Modeling and Analysis of Time Series Data

Chapter 10: Introduction to partially observed Markov process models

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Outline

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   - Prediction and filtering recursions
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Latent process models

- Uncertainty and variability are common features 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. 决定过程可预测,随机过程无法完美预测
- 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 models 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

The density in question

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

dummy variable

只由上一个状态决定

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. 初始状态可以是随机或者未知的
- 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 10.1. 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

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

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

Gaussian AR(1): $X_n = \phi X_{n-1} + \varepsilon_n$, $\varepsilon_n \sim$ iid normal$(0, \sigma^2)$

Here, ε_n is independent of $X_{1:n-1}$ by construction because $X_{1:n-1}$ is a function of $\varepsilon_{1:n-1}$. So X_n given $X_{1:n-1}$ depends only on X_{n-1} by construction, i.e. $\{X_n\}$ has a Markov property

白噪音必须是independent才可以作为Markov Model,
例如Gaussian,但是其他白噪音分布未必

For a general white noise process, $\{\varepsilon_n\}$ are uncorrelated but not independent, so $\{X_n\}$ is not necessarily Markov

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. 可以和时间有关,但不能和之前的状态有关
- $X_{0:N}$ 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 10.2. If $X_{0:N}$ is strict stationary, it is time-homogeneous. Why?

Strict stationary implies all joint and conditional density are invariant, so

$f_{X_n|X_{n-1}}(X_n|X_{n-1}) = f_{X_1|X_0}(X_1,X_0)$ for all n

Question 10.3. Time-homogeneity does not necessarily imply stationarity. Find a counter-example.

Consider a random walk, with or without a drift

$X_n = X_{n-1} + \mu + \varepsilon_n$, $\varepsilon_n \sim$ iid normal $(0, \sigma^2)$

This is non-stationary, but has time-homogeneous transitions

Partially observed Markov process (POMP) models

观测值和模型状态都有可能测不准

- **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 to 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:

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

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

根据当前观测值来获得隐藏状态

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 $g(y_n|x_n)$.

观测矩阵和时间无关

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

基于之前的观测值,估计下一次的状态

$$f_{X_{n+1}|Y_{1:n}}(x_{n+1} \,|\, y^*_{1:n}). \tag{4}$$

- 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?

Advantage: We want to know the range of possibilities and
their relative plausibility

Disadvantage: Harder to compute, harder to interpret
分布概率密度的信息量比点估计更全,但更难计算

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 基于之前的观测值,估计当前的状态

$$f_{X_n|Y_{1:n}}(x_n \,|\, y^*_{1:n}). \tag{5}$$

- 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 filtered through capacitors and resistors to estimate the source signal.

Smoothing

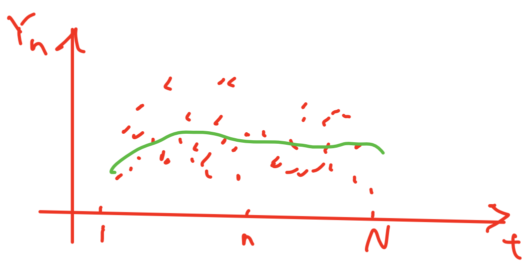
- In the context of a POMP model, smoothing involves finding the conditional distribution of X_n given all the data, $y^*_{1:N}$.

- So, the smoothing calculation is to find

基于过去和未来的信息,获得当前状态分布

$$f_{X_n|Y_{1:N}}(x_n \,|\, y^*_{1:N}). \qquad (6)$$

If X_n is a stochastic model of “trend” (not a trend according to our definition of trend as an expected value) then estimation of X_n is exactly the classic statistical smoothing problem



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 $n \in 1:N$,

[P4] $f_{X_n|Y_{1:n-1}}(x_n \,|\, y^*_{1:n-1}) =$上一个状态的出现概率 * 上一个状态转换到当前状态的概率

$$\int \underline{f_{X_{n-1}|Y_{1:n-1}}(x_{n-1} \,|\, y^*_{1:n-1})}\, \underline{f_{X_n|X_{n-1}}(x_n \,|\, x_{n-1})}\, dx_{n-1}.$$

- For the case $n = 1$, we let $1 : k$ is 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 10.2. 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 $P[X \cap Y \mid Z] = P[X \mid Z]\, P[Y \mid X, Z]$

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

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

z是所有可能的上一个状态

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

Example 3. A conditional form of Bayes' identity is

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

$= f_{XY|Z}(x,y|z)$

The filtering formula

通过贝叶斯获得当前状态的概率

- 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 $n \in 1:N$,

recursive

$f(X_n, Y_n \mid Y_{1:n-1})$

[P5] $$f_{X_n|Y_{1:n}}(x_n \mid y^*_{1:n}) = \frac{f_{X_n|Y_{1:n-1}}(x_n \mid y^*_{1:n-1})\, f_{Y_n|X_n}(y^*_n \mid x_n)}{f_{Y_n|Y_{1:n-1}}(y^*_n \mid y^*_{1:n-1})}.$$

是分子不同X_n的积分

拆解成y_n和y_{1:n-1}

Exercise 10.3. 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**,

$$\text{[P6]} \quad f_{Y_n|Y_{1:n-1}}(y_n^* \,|\, y_{1:n-1}^*) = \int \underbrace{f_{X_n|Y_{1:n-1}}(x_n \,|\, y_{1:n-1}^*)}_{\text{One step prediction result}} \, f_{Y_n|X_n}(y_n^* \,|\, x_n)\, dx_n.$$

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

[P6] shows that $f_{Y_n|Y_{1:n-1}}(y_n^* | y_{1:n-1}^*)$ is the proper normalizing factor for [P5]

Computation of the likelihood and log likelihood

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

$$f_{Y_{1:N}}(y^*_{1:N}) = \prod_{n=1}^{N} f_{Y_n|Y_{1:n-1}}(y^*_n \mid y^*_{1:n-1}). \tag{13}$$

- Equation (13) uses the convention that $1:k$ is the empty set when $k=0$, so the first term in the product is

$$f_{Y_1|Y_{1:0}}(y^*_1 \mid y^*_{1:0}) = f_{Y_1}(y^*_1) \tag{14}$$

- If our model has an unknown parameter θ then (13) gives the **log likelihood function** as a sum of conditional log likelihoods,

$$\ell(\theta) = \log \mathcal{L}(\theta) = \log f_{Y_{1:N}}(y^*_{1:N}\,; \theta) = \sum_{n=1}^{N} \log f_{Y_n|Y_{1:n-1}}(y^*_n \mid y^*_{1:n-1}\,; \theta).$$

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] $$f_{Y_{n:N}|X_n}(y^*_{n:N}\,|\,x_n) = f_{Y_n|X_n}(y^*_n\,|\,x_n)\underline{f_{Y_{n+1:N}|X_n}(y^*_{n+1:N}\,|\,x_n)}.$$

[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**,

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

Exercise 10.4. 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 used for inference in general nonlinear POMP models.

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 $n \in 1:N$,

$$\begin{array}{llll}
\text{[LG1]} & X_n = \mathbb{A}_n X_{n-1} + \epsilon_n, & & \epsilon_n \sim N[0, \mathbb{U}_n], \\
\text{[LG2]} & Y_n = \mathbb{B}_n X_n + \eta_n, & & \eta_n \sim N[0, \mathbb{V}_n].
\end{array}$$

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 $n \in 1:N$.
参数不随着时间变化

The LG-POMP representation of a Gaussian ARMA

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

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

- 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.

隐含状态需要考虑前max(p,q+1)个时间节点的状态

- To do this, we define $d_X = r = \max(p, q+1)$ and

令Y作为隐含状态的直接输出

$$\mathbb{B} = (1, 0, 0, \ldots, 0), \tag{16}$$

$$\mathbb{V} = 0. \tag{17}$$

假定没有观测误差

- We require $\mathbb{A}$ and $\mathbb{U}$ such that Y_n satisfies equation (15).

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

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

We can check that the ARMA equation (15) matches the matrix equation

ARMA模型是LG-POMP的例子

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

This is a time-homogenous LG-POMP, with $\mathbb{A}$, $\mathbb{B}$ and $\mathbb{V}$ as above and

$$
\underline{\mathbb{U} = \sigma^2 (1, \psi_1, \psi_2, \ldots, \psi_{r-1})^{\mathrm{T}} (1, \psi_1, \psi_2, \ldots, \psi_{r-1})}.
$$

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.

可选的POMP模型太多了

- 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. ARMA模型只是LG-POMP的特例
- 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). level is defined to be called trend. "Trend" is like the slope of the real trend (level)
- The model supposes that the level, trend and seasonality are perturbed with Gaussian white noise at each time point,

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

slope of real trend8

Have trend defined on a random process, not a expectation

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

Two common special cases of the basic structural model

- The **local linear trend** model is the basic structural model without the seasonal component, $\{S_n\}$ 没有周期性变化,稳定按照T_n作为slope波动

- 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. 没有slope波动,只有误差导致的随机游走

Initial values for the basic structural model

Try with R choice and explore

- 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$^2_{\text{eps}}$."

It's important to report likelihood

The basic structural model is an LG-POMP model

[BSM1–4] can be put in matrix form,

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

Now, set

$$X_n = (L_n, T_n, S_n, S_{n-1}, S_{n-2}, \dots, S_{n-10})^{\mathrm{T}}, \quad (18)$$

$$Y_n = (1, 0, 1, 0, 0, \dots, 0) X_n + \epsilon_n. \quad (19)$$

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

Spline smoothing and its LG-POMP representation

和HP smoothing一样

- 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)**, which is defined as

通过过滤得到的x序列是隐状态的一种

[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,

$$x_n = \alpha + \beta n, \tag{20}$$

  since $\Delta^2(\alpha + \beta n) = 0$.
- Now consider the linear Gaussian model,

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

- Note that $\Delta^2 X_n = \epsilon_n$. $\log f(\Delta^2 X_{1:N}) = \sum -\frac{\lambda}{2\sigma^2} \Delta X_i^2 - \frac{1}{2} \ln \frac{2\pi\sigma^2}{\lambda}$
- We will show that [SS1] is equivalent to [SS2,SS3].

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

Question 10.4. $\{X_n, Y_n\}$ 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?

将过往的隐含状态同样视为当下隐含状态的一个分量,因此仍然是线性的

$$\tilde{X}_n = \begin{pmatrix} X_n \\ X_{n-1} \end{pmatrix}$$

$$\tilde{X}_{n+1} = \begin{pmatrix} X_{n+1} \\ X_n \end{pmatrix} = \begin{pmatrix} 2 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} X_n \\ X_{n-1} \end{pmatrix} + \begin{pmatrix} \epsilon_n \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} 2 & -1 \\ 1 & 0 \end{pmatrix} \tilde{X}_n + \Sigma_n$$

General approach: take something that is not quite a POMP model, and relied it so it is, e.g. by adding lags to the stable representation

Deriving the penalized spline from the LG-POMP

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

$$f_{X_{1:N}Y_{1:N}}(x_{1:N}, y_{1:N}) = f_{X_{1:N}}(x_{1:N})\, f_{Y_{1:N}|X_{1:N}}(y_{1:N} \,|\, x_{1:N}). \qquad (21)$$

  Taking logs of (21) 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 $\mathrm{normal}[0, \sigma^2/\lambda]$ and $\mathrm{normal}[0, \sigma^2]$. Thus,

都是独立的,所以可以直接当
作正态分布的似然函数拆分

$$\log f_{X_{1:N}Y_{1:N}}(x_{1:N}, y_{1:N}\,; \sigma, \lambda) = \frac{-1}{2\sigma^2}\sum_{n=1}^{N}(y_n - x_n)^2 + \frac{-\lambda}{2\sigma^2}\sum_{n=3}^{N}(\Delta^2 x_n)^2 + C. \qquad (22)$$

C是由参数决定的常数

- 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 (22) 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

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

y出现的概率和x无关,因此可以直接放分母

在对正态分布线性组合做极大似然估计,
因此argmax就是期望

This is the expectation of the smoothing density at n for each n in [1,N]

- 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.

已知X,通过POMP来找最合适的lambda

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

Question 10.5. 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 that the equivalent penalty from some other LG-POMP model?

Historically, the spline penalty was used before people know of the more general connection to POMP models.

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

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

多变量正态分布

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

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

- A matrix square root of this type exists for any covariance matrix, though the choice of $\mathbb{H}$ is not unique.
- We write $X \sim \mathrm{normal}\big[\mu_X, \Sigma_X\big]$. If Σ_X is invertible, X has a probability density function,

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

Joint multivariate normal vectors

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

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

is multivariate normal. In this case, we write

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

where

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

- 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

X是向量,因此还是服从多变量正太分布

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

- We write this as

将多变量正态分布拆解

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

- 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: 隐状态都服从正态分布

$$\text{[KF3]} \qquad X_n \,|\, Y_{1:n-1} = y_{1:n-1} \sim \text{normal}\big[\,\mu_n^P(y_{1:n-1}),\, \Sigma_n^P\,\big],$$

$$\text{[KF4]} \qquad X_n \,|\, Y_{1:n} = y_{1:n} \sim \text{normal}\big[\,\mu_n^F(y_{1:n}),\, \Sigma_n^F\,\big],$$

$$\text{[KF5]} \qquad X_n \,|\, Y_{1:N} = y_{1:N} \sim \text{normal}\big[\,\mu_n^S(y_{1:N}),\, \Sigma_n^S\,\big].$$

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

$$
\begin{array}{lrcl}
\text{[KF6]} & \mu^P_{n+1}(y_{1:n}) & = & \mathbb{A}_{n+1}\mu^F_n(y_{1:n}) \\
\text{[KF7]} & \Sigma^P_{n+1} & = & \mathbb{A}_{n+1}\Sigma^F_n\mathbb{A}^{\mathrm{T}}_{n+1} + \mathbb{U}_{n+1}, \\
\text{[KF8]} & \Sigma^F_n & = & \big([\Sigma^P_n]^{-1} + \mathbb{B}^{\mathrm{T}}_n\mathbb{V}^{-1}_n\mathbb{B}_n\big)^{-1}, \\
\text{[KF9]} & \mu^F_n(y_{1:n}) & = & \mu^P_n(y_{1:n-1}) + \Sigma^F_n\mathbb{B}^{\mathrm{T}}_n\mathbb{V}^{-1}_n\big\{y_n - \mathbb{B}_n\mu^P_n(y_{1:n-1})\big\}.
\end{array}
$$

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, $X \sim \mathrm{normal}(\mu, \Sigma)$, then $\mathbb{A}X + b \sim \mathrm{normal}\big(\mathbb{A}\mu + b, \mathbb{A}\Sigma\mathbb{A}^{\mathrm{T}}\big)$. 转换后的方差+误差
- 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,

$$f_{X_n Y_n | Y_{1:n-1}}(x_n, y_n \,|\, y_{1:n-1}) \tag{23}$$

  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 10.5. 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 *et al.* (2016)
- Chapter 6 of Shumway and Stoffer (2017) gives an approach emphasizing linear Gaussian state space models.

References and Acknowledgements

King AA, Nguyen D, Ionides EL (2016). "Statistical Inference for Partially Observed Markov Processes via the R Package pomp." *Journal of Statistical Software*, **69**(12), 1–43. doi: 10.18637/jss.v069.i12.

Shumway RH, Stoffer DS (2017). *Time Series Analysis and its Applications: With R Examples*. Springer.

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