Exercises 2: Introduction to smoothing

For the next several weeks, we'll consider two age-old problems.

Density estimation: Given a sample $x_1, \ldots, x_n$ from some distribution P, estimate the probability density function p.

Regression: Given pairs $(x_1, y_1), \ldots, (x_n, y_n)$ where $y_i = f(x_i) + \epsilon_i$, with $E(\epsilon_i) = 0$, estimate the regression function f.

This set of exercises will kick us off.

Basic concepts

Bias–variance decomposition

Let $\hat{f}(x)$ be a noisy estimate of some function $f(x)$, evaluated at some point x. Define the mean-squared error of the estimate as

$$\text{MSE}(\hat{f}, f) = \text{E}\{[f(x) - \hat{f}(x)]^2\}\,.$$

Prove that $\text{MSE}(f, \hat{f}) = B^2 + v$, where

$$B = \text{E}\{\hat{f}(x)\} - f(x) \quad \text{and} \quad V = \text{var}\{\hat{f}(x)\}\,.$$

A simple example

Some people refer to the above decomposition as the *bias–variance tradeoff.* Why a tradeoff? Here's a simple example to convey the intuition.

Suppose we observe $x_1, \ldots, x_n$ from some distribution F, and want to estimate $f(0)$, the value of the probability density function at 0. Let h be a small positive number, called the *bandwidth*, and define the quantity

$$\pi_h = P\left(-\frac{h}{2} < X < \frac{h}{2}\right) = \int_{-h/2}^{h/2} f(x) dx\,.$$

Clearly $\pi_h \approx h f(0)$.

(A) Let Y be the number of observations in a sample of size n that fall within the interval $(-h/2, h/2)$. What is the distribution of Y? What are its mean and variance in terms of n and π_h? Propose a simple estimator $\hat{f}(0)$ involving Y.

(B) Suppose we expand $f(x)$ in a second-order Taylor series about 0:

$$f(x) \approx f(0) + x f'(0) + \frac{x^2}{2} f''(0)\,.$$

Use this in the above expression for π_h, together with the bias–variance decomposition, to show that

$$\text{MSE}\{\hat{f}(0), f(0)\} \approx Ah^4 + \frac{B}{nh}$$

for constants A and B that you should (approximately) specify. What happens to the bias and variance when you make h small? When you make h big?

(C) Use this result to derive an expression for the bandwidth that minimizes mean-squared error, as a function of n. You can approximate any constants that appear, but make sure you get the right functional dependence on the sample size.

Curve fitting by linear smoothing

Consider a nonlinear regression problem with one predictor and one response: $y_i = f(x_i) + \epsilon_i$, where the ϵ_i are mean-zero random variables.

(A) Suppose we want to estimate the value of the regression function $y^\star$ at some new point $x^\star$, denoted $\hat{f}(x^\star)$. Assume for the moment that $f(x)$ is linear, and that y and x have already had their means subtracted, in which case $y_i = \beta x_i + \epsilon_i$.

Return to your least-squares estimator for multiple regression. Show that for the one-predictor case, your prediction $\hat{y}^\star = f(x^\star) = \hat{\beta} x^\star$ may be expressed as a *linear smoother*[1] of the following form:

$$\hat{f}(x^\star) = \frac{\sum_{i=1}^n w(x_i, x^\star) y_i}{\sum_{i=1}^n w(x_i, x^\star)}$$

for any $x^\star$. Inspect the weighting function you derived. Briefly describe your understanding of how the resulting smoother behaves, compared with the smoother that arises from an alternate form of the weight function $w(x_i, x^\star)$:

$$w_K(x_i, x^\star) = \begin{cases} 1/K, & x_i \text{ one of the } K \text{ closest sample points to } x^\star\,, \\ 0, & \text{otherwise.} \end{cases}$$

This is referred to as *K-nearest-neighbor smoothing*.

(B) A *kernel function* $K(x)$ is a smooth function satisyfing

$$\int_{\mathbb{R}} K(x)dx = 1\,, \quad \int_{\mathbb{R}} xK(x)dx = 0\,, \quad \int_{\mathbb{R}} x^2 K(x)dx > 0\,.$$

[1] This doesn't mean the weight function $w(\cdot)$ is linear in its argument, but rather than the new prediction is a linear combination of the past outcomes y_i.

A very simple example is the uniform kernel,

$$K(x) = \frac{1}{2} I(x) \quad \text{where} \quad I(x) = \begin{cases} 1, & |x| \leq 1 \\ 0, & \text{otherwise}. \end{cases}$$

Another common example is the Gaussian kernel:

$$K(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} .$$

Kernels are used as weighting functions for taking local averages. Specifically, define the weighting function

$$w(x_i, x^\star) = \frac{1}{h} K\left(\frac{x_i - x^\star}{h}\right) ,$$

where h is the bandwidth. Using this weighting function in a linear smoother is called *kernel regression*.

Write your own R function that will fit a kernel smoother for an arbitrary set of x-y pairs, and arbitrary choice of (positive real) bandwidth h.[2] Set up an R script that will simulate noisy data from some nonlinear function, $y = f(x) + \epsilon$; subtract the sample means from the simulated x and y; and use your function to fit the kernel smoother for some choice of h. Plot the estimated functions for a range of bandwidths large enough to yield noticeable changes in the qualitative behavior of the prediction functions.

Cross validation

Left unanswered so far in our previous study of kernel regression is the question: how does one choose the bandwidth h used for the kernel? Assume for now that the goal is to predict well, not necessarily to recover the truth. (These are related but distinct goals.)

(A) Why not just choose h to minimize the sum of squared errors for the observed data set?

(B) What if you had a fresh data set where you could test your predictions arising from fitting the model to the first data set, with particular choices of h? Presumably a good choice of h would be one that led to smaller predictive errors. This is called *out-of-sample predictive validation*.

Write a function or script that will: (1) accept an old ("training") data set and a new ("testing") data set as inputs; (2) fit the kernel-regression estimator to the training data for specified choices of h;

[2] Coding tip: write things in a modular way. A kernel function is a function accepting a distance and a bandwidth and returning a nonnegative real. A weighting function is a function that accepts a vector of previous x's, a new x, and a kernel function; and that returns a vector of weights. Et cetera. You will appreciate your foresight in writing modular code later in the course!

and (3) return the estimated functions and the realized prediction error on the testing data for each value of h. This should involve a fairly straightforward "wrapper" of the function you've already written.

(C) Imagine a conceptual two-by-two table for the unknown, true state of affairs. The rows of the table are "wiggly function" and "smooth function," and the columns are "highly noisy observations" and "not so noisy observations." Simulate one data set (say, 500 points) for each of the four cells of this table, where the x's take values in the unit interval. Then split each data set into training and testing subsets. You choose the functions.[3] Apply your method to each case, using the testing data to select a bandwidth parameter. Choose the estimate that minimizes the average squared error in prediction, which estimates the mean-squared error:

$$L_n(\hat{f}) = \frac{1}{n} \sum_{i=1}^{n^\star} (y_i^\star - \hat{y}_i^\star)^2 \, ,$$

where $(y_i^\star, x_i^\star)$ are the points in the test set, and $\hat{y}_i^\star$ is your predicted value arising from the model you fit using only the training data. Does your out-of-sample predictive validation method lead to reasonable choices of h for each case?

(D) Splitting a data set into two chunks to choose h by out-of-sample validation has some drawbacks. List at least two. Then consider an alternative: leave-one-out cross validation. Define

$$\text{LOOCV} = \sum_{i=1}^{n} \left(y_i - \hat{y}_i^{(-i)} \right)^2 \, ,$$

where $\hat{y}_i^{(-i)}$ is the predicted value of y_i obtained by omitting the ith pair and fitting the model to the reduced data set.[4] This is contingent upon a particular bandwidth, and is obviously a function of x_i, but these dependencies are suppressed for notational ease. This looks expensive to compute: for each value of h, and for each data point to be held out, fit a whole nonlinear regression model. But you will derive a shortcut!

Observe that for a linear smoother, we can write the whole vector of fitted values as $\hat{y} = Hy$, where H is called the smoothing matrix (or "hat matrix") and y is the vector of observed outcomes.[5] Write $\hat{y}_i$ in terms of H and y, and show that $\hat{y}_i^{(-i)} =$

[3] Trigonometric functions, for example, can be pretty wiggly if you make the period small.

[4] The intuition here is straightforward: for each possible choice of h, you have to predict each data point using all the others. The bandwidth that with the lowest prediction error is the "best" choice by the LOOCV criterion.

[5] Remember that in multiple linear regression this is also true:

$$\hat{y} = X\hat{\beta} = X(X^T X)^{-1} X^T y = Hy \, .$$

$\hat{y}_i - H_{ii} y_i + H_{ii} \hat{y}_i^{(-i)}$. Deduce that, for a linear smoother,

$$\text{LOOCV} = \sum_{i=1}^{n} \left(\frac{y_i - \hat{y}_i}{1 - H_{ii}} \right)^2 .$$

Local polynomial regression

(A) Kernel regression has a nice interpretation as a "locally constant" estimator, obtained from locally weighted least squares. To see this, suppose we observe pairs (x_i, y_i) for $i = 1, \ldots, n$ from our new favorite model, $y_i = f(x_i) + \epsilon_i$ and wish to estimate the value of the underlying function $f(x)$ at some point x by weighted least squares. Our estimate is the scalar[6] quantity

$$\hat{f}(x) = a = \arg\min_{\mathbb{R}} \sum_{i=1}^{n} w_i (y_i - a)^2 ,$$

where the w_i are the normalized weights (i.e. they have been rescaled to sum to 1 for fixed x). Clearly if $w_i = 1/n$, the estimate is simply $\bar{y}$, the sample mean, which is the "best" globally constant estimator. Show (using elementary calculus) that if the unnormalized weights are

$$w_i \equiv w(x, x_i) = \frac{1}{h} K \left(\frac{x_i - x}{h} \right) ,$$

then the solution is exactly the kernel-regression estimator.

(B) A natural generalization of locally constant regression is local polynomial regression. For points u in a neighborhood of the target point x, define the polynomial

$$g_x(u; a) = a_0 + \sum_{k=1}^{D} a_j (u - x)^k$$

for some vector of coefficients $a = (a_0, \ldots, a_D)$. As above, we will estimate the coefficients a in $g_x(u; a)$ at some target point x using weighted least squares:

$$\hat{a} = \arg\min_{R^{D+1}} \sum_{i=1}^{n} w_i \left\{ y_i - g_x(x_i; a) \right\}^2 ,$$

where $w_i \equiv w(x_i, x)$ are the kernel weights defined just above, normalized to sum to one.[7] Derive a concise (matrix) form of the weight vector $\hat{a}$, and by extension, the local function estimate $\hat{f}(x)$ at the target value x.[8] Life will be easier if you define the matrix

[6] Because we are only talking about the value of the function at a specific point x, not the whole function.

[7] We are fitting a different polynomial function for every possible choice of x. Thus $\hat{a}$ depends on the target point x, but we have suppressed this dependence for notational ease.

[8] Observe that at x, $g_x(u; a) = a_0$.

R_x whose (i, j) entry is $(x_i - x)^{j-1}$, and remember that (weighted) polynomial regression is the same thing as (weighted) linear regression with a polynomial basis.

(C) From this, conclude that for the special case of the local linear estimator ($D = 1$), we can write $\hat{f}(x)$ as a linear smoother of the form

$$\hat{f}(x) = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i} \, ,$$

where the unnormalized weights are

$$\begin{aligned} w_i &= K\left(\frac{x - x_i}{h}\right) \{s_2(x) - (x_i - x) s_1(x)\} \\ s_j(x) &= \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right) (x_i - x)^j \, . \end{aligned}$$

(D) What are the mean and variance of the sampling distribution for the local polynomial estimate $\hat{f}(x)$? (Again, this is just a scalar quantity at x, not the whole function.)

(E) Write a new R function that fits the local linear estimator using a Gaussian kernel for a specified choice of bandwidth h. Then load the data in "utilities.csv" into R. This data set shows the monthly gas bill (in dollars) for a single-family home in Minnesota, along with the average temperature in that month (in degrees F), and the number of billing days in that month. Let y be the average daily gas bill in a given month (i.e. dollars divided by billing days), and let x be the average temperature. Fit y versus x using both the kernel-regression (locally constant) and local linear methods using a Gaussian kernel. In each case, choose a bandwidth by leave-one-out cross-validation.

Inspect the results of the models you just fit, paying careful attention to the fit at the far-left and far-right ends of the x axis. Do you see a reason a prefer one method to the other?

(F) Use the results of Part D to construct an approximate point-wise 95% confidence interval for the local linear model (using your chosen bandwidth) for the value of the function at each of the observed points x_i for the utilities data. Plot these confidence bands, along with the estimated function, on top of a scatter plot of the data.