

Linear-Nonlinear Regression

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Linear-in-Parameters Models

We've often brushed over models which are non-linear in parameters. Why?

- Problems linear in parameters generally much easier to estimate; criterion functions often quadratic; normal equations linear.
- Perhaps more important: linear models can nevertheless be very effective for estimating non-linear phenomena.

Estimating non-linear phenomena with linear models

Our basic linear regression model is:

$$y = X\beta + u.$$

But the linearity that's important for estimation here is the linearity in parameters. We can just as well have

$$y = f(X) + u, \quad \text{with } f(X) = \hat{f}(X; \alpha) + \epsilon;$$

where

$$\hat{f}(X; \alpha) = \sum_{k=1}^K \alpha_k \phi_k(X);$$

The (ϕ_k) are *basis* functions with which we can try to approximate f . Note linearity in parameters α !

Stepwise Basis Functions

For a function f defined over an interval $(0, 1)$ define:

K	$\phi_1(x)$	$\phi_2(x)$	$\phi_3(x)$	$\phi_4(x)$
2	$\mathbb{1}\{x \leq \frac{1}{2}\}$	$\mathbb{1}\{x > \frac{1}{2}\}$		
3	$\mathbb{1}\{x \leq \frac{1}{3}\}$	$\mathbb{1}\{\frac{1}{3} > x \leq \frac{2}{3}\}$	$\mathbb{1}\{x > \frac{2}{3}\}$	
4	$\mathbb{1}\{x \leq \frac{1}{4}\}$	$\mathbb{1}\{\frac{1}{4} > x \leq \frac{1}{2}\}$	$\mathbb{1}\{\frac{1}{2} < x \leq \frac{3}{4}\}$	$\mathbb{1}\{x > \frac{3}{4}\}$
\vdots	\vdots	\vdots	\vdots	\vdots

Radial Basis Functions

If $x \in \mathbb{R}^n$, define a set of *centers* $c_k \in \mathbb{R}^n$, and let

$$\phi_k(x) = K(x, c_k) = e^{-\frac{1}{2}\|x - c_k\|^2}.$$

Gram Matrix

This may seem as though we then need to choose a bunch of non-linear parameters, but consider letting $c_k = x_k$, where x_k is the k th observation in a dataset; then we have:

$$\mathbf{K} = \begin{bmatrix} K(x_1, x_1) & K(x_1, x_2) & \cdots & K(x_1, x_N) \\ K(x_2, x_1) & K(x_2, x_2) & \cdots & K(x_2, x_N) \\ \vdots & \vdots & \ddots & \vdots \\ K(x_N, x_1) & K(x_N, x_2) & \cdots & K(x_N, x_N) \end{bmatrix}$$

Other Basis Functions

- Polynomials
- Splines
- Piecewise linear functions
- Periodic functions...

“Over-fitting” & MSE

We can fit any given dataset better by increasing the number of functions in the basis. However, at some point improving the fit for a *given* sample makes the fit worse for a *different* sample.

Mean Squared Error

In a given sample, large deviations from true f are evidence of either a large *bias* or large *variance*.

In this case we can compute the squared bias of this particular estimated function \hat{f} by

$$\text{MSE}(\hat{f}) = \int \left(f(x) - \hat{f}(x) \right)^2 dF(x),$$

where $F(x)$ is the CDF of X .

Leave-one-out estimators

Whatever estimator we have of $\hat{y}(X)$, we presume that can be estimated using observations $j = 1, \dots, N$.

Estimator

An old idea for improving out-of-sample predictive power is the "leave-one-out" estimator. In this case for each observation j we construct a prediction function using every observation *except* j ; i.e.,

$$\hat{y}_{-j}(X) = \hat{f}(X|y_{-j}, X_{-j}) \quad j = 1, \dots, N.$$

That is, \hat{y}_{-j} is estimated using data (y_{-j}, X_{-j}) , but can then be evaluated at any X . Then the usual leave-one-out estimator is

$$\hat{y}(X) = \frac{1}{N} \sum_{j=1}^N \hat{y}_{-j}(X).$$

Note that *every single* $\hat{y}_{-j}(X_j)$ is an out-of-sample prediction, since (y_j, X_j) weren't used to construct \hat{y}_{-j} .

Cross-validation criterion

Let $e_{-j} = y_j - \hat{y}_{-j}(X_j)$. Call this the “leave-one-out error”.

Criterion

Define the *cross-validation* criterion as

$$CV = \frac{1}{N} \sum_{j=1}^N e_{-j}^2.$$

Given the iid sampling assumption it's easy to see that this is an unbiased estimator of the expected squared out-of-sample prediction error.

General Approach

If we have multiple possible models or estimators of the relationship between y and X , say $(\hat{y}^1(X), \dots, \hat{y}^q(X))$ we *select* a model by choosing the one that minimizes the CV criterion.

Parameter Estimation

Rather than selecting among a finite number of discrete “models”, we can also use the CV criterion as the basis for selecting a vector of continuous parameters.

K -fold Cross-Validation

A practical problem is that as N grows large our proposal to choose models by minimizing CV become impractical; typically the computational cost of implementing the estimator becomes $O(N^2)$ or worse. Enter K -fold cross-validation.

- 1 Divide sample of N observations into K different “folds” $d_{(k)}$, each of roughly size N/K .
- 2 Estimate a “leave N/K out” estimator that uses data from $K - 1$ folds to estimate $\hat{y}^{(-k)}(X)$.
- 3 Let

$$e_j^{(k)} = y_j - \hat{y}^{(-k)}(X_j) \quad \text{for } j \in d_{(k)}.$$

- 4 The criteria

$$\text{CV}^{(k)} = \frac{1}{K} \sum_{k=1}^K \frac{1}{N_k} \sum_{j \in d_{(k)}} (e_j^{(k)})^2$$

then approximates the CV criterion. (If $K = N$ the two are identical).

Expected MSE

We can think of the *expected* MSE as the limit we'd reach taking averages in repeated samples. (This can be estimated in a given finite sample by our Cross-Validation measure). If \hat{f}_m is estimated using a sample $m = 1, \dots, M$, then

$$CV_M = \frac{1}{M} \sum_{m=1}^M \text{MSE}(\hat{f}_m) \xrightarrow{p} \text{EMSE}.$$