Nonlinear Regression (Part 3)

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Overview

Last time:

- Linear Smoothers
  - Local Averages
  - Local Regression
  - Penalized Regression

Today:

- Cross-Validation
- Variance Estimation
- Confidence Bands
- Bootstrap Confidence Bands

Nonlinear Regression

- We are given n pairs of observations $(x_1, Y_1), \ldots, (x_n, Y_n)$
- The covariates x_i are fixed
- The **response variable** is related to the **covariate**

$$Y_i = r(x_i) + \epsilon_i \qquad\qquad E(\epsilon_i) = 0, i = 1, \ldots, n$$

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

Choosing the Smoothing Parameter

- The choice of kernel is not too important
- Estimates obtained by using different kernels are usually numerically very similar
- Can be confirmed by theoretical calculations showing that risk is insensitive to choice of kernel
- Choice of bandwidth matters which controls the amount of smoothing
- Small bandwidths give very rough estimates while larger bandwidths give smoother estimates

Choosing the Smoothing Parameter

- If the bandwidth is small
  - $\widehat{r}_n(x_0)$ is an average of a small number of Y_i close to x_0
  - The variance will be relatively large, close to that of an individual Y_i
  - The bias will tend to be small, because a close $r(x_i)$ should be similar to $r(x_0)$
- If the bandwidth is large
  - The variance of $\widehat{r}_n(x_0)$ will be small relative to the variance of any Y_i, because of the effects of averaging
  - 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 $r(x_0)$

Choosing the Smoothing Parameter

- The smoothers depend on some smoothing parameter h
- We define a risk

$$R(h) = \mathrm{E}\left(\frac{1}{n}\sum_{i=1}^{n}(\widehat{r}_n(x_i) - r(x_i))^2\right)$$

- Ideally, we would like to choose h to minimize $R(h)$
- But $R(h)$ depends on unknown function $r(x)$
- Instead we minimize an estimate $\widehat{R}(h)$
- As first guess, we might try minimizing the **training error**

$$\frac{1}{n}\sum_{i=1}^{n}(Y_i - \widehat{r}_n(x_i))^2$$

- This is a poor estimator, because it overfits (undersmoothing)
- We use the data twice: to estimate the function and to estimate the risk

Choosing the Smoothing Parameter

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

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

  with $\widehat{r}_{(-i)}$ estimator obtained by omitting the ith pair (x_i, Y_i)
- Define

$$\widehat{r}_{(-i)} = \sum_{j=1}^{n} Y_j l_{j,(-i)}(x)$$

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

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

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

Choosing the Smoothing Parameter

- We can compute leave-one-out cross-validation without leaving one observation out

$$\widehat{R}(h) = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{Y_i - \widehat{r}_n(x_i)}{1 - L_{ii}}\right)$$

- This is exactly true not an approximation!
- After some algebra, we can see that

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

Variance Estimation

- There are several variance estimators for linear smoothers
- Let $\hat{r}_n(x)$ be a linear smoother
- A consistent estimator (converges in probability to the true value of the parameter) of σ^2 is

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{n}(Y_i - \hat{r}_n(x_i))^2}{n - 2\nu + \tilde{\nu}}$$

- with

$$\nu = \text{tr}(L), \tilde{\nu} = \text{tr}(L^T L) = \sum_{i=1}^{n} \|l(x_i)\|^2$$

- and if r is sufficiently smooth

Variance Estimation

- The expected value of our estimator is

$$E(\widehat{\sigma}^2) = \frac{E(Y^T \Lambda Y)}{\mathrm{tr}(\Lambda)} = \sigma^2 + \frac{\boldsymbol{r}^T \Lambda \boldsymbol{r}}{n - 2\nu + \tilde{\nu}}$$

  with

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

  and

$$E(Y^T Q Y) = \mathrm{tr}(QV) + \mu^T Q \mu$$

  where $V = \mathrm{Var}(Y)$ is covariance matrix of Y and $\mu = E(Y)$ is the mean vector
- Assuming that ν and $\widehat{\nu}$ do not grow too quickly, and that r is smooth, the second term is small for large n
- So $E(\widehat{\sigma}^2) \approx \sigma^2$
- and one can show that $\mathrm{Var}(\widehat{\sigma^2}) \to 0$

Variance Estimation

- Another variance estimator (order x_i's)

$$\widehat{\sigma}^2 = \frac{1}{2(n-1)} \sum_{i=1}^{n-1} (Y_{i+1} - Y_i)^2$$

- Assuming r is smooth

$$Y_{i+1} - Y_i = [r(x_{i+1}) + \epsilon_{i+1}] - [r(x_i) + \epsilon_i] \approx \epsilon_{i+1} - \epsilon_i$$

- Therefore

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

Confidence Bands

- **Variability** bands

$$\widehat{r}_n(x) \pm 2\widehat{\sigma}(x)$$

- There is a problem with that

$$\frac{\widehat{r}_n(x) - r(x)}{\widehat{\sigma}(x)} = \frac{\widehat{r}_n(x) - \bar{r}_n(x)}{\widehat{\sigma}(x)} + \frac{\bar{r}_n(x) - r(x)}{\widehat{\sigma}(x)}$$

  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

$$\frac{\bar{r}_n(x) - r(x)}{\widehat{\sigma}(x)} = \frac{\text{Bias}(\widehat{r}_n(x))}{\sqrt{\text{Variance}(\widehat{r}_n(x))}}$$

Confidence Bands

- The result is that the confidence interval will not be centered around the true function r due to the smoothing bias
- Possible solutions:

1. Accept the fact that confidence band is for $\bar{r}_n$ not r
2. Estimate bias (this is difficult because it involves estimating $r''(x)$)
3. Undersmooth: less smoothing will bias results less, and asymptotically the bias will decrease faster than the variance

- We will go with the first approach

Constructing Confidence Bands

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

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

  and assuming constant variance

$$\mathrm{Var}(\widehat{r}_n(x)) = \sigma^2 \|l(x)\|^2$$

- 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 $a \leq x \leq b$

Constructing Confidence Bands

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

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

- We are left just with the error term

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

- 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 $x_1, \ldots, x_k$

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

Constructing Confidence Bands

- We want to find c for a fixed probability
- We need to compute the distribution of the maximum of a Gaussian process
- This is a well studied problem
  - Hotelling wrote about in 1939 (Tubes and spheres in n-spaces and a class of statistical problems)
  - There is a book treatment on this by Adler and Taylor (Random Fields And Geometry) connecting probability, geometry, and topology
  - In our neuroimaging example, we used permutation test to find maximum voxel clusters

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. $\alpha = 0.05$)

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

Constructing Confidence Bands

- So far we assumed that σ was known
- If unknown, we can use an estimate $\widehat{\sigma}$
- In this setting, one replaces the normal distribution with the t-distribution, however, for large n the previous approach remains a good approximation
- For changing variance $\sigma(x)$ as a function of x,

$$\mathrm{Var}(\widehat{r}_n(x)) = \sum_{i=1}^{n} \sigma^2(x_i) l_i^2(x)$$

- 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

- So far we required coverage bands to cover the function at all x
- We can relax this requirement a bit
- Suppose we are estimating $r(x)$ over an interval $[0, 1]$, then **average coverage** is defined as

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

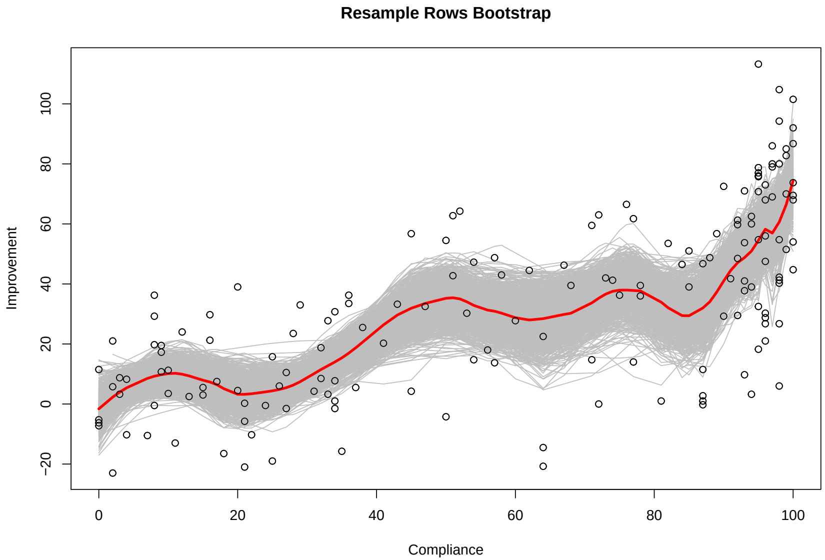
Bootstrap Confidence Bands

- There are at least two different ways to implement the boostrap for regression problems
- Resample rows:
  - Assume both Y and X are random
  - Rows need to be iid
- Resample residuals:
  - Assume that only Y is random and x is fixed
  - Errors need to be iid

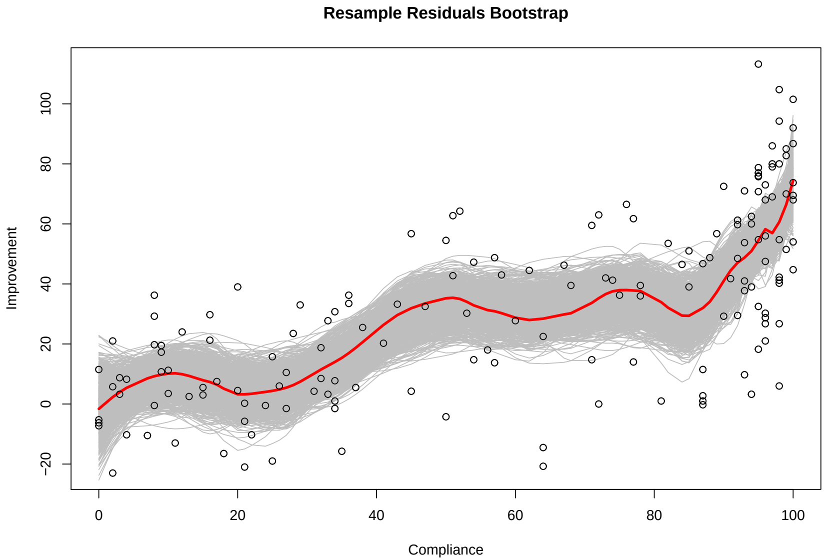
Bootstrap Confidence Bands (Example)

- 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

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