Smoothing

Lessons for the master course in Applied Statistics

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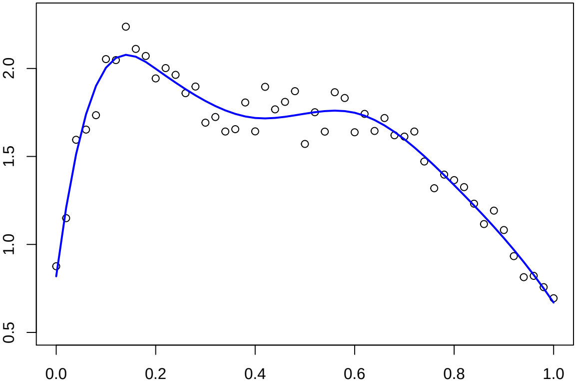
POLITECNICO
MILANO 1863


2.0
1.5
1.0
0.5
0.0
0.2
0.4
0.6
0.8
1.0

SMOOTHING

- Data: $\{(Y_1, x_1), \ldots, (Y_n, x_n)\}$

Model

$$Y = f(x) + \epsilon$$

$f \in \mathcal{F}$ where $\mathcal{F}$ is the appropriate functional space

Smoothing

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$$Y_i = f(x_i) + \epsilon_i \qquad \epsilon_i \sim \text{indep} \quad \mathbb{E}[\epsilon_i] = 0, Var[\epsilon_i] = \sigma^2 < 0$$

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Smoothing problem:

$$\hat{f} = \underset{f \in \mathcal{F}}{\text{argmin}}\, \text{RSS}(f) = \underset{f \in \mathcal{F}}{\text{argmin}} \left\{ \sum_{i=1}^{n} (Y_i - f(x_i))^2 \right\}$$

- Data: $\{(Y_1, x_1), \ldots, (Y_n, x_n)\}$

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ill posed!

Smoothing

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Smoothing problem:

$$\hat{f} = \underset{f \in \mathcal{F}_K}{\text{argmin}}\, \text{RSS}(f) = \underset{f \in \mathcal{F}_K}{\text{argmin}} \left\{ \sum_{i=1}^{n} (Y_i - f(x_i))^2 \right\}$$

1st approach: restrict search to $\mathcal{F}_K$, with $dim(\mathcal{F}_K) = K << n$

Smoothing

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Smoothing problem:

$$\hat{f} = \underset{f \in \mathcal{F}}{\text{argmin}}\, \text{RSS}(f) = \underset{f \in \mathcal{F}}{\text{argmin}} \left\{ \sum_{i=1}^{n} (Y_i - f(x_i))^2 + \mathcal{P}(f) \right\}$$

2nd approach: do not restrict $\mathcal{F}$ but add a roughness penalty

1st approach: $\mathcal{F}$ approximated by $\mathcal{F}_K$, with $dim(\mathcal{F}_K) = K << n$

$$\hat{f} = \underset{f \in \mathcal{F}_K}{\text{argmin}} \ \text{RSS}(f) = \underset{f \in \mathcal{F}_K}{\text{argmin}} \sum_{i=1}^{n} \left(Y_i - f(x_i)\right)^2$$

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- $\psi_1, \ldots, \psi_K$: K basis functions s.t. $\mathcal{F}_K = \mathrm{span}(\psi_1, \ldots, \psi_K)$

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Model

$$Y_i = f(x_i) + \epsilon_i \qquad \rightsquigarrow \qquad Y_i = \sum_{j=1}^{K} c_j \psi_j(x_i) + \epsilon_i$$

1st approach: $\mathcal{F}$ approximated by $\mathcal{F}_K$, with $dim(\mathcal{F}_K) = K << n$

$$\hat{f} = \underset{f \in \mathcal{F}_K}{\operatorname{argmin}} \ \mathrm{RSS}(f) = \underset{f \in \mathcal{F}_K}{\operatorname{argmin}} \sum_{i=1}^{n} \left(Y_i - f(x_i)\right)^2$$

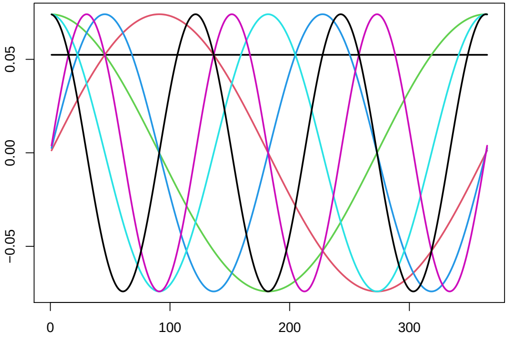
$$= \underset{\boldsymbol{c} \in \mathbb{R}^K}{\operatorname{argmin}} \ \mathrm{RSS}(\boldsymbol{c}) = \underset{\boldsymbol{c} \in \mathbb{R}^K}{\operatorname{argmin}} \sum_{i=1}^{n} \left(Y_i - \sum_{j=1}^{K} c_j \psi_j(x_i)\right)^2$$

- $\psi_1, \ldots, \psi_K$: K basis functions s.t. $\mathcal{F}_K = \mathrm{span}(\psi_1, \ldots, \psi_K)$

Model

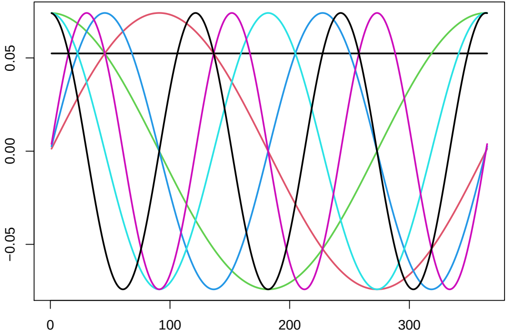
$$Y_i = f(x_i) + \epsilon_i \qquad \rightsquigarrow \qquad Y_i = \sum_{j=1}^{K} c_j \psi_j(x_i) + \epsilon_i$$

Fourier

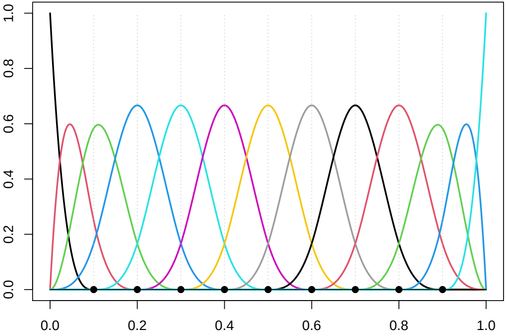


Fourier basis

Fourier

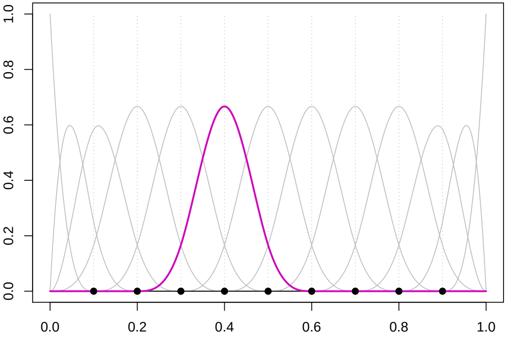


Periodic, localized in frequency, Convenient for differentiation and integration, Computationally efficient (orthogonal)



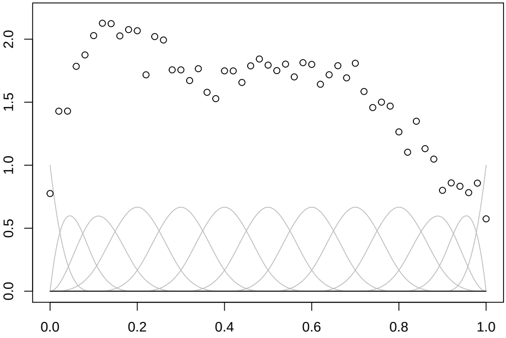
Cubic B-spline basis

B-SPLINE BASIS



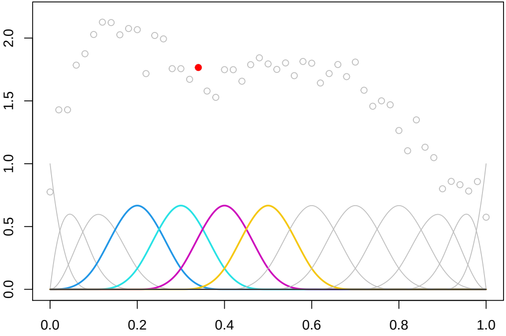
Flexible, localized in space, convenient for differentiation and integration

B-SPLINE BASIS



Computationally efficient (local support, band limited structure of key matrices involved, etc)

B-SPLINE BASIS



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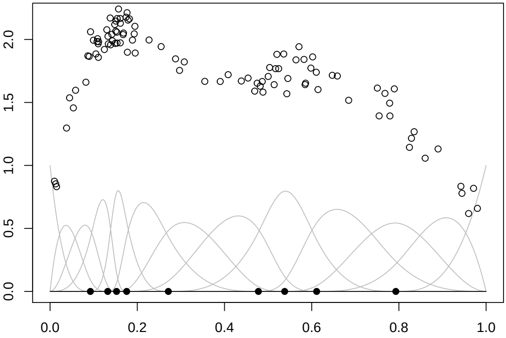
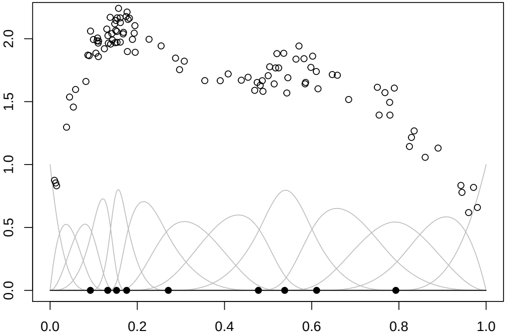
B-spline basis



Knots can be placed along the percentiles of X

B-SPLINE BASIS



Knots replication permits discontinuity in derivatives or function itself

$$\Psi = \begin{bmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_K(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \cdots & \psi_K(x_2) \\ \vdots & \vdots & & \vdots \\ \psi_1(x_n) & \psi_2(x_n) & \cdots & \psi_K(x_n) \end{bmatrix}$$

$$\boldsymbol{\Psi} = \begin{bmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_K(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \cdots & \psi_K(x_2) \\ \vdots & \vdots & & \vdots \\ \psi_1(x_n) & \psi_2(x_n) & \cdots & \psi_K(x_n) \end{bmatrix}$$

$$\boldsymbol{\psi} = (\psi_1, \dots, \psi_K)^\top$$

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$$\boldsymbol{Y} = (Y_1, \ldots, Y_n)^\top$$

$$\boldsymbol{\Psi} = \begin{bmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_K(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \cdots & \psi_K(x_2) \\ \vdots & \vdots & & \vdots \\ \psi_1(x_n) & \psi_2(x_n) & \cdots & \psi_K(x_n) \end{bmatrix} \qquad \boldsymbol{\psi} = (\psi_1, \ldots, \psi_K)^\top$$

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Model

$$\boldsymbol{Y} = \boldsymbol{f} + \boldsymbol{\epsilon} = \Psi \boldsymbol{c} + \boldsymbol{\epsilon}$$

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$$\boldsymbol{c} = (c_1, \ldots, c_K)^\top \qquad \boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_n)^\top$$

Model

$$\boldsymbol{Y} = \boldsymbol{f} + \boldsymbol{\epsilon} = \boldsymbol{\Psi}\boldsymbol{c} + \boldsymbol{\epsilon} \qquad \mathbb{E}[\boldsymbol{\epsilon}] = \boldsymbol{0} \quad Var[\boldsymbol{\epsilon}] = \sigma^2 I_n$$

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$$\hat{f} = \boldsymbol{\psi}^\top \hat{\boldsymbol{c}}$$

$$\hat{\boldsymbol{c}} = \underset{\boldsymbol{c}\in\mathbb{R}^K}{\operatorname{argmin}} \, \mathrm{RSS}(\boldsymbol{c}) = \underset{\boldsymbol{c}\in\mathbb{R}^K}{\operatorname{argmin}} \left\{ (\boldsymbol{Y} - \Psi\boldsymbol{c})^\top (\boldsymbol{Y} - \Psi\boldsymbol{c}) \right\}$$

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$$\hat{\boldsymbol{Y}} = \hat{\boldsymbol{f}} = \Psi\hat{\boldsymbol{c}} = \Psi\left(\Psi^\top\Psi\right)^{-1}\Psi^\top\boldsymbol{Y} = S\boldsymbol{Y}$$

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$$S = \Psi\left(\Psi^\top\Psi\right)^{-1}\Psi^\top : \text{projection matrix (properties: } S^\top S = S)$$

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$$df = K = tr(S) = tr(S^\top S) = tr(2S - S^\top S)$$

$$
\begin{aligned}
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\hat{\boldsymbol{c}} &= \left(\Psi^\top\Psi\right)^{-1}\Psi^\top\boldsymbol{Y} \\
\hat{\boldsymbol{Y}} &= \hat{\boldsymbol{f}} = \Psi\hat{\boldsymbol{c}} = \Psi\left(\Psi^\top\Psi\right)^{-1}\Psi^\top\boldsymbol{Y} = S\boldsymbol{Y} \\
S &= \Psi\left(\Psi^\top\Psi\right)^{-1}\Psi^\top : \text{projection matrix (properties: } S^\top S = S) \\
df &= K = tr(S) = tr(S^\top S) = tr(2S - S^\top S) \\
\hat{\sigma}^2 &= \frac{1}{n-K}(\boldsymbol{Y}-\hat{\boldsymbol{Y}})^\top(\boldsymbol{Y}-\hat{\boldsymbol{Y}}) = \frac{1}{n-tr(S)}(\boldsymbol{Y}-\hat{\boldsymbol{Y}})^\top(\boldsymbol{Y}-\hat{\boldsymbol{Y}})
\end{aligned}
$$

$$\hat{f}(x) = \psi(x)^\top \hat{\boldsymbol{c}} = \psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \boldsymbol{Y}$$

$$\hat{f}'(x) = \psi'(x)^\top \hat{\boldsymbol{c}} \qquad \text{where } \psi' = (\psi'_1, \dots, \psi'_k)^\top$$

$$\hat{f}''(x) = \psi''(x)^\top \hat{\boldsymbol{c}} \qquad \text{where } \psi'' = (\psi''_1, \dots, \psi''_k)^\top$$

Smoothing requires special care when the curve estimate is asked, not only to provide a good smoothing of the data, but also to reflect the differential features

Curve derivatives (or their functions) are very often:
- objects of analysis
- helpful for further processing and data analysis (curve alignment/clustering)

$$\hat{f}(x) = \boldsymbol{\psi}(x)^\top \hat{\boldsymbol{c}} = \boldsymbol{\psi}(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \boldsymbol{Y}$$

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$$\mathbb{E}\big[\hat{f}(x)\big] = \mathbb{E}\big[\psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \boldsymbol{Y}\big] = \psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \Psi \boldsymbol{c} = \psi(x)^\top \boldsymbol{c}$$

$$\hat{f}(x) = \psi(x)^\top \hat{\boldsymbol{c}} = \psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \boldsymbol{Y}$$

$$\mathbb{E}\left[\hat{f}(x)\right] = \mathbb{E}\left[\psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \boldsymbol{Y}\right] = \psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \Psi \boldsymbol{c} = \psi(x)^\top \boldsymbol{c}$$

$$\mathrm{Bias}[\hat{f}(x)] = f(x) - \mathbb{E}[\hat{f}(x)] = f(x) - \psi(x)^\top \boldsymbol{c}$$

$$\hat{f}(x) = \psi(x)^\top \hat{\boldsymbol{c}} = \psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \boldsymbol{Y}$$

$$\mathbb{E}\big[\hat{f}(x)\big] = \mathbb{E}\big[\psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \boldsymbol{Y}\big] = \psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \Psi \boldsymbol{c} = \psi(x)^\top \boldsymbol{c}$$

$$\mathrm{Bias}[\hat{f}(x)] = f(x) - \mathbb{E}[\hat{f}(x)] = f(x) - \psi(x)^\top \boldsymbol{c}$$

Source of bias: discretization

$$\hat{f}(x) = \psi(x)^\top \hat{\boldsymbol{c}} = \psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \boldsymbol{Y}$$

$$\mathbb{E}\big[\hat{f}(x)\big] = \mathbb{E}\big[\psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \boldsymbol{Y}\big] = \psi(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \Psi \boldsymbol{c} = \psi(x)^\top \boldsymbol{c}$$

$$\mathrm{Bias}[\hat{f}(x)] = f(x) - \mathbb{E}[\hat{f}(x)] = f(x) - \psi(x)^\top \boldsymbol{c}$$

$$\text{Source of bias: discretization}$$

$$\mathrm{Var}[\hat{f}(x)] = \mathbb{E}[\{\hat{f}(x) - \mathbb{E}[\hat{f}(x)]\}^2] = \sigma^2 \psi(x)^\top (\Psi^\top \Psi)^{-1} \psi(x)$$

$$\hat{f}(x) = \boldsymbol{\psi}(x)^\top \hat{\mathbf{c}} = \boldsymbol{\psi}(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \mathbf{Y}$$

$$\mathbb{E}\left[\hat{f}(x)\right] = \mathbb{E}\left[\boldsymbol{\psi}(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \mathbf{Y}\right] = \boldsymbol{\psi}(x)^\top (\Psi^\top \Psi)^{-1} \Psi^\top \Psi \mathbf{c} = \boldsymbol{\psi}(x)^\top \mathbf{c}$$

$$\mathrm{Bias}[\hat{f}(x)] = f(x) - \mathbb{E}[\hat{f}(x)] = f(x) - \boldsymbol{\psi}(x)^\top \mathbf{c}$$

Source of bias: discretization

$$\mathrm{Var}[\hat{f}(x)] = \mathbb{E}[\{\hat{f}(x) - \mathbb{E}[\hat{f}(x)]\}^2] = \sigma^2 \boldsymbol{\psi}(x)^\top (\Psi^\top \Psi)^{-1} \boldsymbol{\psi}(x)$$

$$\widehat{\mathrm{Var}[\hat{f}(x)]} = \mathbb{E}[\{\hat{f}(x) - \mathbb{E}[\hat{f}(x)]\}^2] = \hat{\sigma}^2 \boldsymbol{\psi}(x)^\top (\Psi^\top \Psi)^{-1} \boldsymbol{\psi}(x)$$

Number of bases K controls Bias-Variance trade-off.

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$$
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GCV(K) &= \frac{n}{(n-K)} \frac{1}{(n-K)} (\boldsymbol{Y} - \hat{\boldsymbol{Y}})^\top (\boldsymbol{Y} - \hat{\boldsymbol{Y}}) \\
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Number of bases K controls Bias-Variance trade-off.

K can be selected by AiC, C_p Mallows, cross-validation, Generalized Cross Validation:

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Hopefully the chosen value of K is close to that minimizing

$$\mathrm{MSE}[\hat{f}(x)] = \mathbb{E}[\{\hat{f}(x) - f(x)\}^2] = \mathrm{Bias}^2[\hat{f}(x)] + \mathrm{Var}[\hat{f}(x)]$$

Under regularity conditions, as $n \to \infty$ and $K(n) \to \infty$ with appropriate rates

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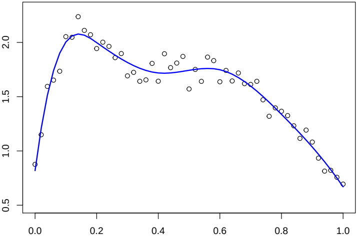
- Test on $H_0 : f(x) = f_0(x)$ vs $H_1 : f(x) \neq f_0(x)$ of approx level α

  Reject H_0 if $|\hat{f}(x) - f_0(x)| > z_{1-\alpha/2}\sqrt{\widehat{\mathrm{Var}[\hat{f}(x)]}}$

Caveats:

- This inference is only pointwise!



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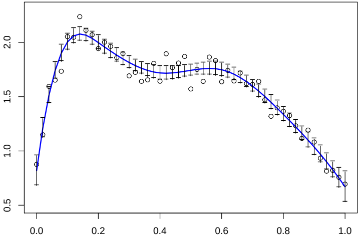

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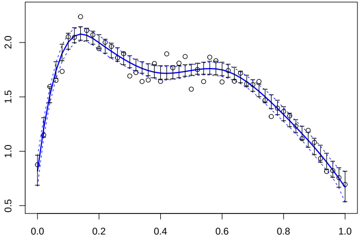

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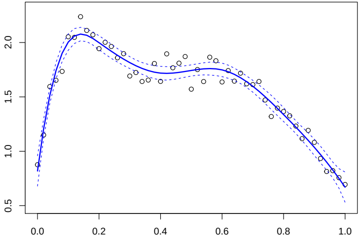

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You cannot interpret the smooth dashed bands as delimiters of a region that includes the true overall f with a given confidence.

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  - $\mathbb{P}$(type I error) > α

Various alternative approaches, including bootstrap, as well as undersmoothing or oversmoothing approaches (see, e.g., review in Hall and Horowitz 2013)

2nd approach: Do not restrict $\mathcal{F}$ but
minimize RSS + roughness penalty

$$\hat{f} = \underset{f \in \mathcal{F}}{\operatorname{argmin}}\ \mathrm{RSS}_\lambda(f) = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \left\{ \sum_{i=1}^{n} (Y_i - f(x_i))^2 + \lambda \mathcal{P}(f) \right\} \qquad \lambda > 0$$

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THM: If (a, b) s.t. $a < x_{[1]} < x_{[2]} < \ldots < x_{[n]} < b$, $\mathcal{F} = H^2(a, b)$, and $\mathcal{P}(f) = \int_a^b (f''(x))^2 dx$ then $\hat{f}$ is a natural cubic splines over (a, b) with knots at $x_{[1]}, x_{[2]}, \ldots, x_{[n]}$.

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Ex: For $\mathcal{P}(f) = \int (f'')^2$ then (j, ℓ)-entry of P is $\int_a^b \psi_j''(x) \psi_\ell''(x)\, dx$

2nd approach: $\hat{f} \in \mathcal{F}_K$, with $dim(\mathcal{F}_K) = K \approx n$
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For large datasets, it may be convenient to employ a mixed approach, where one considers a roughness penalty, but also reduces the dimensionality of the data estimation problem by considering a basis of dimension K, where K is still large but somehow smaller than n.

$$\hat{\boldsymbol{c}} \quad = \quad \left(\Psi^\top \Psi + \lambda P\right)^{-1} \Psi^\top \boldsymbol{Y}$$

Penalized smoothing
Expression of the estimator

$$\hat{\boldsymbol{c}} = \left(\Psi^\top \Psi + \lambda P\right)^{-1} \Psi^\top \boldsymbol{Y}$$

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PENALIZED SMOOTHING

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Physics-informed penantly: $\mathcal{P}(f) = \int (Lf - u)^2$
$Lf = u$ encodes available problem-specific information