Shape Restricted Splines via Constrained Optimization: Computation and Statistical Analysis

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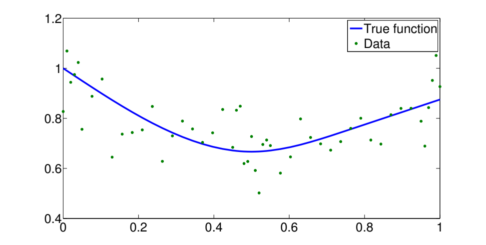
Outline

Shape Constrained Curve-fitting/Estimation

Motivation

1. Various static or dynamic models of biologic, engineering and economic systems contain shape constrained functions
2. Example: convex shape constraint



Applications

- Biology: dose response, drug combination, and genetic networks
- Engineering: path planning, lifetime estimation in reliability engr.
- Statistics: isotonic regression, log-concave density estimation

Focused Topics

Topic I: Computation of shape constrained smoothing splines

1. Formulated as a constrained optimal control or constrained optimization problem with nonsmooth features
2. Efficient numerical schemes

Topic II: Statistical analysis of shape constrained estimators

1. Convergence of an estimator to the true function: consistency and convergence rate
2. Optimal rate estimation and minimax optimal estimation

T. Robertson, F.T. Wright, and R.L. Dykstra. *Order Restricted Statistical Inference*. John Wiley & Sons Ltd., 1988.

Smoothing Splines

Smoothing spline model: unconstrained case

1. Classical smoothing splines (Wahba): $\min_{f \in \mathcal{S}} J(f)$, where $f : [0,1] \to \mathbb{R}$, $(t_i, y_i)_{i=1}^n$ are samples, and

$$J(f) := \frac{1}{n} \sum_{i=1}^{n} \Big(f(t_i) - y_i \Big)^2 + \lambda \int_0^1 \Big(f^{(m)}(t) \Big)^2 dt$$

2. Control theoretical splines (Egerstedt and Martin)

$$\min \frac{1}{n} \sum_{i=1}^{n} \Big(f(t_i) - y_i \Big)^2 + \lambda \int_0^1 u^2(t) dt$$

where

$$\dot{x}(t) = Ax(t) + bu(t), \quad f(t) = c^T x(t), \quad A \in \mathbb{R}^{\ell \times \ell}, \quad b, c \in \mathbb{R}^{\ell}.$$

Example: when $m = 2$, $A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$, $b = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $c = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, and $u(t) = f''(t)$.

Shape Constrained Smoothing Splines

Example: convex smoothing spline

- $\min J(f) := \frac{1}{n}\sum_{i=1}^{n}\big(f(t_i)-y_i\big)^2+\lambda\int_0^1\big(f^{(2)}(t)\big)^2dt,\quad f^{(2)}\geq 0\ a.e.\ [0,1]$
- equivalently, $\min J(f) := \frac{1}{n}\sum_{i=1}^{n}\big(f(t_i)-y_i\big)^2+\lambda\int_0^1 u^2(t)dt$ subject to

$$\dot{x}(t)=Ax(t)+bu(t),\quad f(t)=c^Tx(t),\quad u(t)\in\Omega:=\mathbb{R}_+\ a.e.\ [0,1]$$

Formulation of shape constrained smoothing spline

Given a (constrained) linear control system $\Sigma(A,B,C,\Omega)$ on $\mathbb{R}^\ell$:

$$\dot{x}=Ax+Bu,\qquad u\in\mathcal{W}:=\{u\in L_2([0,1];\mathbb{R}^m)\,|\,u(t)\in\Omega\ a.e.\},$$

where $A\in\mathbb{R}^{\ell\times\ell}$, $B\in\mathbb{R}^{\ell\times m}$, $C\in\mathbb{R}^{p\times\ell}$, $\Omega\subseteq\mathbb{R}^m$ is closed and convex. Given $\{(t_i,y_i)\}_{i=1}^n$ and weights $w_i>0$ with $\sum_{i=1}^n w_i=1$, define the cost functional

$$J(u,x_0)\ :=\ \sum_{i=1}^{n}w_i\big\|y_i-Cx(t_i;u,x_0)\big\|_2^2+\lambda\int_0^1\|u(t)\|_2^2dt$$

A shape constrained smoothing spline $\widehat{f}$ is determined by an optimal solution of $\inf J(u,x_0)$ subject to $\Sigma(A,B,C,\Omega)$, i.e., $\widehat{f}(t)=Cx(t;u^*,x_0^*)$.

Optimality Conditions

Existence and uniqueness of optimal solution

Suppose

$$\mathbf{H.1}: \ \text{rank} \begin{pmatrix} Ce^{At_1} \\ Ce^{At_2} \\ \vdots \\ Ce^{At_n} \end{pmatrix} = \ell.$$

Then there exists a unique optimal solution $(u^*, x_0^*) \in \mathcal{W} \times \mathbb{R}^\ell$ for any (t_i, y_i), (w_i), and $\lambda > 0$.

Optimality conditions in term of VI

$$\begin{aligned} u^*(t) &= \Pi_\Omega\Big(-\lambda^{-1}\sum_{i=1}^n w_i P_i^T(t)\big(\widehat{f}(t_i) - y_i\big)\Big), \quad \text{and} \\ 0 &= \sum_{i=1}^n w_i\big(Ce^{A_i t_i}\big)^T\big(\widehat{f}(t_i) - y_i\big), \end{aligned}$$

where $\widehat{f}(t_i) = Cx(t_i; u^*(t_i), x_0^*)$, and $P_i(t) := Ce^{A(t_i - t)}B \cdot \mathbf{I}_{[0,t_i]}$.

More on Optimality Conditions

Facts

1. On each $[t_k, t_{k+1})$, $u^*(t)$ depends on $\widehat{f}(t_i)$ with $t_i < t_k$ only.
2. The optimal initial condition x_0^* completely determines u^* and $\widehat{f}$ on $[0,1]$ (may write $\widehat{f}$ as $\widehat{f}(t, x_0^*)$)
3. Given (t_i, y_i) and (w_i) and λ, define $H_{y,n} : \mathbb{R}^\ell \to \mathbb{R}^\ell$

$$H_{y,n}(z) := \sum_{i=1}^{n} w_i \big(Ce^{A_i t_i}\big)^T \Big(\widehat{f}(t_i, z) - y_i\Big)$$

   Then the equation $H_{y,n}(z) = 0$ has a unique solution (under **H.1**), which is the optimal initial condition x_0^*.

Nonsmoothness of $\widehat{f}(t, \cdot)$ and $H_{y,n}$

1. If Π_Ω is directionally differentiable on $\mathbb{R}^m$, then $\widehat{f}(t, z)$ is B-differentiable in z for any fixed $t \in [0,1]$;
2. If Π_Ω is semismooth on $\mathbb{R}^m$, then $\widehat{f}(t, z)$ is semismooth in z for any fixed $t \in [0,1]$.

Boundedness of Level Sets

Level set of $H_{y,n}$

Given $z_* \in \mathbb{R}^\ell$, define $S_{z_*} := \big\{ z \in \mathbb{R}^\ell \,|\, \|H_{y,n}(z)\| \le \|H_{y,n}(z_*)\| \big\}$

Proposition (Boundedness of level sets)

Let $\Omega \subseteq \mathbb{R}^m$ be closed and convex. For any given $(t_i, y_i), (w_i), \lambda > 0$ and z_* such that **H.1** holds, the level set S_{z_*} is bounded.

Sketch of the proof

Suppose not. Then there exists (z_k) in S_{z_*} with $\|z_k\| \to \infty$ and $z_k/\|z_k\| \to v_* \neq 0$. It can be shown

$$\lim_{k\to\infty} \frac{H_{y,n}(z_k)}{\|z_k\|} = \widetilde{H}_{\widetilde{y},n}(v_*)\big|_{\widetilde{y}=0},$$

where $\widetilde{H}_{\widetilde{y},n}(z) = \sum_{i=1}^n w_i (Ce^{A_i t_i})^T \big(\widetilde{f}(t_i, z) - \widetilde{y}_i\big)$, $\widetilde{f}$ is obtained from the linear control system $\Sigma(A, B, C, \Omega^\infty)$, and $\widetilde{y}_i = 0, \forall i$. Since $\widetilde{H}_{0,n}(z) = 0$ has a unique solution $z = 0$, $\widetilde{H}_{0,n}(v_*) \neq 0$ and $\|H_{y,n}(z_k)\| \to \infty$, contradiction.

Solving $H_{y,n}(z) = 0$ for Polyhedral Ω (I)

Notation

- Define $F(z) := B \circ \Pi_\Omega \circ B^T$
- For each $k = 1, 2, \ldots, n-1$, let

$$v_k(z) := \frac{1}{\lambda} \sum_{i=1}^{k} w_i \big(Ce^{A_i t}\big)^T \Big(\widehat{f}(t_i, z) - y_i\Big), \quad q(t, v) := e^{-A^T t} v$$

Then $Bu^*(t, z) = F(q(t, v_k(z)))$ for all $t \in [t_k, t_{k+1})$.

Non-degenerate case

1. $F : \mathbb{R}^\ell \to \mathbb{R}^\ell$ is continuous and piecewise affine, and admits a polyhedral subdivision Ξ.
2. For any v and k, $q(t, v)$ has finitely many switchings on Ξ in $[t_k, t_{k+1}]$.
3. $q(t, v)$ is called non-degenerate on $[t_k, t_{k+1}]$ if it is in the interior of a polyhedron of Ξ between any consecutive switching times; otherwise, $q(t, v)$ is called degenerate.

Solving $H_{y,n}(z) = 0$ for Polyhedral Ω (II)

More assumptions and notation

- Let $\rho_1 > 0$ and $\rho_2 > 0$ be such that $\|Ce^{A(t-s)}\|_\infty \leq \rho_1, \forall\, t, s \in [0,1]$ and $\max_i \|E_i\|_\infty \leq \rho_2$, where each matrix E_i corresponds to an affine piece of F.
- Assumption **H.2**: there exist $\rho_t > 0$ and $\mu \geq \nu > 0$ such that for all n,

$$\max_{0 \leq i \leq n-1} |t_{i+1} - t_i| \leq \frac{\rho_t}{n}, \qquad \frac{\nu}{n} \leq w_i \leq \frac{\mu}{n}, \quad \forall\, i.$$

Theorem (Non-degenerate case)

Let Ω be a polyhedron in $\mathbb{R}^m$. Assume that **H.1** – **H.2** hold and $\lambda \geq \mu^2 \rho_1^2 \rho_2 \rho_t / (4\nu)$. Suppose that $q(t, v_k(z))$ is non-degenerate on $[t_k, t_{k+1}]$ for each $k = 1, 2 \ldots, n-1$. Then there exists a unique direction vector $d \in \mathbb{R}^\ell$ such that

$$H_{y,n}(z) + H'_{y,n}(z; d) = 0.$$

Solving $H_{y,n}(z) = 0$ for Polyhedral Ω (III)

Proposition (Degenerate case)

Assume additionally that (C, A) is an observable pair. If $q(t, v_k(z))$ is degenerate on $[t_k, t_{k+1}]$ for some $k \in \{1, \ldots, n-1\}$, then for any $\varepsilon > 0$, there exists $d \in \mathbb{R}^\ell$ with $0 < \|d\| \leq \varepsilon$ such that $q(t, v_k(z+d))$ is non-degenerate on $[t_k, t_{k+1}]$ for each $k = 1, \ldots, n-1$.

Modified Nonsmooth Newton's Method w. Line Search

- Apply the modified nonsmooth Newton's method with line search based on (Pang, 1990) to solve $H_{y,n}(z) = 0$
- Numerical convergence is proved under suitable conditions

J.-S. Pang. Newton's method for B-differentiable equations. *Mathematics of Operations Research*, Vol. 15, pp. 311–341, 1990.

Numerical Results: Example I

Consider $y_i - f(t_i) \sim \mathcal{N}(0, \sigma^2)$

Example 1: Convex constraint w. unevenly spaced design pts

$$f(t) = \begin{cases} \frac{4}{3}t^3 - t + 1 & \text{if } t \in [0, \frac{1}{2}) \\ -\frac{8}{3}t^3 + 6t^2 - 4t + \frac{3}{2} & \text{if } t \in [\frac{1}{2}, \frac{3}{4}) \\ \frac{1}{2}t + \frac{3}{8} & \text{if } t \in [\frac{3}{4}, 1] \end{cases}$$

$$u(t) = f''(t) = \begin{cases} 8t & \text{if } t \in [0, \frac{1}{2}) \\ 12 - 16t & \text{if } t \in [\frac{1}{2}, \frac{3}{4}) \in \Omega := [0, \infty), \\ 0 & \text{if } t \in [\frac{3}{4}, 1] \end{cases}$$

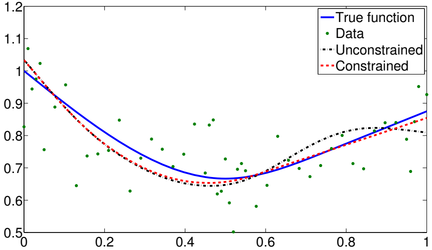
$$z^0 = (2, 3)^T, \qquad \sigma = 0.1, \qquad \frac{\sigma}{|f_{\max} - f_{\min}|} = 30\%, \qquad \lambda = 10^{-4},$$

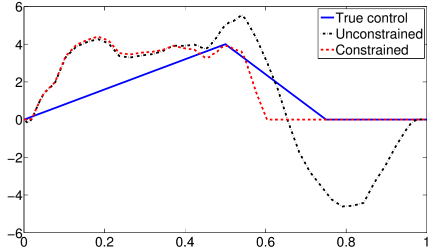
Design points (t_i):

$$\Big\{0, \frac{1}{2n}, \ldots, \frac{1}{20}, \frac{1}{20} + \frac{4}{3n}, \ldots, \frac{9}{20}, \frac{9}{20} + \frac{1}{2n}, \ldots, \frac{11}{20}, \frac{11}{20} + \frac{4}{3n}, \ldots, \frac{19}{20}, \frac{19}{20} + \frac{1}{2n}, \ldots, 1$$

$$x_0 = (1, -1)^T, \qquad A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 1 \end{bmatrix}^T, \qquad C = \begin{bmatrix} 1 & 0 \end{bmatrix}$$

Numerical Results: Example I with $n = 50$





Numerical Results: Example II

Example 2: General dynamics and constraint with unevenly spaced design points $u(t) \in \Omega := [8, \infty)$

$$f(t) = \begin{cases} 11.60967t(e^{-t} + e^{-2t}) - 27.21935e^{-t} + 25.21945e^{-2t} + 2 & \text{if } t \in [0, \frac{1}{4}) \\ -6.23368e^{-t} + 3.25670e^{-2t} + 3 & \text{if } t \in [\frac{1}{4}, \frac{1}{2}) \\ -11.60967t(e^{-t} + e^{-2t}) + 18.22245e^{-t} - 21.69226e^{-2t} + 3 & \text{if } t \in [\frac{1}{2}, \frac{3}{4}) \\ -3.34450e^{-t} + 1.30615e^{-2t} + 2 & \text{if } t \in [\frac{3}{4}, 1] \end{cases}$$

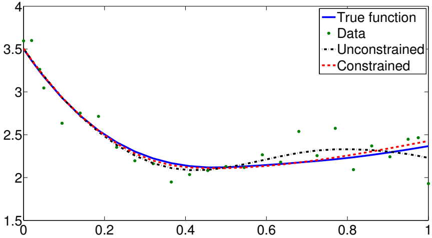
$$u(t) = f''(t) + 3f'(t) + 2f(t) = \begin{cases} 23.21935(e^{-t} - e^{-2t}) + 8 & \text{if } t \in [0, \frac{1}{4}) \\ 12 & \text{if } t \in [\frac{1}{4}, \frac{1}{2}) \\ -38.28223e^{-t} + 63.11673e^{-2t} + 6 & \text{if } t \in [\frac{1}{2}, \frac{3}{4}) \\ 8 & \text{if } t \in [\frac{3}{4}, 1] \end{cases}$$

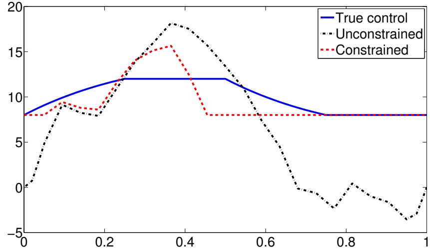
$$z^0 = (0, 1/2)^T, \qquad \sigma = 0.2, \qquad \frac{\sigma}{|f_{\max} - f_{\min}|} = 14.5\%, \qquad \lambda = 10^{-4},$$

$$\text{Design points } (t_i) = \left\{0, \frac{1}{2n}, \frac{2}{2n}, \ldots, \frac{1}{20}, \frac{1}{20} + \frac{9}{8n}, \ldots, \frac{19}{20}, \frac{19}{20} + \frac{1}{2n}, \ldots, 1\right\},$$

$$x_0 = (7/2, -7)^T, \qquad A = \begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 1 \end{bmatrix}^T, \qquad C = \begin{bmatrix} 1 & 0 \end{bmatrix}$$

Numerical Results: Example II with $n = 25$





Numerical Performance

Constrained vs. unconstrained smoothing splines

Shape constrained smoothing splines outperform their unconstrained counterparts

		$\|f - \widehat{f}\|_{L_2}$		$\|f - \widehat{f}\|_{L_\infty}$		$\|x(0) - \widehat{x}_0\|_2$	
		const.	unconst.	const.	unconst.	const.	unconst.
I	$n = 25$	0.00696	0.00723	0.06809	0.07216	0.25985	0.30825
	$n = 50$	0.00351	0.00362	0.04971	0.05218	0.19141	0.22549
	$n = 100$	0.00177	0.00180	0.03487	0.03588	0.14021	0.15958
II	$n = 25$	0.01302	0.01492	0.12639	0.15609	0.76778	1.45583
	$n = 50$	0.00704	0.00791	0.09998	0.12474	0.70899	1.41832
	$n = 100$	0.00387	0.00436	0.08048	0.10519	0.75410	1.54277

Numerical convergence of modified Newton's method

- Depends heavily on examples but appears to be superlinear
- Typically ranges between 10 and 30 iterations
- Iterations for convergence increase slightly with sample size n

Shape Constrained Regression

Regression model

$$y_i = f(t_i) + \varepsilon_i, \quad i = 1, 2, \ldots, n,$$

where $f : [0,1] \to \mathbb{R}$ is the underlying true function subject to the constraint $f \in \mathcal{C}$, t_i are design points, y_i are samples, and ε_i are i.i.d. random variables with $\varepsilon_i \sim N(0, \sigma^2)$.

Constraints

1. Shape constraint: $f \in \mathcal{S}$, where for some $m \in \mathbb{N}$,

   $$\mathcal{S} := \left\{ f : [0,1] \to \mathbb{R} \,|\, (f^{(m-1)}(t_1) - f^{(m-1)}(t_2)) \cdot (t_1 - t_2) \geq 0, \forall\, t_1, t_2 \in [0,1] \right\}.$$

2. Smoothness constraint: f is in the Hölder class $H(r, L)$ with $r \in (m-1, m]$, $L > 0$, i.e., the family of $\ell := (m-1)$ times continuously differentiable functions whose ℓ-th derivative is uniformly Hölder continuous with exponent $\gamma := r - \ell \in (0,1]$, i.e.,

   $$|f^{(\ell)}(t_1) - f^{(\ell)}(t_2)| \leq L \cdot |t_1 - t_2|^{\gamma}, \quad \forall\, t_1, t_2 \in [0,1].$$

Minimax Optimal Estimation

Key issues on a given function class $\mathcal{C}$

- What is the "best rate" of convergence of estimators uniformly on $\mathcal{C}$?
- How can one construct an estimator that achieves the "best rate" of convergence on $\mathcal{C}$? (minimax upper bound)
- Is the "best rate" of convergence strict on $\mathcal{C}$ for any permissible estimator? (minimax lower bound)

Optimal rate of convergence on $H(r, L)$ in the sup-norm

$$\inf_{\widehat{f}} \sup_{f \in H(r,L)} \mathbb{E}\left(\|\widehat{f} - f\|_\infty\right) \asymp L^{\frac{1}{2r+1}} \sigma^{\frac{2r}{2r+1}} \left(\frac{\log n}{n}\right)^{\frac{r}{2r+1}},$$

where $\widehat{f}$: estimate of a true function f, and $a \asymp b$: a/b is bounded by two positive constants from below and above for all n sufficiently large.

Motivating question

For a given $m \in \mathbb{N}$, what are the minimax upper and lower bounds over $\mathcal{S}_H(r, L) := H(r, L) \cap \mathcal{S}$ as $n \to \infty$ (when the sup-norm is used)?

Constrained B-spline Estimator (I)

Constrained B-spline estimator

$$\widehat{f}(t) = \sum_{k=1}^{K_n+m-1} \widehat{b}_k B_k(t)$$

where $t_i = i/n$, B_k are B-splines of $(m-1)$th degree with knots $\kappa_i = i/K_n$, and the optimal spline coefficient $\widehat{b} = \{\widehat{b}_k, k = 1, \ldots, K_n + m - 1\}$ is

$$\widehat{b} = \arg \min_{D_m b \geq 0} \sum_{i=1}^{n} \left[y_i - \sum_{k=1}^{K_n+m-1} b_k B_k(t_i) \right]^2$$

Here $D_m \in \mathbb{R}^{(K_n-1)\times(K_n+m-1)}$ corresponds to the m-th difference operator.

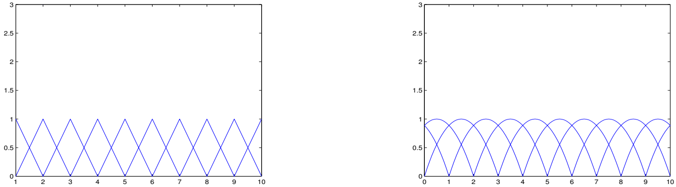


Figure: Left: B-splines of degree 1; Right: B-splines of degree 2

Constrained B-spline Estimator (II)

Quadratic program for optimal spline coefficients

$$\widehat{b} = \arg \min_{D_m b \geq 0} \frac{1}{2} b^T \Lambda_{K_n} b - b^T \bar{y},$$

where

$$\Lambda_{K_n} = \frac{1}{\beta_n} X^T X, \quad \bar{y} = \frac{1}{\beta_n} X^T y, \quad y = (y_1, \ldots, y_n)^T.$$

Here $\beta_n := \sum_{i=1}^n B_k^2(t_i)$ for any $k = m, \ldots, K_n$, and $X = \left[B_k(t_j)\right]_{j,k}$.

Key questions for statistical asymptotic analysis

Since the number of knots K_n depends on n and $K_n \to \infty$ as $n \to \infty$, it is desired to know how to choose K_n for favorable asymptotic properties:

- uniform convergence on $[0, 1]$, including consistency on the boundary (and in the interior)
- optimal convergence rate

Piecewise Linear Formulation of $\widehat{b}$

Properties of $\widehat{b}$ for fixed K_n

1. Optimality condition:

$$\Lambda_{K_n}\widehat{b} - \bar{y} - D_m^T\lambda = 0, \qquad 0 \le \lambda \perp D_m\widehat{b} \ge 0.$$

2. $\widehat{b} : \mathbb{R}^{K_n+m-1} \to \mathbb{R}^{K_n+m-1}$ is a continuous, piecewise linear function of $\bar{y}$ with 2^{K_n-1} linear selection functions (may write $\widehat{b}$ as $\widehat{b}^{(K_n)}$)
3. $\widehat{b}$ is Lipschitz in $\bar{y}$, and the Lipschitz constant may depend on K_n and a norm (e.g., the ℓ_∞-norm).

Formulation of linear pieces of $\widehat{b}$

1. For each $\bar{y}$, define the index set

$$\alpha := \{i \,|\, (D_m\widehat{b}(\bar{y}))_i = 0\} \subseteq \{1, \ldots, K_n - 1\}$$

2. For each α, a row linearly independent matrix F_α exists such that

$$\widehat{b}(\bar{y}) = F_\alpha^T (F_\alpha \Lambda_{K_n} F_\alpha^T)^{-1} F_\alpha \bar{y}$$

Uniform Lipschitz Property of $\widehat{b}$

Theorem (Uniform Lipschitz property)

The family of piecewise linear functions $\{\widehat{b}^{(K_n)} \mid K_n \in \mathbb{N}\}$ is uniformly Lipschitz in the ℓ_∞-norm, i.e., there exists a constant $L_m > 0$ s.t.

$$\sup_{K_n \in \mathbb{N}} \sup_{u \neq v \in \mathbb{R}^{K_n+m-1}} \frac{\left\|\widehat{b}^{(K_n)}(u) - \widehat{b}^{(K_n)}(v)\right\|_\infty}{\|u-v\|_\infty} \leq L_m$$

Sufficient condition for uniform Lipschitz property

In light of the piecewise linear formulation of $\widehat{b}^{(K_n)}$, it suffices to show

$$\sup_{K_n,\alpha} \|F_\alpha^T (F_\alpha \Lambda_{K_n} F_\alpha^T)^{-1} F_\alpha\|_\infty < \infty$$

T. Lebair and J. Shen. Uniform Lipschitz property of constrained B-splines subject to general shape constraints. 2014.

Proof of Uniform Lipschitz Property

Sketch of the proof

1. Cornerstone result

Theorem (de Boor's Conjecture (Shadrin, 2001))

Let $\mathcal{T} = (t_k)_{k=0}^n$ be a knot sequence on $[a, b]$, let $N_{m,k}^{\mathcal{T},E} := (\widetilde{N}_k)_{k=1}^{n+m-1}$ be B-splines of degree $(m-1)$ defined by $\mathcal{T}$ and some extension E. Let $\widetilde{M}_k := \|\widetilde{N}_k\|_{L_1}^{-1} \cdot \widetilde{N}_k$ for each k, and G be the Grammian matrix given by $G_{ij} = \langle \widetilde{M}_i, \widetilde{N}_j \rangle$. Then $\|G^{-1}\|_\infty$ is bounded independent of a, b, n, and $\mathcal{T}$.

2. Main idea: for any K_n and α, relate $F_\alpha^T (F_\alpha \Lambda_{K_n} F_\alpha^T)^{-1} F_\alpha$ to a suitable Grammian defined by some B-splines with certain knot sequence satisfying the shape constraint, and apply the above theorem to obtain a uniform bound on $\|F_\alpha^T (F_\alpha \Lambda_{K_n} F_\alpha^T)^{-1} F_\alpha\|_\infty$.

A.Y. Shadrin. The L_∞-norm of the L_2-spline projector is bounded independently of the knot sequence: A proof of de Boor's conjecture. *Acta Mathematica*, Vol. 187(1), pp. 59–137, 2001.

Implications of Uniform Lipschitz Property (I)

Uniform convergence and optimal estimation on $\mathcal{S}_H(r, L)$

1. Asymptotic performance in the sup-norm:

$$\mathbb{E}(\|\widehat{f} - f\|_\infty) \quad = \quad O\left(L K_n^{-r} + \sigma \sqrt{\frac{K_n \log n}{n}} \right)$$

2. Optimal rate of convergence in the sup-norm (minimax upper bound): Let $K_n = \left\lceil \left(\frac{L}{\sigma}\right)^{\frac{2}{2r+1}} \left(\frac{n}{\log n}\right)^{\frac{1}{2r+1}} \right\rceil$, then $\exists$ a constant $C > 0$ s.t.

$$\sup_{f \in \mathcal{S}_H(r,L)} \mathbb{E}\left(\|\widehat{f} - f\|_\infty\right) \quad \leq \quad C \cdot L^{\frac{1}{2r+1}} \sigma^{\frac{2r}{2r+1}} \left(\frac{\log n}{n}\right)^{\frac{r}{2r+1}}, \ \forall\, n$$

3. $\widehat{f}$ is consistent on the boundary of $[0, 1]$ as $K_n, n \to \infty$

X. Wang and J. Shen. Uniform convergence and rate adaptive estimation of convex functions via constrained optimization. *SIAM Journal on Control and Optimization*, Vol. 51(4), pp. 2753–2787, 2013.

Implications of Uniform Lipschitz Property (II)

Let $\overline{f}$ be the estimator based on noise free data, i.e.,

$$\overline{f}(t) = \sum_{k=1}^{K_n+m-1} \overline{b}_k B_k(t), \quad \text{where } \overline{b} := \arg \min_{D_m b \geq 0} \frac{1}{2} b^T \Lambda_{K_n} b - b^T \mathbb{E}(\bar{y})$$

Pointwise uniform bound

1. There exist positive constants C_1 and C_2 such that for any $t_0 \in (0, 1)$,

$$\mathbb{E}\big(|\widehat{f}(t_0) - \overline{f}(t_0)|^2\big) \leq C_1 \cdot \sigma^2 \frac{K_n}{n}$$
$$\mathbb{E}\big(|\widehat{f}(t_0) - \overline{f}(t_0)|^4\big) \leq C_2 \cdot \sigma^4 \left(\frac{K_n}{n}\right)^2$$

2. For any $t_0 \in (0, 1)$ and any $m - 1 \leq r' \leq r$,

$$\sup_{f \in \mathcal{S}_H(r,L)} \mathbb{E}\big(|\widehat{f}(t_0) - f(t_0)|^2\big) = O\left(C_1 \cdot \sigma^2 \frac{K_n}{n} + C_1' \frac{L^2}{K_n^{2r'}}\right)$$

Implications of Uniform Lipschitz Property (III)

Adaptive constrained estimation on $\mathcal{S}_H(r, L)$

1. Assume that the Hölder order $r \in [m-1, m]$ is unknown
2. Develop a constrained spline based adaptive estimator that achieves the optimal sup-norm risk:

$$\sup_{r\in[m-1,m]} \sup_{f\in\mathcal{S}_H(r,L)} \mathbb{E}\Big(\|\widehat{f}_{(\hat{r})} - f\|_\infty\Big) \leq \pi_2 \, L^{\frac{1}{2r+1}} \sigma^{\frac{2r}{2r+1}} \Big(\frac{\log n}{n}\Big)^{\frac{r}{2r+1}}.$$

3. Develop an adaptive estimator that achieves the optimal pointwise risk:

$$\sup_{r\in[m-1,m]} \sup_{f\in\mathcal{S}_H(r,L)} \mathbb{E}\Big(|\widetilde{f}(x_0) - f(x_0)|^2\Big) \leq \pi_3 L^{\frac{2}{(2r+1)}} \sigma^{\frac{4r}{(2r+1)}} n^{-\frac{2r}{(2r+1)}}.$$

Minimax Lower Bound

Background

Based on information theoretical results on probability measure distance.

Construction for lower bound

Construct a family of shape constrained functions $f_{j,n}, j = 0, 1, \ldots, M_n$ s.t.

(C1) each $f_{j,n} \in \mathcal{C}_H(r, L)$, $j = 0, 1, \ldots, M_n$;

(C2) once $j \neq k$, $\|f_{j,n} - f_{k,n}\|_\infty \geq 2s_n > 0$, where $s_n \asymp (\log n/n)^{r/(2r+1)}$;

(C3) there exists a fixed constant $c_0 \in (0, 1/8)$ s.t. for all large n,

$$\frac{1}{M_n}\sum_{j=1}^{M_n} K(P_j, P_0) \leq c_0 \log(M_n),$$

where P_j: distribution of $(Y_{j,1}, \ldots, Y_{j,n})$, $Y_{j,i} = f_{j,n}(X_i) + \xi_i$, $i = 1, \ldots, n$ with $X_i = i/n$ and ξ_i: iid r.v., and $K(P, Q)$: Kullback divergence between two probability measures P and Q.

T. Lebair, J. Shen, and X. Wang. Minimax optimal estimation of convex functions in the sup-norm. 2013.

Conclusions

Summary

1. Computation of general shape constrained smoothing splines via a nonsmooth Newton's method
2. Statistical analysis of constrained B-spline estimation: uniform Lipschitz property

Future research

1. Numerical issues: constrained smoothing splines subject to additional constraints
2. Statistical issues: minimax analysis under general constraints
3. Multivariable shape constrained estimation and computation

Thank you!