Nonlinear Regression (Part 3)

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Stanford University, Spring 2016, STATS 205

Overview

Last time:

- Linear Smoothers

Today:

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    - Local Averages

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- Bootstrap Confidence Bands

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  with r being the **regression function**
- For now, assume that variance $\mathrm{Var}(\epsilon_i) = \sigma^2$ is independent of x

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- Small bandwidths give very rough estimates while larger bandwidths give smoother estimates

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  - The bias will be higher, because we are now using observations x_i further from x_0, and there is no guarantee that $r(x_i)$ will be close to $r(x_0)$

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- We use the data twice: to estimate the function and to estimate the risk

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- A better idea is to use leave-one-out cross-validation

$$\text{cv} = \widehat{R}(h) = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \widehat{r}_{(-i)}(x_i))^2$$

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- and we set the weight on x_i to 0 and renormalize the other weights to sum to one

$$l_{j,(-i)}(x) = \begin{cases} 0 & \text{if } j = i \\ \frac{l_j(x)}{\sum_{k \neq i} l_k(x)} & \text{if } j \neq i \end{cases}$$

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- Cross-validation is approximately the predictive risk (predicting the left-one-out observation)

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- After some algebra, we can see that

$$\widehat{r}(x_i) = (1 - L_{ii})\widehat{r}_{(-i)}(x_i) + L_{ii}Y_i$$

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- and if r is sufficiently smooth

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with

$$\Lambda = (I - L)^T (I - L)$$

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- and one can show that $\mathrm{Var}(\widehat{\sigma^2}) \to 0$

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- Therefore

$$\mathrm{E}(Y_{i+1} - Y_i) \approx \mathrm{E}(\epsilon_{i+1}) + \mathrm{E}(\epsilon_i) = 2\sigma^2$$

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with $\bar{r}_n(x)$ being the mean
- First term converges to a normal
- If we do a good job trading off bias and variance, the second term doesn't vanish with large n
$$\frac{\bar{r}_n(x) - r(x)}{\widehat{\sigma}(x)} = \frac{\text{Bias}(\widehat{r}_n(x))}{\sqrt{\text{Variance}(\widehat{r}_n(x))}}$$

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- We will go with the first approach

Constructing Confidence Bands

- For linear smoother $\widehat{r}_n(x)$ with

$$\bar{r}(x) = \mathrm{E}(\widehat{r}_n(x)) = \sum_{i=1}^{n} l_i(x) r(x_i)$$

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- Consider confidence bands

$$\mathcal{I}(x) = (\widehat{r}_n(x) - c\widehat{\sigma}\|l(x)\|, \widehat{r}_n(x) + c\widehat{\sigma}\|l(x)\|)$$

  for some c and $a \leq x \leq b$

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- For now, suppose that σ is known, then probability of estimate not in confidence band in at least one position x

$$\mathrm{P}(\bar{r}(x) \notin \mathcal{I}(x) \text{ for some } x \in [a, b]) = \mathrm{P}\left(\max_{x \in [a,b]} \frac{|\widehat{r}(x) - \bar{r}|}{\sigma \| l(x) \|} > c \right)$$

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- We are left just with the error term

$$= P\left(\max_{x\in[a,b]} \frac{|\sum_i \epsilon_i l_i(x)|}{\sigma\|l(x)\|} > c\right) = P\left(\max_{x\in[a,b]} |W(x)| > c\right)$$

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- This is a Gaussian process: a random function such that the vector $(W(x_1), \ldots, W(x_k))$ has a multivariate normal distribution, for any finite set of points $x_1, \ldots, x_k$

$$W(x) = \sum_{i=1}^{n} Z_i T_i(x), \quad Z_i = \epsilon_i/\sigma \sim N(0,1), \quad T_i(x) = l_i(x)\|l(x)\|$$

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  - In our neuroimaging example, we used permutation test to find maximum voxel clusters

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$$\mathrm{P}\left(\max_x \left|\sum_{i=1}^n Z_i T_i(x)\right| > c\right) \approx 2(1-\Phi(c)) + \frac{\kappa_0}{\pi} e^{-c^2/2}$$

for large c, $\kappa_0 = \int_a^b \|T'(x)\| dx$, and $T'(x) = \partial T_i(x)/\partial x$

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- Intuition: The task is to calculate the volume of this tube

Constructing Confidence Bands

- One can show that (cdf of the standard normal Φ)

$$\mathrm{P}\left(\max_x \left|\sum_{i=1}^n Z_i T_i(x)\right| > c\right) \approx 2(1-\Phi(c)) + \frac{\kappa_0}{\pi} e^{-c^2/2}$$

for large c, $\kappa_0 = \int_a^b \|T'(x)\| dx$, and $T'(x) = \partial T_i(x)/\partial x$

- Think of $T(x)$ as a curve in R^n, and c as defining a tube around it with radius c
- Intuition: The task is to calculate the volume of this tube
- We choose c by solving for α (e.g. $\alpha = 0.05$)

$$2(1-\Phi(c)) + \frac{\kappa_0}{\pi} e^{-c^2/2} = \alpha$$

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- Then this confidence is used

$$\mathcal{I}(x) = \widehat{r}_n(x) \pm c \sqrt{\sum_{i=1}^{n} \widehat{\sigma}^2(x_i) l_i^2(x)}$$

with c computed the same way

Average Coverage

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- Suppose we are estimating $r(x)$ over an interval $[0, 1]$, then **average coverage** is defined as

$$C = \int_0^1 \mathrm{P}(r(x) \in [d(x), u(x)])dx$$

Bootstrap Confidence Bands

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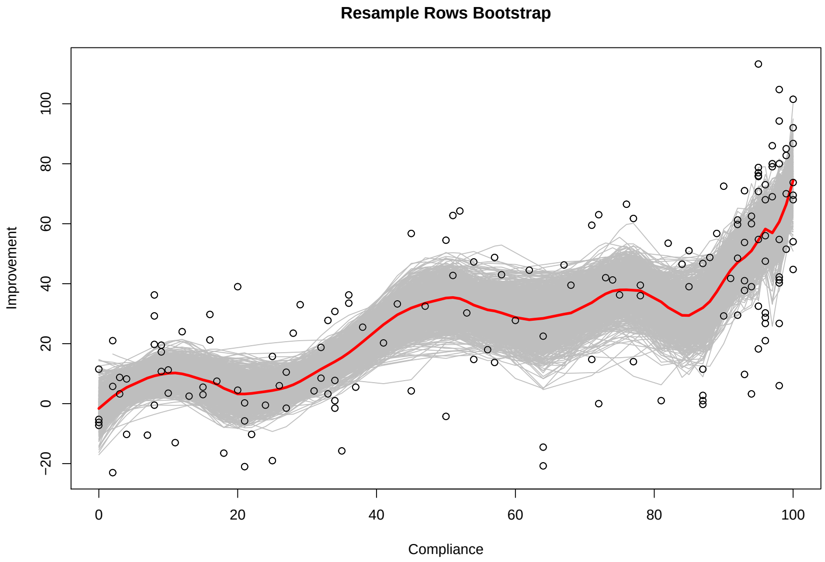
Bootstrap Confidence Bands (Example)

- Experiment with $n = 164$ men to see if the drug cholostyramine lowered blood cholesterol levels

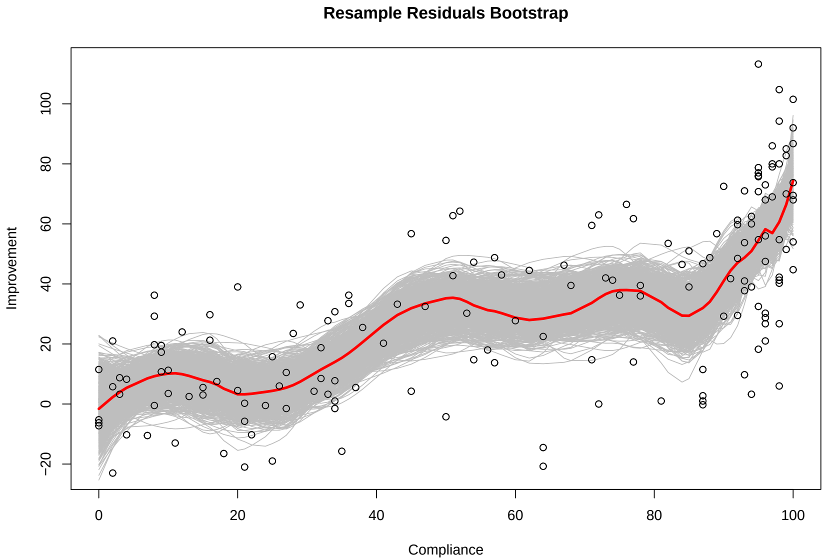
Bootstrap Confidence Bands (Example)

- Experiment with $n = 164$ men to see if the drug cholostyramine lowered blood cholesterol levels
- They were supposed to take six packets of cholostyramine per day, but many actually took much less

Bootstrap Confidence Bands (Example)



Bootstrap Confidence Bands (Example)



References

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References

- Wasserman (2006). All of Nonparametric Statistics
- Efron and Tibshirani (1994). An Introduction to the Bootstrap