MP6], being careful to note when you use the Markov property [MP1].

## Computation of the likelihood

- The likelihood of the entire dataset,  $y_{1:N}^*$  can be found from [MP6], using the identity

$$[MP7] \quad f_{Y_{1:N}}(y_{1:N}^*) = \prod_{n=1}^N f_{Y_n|Y_{1:n-1}}(y_n^* | y_{1:n-1}^*). \quad (14)$$

- As above, this formula [MP7] requires the convention that  $1 : k$  is the empty set when  $k = 0$ , so the first term in the product is

$$f_{Y_1|Y_{1:0}}(y_1^* | y_{1:0}^*) = f_{Y_1}(y_1^*). \quad (15)$$

- If our model has an unknown parameter  $\theta$ , the likelihood identity [MP7] lets us evaluate the log likelihood function,

$$\ell(\theta) = \log f_{Y_{1:N}}(y_{1:N}^*; \theta). \quad (16)$$

## The smoothing formulas

- 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 forwards in time (we use the solution at time  $t_{n-1}$  to carry out the computation at time  $t_n$ ).
- There are similar **backwards recursion formulas**,

$$[MP8] \quad f_{Y_{n:N}|X_n}(y_{n:N}^* | x_n) = f_{Y_n|X_n}(y_n^* | x_n) f_{Y_{n+1:N}|X_n}(y_{n+1:N}^* | x_n).$$

$$\begin{aligned} [MP9] \quad f_{Y_{n+1:N}|X_n}(y_{n+1:N}^* | x_n) \\ = \int f_{Y_{n+1:N}|X_{n+1}}(y_{n+1:N}^* | x_{n+1}) f_{X_{n+1}|X_n}(x_{n+1} | x_n) dx_{n+1}. \end{aligned} \quad (17)$$

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

$$[MP10] \quad f_{X_n|Y_{1:N}}(x_n | y_{1:N}^*) = \frac{f_{X_n|Y_{1:n-1}}(x_n | y_{1:n-1}^*) f_{Y_{n:N}|X_n}(y_{n:N}^* | x_n)}{f_{Y_{n:N}|Y_{1:n-1}}(y_{n:N}^* | y_{1:n-1}^*)}. \quad (18)$$

**Question 10.7.** Show how [MP8], [MP9] and [MP10] follow from the basic properties of conditional densities combined with the Markov property.

### An algebraic trick: Using un-normalized identities

- Sometimes we can avoid calculating a normalizing constant for a density, since it can be worked out later using the property that the probability density function must integrate to 1.
- The denominators  $f_{Y_n|Y_{1:n-1}}(y_n^* | y_{1:n-1}^*)$  and  $f_{Y_{n:N}|Y_{1:n-1}}(y_{n:N}^* | y_{1:n-1}^*)$ , in equations [MP5] and [MP10] respectively, may sometimes be hard to compute.
- We can simplify [MP5] and [MP10] using the proportionality relationship  $\propto$ . This gives,

$$[\text{MP5}'] \quad f_{X_n|Y_{1:n}}(x_n | y_{1:n}^*) \propto f_{X_n|Y_{1:n-1}}(x_n | y_{1:n-1}^*) f_{Y_n|X_n}(y_n^* | x_n),$$

$$[\text{MP10}'] \quad f_{X_n|Y_{1:N}}(x_n | y_{1:N}^*) \propto f_{X_n|Y_{1:n-1}}(x_n | y_{1:n-1}^*) f_{Y_{n:N}|X_n}(y_{n:N}^* | x_n).$$

- The normalizing “constant” avoided in equations [MP5'] and [MP10'] does depend on  $y_{1:N}^*$ . However, the data are fixed constants. The variable in these equations is  $x_n$ .

### Linear Gaussian POMP (LG-POMP) models

- Linear Gaussian partially observed Markov process (LG-POMP) models have many applications
- 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.
- The computations for smoothing splines can be written as an LG-POMP model, enabling computationally efficient spline smoothing.
- 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.
- LG-POMP models are widely used in engineering, especially for control applications. If a scientific and engineering application is not too far from linear and Gaussian, you save a lot of effort if an LG-POMP model is appropriate. General nonlinear POMP models usually involve intensive Monte Carlo computation.

### The general LG-POMP model

Suppose the latent process,  $X_{0:N}$ , and the observation process  $\{Y_n\}$ , takes 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,  $\mathbb{A}_{1:N}$ ,
- A sequence of  $d_X \times d_X$  covariance matrices,  $\mathbb{U}_{0:N}$ ,
- A sequence of  $d_Y \times d_X$  matrices,  $\mathbb{B}_{1:N}$
- A sequence of  $d_Y \times d_Y$  covariance matrices,  $\mathbb{V}_{1:N}$ .

We initialize with  $X_0 \sim N[0, \mathbb{U}_0]$  and then define the entire LG-POMP model by a recursion for  $n \in 1 : N$ ,

$$[\text{LG1}] \quad X_n = \mathbb{A}_n X_{n-1} + \epsilon_n, \quad \epsilon_n \sim N[0, \mathbb{U}_n],$$

$$[\text{LG2}] \quad Y_n = \mathbb{B}_n X_n + \eta_n, \quad \eta_n \sim N[0, \mathbb{V}_n]. \quad (19)$$

Often, but not always, we will have a **time-homogeneous** LG-POMP model, with  $\mathbb{A}_n = \mathbb{A}$ ,  $\mathbb{B}_n = \mathbb{B}$ ,  $\mathbb{U}_n = \mathbb{U}$  and  $\mathbb{V}_n = \mathbb{V}$  for  $n \in 1 : N$ .



### The LG-POMP representation of a Gaussian ARMA

Suppose  $\{Y_n\}$  is a Gaussian ARMA(p,q) model with noise process  $\omega_n \sim N[0, \sigma^2]$  and specification

$$[LG3] \quad Y_n = \sum_{j=1}^p \phi_j Y_{n-j} + \omega_n + \sum_{k=1}^q \psi_k \omega_{n-k}.$$

Set  $r = \max(p, q + 1)$  so that  $\{Y_n\}$  is also ARMA(r,r-1). Our LG-POMP representation has  $d_X = r$ , with

$$\mathbb{B}_n = \mathbb{B} = (1, 0, 0, \dots, 0) \quad (20)$$

and

$$\mathbb{V}_n = \mathbb{V} = 0. \quad (21)$$

Therefore,  $Y_n$  is the first component of  $X_n$ , observed without measurement error.

Now, define

$$X_n = \begin{pmatrix} Y_n \\ \phi_2 Y_{n-1} + \dots + \phi_r Y_{n-r+1} + \psi_1 \omega_n + \dots + \psi_{r-1} \omega_{n-r+2} \\ \phi_3 Y_{n-1} + \dots + \phi_r Y_{n-r+1} + \psi_2 \omega_n + \dots + \psi_{r-1} \omega_{n-r+3} \\ \vdots \\ \phi_r Y_{n-1} + \psi_{r-1} \omega_t \end{pmatrix} \quad (22)$$

We can check that the ARMA equation [LG3] corresponds to the matrix equation

$$X_n = \mathbb{A} X_{n-1} + \begin{pmatrix} 1 \\ \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{r-1} \end{pmatrix} \omega_n. \text{ where } \mathbb{A} = \begin{pmatrix} \phi_1 & 1 & 0 & \dots & 0 \\ \phi_2 & 0 & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \phi_{r-1} & 0 & \dots & 0 & 1 \\ \phi_r & 0 & \dots & 0 & 0 \end{pmatrix}$$

This is in the form of a time-homogenous LG-POMP, with  $\mathbb{A}$ ,  $\mathbb{B}$  and  $\mathbb{V}$  defined above, and

$$\mathbb{U}_n = \mathbb{U} = \sigma^2 (1, \psi_1, \psi_2, \dots, \psi_{r-1})^\top (1, \psi_1, \psi_2, \dots, \psi_{r-1}). \quad (23)$$

### 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  $r^2$  parameters and the ARMA model has order  $r$  parameters, so we might expect there are many ways to parameterize the ARMA model as a special case of the much larger LG-POMP model.
- The same can be true of non-Gaussian POMPs, but it is easier to see in the Gaussian case.

### The basic structural model and its LG-POMP representation

- The **basic structural model** is an econometric model used for forecasting.
- The basic structural model supposes that the observation process  $Y_{1:N}$  is 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 all these quantities are perturbed with Gaussian white noise at each time point. So, we have the following model equations

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

- We suppose  $\epsilon_n \sim N[0, \sigma_\epsilon^2]$ ,  $\xi_n \sim N[0, \sigma_\xi^2]$ ,  $\zeta_n \sim N[0, \sigma_\zeta^2]$ , and  $\eta_n \sim N[0, \sigma_\eta^2]$ .

### 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  $\sigma_{\text{eps}}^2$ .”

To put [BSM1-4] in the form of an LG-POMP model, we set

$$[\text{BSM5}] \quad X_n = (L_n, T_n, S_n, S_{n-1}, S_{n-2}, \dots, S_{n-10})^\top.$$

Then, we have

$$[\text{BSM6}] \quad Y_n = (1, 0, 1, 0, 0, \dots, 0)X_n + \epsilon_n,$$

$$\begin{pmatrix} L_n \\ T_n \\ S_n \\ S_{n-1} \\ S_{n-2} \\ \vdots \\ S_{n-10} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & -1 & -1 & -1 & \dots & -1 \\ 0 & 0 & 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 1 & 0 & \dots & 0 \\ \vdots & & & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} L_{n-1} \\ T_{n-1} \\ S_{n-1} \\ S_{n-2} \\ S_{n-3} \\ \vdots \\ S_{n-11} \end{pmatrix} + \begin{pmatrix} \xi_n \\ \zeta_n \\ \eta_n \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

From [BSM5] and [BSM6], we can read off the matrices  $\mathbb{A}$ ,  $\mathbb{B}$ ,  $\mathbb{U}$  and  $\mathbb{V}$  in the LG-POMP representation of the basic structural model.

## Spline smoothing and its LG-POMP representation

- Spline smoothing is a standard method to smooth scatter plots and time plots. For example, `smooth.spline` 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)**, which is defined as

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

- 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**,  $\lambda$ , 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,

$$x_n = \alpha + \beta n, \tag{24}$$

since  $\Delta^2(\alpha + \beta n) = 0$ .

- Now consider the model,

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

- Note that  $\Delta^2 X_n = \epsilon_n$ .

### Constructing a linear Gaussian POMP (LG-POMP) model from [SS2]

**Question 10.8.**  $\{X_n, Y_n\}$  defined in [SS2] is not quite an LG-POMP model. However, we can use  $\{X_n\}$  and  $\{Y_n\}$  to build an LG-POMP model. How?

- The joint density of  $X_{1:N}$  and  $Y_{1:N}$  in [SS2] can be written as

$$f_{X_{1:N} Y_{1:N}}(x_{1:N}, y_{1:N}) = f_{X_{1:N}}(x_{1:N}) f_{Y_{1:N} | X_{1:N}}(y_{1:N} | x_{1:N}). \tag{25}$$

- Taking logs,

$$\log f_{X_{1:N} Y_{1:N}}(x_{1:N}, y_{1:N}) = \log f_{X_{1:N}}(x_{1:N}) + \log f_{Y_{1:N} | X_{1:N}}(y_{1:N} | x_{1:N}). \quad (26)$$

- Suppose the initial conditions are irrelevant (either unknown parameters or an improper Gaussian distribution with infinite variance). Noting that  $\{\Delta^2 X_n, n \in 1 : N\}$  and  $\{Y_n - X_n, n \in 1 : N\}$  are collections of independent Normal random variables with mean zero and variances  $\sigma^2/\lambda$  and  $\sigma^2$  respectively, we have

$$\begin{aligned} [SS3] \quad \log f_{X_{1:N} Y_{1:N}}(x_{1:N}, y_{1:N}; \sigma, \lambda) = \\ \frac{-1}{2\sigma^2} \sum_{n=1}^N (y_n - x_n)^2 + \frac{-\lambda}{2\sigma^2} \sum_{n=3}^N (\Delta^2 x_n)^2 + C. \end{aligned}$$

- In [SS3],  $C$  is a constant depending on  $\sigma$  and  $\lambda$  but not  $x_{1:N}$  or  $y_{1:N}$ .
- Comparing [SS3] 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 in [SS1].
- For a Gaussian density, the mode (i.e., the maximum of the density) is equal to the expected value. Therefore, we have

$$\begin{aligned} \arg \min_{x_{1:N}} \text{PSS}(x_{1:N}; \lambda), &= \arg \max_{x_{1:N}} f_{X_{1:N} Y_{1:N}}(x_{1:N}, y_{1:N}^*; \sigma, \lambda), \\ &= \arg \max_{x_{1:N}} \frac{f_{X_{1:N} Y_{1:N}}(x_{1:N}, y_{1:N}^*; \sigma, \lambda)}{f_{Y_{1:N}}(y_{1:N}^*; \sigma, \lambda)}, \\ &= \arg \max_{x_{1:N}} f_{X_{1:N} | Y_{1:N}}(x_{1:N} | y_{1:N}^*; \sigma, \lambda), \\ &= \mathbb{E}[X_{1:N} | Y_{1:N} = y_{1:N}^*; \sigma, \lambda]. \end{aligned}$$

- The smoothing calculation for an LG-POMP model involves finding the 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, we might propose that the smoothing parameter  $\lambda$  could be selected by maximum likelihood for the POMP model.

**Question 10.9.** Why do we use  $\Delta^2 X_n = \epsilon_n$  for our smoothing model?

- Seeing that the smoothing spline arrives from the particular choice of LG-POMP model in equation [SS2] could make you wonder why we choose that model. Any ideas?

- Even if this LG-POMP model is sometimes reasonable, presumably there are other occasions when a different LG-POMP model would be a superior choice for smoothing.

### The Kalman filter

- We find exact versions of the prediction, filtering and smoothing formulas [MP4–10] for the linear Gaussian partially observed Markov process (LG-POMP) model [LG1,LG2].
- In the linear Gaussian case, the conditional probability density functions in [MP4–10] are specified by the conditional mean and conditional variance.

### Review of the multivariate normal distribution

- A random variable  $X$  taking values in  $\mathbb{R}^{d_X}$  is **multivariate normal** with mean  $\mu_X$  and variance  $\Sigma_X$  if we can write

$$X = \mathbb{H}Z + \mu_X,$$

where  $Z$  is a vector of  $d_X$  independent identically distributed  $N[0, 1]$  random variables and  $\mathbb{H}$  is a  $d_X \times d_X$  matrix square root of  $\Sigma_X$ , i.e.,

$$\mathbb{H}\mathbb{H}^T = \Sigma_X.$$

- The choice of  $\mathbb{H}$  is not unique, and a matrix square root of this type exists for any covariance matrix because covariance matrices are positive semi-definite.
- We write  $X \sim N[\mu_X, \Sigma_X]$ .
- $X \sim N[\mu_X, \Sigma_X]$  has a probability density function if and only if  $\Sigma_X$  is invertible. This density is given by

$$f_X(x) = \frac{1}{(2\pi)^{d_X/2} |\Sigma_X|} \exp \left\{ -\frac{(x - \mu_X)^T \Sigma_X^{-1} (x - \mu_X)}{2} \right\}.$$

### Jointly multivariate normal vectors

$X$  and  $Y$  are **jointly multivariate normal** if the combined vector

$$W = \begin{pmatrix} X \\ Y \end{pmatrix}$$

is multivariate normal. In this case, we write

$$\mu_W = \begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix}, \quad \Sigma_W = \begin{pmatrix} \Sigma_X & \Sigma_{XY} \\ \Sigma_{YX} & \Sigma_Y \end{pmatrix},$$

where

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

- For jointly 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

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

- We write this as

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

- In general, the conditional variance of  $X$  given  $Y = y$  will depend on  $y$  (remind yourself of the definition of conditional variance). In the special case where  $X$  and  $Y$  are jointly multivariate normal, this conditional variance happens not to depend on the value of  $y$ .
- If  $\Sigma_Y$  is not invertible, to make [KF1] work we have to interpret  $\Sigma_Y^{-1}$  as a generalized inverse.

### Notation for the Kalman filter recursions

To write the Kalman filter, we define the following notation, Since the system is Gaussian, the filtering and prediction distributions are defined by their mean and variance.

$$\begin{aligned} X_n | Y_{1:n-1} = y_{1:n-1} &\sim N[\mu_n^P(y_{1:n-1}), \Sigma_n^P], \\ [KF2] \quad X_n | Y_{1:n} = y_{1:n} &\sim N[\mu_n^F(y_{1:n}), \Sigma_n^F], \\ X_n | Y_{1:N} = y_{1:N} &\sim N[\mu_n^S(y_{1:N}), \Sigma_n^S]. \end{aligned}$$

To relate this notation to the general POMP recursion formulas, given data  $y_{1:N}^*$ , we define the following terminology:

$\mu_n^P(y_{1:n-1}^*) = \mathbb{E}[X_n | Y_{1:n-1} = y_{1:n-1}^*]$  is the **one-step prediction mean** for time  $t_n$ . It is an arbitrary decision we have made to call this the prediction for time  $t_n$  (the time for which the prediction is being made) rather than for time  $t_{n-1}$  (the time at which the prediction for time  $t_n$  becomes available).  
 $\Sigma_n^P(y_{1:n-1}^*) = \text{Var}(X_n | Y_{1:n-1} = y_{1:n-1}^*)$  is the **one-step prediction variance** for time  $t_n$ .

For a Gaussian model, this conditional variance does not depend on  $y_{1:n}^*$ . To make this terminology work for general POMP models we see later, we include possible dependence on  $y_{1:n-1}^*$ .

Other related quantities use the same notation:

- $\mu_n^F(y_{1:n}^*) = \mathbb{E}[X_n | Y_{1:n} = y_{1:n}^*]$  is the **filter mean** for time  $t_n$ .
- $\Sigma_n^F(y_{1:n}^*) = \text{Var}(X_n | Y_{1:n} = y_{1:n}^*)$  is the **filter variance** for time  $t_n$ .
- $\mu_n^S(y_{1:N}^*) = \mathbb{E}[X_n | Y_{1:N} = y_{1:N}^*]$  is the **smoothing mean** for time  $t_n$ .
- $\Sigma_n^S(y_{1:N}^*) = \text{Var}(X_n | Y_{1:N} = y_{1:N}^*)$  is the **smoothing variance** for time  $t_n$ .

### The Kalman matrix recursions

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

$$[KF3] \quad \mu_{n+1}^P(y_{1:n}) = \mathbb{A}_{n+1} \mu_n^F(y_{1:n}), \quad (27)$$

$$[KF4] \quad \Sigma_{n+1}^P = \mathbb{A}_{n+1} \Sigma_n^F \mathbb{A}_{n+1}^T + \mathbb{U}_{n+1}. \quad (28)$$

$$[KF5] \quad \Sigma_n^F = ([\Sigma_n^P]^{-1} + \mathbb{B}_n^T \mathbb{V}_n^{-1} \mathbb{B}_n)^{-1}. \quad (29)$$

$$[KF6] \quad \mu_n^F(y_{1:n}) = \mu_n^P(y_{1:n-1}) + \Sigma_n^F \mathbb{B}_n^T \mathbb{V}_n^{-1} \{y_n - \mathbb{B}_n \mu_n^P(y_{1:n-1})\}. \quad (30)$$

### Toward deriving the Kalman matrix recursions

- The prediction recursions [KF3] and [KF4] are relatively easy to demonstrate, but it is a good exercise to go through the algebra to your own satisfaction.
- A useful trick for the algebra is to notice that the conditioning identities [KF1] for joint Gaussian random variables continue to hold if left and right are both conditioned on some additional jointly Gaussian variable, such as  $Y_{1:n-1}$ .

KF5 and [KF6] can be deduced by completing the square in an expression for the joint density,

$$[test] f_{X_n Y_n | Y_{1:n-1}}(x_n, y_n | y_{1:n-1}) \quad (31)$$

and noticing that the marginal density of  $X_n$  given  $Y_{1:n}$  is proportional to the joint density, with a normalizing constant that must allow the marginal density to integrate to one.


**Question 10.10.** Derive some or all of these equations.

- These 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 [MP10], is called **Kalman smoothing**.

### Further reading

- The approach in this chapter is aligned with King *et al.* (2016)
- Chapter 6 of Shumway and Stoffer (2017) gives an approach emphasizing linear Gaussian state space models.

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