Slide 1

Partial Splines

Let $\{\psi_\mu\}_{\mu=1}^q$ be known functions on $\mathcal{X}$. The minimizer of

$$\frac{1}{n}\sum_{i=1}^n\Big(Y_i-\sum_{\mu=1}^q\beta_\mu\psi_\mu(x_i)-\eta(x_i)\Big)^2+\lambda J(\eta)$$

w.r.t. β_μ and $\eta\in\mathcal{H}=\{f:J(f)<\infty\}$ is called a *partial spline.*

Write $\mathcal{H}=\mathcal{N}_J\oplus\mathcal{H}_J$, where $\mathcal{N}_J=\text{span}\{\phi_\nu,\nu=1,\dots,m\}$. A partial spline is simply a regular spline that minimizes

$$\frac{1}{n}\sum_{i=1}^n(Y_i-\tilde{\eta}_0(x_i)-\eta_1(x_i))^2+\lambda J(\eta_1)$$

for $\tilde{\eta}_0\in\tilde{\mathcal{H}}_0=\text{span}\{\phi_\nu,\psi_\mu\}$ and $\eta_1\in\mathcal{H}_J$.

- These and similar models are also called semiparametric models.

Slide 2

Periodic Splines

Consider $f\in\mathcal{P}[0,1]$ permitting a Fourier expansion

$$f(x)=a_0+\textstyle\sum_{\mu=1}^\infty(a_\mu\cos 2\pi\mu x+b_\mu\sin 2\pi\mu x),$$

where $\sum_{\mu=1}^\infty(a_\mu^2+b_\mu^2)<\infty$; this includes all continuous functions. One has $\int_0^1(f^{(m)})^2dx=\frac{1}{2}\sum_{\mu=1}^\infty(a_\mu^2+b_\mu^2)(2\pi\mu)^{2m}$.

In the space $\mathcal{H}=\{f:f\in\mathcal{P}[0,1],f^{(m)}\in\mathcal{L}_2[0,1]\}$ with an IP $(f,g)=\big(\int_0^1 fdx\big)\big(\int_0^1 gdx\big)+\int_0^1 f^{(m)}g^{(m)}dx$, the RK is given by

$$\begin{aligned}R(x,y)&=1+\sum_{\mu=1}^\infty\frac{2}{(2\pi\mu)^{2m}}(\cos 2\pi\mu x\cos 2\pi\mu y+\sin 2\pi\mu x\sin 2\pi\mu y)\\&=1+\sum_{\mu=1}^\infty\frac{2\cos 2\pi\mu(x-y)}{(2\pi\mu)^{2m}}=1+(-1)^{m-1}k_{2m}(x-y);\end{aligned}$$

a one-way ANOVA is built in with $Af=\int_0^1 fdx$.

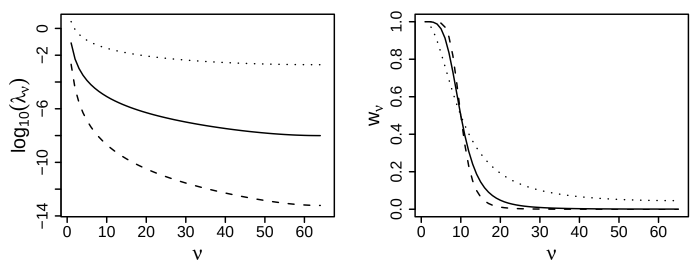
Slide 3

Splines as Low-Pass Filters

A periodic polynomial spline is the minimizer in $\mathcal{P}[0,1]$ of

$$\frac{1}{n}\sum_{i=1}^{n}(Y_i-\eta(x_i))^2+\lambda\int_0^1(\eta^{(m)})^2dx.$$

With equally spaced data, the DFT of $\mathbf{Y}$ and $\hat{\mathbf{Y}}$ satisfy $\tilde{\hat{Y}}_\nu = w_\nu \tilde{Y}_\nu$, where $w_1=1$, $w_\nu=\lambda_{\nu-1}/(\lambda_{\nu-1}+n\lambda)$, $\nu=2,\dots,n$.



Slide 4

L-Splines

Given a general differential operator L and a weight function $h(x)>0$, the minimizer of

$$\frac{1}{n}\sum_{i=1}^{n}(Y_i-\eta(x_i))^2+\lambda\int_0^1(L\eta)^2(x)h(x)dx$$

is called an L-spline; the polynomial splines are special cases.

In applications where $\mathcal{N}_L=\{f: Lf=0\}$ provides a more natural parametric model than a low-order polynomial, an L-spline other than a polynomial spline often provides a better estimate.

Given an RK in $\mathcal{H}_L=\{f:\int_0^1(Lf)^2hdx<\infty\}\ominus\mathcal{N}_L$ with the IP $(f,g)=\int_0^1(Lf)(Lg)hdx$, and a basis of $\mathcal{N}_L$, an L-spline can be readily computed by the generic algorithms.

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Trigonometric Splines

Consider $f \in \mathcal{P}[0,1]$ with $\int_0^1 f dx = a_0 = 0$. The operator $L_2 = D^2 + (2\pi)^2$ has a null space $\mathcal{N}_L = \text{span}\{\cos 2\pi x, \sin 2\pi x\}$.

To the square norm $(\int_0^1 f(x)\cos 2\pi x dx)^2 + (\int_0^1 f(x)\sin 2\pi x dx)^2$ in $\mathcal{N}_L$ corresponds the RK $\cos 2\pi x \cos 2\pi y + \sin 2\pi x \sin 2\pi y$. Take $h(x) = 1$, define $\mathcal{H} = \{f : f \in \mathcal{P}[0,1], a_0 = 0, \int_0^2 (L_2 f)^2 dx < \infty\}$, and consider $\mathcal{H}_L = \mathcal{H} \ominus \mathcal{N}_L$. To the IP $(f,g) = \int_0^1 (L_2 f)(L_2 g) dx$ in $\mathcal{H}_L$ corresponds the RK

$$R_2(x,y) = \sum_{\mu=2}^{\infty} \frac{2\cos 2\pi\mu(x-y)}{(2\pi)^4(\mu^2-1)^2}.$$

Compare $\int_0^1 (L_2 f)^2 dx = (2\pi)^4 \sum_{\mu=2}^{\infty} (a_\mu^2 + b_\mu^2)(\mu^2-1)^2$ with $\int_0^1 \ddot{f}^2 dx = (1/2)(2\pi)^4 \sum_{\mu=1}^{\infty} (a_\mu^2 + b_\mu^2)\mu^4$, in $\mathcal{H}_L$.

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Trigonometric Splines

Consider $f \in \mathcal{P}[0,1]$, and the operator $L_3 = D(D^2 + (2\pi)^2)$ with a null space $\mathcal{N}_L = \text{span}\{1, \cos 2\pi x, \sin 2\pi x\}$.

To $(f,f) = (\int_0^1 f^2 dx) + (\int_0^1 f(x)\cos 2\pi x dx)^2 + (\int_0^1 f(x)\sin 2\pi x dx)^2$ in $\mathcal{N}_L$ corresponds the RK $1 + \cos 2\pi x \cos 2\pi y + \sin 2\pi x \sin 2\pi y$. Take $h(x) = 1$, define $\mathcal{H} = \{f : f \in \mathcal{P}[0,1], \int_0^2 (L_3 f)^2 dx < \infty\}$, and consider $\mathcal{H}_L = \mathcal{H} \ominus \mathcal{N}_L$. To the IP $(f,g) = \int_0^1 (L_3 f)(L_3 g) dx$ in $\mathcal{H}_L$ corresponds the RK

$$R_3(x,y) = \sum_{\mu=2}^{\infty} \frac{2\cos 2\pi\mu(x-y)}{(2\pi)^6\mu^2(\mu^2-1)^2}.$$

Compare $\int_0^1 (L_3 f)^2 dx = (2\pi)^6 \sum_{\mu=2}^{\infty} (a_\mu^2 + b_\mu^2)\mu^2(\mu^2-1)^2$ with $\int_0^1 (f^{(3)})^2 dx = (1/2)(2\pi)^6 \sum_{\mu=1}^{\infty} (a_\mu^2 + b_\mu^2)\mu^6$, in $\mathcal{H}_L$.

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Exponential Splines

Consider $L = D(D-\theta)$, which has a null space $\mathcal{N}_L = \text{span}\{1, e^{\theta x}\}$.

Write $\phi_1(x) = 1$ and $\phi_2(x) = (e^{\theta x} - 1)/\theta$, and consider the transform $\tilde{x} = \phi_2(x)$. It can be shown that $dx/d\tilde{x} = e^{-\theta x}$ and that $d^2x/d\tilde{x}^2 = -\theta e^{-2\theta x}$. It follows that

$$\frac{d^2 f}{d\tilde{x}^2} = \frac{d^2 f}{dx^2}\left(\frac{dx}{d\tilde{x}}\right)^2 + \frac{df}{dx}\frac{d^2 x}{d\tilde{x}^2} = e^{-2\theta x} D_x(D_x - \theta)f,$$

hence $\int_0^1 (d^2 f/d\tilde{x}^2)^2 d\tilde{x} = \int_0^1 \{(Lf)(x)\}^2 e^{-\theta x} dx$. It is seen that an L-spline with $L = D(D-\theta)$ and $h(x) = e^{-\theta x}$ is a cubic spline in $\tilde{x}$.

Exponential splines with $\theta > 0$ can be used to model growth curves. The parameter θ is an extra smoothing parameter. Cubic splines correspond to $\theta = 0$.

Slide 8

Thin-Plate Splines

A thin-plate spline is the minimizer of

$$\frac{1}{n}\sum_{i=1}^{n}(Y_i - f(x_i))^2 + \lambda J_m^d(f)$$

for $x_i \in (-\infty, \infty)^d$, where $J_m^d(f)$ is given by

$$\sum_{\alpha_1+\cdots+\alpha_d=m} \frac{m!}{\alpha_1!\cdots\alpha_d!} \int\cdots\int \left(\frac{\partial^m f}{\partial x_{\langle 1\rangle}^{\alpha_1}\cdots\partial x_{\langle d\rangle}^{\alpha_d}}\right)^2 dx_{\langle 1\rangle}\cdots dx_{\langle d\rangle},$$

for $2m > d$. The null space $\mathcal{N}_J$ of $J_m^d(f)$ consists of polynomials of up to $(m-1)$ total order, of dimension $M = \binom{d+m-1}{d}$.

The functional $J_m^d(f)$ is invariant under shift and rotation of the coordinates, so thin-plate splines are appropriate for modeling geographic or spatial effects.

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Thin-Plate Splines

Let ψ_ν be a set of polynomials that span $\mathcal{N}_J$. Define an IP

$$(f,g)_0 = \sum_{i=1}^N p_i f(u_i) g(u_i),$$

where $u_i \in (-\infty,\infty)^d$, $p_i > 0$, $\sum_{i=1}^N p_i = 1$ are specified such that the Gram matrix with the (ν,μ)th entry $(\psi_\nu,\psi_\mu)_0$ is nonsingular.

Let ϕ_ν, $\nu = 1,\ldots,M$, be an orthonormal basis with $\phi_1(x) = 1$ and $(\phi_\nu,\phi_\mu)_0 = \delta_{\nu,\mu}$; $\sum_{\nu=1}^M \phi_\nu(x)\phi_\nu(y)$ is the RK in $\mathcal{N}_J$. In the space $\mathcal{H}_J = \{f : J_m^d(f) < \infty\} \ominus \mathcal{N}_J$ with $J_m^d(f)$ as the square norm, the RK is given by

$$R_J(x,y) = (I - P_{(x)})(I - P_{(y)})E(|x-y|),$$

where $(Pf)(x) = \sum_{\nu=1}^M (f,\phi_\nu)_0 \phi_\nu(x)$ is the projection operator onto $\mathcal{N}_J$ and $E(x) = \theta_{m,d}\, x^{2m-d} (\log x)^{I_{[d \text{ even}]}}$ for some constants $\theta_{m,d}$.

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Thin-Plate Splines

In the above construction, a onw-way ANOVA decomposition is built in with $Af = \sum_{i=1}^N p_i f(u_i)$, with $\mathrm{span}\{\phi_\nu, \nu = 2,\ldots,M\}$ containing the parametric "contrast" and $\mathcal{H}_J$ containing the nonparametric "contrast".

Thin-plate marginals can be used to construct tensor product RKHS, and the resulting PLS estimates are known as the *tensor product thin-plate splines.*

Thin-plate marginals with $d > 1$ are mathematically multivariate but conceptually univariate. For $d = 1$, the thin-plate splines reduce to polynomial splines.