Constrained Functions

Text: Chapter 6
There are some situations in which we want to include known restrictions about \( x(t) \).
- \( x(t) \) is always positive
- \( x(t) \) is always increasing (or decreasing)
- \( x(t) \) is a density

Idea: Enforce these conditions by transforming \( x(t) \).

Positive Smoothing

We know that angular acceleration must be positive:

\[
a(t) = \sqrt{[D^2x(t)]^2 + [D^2y(t)]^2}
\]

But negative values can occur because of smoothing/basis bias.

Estimating a Positive Smooth

We now want to minimize

\[
PENSSE_\lambda(W) = \sum_{i=1}^{n} \left( y_i - e^{W(t_i)} \right)^2 + \lambda \int [LW(t)]^2 \, dt
\]

This does not have an explicit formula.
But it is convex – there is only one minimum.
Requires numerical optimization, but this is generally fast.
Positive Smoothing Vancouver Precipitation
Constraints imply smoothness (of a certain type) – tend to need less smoothing on $W$.

Monotone Smoothing

Berkeley growth study – heights aged 1 - 18

We need $x(t)$ always increasing:

$$Dx(t) > 0$$

suggests

$$Dx(t) = e^{W(t)} \rightarrow x(t) = \alpha + \int_{t_0}^{t} e^{W(s)} ds$$

again, $W(t) = \Phi(t) c$

Estimating a Monotone Smooth

We now want to minimize

$$\text{PENSSE}_\lambda(W) = \sum_{i=1}^{n} \left( y_i - \alpha - \int_{t_0}^{t_i} e^{W(s)} ds \right)^2 + \lambda \int [LW(t)]^2 dt$$

- No explicit formula
- No good formula for the integral
- Still a convex problem; numerics work fairly quickly

Note, $LW(t) = D^2 W(t)$ suggests that any $x(t) = \alpha + e^{\beta t}$ is smooth.
Density Estimation

Position of Beetles in Angles

\[ x(t) \text{ a density } \Rightarrow \text{positive, integrates to 1} \]

\[ x(t) = \frac{e^{W(t)}}{\int e^{W(t)} dt} \]

But we observe only \( t_1, \ldots, t_n \).
Need to find an objective to minimize.

Penalized Likelihood

Likelihood of \( W(t) \) is probability of seeing \( t_1, \ldots, t_n \) if \( W \) is true.
Easier to work with log likelihood

\[ l(W|t_1, \ldots, t_n) = \sum_{i=1}^{n} \left( W(t_i) - \log \int e^{W(t)} dt \right) \]

Minimize the penalized negative log likelihood:

\[ \text{PENLOGLIK}_\lambda(W) = -\sum_{i=1}^{n} W(t_i) + n \log \int e^{W(t)} dt + \lambda \int [LW(t)]^2 dt \]

Usual comments about numerics apply.

Thinking about Smoothness

What is an appropriate measure of smoothness for densities?

\[ x(t) = Ce^{W(t)} \]

Compare to Normal density

\[ f(t) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(t-\mu)^2}{\sigma^2}} \]

then \( W(t) = t^2 \) should be smooth \( \Rightarrow \) \( LW(t) = D^3 W(t) \).
Alternatively, \( LW(t) = D^2 W(t) \) \( \Rightarrow \) exponential distribution is smooth – useful for positive data.
Rough to Smooth Densities

Every 10th beetle

Binary data: $y_i \in \{0, 1\}$; want to measure $p(t_i) = P(y_i = 1|t_i)$.
- Count data; want a Poisson intensity at each $t_i$.
- Measurements of event times $t_1, \ldots, t_n$; Poisson-process intensity can change over time.

In each case we can write down a log likelihood of observed data given (some transformation of) $W(t)$ and apply a smoothing penalty.

These are discussed in the text, but not implemented in software.
Mathematical theory justifies process.

Examining the Berkeley Growth Data

54 girls recorded at 31 unequally-spaced times

Looking at Derivatives

The pubertal growth spurt is much more evident when we look at velocity.

A pre-pubertal mini-spurt may also be seen in acceleration.
The Case for Registration

The fact that growth spurts are not aligned makes thinking about a mean more difficult.

Aligning the curves reduces variation by 25%

Phase Plane Plots

Plotting velocity versus acceleration gives us an idea of the potential versus kinetic energy in a system.

Summary

Can put constraints to force

- $x(t) > 0$ by $x(t) = e^{W(t)}$
- $x(t)$ monotone by $x(t) = \alpha + \int_0^t e^{W(s)} ds$
- $x(t)$ a density by $x(t) = e^{W(t)} / \int e^{W(t)} dt$

Extension: penalized maximum likelihood for $x(t)$ not directly observed.

Requires nonlinear optimization, but still relatively fast.