Adaptive Piecewise Polynomial Estimation via Trend Filtering

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Introduction

- Univariate nonparametric estimation:

$$y_i = f_0(x_i) + \epsilon_i \quad i = 1, \ldots, n$$

  How to estimate f_0?

- Fixed design (x_i are nonrandom),
  i.i.d. noise ϵ_i with $\mathbb{E}(\epsilon_i) = 0, \mathrm{Var}(\epsilon_i) = \sigma^2$
- Linear smoothers & nonlinear smoothers

Linear Smoothers

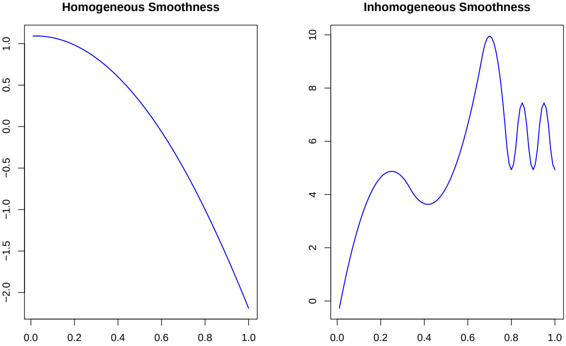
- Many well-known methods are linear smoothers:
  - Regression splines/smoothing splines [De Boor et al., 1978, Wahba, 1990, Green and Silverman, 1993]
  - K nearest neighbor (KNN) smoother[Györfi et al., 2006]
  - Kernel smoothers[Friedman et al., 2001, Loader, 2006]
  - RKHS[Smola and Schölkopf, 1998, Wahba, 1990]
  - Sieves[Shen and Wong, 1994, Wong and Shen, 1995]
- Linear smoothers have fit linear in y,

$$\hat{u} = (\hat{f}(x_1), \hat{f}(x_2), \ldots, \hat{f}(x_n)) = S_\lambda y$$

  where S_λ is smoothing matrix, λ is the smoothness index, e.g. k in KNN or bandwidth h in kernel smoothing
- **Nice properties**: Closed form $df = \mathrm{tr}(S_\lambda)$, efficient CV

Linear Smoothers

- **Defect:** linear smoothers are not **locally adaptive**, i.e. they cannot represent heterogeneous signals well



- Left panel: **homogeneous** smoothness; Right panel: **heterogeneous** smoothness

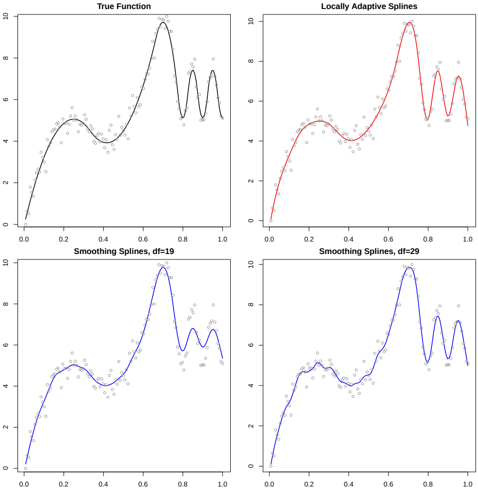
Smoothing Spline

$$\underset{f \in \mathcal{W}_{(k+1)/2}}{\text{minimize}} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \int_0^1 (f^{((k+1)/2)}(t))^2 dt$$

where $\mathcal{W}_{(k+1)/2}$ is the Sobolev space, λ controls the degrees of freedom

- Most commonly used: cubic smoothing spline ($k = 3$)
- $\mathcal{W}_2$ is infinite-dimensional, but solution is natural cubic spline (finite-dimensional)

Smoothing Spline



- Small df: **over-smooth**; large df: **under-smooth**

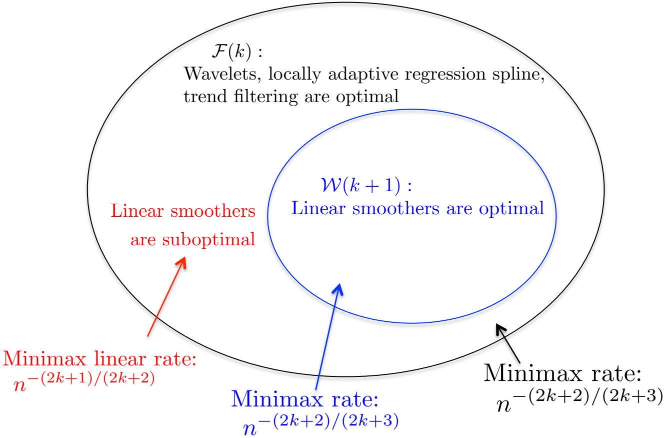
Minimax Convergence Rate

- In nonparametric statistics, we usually consider the **minimax** convergence rate:

$$\min_{\hat{f}} \max_{f_0 \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (f_0(x_i) - \hat{f}(x_i))^2$$

  where $\mathcal{F}$ is some smooth function class, e.g. Sobolev $\mathcal{W}(k)$, bounded TV $\mathcal{F}(k)$, Hölder $H(k)$, etc.
- Minimax rate is the best achievable rate over $\mathcal{F}$
- Estimators that achieve minimax rate are called **(minimax) optimal**

Minimax Convergence Rate

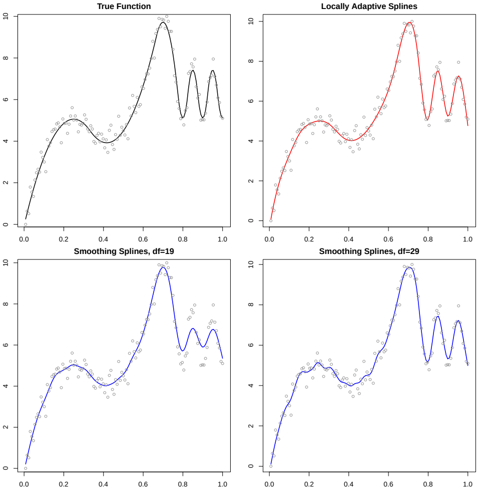


- Linear smoothers are **sub-optimal** in bounded TV class $\mathcal{F}(k)$! (e.g. for $k=0$, linear $n^{-1/2}$ v.s. nonlinear $n^{-2/3}$)

Nonlinear Smoothers

- Three methods:
  - Wavelet smoother[Johnstone, 2011, Mallat, 2008, Donoho and Johnstone, 1994]
  - Locally adaptive spline[Mammen et al., 1997]
  - Trend filtering[Kim et al., 2009]
- In 90's, wavelet smoother and locally adaptive spline were proved to be minimax optimal ($n^{-(2k+2)/(2k+3)}$) over bounded TV class $\mathcal{F}(k)$
- 20 years later, this paper proves trend filtering is also minimax-optimal

Nonlinear Smoothers



- Nonlinear smoothers are **locally adaptive**!

Nonlinear Smoothers

Why another nonlinear smoother???

- Wavelet method has stringent conditions: inputs $(x_1, \ldots, x_n)$ are evenly spaced, sample size n power of 2, boundary issues, etc.
- Locally adaptive spline is hard to compute for order $k \geq 2$, also hard to choose the location of the knots
- Trend filtering is **minimax optimal, locally adaptive**, and **computationally efficient**!

Trend Filtering

$$\underset{u \in \mathbb{R}^n}{\text{minimize}} \; \frac{1}{2}\|y - u\|_2^2 + \lambda \|D^{(k+1)} u\|_1$$

where $D^{(k+1)}$ is the $(k+1)$-st discrete difference operator, inputs $(x_1, \ldots, x_n)$ assumed to be evenly-spaced (**for simplicity, not must**).

- For $k = 0$,

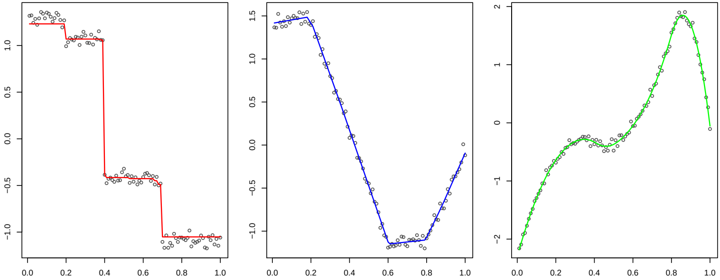
$$D^{(1)} = \begin{bmatrix} -1 & 1 & 0 & \ldots & 0 & 0 \\ 0 & -1 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & -1 & 1 \end{bmatrix} \in \mathbb{R}^{(n-1)\times n}$$

- This recovers the 1d TV denoising[Rudin et al., 1992], fused lasso problem[Tibshirani et al., 2005]

Trend Filtering

- For higher orders, $D^{(k+1)} \equiv D^{(1)} \cdot D^{(k)}$, can be seen as a discrete analogue of $(k+1)$th order **derivative**

Will the solution of TF be piecewise polynomials/splines?



- Need a **continuous representation** of trend filtering!

(Generalized) Lasso Type Problem

- Generalized Lasso problem:

$$\underset{\beta \in \mathbb{R}^n}{\text{minimize}} \frac{1}{2}\|y - X\beta\|_2^2 + \lambda\|D\beta\|_1$$

  thus TF is generalized Lasso with $X = \mathbb{I}_n, D = D^{(k+1)}$.

- Can be recast as an ordinary Lasso problem

$$\hat{\alpha} = \underset{\alpha \in \mathbb{R}^n}{\arg\min} \frac{1}{2}\|y - H\alpha\|_2^2 + \lambda \sum_{j=k+2}^{n} |\alpha_j|$$

  with some sparse design H, and the TF fit is $\hat{u} = H\hat{\alpha}$

Algorithms

1. Lasso solver:

$$\hat{\alpha} = \underset{\alpha \in \mathbb{R}^n}{\arg\min} \frac{1}{2}\|y - H\alpha\|_2^2 + \lambda \sum_{j=k+2}^{n} |\alpha_j|$$

2. Generalized Lasso path algorithm [Harchaoui and Lévy-Leduc, 2010, Tibshirani et al., 2011]:

$$\underset{\beta \in \mathbb{R}^n}{\text{minimize}} \frac{1}{2}\|y - X\beta\|_2^2 + \lambda\|D\beta\|_1$$

3. Primal-dual interior point algorithm[Kim et al., 2009]

Continuous Representation of TF

- Lasso form: $\hat{\alpha} = \arg\min_{\alpha \in \mathbb{R}^n} \frac{1}{2}\|y - H\alpha\|_2^2 + \lambda \sum_{j=k+2}^{n} |\alpha_j|$
- Goal is to find a set of basis functions $(h_1, \ldots, h_n)$ such that $H_{ij} = h_j(x_i)$
- **Falling factorial basis**[Wang et al., 2014]:

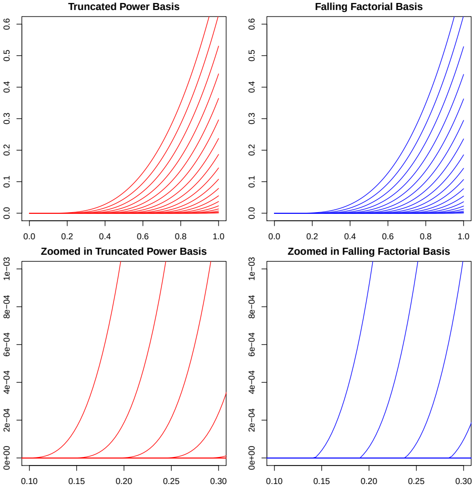
$$h_1(x) = 1, \quad h_2(x) = x, \ldots, h_{k+1}(x) = x^k,$$

$$h_{k+1+j}(x) = \prod_{l=1}^{k}(x - x_{j+l})\mathbb{1}_{[x \geq x_{j+k}]}, \quad \text{for } j = 1, \ldots, n-k-1$$

- Truncated power basis:

$$g_1(x) = 1, \quad g_2(x) = x, \ldots, g_{k+1}(x) = x^k,$$
$$g_{k+1+j}(x) = (x - t_j)^k \mathbb{1}_{[x \geq t_j]}, \quad \text{for } j = 1, \ldots, n-k-1$$

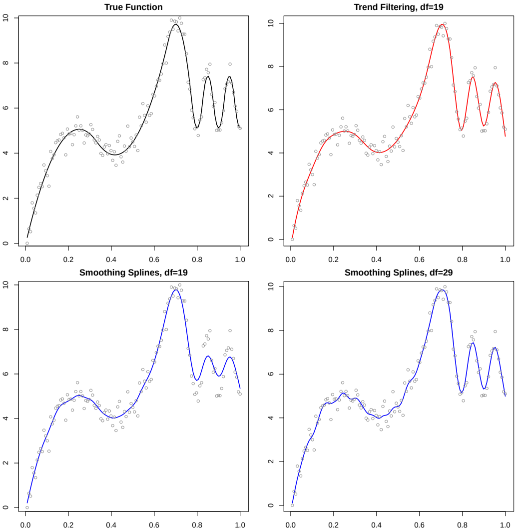
Fall Factorial Basis v.s. Truncated Power Basis



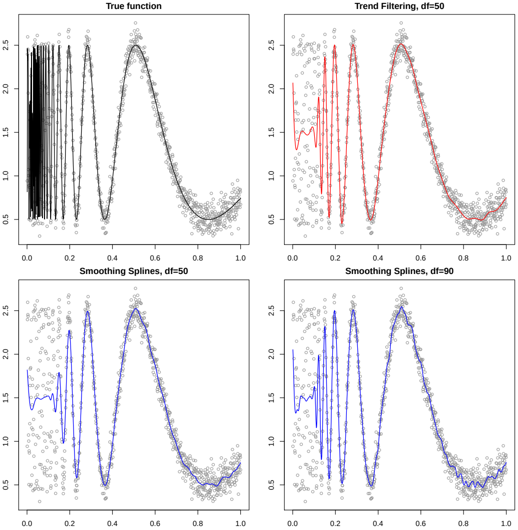
- Conclusion: $k = 0, 1$, TF is constant/linear spline;
  $k \geq 2$, TF is piecewise polynomial

Empirical Comparison with Smoothing Spline

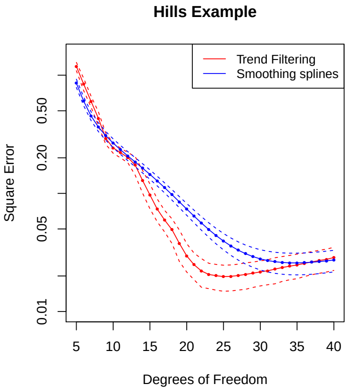
- Heterogeneous "hills" signal

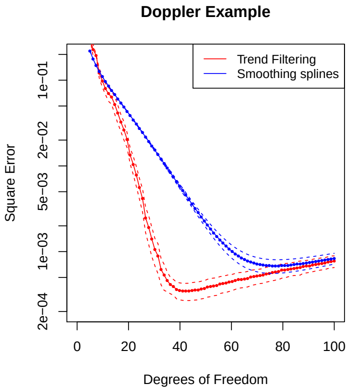


- Heterogeneous Doppler signal



Quantitative Comparison with Smoothing Spline





- In terms of MSE, trend filtering is superior to smoothing spline.

Comparison with Locally Adaptive Spline

$$\underset{f \in \mathcal{G}_K}{\text{minimize}} \frac{1}{2} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \cdot \text{TV}(f^{(k)})$$

where $\mathcal{G}_k$ is the set of splines with knots as a subset of $\{x_1, \ldots, x_n\}$, $TV(\cdot)$ is the total variation penalty

- Equivalent to the following Lasso problem:

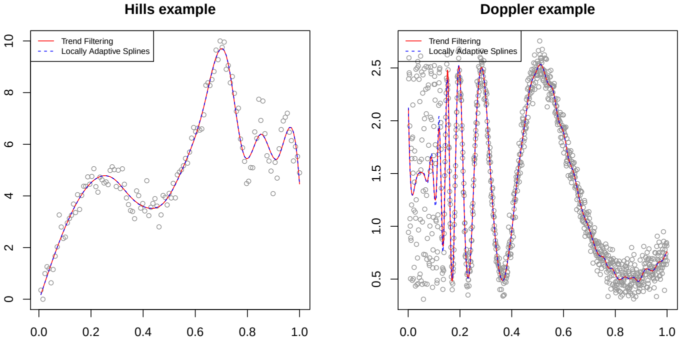
$$\hat{\theta} = \underset{\theta \in \mathbb{R}^n}{\arg\min} \frac{1}{2} \|y - \boldsymbol{G}\theta\|_2^2 + \lambda \sum_{j=k+2}^{n} |\theta_j|$$

- Compare with TF:

$$\hat{\alpha} = \underset{\alpha \in \mathbb{R}^n}{\arg\min} \frac{1}{2} \|y - \boldsymbol{H}\alpha\|_2^2 + \lambda \sum_{j=k+2}^{n} |\alpha_j|$$

Comparison with Locally Adaptive Spline

- For $k = 0, 1$, $G = H$, thus trend filtering and locally adaptive spline give the same fit
- For $k \geq 2$, $G \neq H$, trend filtering and locally adaptive spline give different but extremely similar fit



Real Data Example

Still working on this slide

Convergence Rate of Trend Filtering

Theorem

For a fixed order k and constant $C > 0$, then over the kth order bounded TV class $\mathcal{F}(k, C) \equiv \{f_0 : TV(f_0^{(k)}) \leq C\}$, with tuning parameter chosen as $\lambda \asymp n^{1/(2k+3)}$, the fit of kth order trend filtering $\hat{u}$ satisfies

$$\sup_{f_0 \in \mathcal{F}(k,C)} \mathbb{E}[\frac{1}{n} \sum_{i=1}^{n} (\hat{u}_i - f_0(x_i))^2] \asymp n^{-(2k+2)/(2k+3)}$$

Convergence Rate of Trend Filtering

Idea is simple:

- Trend filtering and locally adaptive spline converge to each other at minimax rate
- Locally adaptive spline converges to the true function at minimax rate[Mammen et al., 1997]
- Hence trend filtering also converges at minimax rate

More Recent Results on Trend Filtering

- [Wang et al., 2016] extends the notion of univariate trend filtering onto trend filtering on graphs
- [Wang et al., 2014] explores in depth the falling factorial basis used by the continuous representation of trend filtering.
- [Sadhanala and Tibshirani, 2017] and [Petersen et al., 2014] both extend trend filtering to high dimensions under the framework of additive model
- [Maidstone et al., 2017] explores linear trend filtering ($k = 1$) with ℓ_0 penalty

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Thank you for listening!

Questions?