Penalized Splines, Mixed Models, and Recent Large-Sample Results

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Two parts

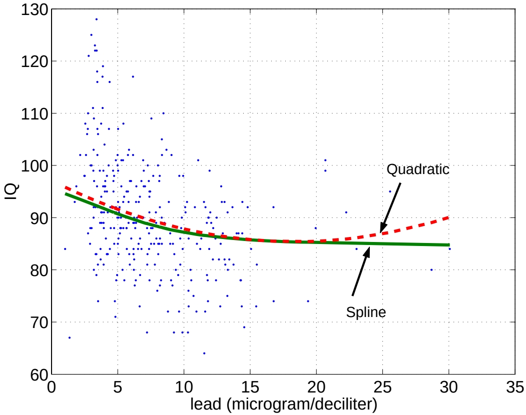
- Old: overview of the book *Semiparametric Regression* by Ruppert, Wand, and Carroll (2003)
- New: asymptotics of penalized splines

Intellectual impairment and blood lead

Example I (courtesy of Rich Canfield, Nutrition, Cornell)

- blood lead and intelligence measured on children
- Question: how do low doses of lead affect IQ?
  - important since doses are decreasing with lead now out of gasoline
- several IQ measurements per child
  - so longitudinal
- nine "confounders"
  - e. g., maternal IQ
  - need to adjust for them
- effect of lead appears nonlinear
  - important conclusion

Dose-response curve



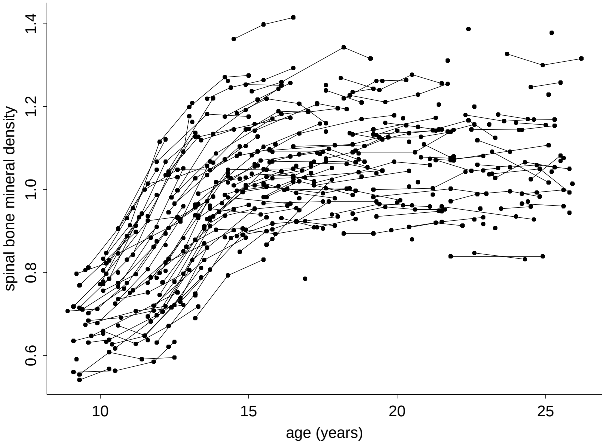
Thanks to Rich Canfield for data and estimates

Spinal bone mineral density example

Example II (in Ruppert, Wand, Carroll (2003), *Semiparametric Regression*

- age and spinal bone mineral density measured on girls and young women
- several measurements on each subject
- increasing but nonlinear curves

Spinal bone mineral density data



What is needed to accommodate these examples

We need a model with

- potentially many variables
- possibility of nonlinear effects
- random subject-specific effects

The model should be one that can be fit with readily available software such as SAS, Splus, or R.

Underlying philosophy

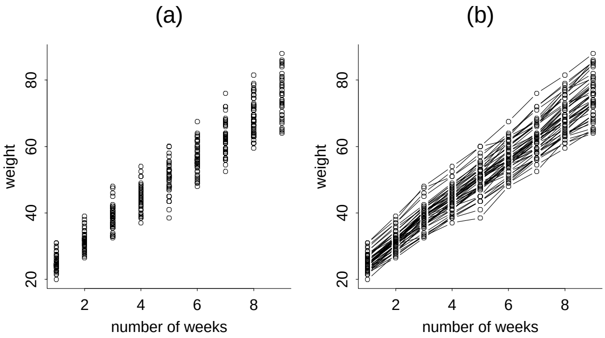
1. minimalist statistics
   - keep it as simple as possible
2. build on classical parametric statistics
3. modular methodology
   - so we can add components to accommodate special features in data sets

Outline of the approach

- Start with linear mixed model
  - allows random subject-specific effects
  - fine for variables that enter linearly
- Expand the basis for those variables that have nonlinear effects
  - we will use a spline basis
  - treat the spline coefficients as random effects to induce empirical Bayes shrinkage = smoothing
- End result
  - linear mixed model from a software perspective, but
  - nonlinear from a modeling perspective

Example: pig weights (random effects)

Example III (from Ruppert, Wand, and Carroll (2003))



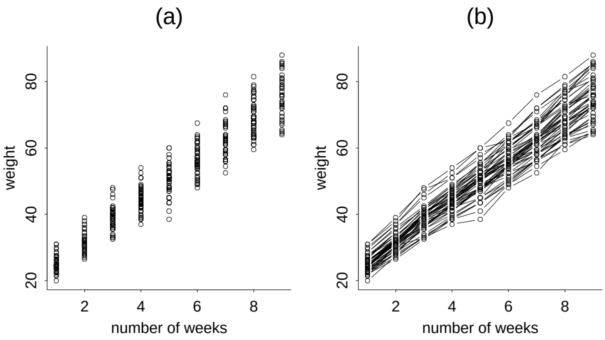
Random intercept model

$$Y_{ij} = (\beta_0 + b_{0i}) + \beta_1 \texttt{week}_j$$

- Y_{ij} = weight of ith pig at the jth week
- β_0 is the average intercept for pigs
- b_{0i} is an offset for ith pig
- So $(\beta_0 + b_{0i})$ is the intercept for the ith pig

Are random intercepts enough?

Example III



Random lines model

$$Y_{ij} = (\beta_0 + b_{0i}) + (\beta_1 + b_{1i})\,\texttt{week}_j$$

- β_1 is the average slope
- b_{ii} is an adjustment to slope of the ith pig
- So $(\beta_1 + b_{1i})$ is the slope for the ith pig
- b_{0i} and b_{1i} seem positively correlated
  - makes sense: faster growing pigs should be larger at the start of data collection

General form of linear mixed model

- Model is:
$$Y_i = \mathbf{X}_i^\mathsf{T} \boldsymbol{\beta} + \mathbf{Z}_i^\mathsf{T} \mathbf{b} + \epsilon_i$$
- $\mathbf{X}_i = (X_{i1}, \ldots, X_{ip})$ and $\mathbf{Z}_i = (Z_{i1}, \ldots, Z_{iq})$ are vectors of predictor variables
- $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)$ is a vector of fixed effects
- $\mathbf{b} = (b_1, \ldots, b_q)$ is a vector of random effects
  - $\mathbf{b} \sim MVN\{0, \Sigma(\theta)\}$
  - θ is a vector of variance components

Estimation in linear mixed models

- $\boldsymbol{\beta}$ and $\boldsymbol{\theta}$ are the parameter vectors
  - estimated by
    - ML (maximum likelihood), or
    - REML (maximum likelihood with degrees of freedom correction)
- $\mathbf{b}$ is a vector of random variables
  - predicted by a BLUP (Best linear unbiased predictor)
  - BLUP is shrunk towards zero (mean of $\mathbf{b}$)
  - amount of shrinkage depends on $\widehat{\boldsymbol{\theta}}$

Estimation in linear mixed models, cont.

- Random intercepts example:

$$Y_{ij} = (\beta_0 + b_{0i}) + \beta_1 \texttt{week}_j$$

  - high variability among the intercepts $\Rightarrow$ less shrinkage of b_{0i} towards 0
    - extreme case: intercepts are fixed effects
  - low variability among the intercepts $\Rightarrow$ more shrinkage
    - extreme case: common intercept (another fixed effects model)

Comparison between fixed and random effects modeling

- fixed effects models allow only the two extremes:
  - no shrinkage
  - common intercept
- mixed effects modeling allows all possibilities between these extremes

Splines

- polynomials are excellent for local approximation of functions
- in practice, polynomials are relatively poor at global approximation
- a spline is made by joining polynomials together
    - takes advantage of polynomials strengths without inheriting their weaknesses
- splines have "maximal smoothness"

Piecewise linear spline model

"Positive part" notation:

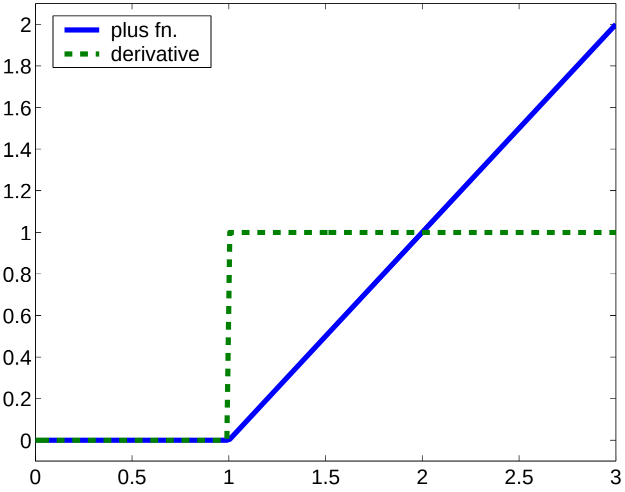
$$x_+ = x, \text{ if } x > 0 \quad (1)$$
$$= 0, \text{ if } x \leq 0 \quad (2)$$

Linear spline:

$$m(x) = \left\{\beta_0 + \beta_1 x\right\} + \left\{b_1(x - \kappa_1)_+ + \cdots + b_K(x - \kappa_K)_+\right\}$$

- $\kappa_1, \ldots, \kappa_K$ are "knots"
- $b_1, \ldots, b_K$ are the spline coefficients

Linear "plus" function with $\kappa = 1$

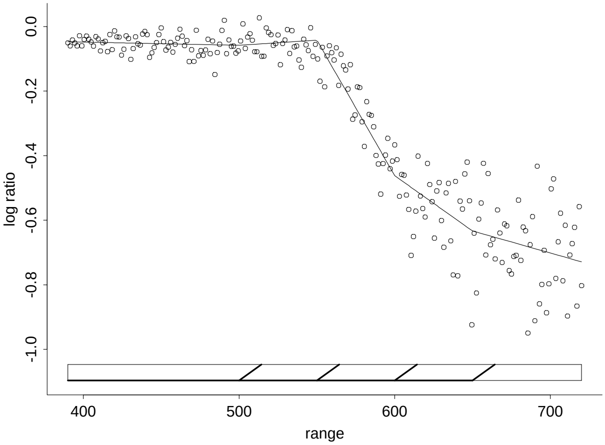


Linear spline

$$m(x) = \beta_0 + \beta_1 x + b_1(x-\kappa_1)_+ + \cdots + b_K(x-\kappa_K)_+$$

- slope jumps by b_k at κ_k, $k = 1, \ldots, K$

Fitting LIDAR data with plus functions

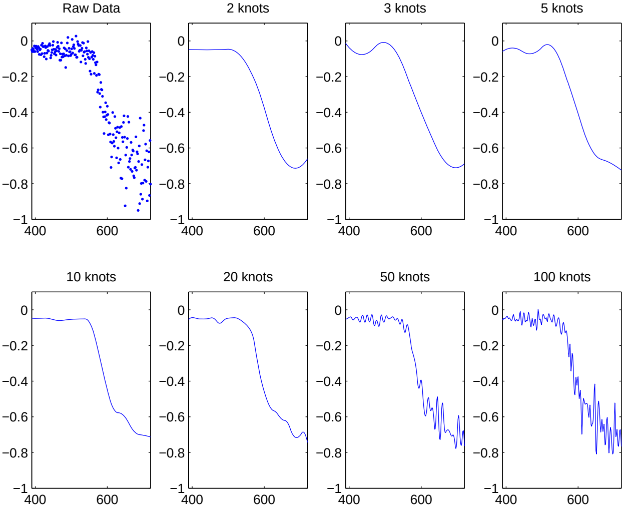


Generalization: higher degree splines

$$m(x) = \beta_0 + \beta_1 x + \cdots + \beta_p x^p$$
$$+ b_1 (x - \kappa_1)_+^p + \cdots + b_K (x - \kappa_K)_+^p$$

- pth derivative jumps by $p!\, b_k$ at κ_k
- first $p - 1$ derivatives are continuous

LIDAR data: ordinary Least Squares



Penalized least-squares

- Use matrix notation:

$$m(X_i) = \beta_0 + \beta_1 X_i + \cdots + \beta_p X_i^p$$
$$+ b_1 (X_i - \kappa_1)_+^p + \cdots + b_K (X_i - \kappa_K)_+^p$$
$$= \mathbf{X}_i^{\mathsf{T}} \boldsymbol{\beta}_X + \mathbf{B}^{\mathsf{T}}(X_i)\mathbf{b}$$

- Minimize

$$\sum_{i=1}^{n} \left\{ Y_i - (\mathbf{X}_i^{\mathsf{T}} \boldsymbol{\beta}_X + \mathbf{B}^{\mathsf{T}}(X_i)\mathbf{b}) \right\}^2 + \lambda\, \mathbf{b}^{\mathsf{T}} \mathbf{D} \mathbf{b}.$$

Penalized least-squares, cont.

- From previous slide: minimize

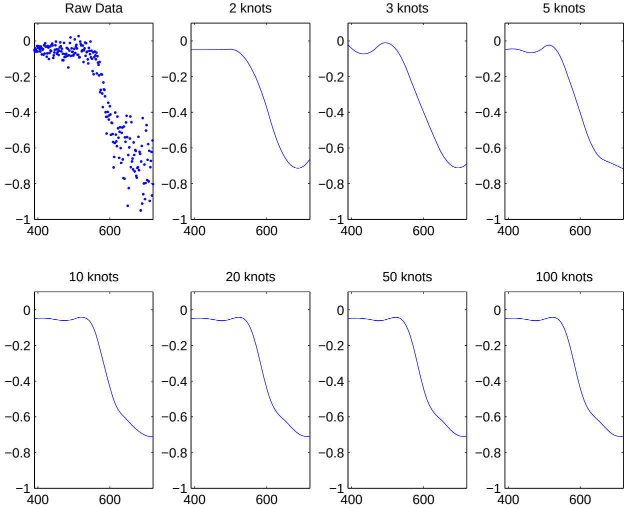
$$\sum_{i=1}^{n}\left\{Y_i-(\mathbf{X}_i^{\mathsf{T}}\boldsymbol{\beta}_X+\mathbf{B}^{\mathsf{T}}(X_i)\mathbf{b})\right\}^2+\lambda\,\mathbf{b}^{\mathsf{T}}\mathbf{D}\mathbf{b}.$$

- $\lambda\,\mathbf{b}^{\mathsf{T}}\mathbf{D}\mathbf{b}$ is a penalty that prevents overfitting
- $\mathbf{D}$ is a positive semidefinite matrix
  - so the penalty is non-negative
  - Example:

$$\mathbf{D}=\mathbf{I}$$

- λ controls that amount of penalization
- the choice of λ is crucial

Penalized Least Squares

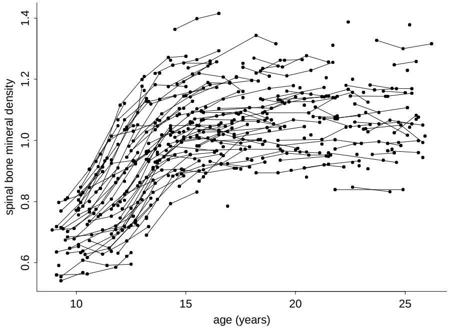


Selecting λ

To choose λ use:

1. one of several model selection criteria:
   - cross-validation (CV)
   - generalized cross-validation (GCV)
   - AIC
   - C_P
2. ML or REML in mixed model framework
   - convenient because one can add other random effects
   - also can use standard mixed model software

Return to spinal bone mineral density study



$$\texttt{SBMD}_{i,j} = U_i + m(\texttt{age}_{i,j}) + \epsilon_{i,j},$$

$$i = 1, \ldots, m = 230, \quad j = i, \ldots, n_i.$$

Fixed effects

$$\mathbf{X} = \begin{bmatrix} 1 & \text{age}_{11} \\ \vdots & \vdots \\ 1 & \text{age}_{1n_1} \\ \vdots & \vdots \\ 1 & \text{age}_{m1} \\ \vdots & \vdots \\ 1 & \text{age}_{mn_m} \end{bmatrix}$$

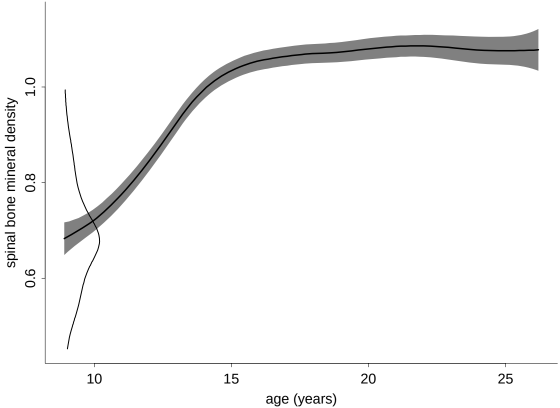
Random effects

$$\mathbf{Z} = \begin{bmatrix} 1 & \cdots & 0 & (\text{age}_{11} - \kappa_1)_+ & \cdots & (\text{age}_{11} - \kappa_K)_+ \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \cdots & 0 & (\text{age}_{1n_1} - \kappa_1)_+ & \cdots & (\text{age}_{1n_1} - \kappa_K)_+ \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & (\text{age}_{m1} - \kappa_1)_+ & \cdots & (\text{age}_{m1} - \kappa_K)_+ \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & (\text{age}_{mn_m} - \kappa_1)_+ & \cdots & (\text{age}_{mn_m} - \kappa_K)_+ \end{bmatrix}$$

Random effects

$$\mathbf{u} = \begin{bmatrix} U_1 \\ \vdots \\ U_m \\ b_1 \\ \vdots \\ b_K \end{bmatrix}$$

Random effects



Variability bars on $\widehat{m}$ and estimated density of U_i

Modeling the blood lead and IQ data

For the jth measurements on the ith subject:

$$\mathrm{IQ}_{ij} = b_i + m(\mathrm{lead}_{ij}) + \beta_1 X_{ij}^1 + \cdots + \beta_L X_{ij}^L + \epsilon_{ij}$$

- $m(\cdot)$ is a spline
  - include the population average intercept
- b_i is a random subject-specific intercept
  - $E(b_i) = 0$
  - model assumes parallel curves
- X_{ij}^{ℓ} is the value of the ℓth confounder, $\ell = 1, \ldots, L$

Summary (overview of semiparametric regression)

- Semiparametric philosophy
  - use nonparametric models where needed
  - but only where needed
- LMMs and GLMMs are fantastic tools, but (apparently) totally parametric
- By basis expansion, LMMs and GLMMs become semiparametric
- Low-rank splines eliminate computational bottlenecks
- Smoothing parameters can be estimated as ratios of variance components

Asymptotic theory: framework

Li and Ruppert (2008, *Biometrika*)

- p-degree spline model:

$$f(x) = \sum_{k=1}^{K+p} b_k B_k(x), \quad x \in (0, 1)$$

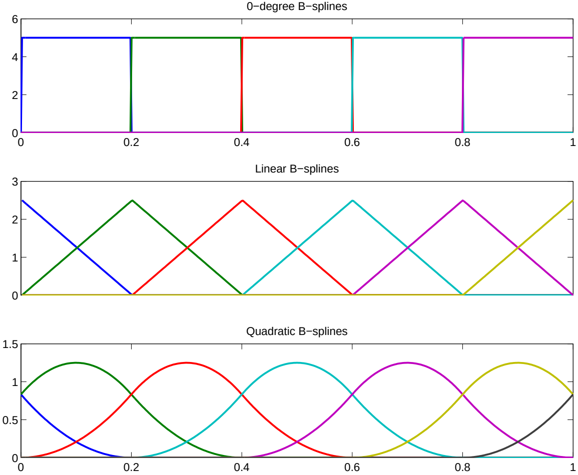
- pth degree B-spline basis:

$$\{B_k : k = 1, \ldots, K + p\}$$

- knots:

$$\kappa_0 = 0 < \kappa_1 < \ldots < \kappa_K = 1$$

B-splines


0−degree B−splines
Linear B−splines
Quadratic B−splines
0
0.2
0.4
0.6
0.8
1
6
4
2
3
1.5
0.5

Outline of asymptotic theory

1. First: summary
2. Go through the case $p = 0$, $m = 1$, equally-spaced x_i carefully
3. Then do $p = 0$ and $m = 2$
4. Discuss higher order cases and unequally-spaced data

Summary of main results

- Penalized spline estimators are approximately binned Nadaraya-Watson kernel estimators
  - Penalized splines are not design-adaptive in the sense of Fan (1992)
- The order of the N-W kernel depends solely on m (order of penalty)
  - this was surprising to us
  - order of kernel is $2m$ in the interior
  - order is m at boundaries

Summary of main results, continued

- The spline degree p does not affect the asymptotic distribution, but
  - p determines the type of binning and the minimum rate at which $K \to \infty$
  - $p = 0 \Rightarrow$ usual binning
  - $p = 1 \Rightarrow$ linear binning
  - a higher value of p means that less knots are needed (because there is less binning bias)

Penalized least-squares

- Penalized least-squares minimizes

$$\sum_{i=1}^{n}\left\{y_i - \sum_{k=1}^{K+p}\widehat{b}_k B_i(x_i)\right\}^2 + \lambda \sum_{k=m+1}^{K+p}\{\Delta^m(\widehat{b}_k)\}^2,$$

- $\Delta b_k = b_k - b_{k-1}$ and $\Delta^m = \Delta(\Delta^{m-1})$
  - $m = 1 \Rightarrow$ constant functions are unpenalized
  - $m = 2 \Rightarrow$ linear functions are unpenalized

$p = 0, \; m = 1$

Assume:

- $x_1 = 1/n, x_2 = 2/n, \ldots, x_n = 1$
- $\kappa_0 = 0, \kappa_1 = 1/K, \kappa_2 = 2/K, \ldots, \kappa_K = 1$
- $B_k(x) = I\{\kappa_{k-1} < x \leq \kappa_k\}$, $1 \leq k \leq K$ (kth bin indicator)
- assume that $n/K := M$ is an integer
- then $X^{\mathsf{T}}X = MI_K$ where I_K

$p = 0, \ m = 1$, continued

Assume further:

- $m = 1$

Then

$$D^{\mathsf{T}} D = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix},$$

$p = 0,\ m = 1$, PLS estimator

The Penalized LS estimator solves:

$$\Lambda \widehat{\mathbf{b}} = \mathbf{z} = \overline{\mathbf{y}}/(1+2\lambda) \quad (\overline{\mathbf{y}} = \text{ bin averages})$$

where

$$\Lambda = \begin{pmatrix} \theta & \eta & 0 & 0 & \cdots & 0 & 0 \\ \eta & 1 & \eta & 0 & \cdots & 0 & 0 \\ 0 & \eta & 1 & \eta & \cdots & 0 & 0 \\ 0 & 0 & \eta & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & \eta \\ 0 & 0 & 0 & 0 & \cdots & \eta & \theta \end{pmatrix}, \quad \eta = -\frac{\lambda}{1+2\lambda}$$

$p = 0, \; m = 1$, PLS estimator, page 2

Let $\rho \in (0,1)$ be a root of

$$\eta + \rho + \eta\rho^2 = 0.$$

Then

$$\rho = \frac{1 - \sqrt{1 - 4\eta^2}}{-2\eta} = \frac{1 + 2\lambda - \sqrt{1 + 4\lambda}}{2\lambda}.$$

Define

$$T_i = (\rho^{i-1}, \rho^{i-2}, \ldots, \rho, 1, \rho, \rho^2, \ldots, \rho^{K-i})^{\mathsf{T}}$$

T_i is orthogonal to all columns of Λ except the first, last, and ith (so T_i is the ith row of Λ, except for a geometrically convergent error)

Finite-sample kernel

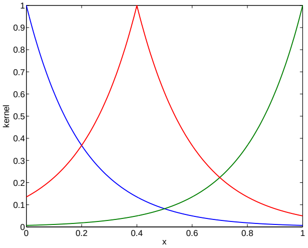
Finite-sample kernel defined by:

$$\widehat{f}(x) = \sum_{j=1}^{K} H(x, \overline{x}_j)\overline{y}_i$$

$$\frac{T_i^{\mathsf{T}}}{1+2\lambda} = \frac{(\rho^{i-1}, \rho^{i-2}, \ldots, \rho, 1, \rho, \rho^2, \ldots, \rho^{K-i})}{1+2\lambda}$$

is the finite-sample kernel (ignoring asymptotically negligible boundary effects).

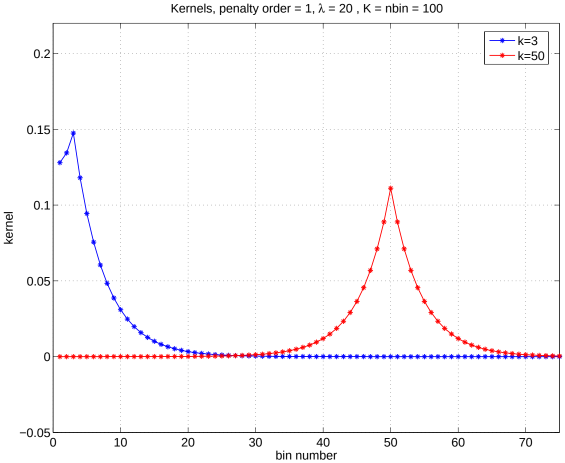
Three kernels corresponding to first-order penalty



- x is an "estimation point" (here fixed at 0.4)

- finite-sample kernel is linear combination of three kernels
  - double exponential kernel centered at x
  - boundary kernels are $\exp(-x)$ and $\exp(x)$
- weights for the boundary kernels are asymptotically negligible in interior

Finite-sample kernels, first-order penalty



Connection with smoothing splines

We get the same equivalent kernels (Silverman, 1985) as for smoothing splines with a penalty on the first derivative

Finding $\widehat{b}_i$ – interior case

- Suppose $i/K \to x \in (0,1)$ (non-boundary case)
- After some algebra:

$$\widehat{b}_i \sim \frac{\sum_{j=1}^{K} \rho^{|i-j|} \overline{y}_j}{\sum_{j=1}^{K} \rho^{|i-j|}}.$$

- Note that

$$\widehat{f}(x) = \widehat{b}_i$$

for x in the ith bin

Equivalence to N-W kernel estimator

- After some more algebra

$$\rho^{|i-j|} \sim \exp\left\{-\frac{|\overline{x}_i - \overline{x}_j|}{hn^{-1/5}}\right\}$$

- Thus, $\widehat{f}_n$ is asymptotically equivalent to the Nadaraya-Watson estimator with
  - double exponential kernel $H(x) = (1/2)\exp(-|x|)$
  - bandwidth $hn^{-1/5}$

Nadaraya-Watson kernel estimators

Model:

$$y_i = f(x_i) + \epsilon_i$$

Nadaraya-Watson estimator:

$$\widehat{f}(x) = \frac{\sum_{i=1}^{n} H\{(x_i - x)/h_n\} y_i}{\sum_{i=1}^{n} H\{(x_i - x)/h_n\}}$$

- $H(\cdot)$ is called the kernel function
- h_n is the bandwidth

Binned Nadaraya-Watson kernel estimators

Binned Nadaraya-Watson estimator:

- range of the x_i divided into K subintervals (bins)
- $\overline{x}_j$ is average of x_i in ith bin
- $\overline{y}_j$ is average of y_i such that x_i is in the ith bin

$$\widehat{f}(x) = \frac{\sum_{j=1}^{K} H\{(\overline{x}_j - x)/h_n\}\overline{y}_j}{\sum_{j=1}^{K} H\{(\overline{x}_i - x)/h_n\}}$$

P-spline equivalent to a Nadaraya-Watson kernel estimator

- Thus, $\widehat{f}_n$ is asymptotically equivalent to a binned Nadaraya-Watson estimator with
  - double exponential kernel $H(x) = (1/2)\exp(-|x|)$
  - bandwidth $hn^{-1/5}$
- binning bias is negligible if $K = Cn^{\gamma}$ for $\gamma > 2/5$ and $C > 0$
- "negligible" means $o(n^{-2/5})$

Selecting λ to achieve desired bandwidth

- To get bandwidth $hn^{-1/5}$ we need λ chosen as

$$\lambda \sim \{(Cn^{\gamma})(hn^{-1/5})\}^2 = (\#\text{ knots } \times \text{ bandwidth})^2$$

Asymptotic Distribution

For $x \in (0,1)$, as $n \to \infty$ we have

$$n^{2/5}\{\hat{f}_n(x) - f(x)\} \Rightarrow N\{\mathcal{B}(x), \mathcal{V}(x)\}$$

where

- $\mathcal{B}(x) = h^2 f^{(2)}(x)$
- $\mathcal{V}(x) = 4^{-1} h^{-1} \sigma^2(x)$

Some folklore

- Folklore: The number of knots is not important, provided that it is large enough.
  - Confirmation:

$$K \sim Cn^{\gamma} \text{ with } C > 0 \text{ and } \gamma > 2/5. \tag{3}$$

- Folklore: The value of the penalty parameter is crucial.
  - Confirmation:

$$\lambda \sim C^2 h^2 n^{2\gamma - 2/5} = (\#\text{ knots } \times \text{ bandwidth})^2 \tag{4}$$

  for some $h > 0$.

- Folklore: Modeling bias is small.
  - Confirmation: Modeling bias does not appear in asymptotic bias provided (3) and (4) hold.

Order of a kernel and bias

Moments: kth moment is $\int x^k H(x)\,dx$

Order of kernel: A kernel is of kth order if the first non-zero moment is the kth

- Non-negative kernel: order is at most 2

Bias: bias $= O\{(\text{bandwidth})^k\}$

Variance:

variance $= O\left(\frac{1}{n \times \text{bandwidth}}\right)$

and

optimal RMSE $= O(n^{-k/(2k+1)})$

2nd order-penalty gives 4th order kernel (in interior)

Now let $m = 2$ (2nd order difference penalty)

- Assume:
  - $K \sim Cn^{\gamma}$ with $C > 0$ and $\gamma > 4/9$
  - $\lambda \sim 4C^4 h^4 n^{4\gamma - 4/9} \sim 4(Khn^{-1/9})^4$.

Then for any $x \in (0,1)$, when $n \to \infty$, we have

$$n^{4/9}\{\widehat{f}_n(x) - f(x)\} \Rightarrow N\{\mathcal{B}_1(x), \mathcal{V}_1(x)\},$$

where

- $\mathcal{B}_1(x) = (1/24)h^4 f^{(4)}(x) \int x^4 T(x)\,dx$
- $\mathcal{V}_1(x) = h^{-1}\{\int T^2(x)\,dx\}\,\sigma^2(x)$
  - $T(x)$ is a fourth order kernel

Mathematical approach

Main technical device uses roots of the polynomial

$$w(\xi) = \lambda(1-4\xi+6\xi^2-4\xi^3+\xi^4)+\xi^2 = \lambda(1-\xi)^4+\xi^2, \ \lambda > 0$$

- No real roots and no roots of modulus one
- Roots are: r, conj(r), r^{-1}, conj$(r)^{-1}$ (all distinct)
- Use the conjugate pair with modulus less than one

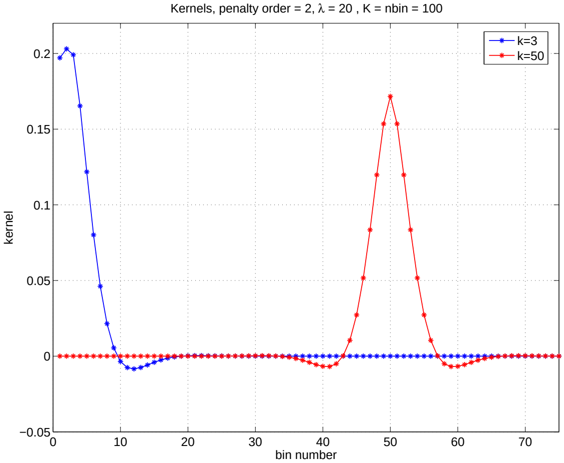
Asymptotic Kernel

- The asymptotic kernel is a linear combination of

$$\exp(-|x|)\cos(x) \quad \text{and} \quad \exp(-|x|)\sin(|x|)$$

- Same equivalent kernel (Silverman, 1985) as for smoothing splines with a penalty on the second derivative

Finite-sample kernels, second-order penalty



Linear splines need less knots

Assume $m = 1$ (1st-order difference penalty).

- If $p = 1$ (linear), then require
$$K \sim Cn^{\gamma} \text{ with } C > 0 \text{ and } \gamma > 1/5$$
- When p was 0 (piecewise constant), we required $\gamma > 2/5$
- Otherwise, results are the same as for 0-degree and linear splines

A similar result holds for $m = 2$.

Conjectures

- Conjecture: For x in the interior:

  P-spline $\sim$ N-W estimator with an $2m$-order kernel

  - Recall: m is order of difference penalty
  - Kernel order independent of $p =$ degree of spline
  - Shown to hold for $m = 1, 2$ and $p = 0, 1$
- $p = 1$ requires less knots than $p = 0$
  - What happens for $p > 1$?
  - Conjecture: Still less knots are needed
- Conjectures are nearly proved: Li, Apanosovich, Ruppert (2009)

Unequally spaced X

- Assume $G(x_t) = t/n$ for a smooth G with $g = G'$
- Fit a spline to (Y_t, u_t) with regression function $f \circ G^{-1}$
  - evaluate this estimate at $G(x)$ to estimate $f(x)$
- Equally spaced knots for (Y_t, u_t) implies knots at sample quantiles for (Y_t, x_t)
- asymptotic bias is

$$h^2 (f \circ G^{-1})^{(2)}\{G(x)\} = \frac{h^2}{g^2(x)} \left\{ f^{(2)}(x) - \frac{f'(x)g'(x)}{g(x)} \right\}$$

- Nadaraya-Watson bias is

$$h^2 \left\{ f^{(2)}(x) + \frac{2f'(x)g'(x)}{g(x)} \right\}$$

We use only one of two potential smoothing parameters

Both K and λ are potential smoothing parameters

- In our asymptotic theory, only λ plays the role of a smoothing parameter
- Could develop a theory where only K plays this role
  - would be similar to regression spline ($\lambda = 0$) theory
- One could also choose K and λ so that both have a non-negligible effect
- Our theory mimics actual practice

Summary (asymptotics)

- P-spline estimators ≈ binned N-W kernel estimators
- The number of knots unimportant if above a minimum
- Degree of spline
  - determines minimum convergence rate for number of knots
  - does not affect rate of convergence
- Order of penalty determines
  - order of equivalent kernel
  - convergence rate of estimator
- mth order penalty ⇔ smoothing spline with penalty on mth difference

Thanks for your attention