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 want to ensure that $x(t) > 0$.

Observation:

$$e^w : (-\infty, \infty) \to (0, \infty)$$

So try the transformation

$$x(t) = e^{W(t)}$$

with

$$W(t) = \Phi(t)\mathbf{c}$$

and penalize the roughness of $W(t)$

Estimating a Positive Smooth

We now want to minimize

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

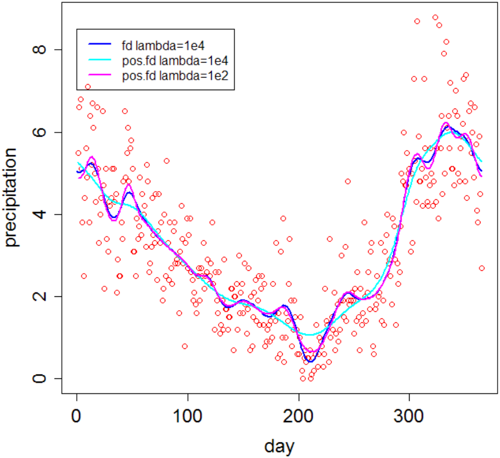
This does not have an explicit formula.

But it is convex – there is only one minimum.

Requires numerical optimization, but this is generally fast.

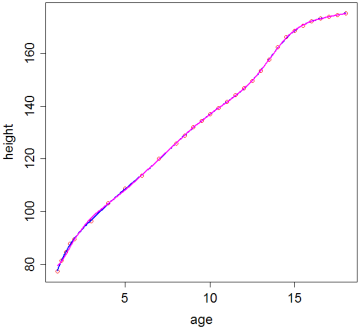
Positive Smoothing Vancouver Precipitation

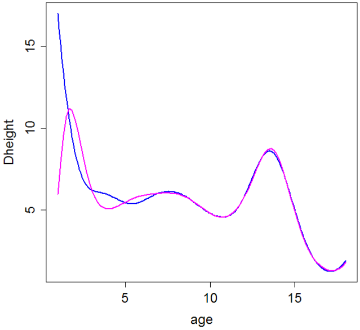
Constraints imply smoothness (of a certain type) – tend to need less smoothing on W.



Monotone Smoothing

Berkeley growth study – heights aged 1 - 18





Monotone Smoothing

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, $W(t) = \Phi(t)\mathbf{c}$

Estimating a Monotone Smooth

We now want to minimize

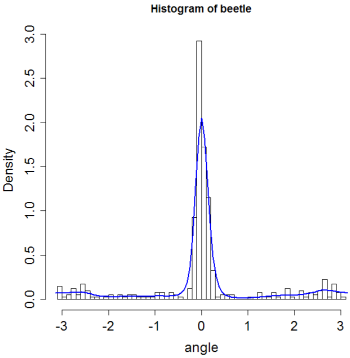
$$\mathrm{PENSSE}_\lambda(W) = \sum_{i=1}^{n} \left(y_i - \alpha - \int_{t_0}^{t_i} e^{W(s)} ds \right)^2 + \lambda \int [LW(t)]^2 \, dt$$

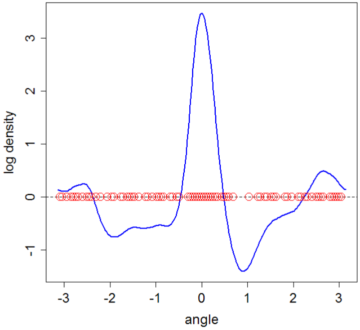
- No explicit formula
- No good formula for the integral
- Still a convex problem; numerics work fairly quickly

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





Density Estimation

$x(t)$ a density $\Rightarrow$ positive, integrates to 1

$$x(t) = e^{W(t)} / \int e^{W(t)} dt$$

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?

$$x(t) = Ce^{W(t)}$$

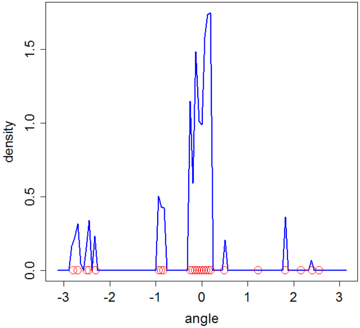
Compare to Normal density

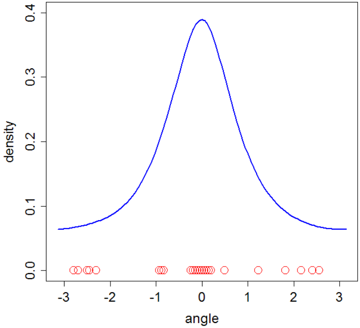
$$f(t) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(t-\mu)^2/\sigma^2}$$

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





Summary

Can put constraints to force

- $x(t) > 0$ by $x(t) = e^{W(t)}$
- $x(t)$ monotone by $x(t) = \alpha + \int_{t_0}^{t} e^{W(s)} ds$
- $x(t)$ 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.