Adaptive Piecewise Polynomial Estimation via Trend Filtering

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Overview

1. (The k^{th} Order) Trend Filtering
2. Comparison to smoothing spline
3. Comparison to locally adaptive regression spline
4. Rate of Convergence
5. Extensions

(The k^{th} Order) Trend Filtering

Motivation

l_1 **Trend Filtering (Kim, 2009):**

- An l_1 filtering or smoothing method for trend estimation in time series data.
- Suited to analyze time series with an underlying piecewise linear trend.
- A special type of basis pursuit problem.

Motivation

Prior Works in Nonparametric Regression:

- **Smoothing Splines:** Not locally adaptive.
- **Locally Adaptive Regression Spline:** Computational Expensive ($O(n^3)$)

Setup(Tibshirani, 2014)

- **Usual Setup in Nonparametric Regression :**
  Assume n observations $y_1, \cdots y_n \in R$ and n input points $x_1, x_2, \cdots, x_n \in R$ from the model:

$$y_i = f_0(x_i) + \epsilon_i, \quad i = 1, 2, \cdots, n, \tag{1}$$

  where f_0 is the underlying function and $\epsilon_1, \cdots, \epsilon_n$ are independent.

- **Further Setup Here:**
  Assume the n input points are ordered and evenly spaced over [0,1], i.e., $x_i = i/n$ for $i = 1, \cdots, n$

Definition

The k^{th} order trend filtering estimate $\hat{\beta} = (\hat{f}_0(x_1), \cdots, \hat{f}_0(x_n))$ is defined as the following:

$$\hat{\beta} = \underset{\beta \in R^n}{argmin} \frac{1}{2}\|y - \beta\|_2^2 + \frac{n^k}{k!}\lambda\|D^{(k+1)}\beta\|_1, \quad (2)$$

where $y = (y_1, \cdots, y_n)^T$ and $D^{(k+1)} \in R^{(n-k)\times n}$ is the discrete difference operator of order $k+1$ defined in the next slide.

Notice: Trend filtering estimators are ONLY defined over the discrete set of inputs.

Definition

The discrete difference operator $D^{(k+1)}$ is defined recursively as:

$$D^{(k+1)} = D^{(1)} \cdot D^{(k)} \in R^{(n-k)\times n} \tag{3}$$

where $D^{(1)}$ is defined as:

$$D^{(1)} = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & & & & & \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix} \in R^{(n-k-1)\times(n-k)} \tag{4}$$

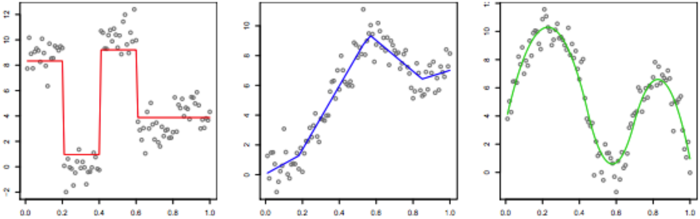
Definition

More discrete difference operators:

$$D^{(2)} = \begin{bmatrix} 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ 0 & 0 & 1 & -2 & \cdots & 0 \\ \vdots & & & & & \end{bmatrix} \tag{5}$$

$$D^{(3)} = \begin{bmatrix} -1 & 3 & -3 & 1 & \cdots & 0 \\ 0 & -1 & 3 & -3 & \cdots & 0 \\ 0 & 0 & -1 & 3 & \cdots & 0 \\ \vdots & & & & & \end{bmatrix} \tag{6}$$

Examples



Linear interpolated trend filtering examples for constant, linear and quadratic orders (k=0,1,2, respectively)

Inference

The inference in continuous domain for trend filtering lies in its equivalence at the input points to the lasso problem:

$$\hat{\alpha} = \underset{\alpha \in R^n}{argmin} \frac{1}{2}\|y - H\alpha\|_2^2 + \lambda \sum_{j=k+2}^{n} |\alpha_j| \tag{7}$$

The solutions satisfy $\hat{\beta} = H\hat{\alpha}$, where $H \in R^{n \times n}$ is a basis matrix, $H_{ij} = h_j(x_i), i, j = 1, \cdots, n$,

$$\begin{aligned} h_j(x) &= \prod_{l=1}^{j-1}(x - x_l), j = 1, \cdots, k+1, \\ h_{k+1+j}(x) &= \prod_{l=1}^{k}(x - x_{j+l}) \cdot 1\{x \geq x_{j+k}\}, j = 1, \cdots, n-k-1. \end{aligned} \tag{8}$$

Properties

- **Recursive Decomposition:** For $k \geq 1$,

$$H^{(k)} = H^{(k-1)} \cdot \begin{bmatrix} I_k & 0 \\ 0 & \frac{k}{n} L_{n-k} \end{bmatrix} \tag{9}$$

  where L_{n-k} denotes the $(n-k) \times (n-k)$ lower triangular matrix of 1s.

- **Inverse Basis:**

$$(H^{(k)})^{-1} = \begin{bmatrix} C \\ \frac{1}{k!} \cdot D^{(k+1)} \end{bmatrix} \tag{10}$$

  It shows that the last n-k-1 rows of $(H^{(k)})^{-1}$ are given exactly by $D^{(k+1)}/k!$

Properties

- **Other Properties:**
  - Efficient Computation – $O(n^{1.5})$
  - Locally Adaptive Polynomial Approximation
  - Minimax Convergence Rate

Comparison to smoothing spline

kth order smoothing spline

The kth (k is an odd number) order smoothing spline estimate is defined as

$$\hat{f} = \underset{f \in \mathcal{W}_{(k+1)/2}}{argmin} \sum_{i=1}^{n} \|y_i - f(x_i)\|_2^2 + \lambda \int_0^1 (f^{(\frac{k+1}{2})}(t))^2 dt, \qquad (11)$$

where $f^{(\frac{k+1}{2})}(t)$ is the derivative of f of order $(k+1)/2$, $\lambda \geq 0$ is a tuning parameter, and the domain of minimization here is Sobolev space $\mathcal{W}_{(k+1)/2} = \{f : [0,1] \rightarrow R :$
f is (k+1)/2 times differentiable, and $\int_0^1 (f^{(\frac{k+1}{2})}(t))^2 dt < \infty\}$

kth order smoothing spline

It can be shown that the infinite-dimensional problem (11) has a unique minimizer[see,e.g.Wahha(1990)] and the minimizer is linear combination of n basis function. Hence to solve problem (11), we can solve for coefficients $\theta \in R^n$ in this basis expansion:

$$\hat{\theta} = \underset{\theta \in R^n}{argmin} \|y - N\theta\|_2^2 + \lambda \theta^T \Omega \theta, \tag{12}$$

If $\eta_1, \cdots, \eta_n$ denotes a collection of basis functions for the set of kth degrees natural splines with knots $x_1, \cdots, x_n$, then

$$N_{ij} = \eta_j(x_i) \text{ and } \Omega_{ij} = \int_0^1 \eta_i^{(\frac{k+1}{2})}(t)\eta_j^{(\frac{k+1}{2})}(t)dt \quad \text{for all } i, j \tag{13}$$

kth order smoothing spline

The solution to problem (11) at given input points $x_1, \cdots, x_n$ and the solution to problem (12) are connected by

$$(\hat{f}(x_1), \cdots, \hat{f}(x_n)) = N\hat{\theta} \qquad (14)$$

More generally,

$$\hat{f}(x) = \sum_{j=1}^{n} \hat{\theta}_j \eta_j(x). \qquad (15)$$

Generalized ridge representation

To compare smoothing spline with trend filtering, we rewrite the smoothing spline fitted values as:

$$\begin{aligned} N\hat{\theta} &= N(N^T + \lambda\Omega)^{-1}N^T y \\ &= N(N^T(I + \lambda N^{-T}\Omega N^{-1})N)^{-1}N^T y \\ &= (I + \lambda K)^{-1} y \end{aligned} \tag{16}$$

where $K = N^{-T}\Omega N^{-1}$. Then $\hat{u} = N\hat{\theta}$ is solution of the minimization problem

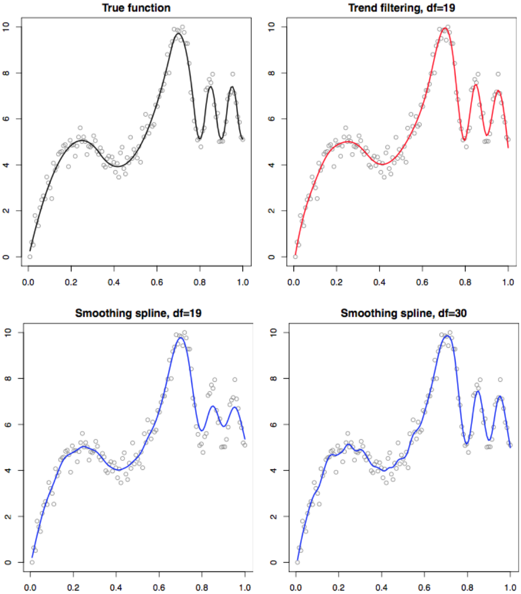
$$\begin{aligned} \hat{u} &= \underset{u \in R^n}{argmin} \|y - u\|_2^2 + \lambda u^T K u \\ &= \underset{u \in R^n}{argmin} \|y - u\|_2^2 + \lambda \|K^{1/2} u\|_2^2 \end{aligned} \tag{17}$$

Empirical comparison

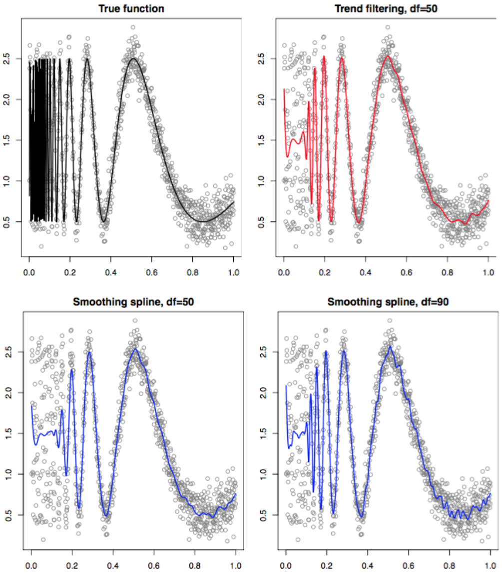
The form of problem (17) is similar to trend filtering and there are two differences:

- $K^{1/2}u$ is similar to $D^{(k)}u$ but strictly different. For example, for $k = 3$ and input points $x_i = \frac{i}{n}$, it can be shown that $K^{1/2}u = C^{-1/2}D^{(2)}u$ where $D^{(2)}$ is second order derivative operator, can $C \in R^{n \times n}$ is a tridiagonal matrix.
- Smoothing spline utilizes l_2 penalty while trend filtering uses l_1 penalty. Thus later one shrinks some components of $D\hat{u}$ to zero, which therefore exhibits a finer degree of local adaptivity.

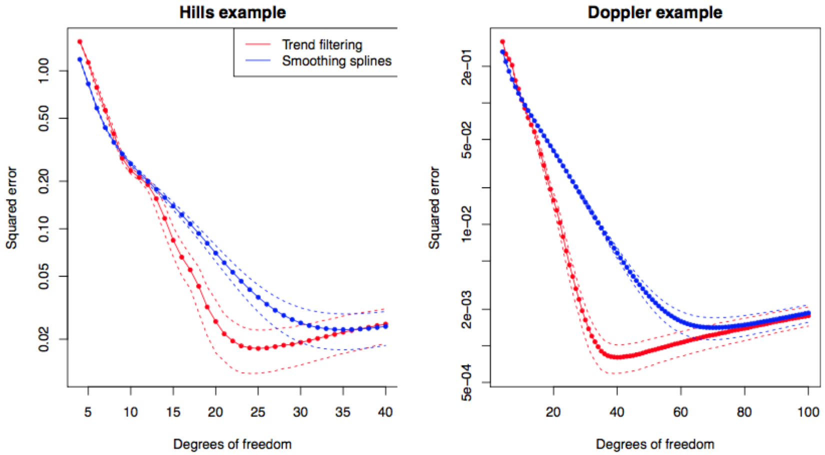
Empirical comparison



Empirical comparison



Empirical comparison



Computation comparison

- By choosing B-spline basis functions, the matrix $N^T N + \lambda\Omega$ is banded, and so the smoothing spline fitted values can be computed in $O(n)$ operations.
- Primal-dual interior point method is one option to solve trend filtering problem with fixed value of λ. This algorithm solves a sequence of banded linear system and the worst number of iterations scales as $O(n^{1/2})$. Hence interior point method is in $O(n^{3/2})$ worst-case complexity.
- The dual path algorithm of Tibshirani & Taylor (2011) constructs solution path as λ varies from ∞ to 0. The computation requires $O(n)$ operations.

Comparison to locally adaptive regression spline

Locally adaptive regression spline

Given arbitrary integer k, we first define the knot superset

$$T = \begin{cases} \{x_{k/2+2}, \cdots, x_{n-k/2}\} & \text{if } k \text{ is even,} \\ \{x_{(k+1)/2+1}, \cdots, x_{n-(k+1)/2}\} & \text{if } k \text{ is odd.} \end{cases} \tag{18}$$

which excludes the points near boundaries of inputs $\{x_1, \cdots, x_n\}$. We then define the kth order locally adaptive regression spline estimate as

$$\hat{f} = \underset{f \in \mathcal{G}_k}{argmin} \frac{1}{2} \sum_{i=1}^{n} \|y_i - f(x_i)\|_2^2 + \lambda TV(f^{(k)}) \tag{19}$$

where $f^{(k)}$ is now the kth weak derivative of f, $TV(\cdot)$ denotes the total variation operator.

Locally adaptive regression spline

$\mathcal{G}_k$ is the set

$$\mathcal{G}_k = \{f : [0,1] \to R : f \text{ is kth degree spline with knots contained in T}\} \tag{20}$$

Total variation of a function $f : [0,1] \to R$ is defines as:

$$TV(f) = \sup\{\sum_{i=1}^{p} |f(z_{i+1}) - f(z_i)| : z_1 < \cdots < z_p \text{ is partition of } [0,1]\}, \tag{21}$$

and this reduces to $TV(f) = \int_0^1 |f'(t)| dt$ if f is (strongly) differentiable.

Generalized lasso representation

$\mathcal{G}_k$ is spanned by n basis function $\{g_1, \cdots, g_n\}$. Each g_j is kth degree spline with knots in T, we know that its kth weak derivative is piecewise constant and right-continuous, with jump point contained in T; therefore, writing $t_0 = 0$ and $T = \{t_1, \cdots, t_{n-k-1}\}$, we have

$$TV(g_j) = \sum_{i=1}^{n-k-1} |g_j^{(k)}(t_i) - g_j^{(k)}(t_{i-1})|. \tag{22}$$

Similarly, any linear combination of $g_1, \cdots, g_n$ has total variation:

$$TV(\sum_{j=1}^{n} \theta_j g_j) = \sum_{i=1}^{n-k-1} \left| \sum_{i=1}^{n-k-1} \left[g_j^{(k)}(t_i) - g_j^{(k)}(t_{i-1}) \right] \cdot \theta_j \right|. \tag{23}$$

Generalized lasso representation

Hence problem (19) can be expressed in terms of $\theta \in R^n$,

$$\hat{\theta} = \underset{\theta \in R^n}{argmin} \frac{1}{2}\|y - G\theta\|_2^2 + \lambda\|C\theta\|_1, \tag{24}$$

where

$$G_{ij} = g_j(t_i) \quad \text{for } i, j = 1, \cdots, n, \tag{25}$$

$$C_{ij} = g_j^{(k)}(t_i) - g_j^{(k)}(t_{i-1}) \quad \text{for } i = 1, \cdots, n-k-1, j = 1, \cdots, n \tag{26}$$

Generalized lasso representation

Given $\hat{\theta}$, the estimates of the locally adaptive spline over the input points are given by:

$$(\hat{f}(x_1), \cdots, \hat{f}(x_n)) = G\hat{\theta} \tag{27}$$

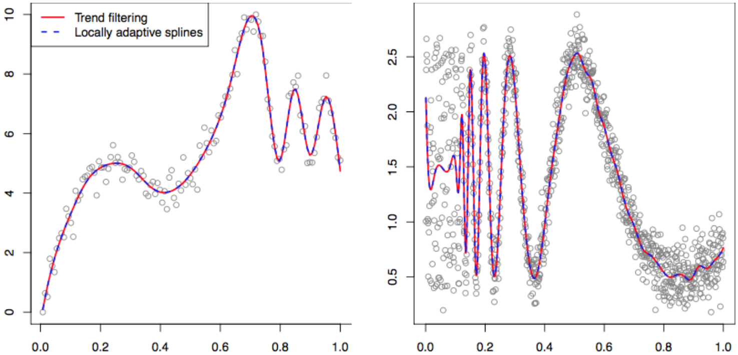
or, at an arbitrary point $x \in [0,1]$ by

$$\hat{f}(x) = \sum_{j=1}^{n} \hat{\theta}_j g_j(x). \tag{28}$$

By taking $g_1, \cdots, g_n$ to be truncated power basis, we can turn (a block of) C into identity, and problem (24) into a lasso problem.

Empirical comparison

- When introducing trend filtering, we showed that trend filtering problem can be written as a lasso problem with design matrix H. $H = G$ for $k < 2$.
- Although $G \neq H$ for $k \geq 2$, the estimates of two methods are practically similar and difficult to distinguish by eyes.



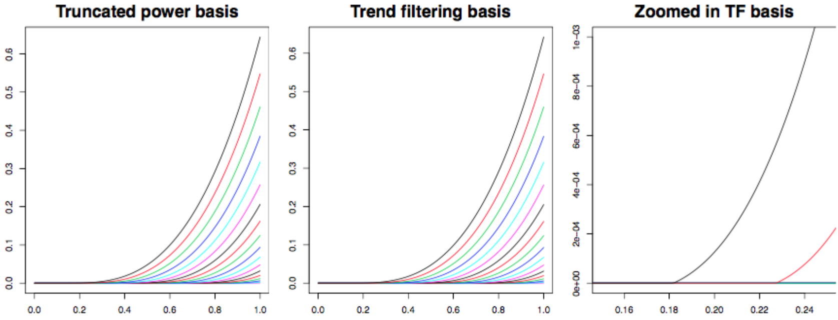
Empirical comparison

The difference of the basis functions:

The kth order truncated power basis is given by:

$$\begin{aligned} g_1(x) = 1,\ g_2(x),\ \cdots, g_{k+1}(x) = x^k, \\ g_{k+1+j} = (x - t_j)^k \cdot 1\{x \geq t_j\}, j = 1, \cdots, n-k-1. \end{aligned} \tag{29}$$

Empirical comparison



Computation comparison

- There is no specialized method for the locally adaptive regression spline.
- Choosing either B-spline or truncated power basis, we are more or less stuck with solving a generalized lasso problem with dense design matrix.

Rate of Convergence

Rate of Convergence

- It has been shown that Locally adaptive regression splines converges at the minimax rate (Mammen & van de Geer 1997).
- As $n \to \infty$, trend filtering estimates lies close enough to locally adaptive regression spline estimates, thus sharing their favorable asymptotic properties.

Extensions

Extensions

- Unevenly spaced inputs

$$D^{(x,k+1)} \cdot \text{diag}\left(\frac{k}{x_{k+1} - x_1}, \frac{k}{x_{k+2} - x_2}, \cdots, \frac{k}{x_n - x_{n-k}}\right) \cdot D^{(x,k)}$$

  $D^{(x,k+1)}$ can still be thought of as a difference operator of order $k+1$, but adjusted to account for the unevenly spaced inputs $x_1, \cdots, x_n$.

- Sparse trend filtering

$$\hat{\beta} = \underset{\beta \in R^n}{minimize} \frac{1}{2}\|y - \beta\|_2^2 + \lambda_1 \|D^{(k+1)}\beta\|_1 + \lambda_2 \|\beta\|_1$$

- Mixed trend filtering

$$\hat{\beta} = \underset{\beta \in R^n}{minimize} \frac{1}{2}\|y - \beta\|_2^2 + \lambda_1 \|D^{(k_1+1)}\beta\|_1 + \lambda_2 \|D^{(k_2+1)}\beta\|_1$$

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