MS&E 226: "Small" Data

Lecture 6: Model complexity scores (v3)

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Estimating prediction error

Estimating prediction error

We saw how we can estimate prediction error using validation or test sets.

But what can we do if we don't have enough data to estimate test error?

In this set of notes we discuss how we can use *in-sample* estimates to measure model complexity.

Training error

The first idea for estimating prediction error of a fitted model might be to look at the sum of squared error in-sample:

$$\mathsf{Err}_{\mathsf{tr}} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{f}(\mathbf{X}_i))^2 = \frac{1}{n}\sum_{i=1}^{n} r_i^2.$$

This is called the *training error*; it is the same as $1/n\times$ *sum of squared residuals* we studied earlier.

Training error vs. prediction error

Of course, based on our discussion of bias and variance, we should expect that training error is *too optimistic* relative to the error on a new test set.

To formalize this, we can compare Err_{tr} to Err_{in}, the in-sample prediction error:

$$\text{Err}_{\text{in}} = \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}[(Y - \hat{f}(\vec{X}))^2 | \mathbf{X}, \mathbf{Y}, \vec{X} = \mathbf{X}_i].$$

This is the prediction error if we received new samples of Y corresponding to each covariate vector in our existing data.

Training error vs. test error

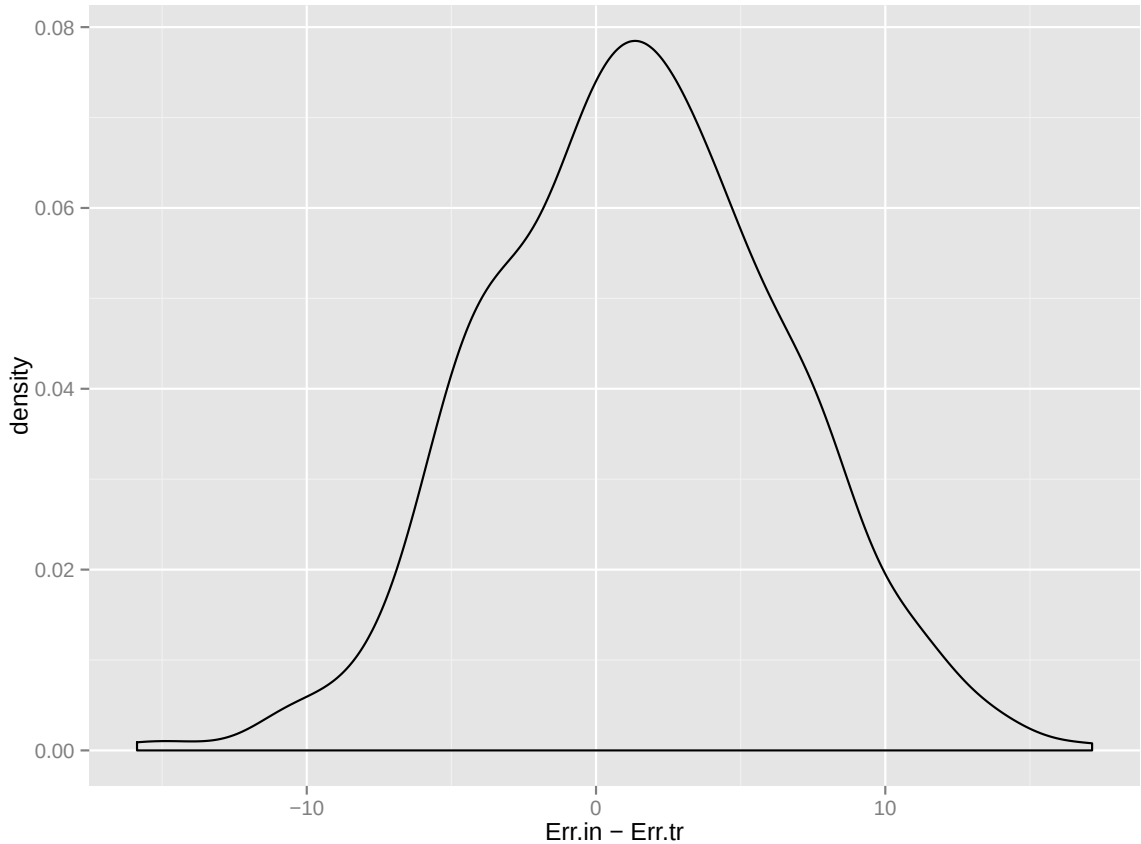
Let's first check how these behave relative to each other.

Use the same type of simulation as before:

- Generate 100 $X_1, X_2 \sim N(0, 1)$, i.i.d.
- Let $Y_i = 1 + X_{i1} + 2X_{i2} + \varepsilon_i$, where $\varepsilon_i \sim N(0, 5)$, i.i.d.
- Fit a model $\hat{f}$ using OLS, and the formula `Y ~ 1 + X1 + X2`.
- Compute training error of the model.
- Generate another 100 *test samples* of Y corresponding to each row of $\mathbf{X}$, using the same population model.
- Compute in-sample prediction error of the fitted model on the test set.
- Repeat in 500 "parallel universes", and create a plot of the results.

Training error vs. test error

Results:



Mean of $\text{Err}_{\text{in}} - \text{Err}_{\text{tr}} = 1.42$.

Training error vs. test error

If we could somehow *correct* $\mathsf{Err}_{\mathsf{tr}}$ to behave more like $\mathsf{Err}_{\mathsf{in}}$, we would have a way to estimate prediction error on new data (at least, for covariates $\mathbf{X}_i$ we have already seen).

Here is a key result towards that correction.[1]

Theorem

$$\mathbb{E}[\mathsf{Err}_{\mathsf{in}}|\mathbf{X}] = \mathbb{E}[\mathsf{Err}_{\mathsf{tr}}|\mathbf{X}] + \frac{2}{n}\sum_{i=1}^{n}\mathrm{Cov}(\hat{f}(\mathbf{X}_i), Y_i|\mathbf{X}).$$

In particular, if $\mathrm{Cov}(\hat{f}(\mathbf{X}_i), Y_i|\mathbf{X}) > 0$, *then training error underestimates test error.*

[1] This result holds more generally for other measures of prediction error, e.g., 0-1 loss in binary classification.

Training error vs. test error: Proof [$*$]

Proof: If we expand the definitions of $\mathsf{Err}_{\mathsf{tr}}$ and $\mathsf{Err}_{\mathsf{in}}$, we get:

$$\mathsf{Err}_{\mathsf{in}} - \mathsf{Err}_{\mathsf{tr}} = \frac{1}{n}\sum_{i=1}^{n}\Big(\mathbb{E}[Y^2|\vec{X} = \mathbf{X}_i] - Y_i^2 - 2(\mathbb{E}[Y|\vec{X} = \mathbf{X}_i] - Y_i)\hat{f}(\mathbf{X}_i)\Big)$$

Now take expectations over $\mathbf{Y}$. Note that:

$$\mathbb{E}[Y^2|\mathbf{X}, \vec{X} = \mathbf{X}_i] = \mathbb{E}[Y_i^2|\mathbf{X}],$$

since both are the expectation of the square of a random outcome with associated covariate $\mathbf{X}_i$. So we have:

$$\mathbb{E}[\mathsf{Err}_{\mathsf{in}} - \mathsf{Err}_{\mathsf{tr}}|\mathbf{X}] = -\frac{2}{n}\sum_{i=1}^{n}\mathbb{E}\Big[(\mathbb{E}[Y|\vec{X} = \mathbf{X}_i] - Y_i)\hat{f}(\mathbf{X}_i)\Big|\mathbf{X}\Big].$$

Training error vs. test error: Proof [$*$]

Proof (continued): Also note that $\mathbb{E}[Y|\vec{X} = \mathbf{X}_i] = \mathbb{E}[Y_i|\mathbf{X}]$, for the same reason. Finally, since:

$$\mathbb{E}[Y_i - \mathbb{E}[Y_i|\mathbf{X}]|\mathbf{X}] = 0,$$

we get:

$$\mathbb{E}[\mathsf{Err}_{\mathsf{in}} - \mathsf{Err}_{\mathsf{tr}}|\mathbf{X}] = \frac{2}{n}\sum_{i=1}^{n}\Big(\mathbb{E}\Big[(Y_i - \mathbb{E}[Y|\vec{X} = \mathbf{X}_i])\hat{f}(\mathbf{X}_i)\Big|\mathbf{X}\Big] - \mathbb{E}[Y_i - \mathbb{E}[Y_i|\mathbf{X}]|\mathbf{X}]\mathbb{E}[\hat{f}(\mathbf{X}_i)\Big|\mathbf{X}]\Big),$$

which reduces to $(2/n)\sum_{i=1}^{n}\mathrm{Cov}(\hat{f}(\mathbf{X}_i), Y_i|\mathbf{X})$, as desired.

The theorem's condition

What does $\mathrm{Cov}(\hat{f}(\mathbf{X}_i), Y_i|\mathbf{X}) > 0$ mean?

In practice, for any "reasonable" modeling procedure, we should expect our predictions to be positively correlated with our outcome.

Example: Linear regression

Assume a linear population model $Y = \vec{X}\boldsymbol{\beta} + \varepsilon$, where $\mathbb{E}[\varepsilon|\vec{X}] = 0$, $\mathrm{Var}(\varepsilon) = \sigma^2$, and errors are uncorrelated.

Suppose we use a subset S of the covariates and fit a linear regression model by OLS.

Recall that the bias-variance tradeoff is:

$$\mathbb{E}[\mathsf{Err}_{\mathsf{in}}|\mathbf{X}] = \sigma^2 + \frac{1}{n}\sum_{i=1}^{n}(\mathbf{X}_i\boldsymbol{\beta} - \mathbb{E}[\hat{f}(\mathbf{X}_i)|\mathbf{X}])^2 + \frac{|S|}{n}\sigma^2.$$

But this is hard to use to precisely estimate prediction error in practice, because we can't compute the bias.

Example: Linear regression

The theorem gives us another way forward. For linear regression with a linear population model we have:

$$\sum_{i=1}^{n} \mathrm{Cov}(\hat{f}(\mathbf{X}_i), Y_i | \mathbf{X}) = |S|\sigma^2.$$

In other words, in this setting we have:

$$\mathbb{E}[\mathsf{Err}_{\mathsf{in}} | \mathbf{X}] = \mathbb{E}[\mathsf{Err}_{\mathsf{tr}} | \mathbf{X}] + \frac{2|S|}{n}\sigma^2.$$

Model complexity for linear regression

A model complexity score

The last result suggests how we might measure model complexity:

- Estimate σ^2 using the sample standard deviation of the residuals *on the full fitted model*, i.e., with $S = \{1, \ldots, p\}$; call this $\hat{\sigma}^2$.[2]
- For a given model using a set of covariates S, compute:

$$C_p = \mathsf{Err}_{\mathsf{tr}} + \frac{2|S|}{n}\hat{\sigma}^2.$$

This is called *Mallow's C_p statistic*. It is an estimate of the prediction error.

[2] For a model with low bias, this will be a good estimate of σ^2.

A model complexity score

$$C_p = \mathsf{Err}_{\mathsf{tr}} + \frac{2|S|}{n}\hat{\sigma}^2.$$

How to interpret this?

- The first term measures fit to the existing data.
- The second term is a penalty for *model complexity*.

So the C_p statistic balances underfitting and overfitting the data (bias and variance).

AIC, BIC

Other model complexity scores:

- *Akaike information criterion* (AIC). In the linear population model with *normal* ε, this is equivalent to:

$$\frac{n}{\hat{\sigma}^2}\left(\mathsf{Err}_{\mathsf{tr}} + \frac{2|S|}{n}\hat{\sigma}^2\right).$$

- *Bayesian information criterion* (BIC). In the linear population model with normal ε, this is equivalent to:

$$\frac{n}{\hat{\sigma}^2}\left(\mathsf{Err}_{\mathsf{tr}} + \frac{|S|\ln n}{n}\hat{\sigma}^2\right).$$

Both are more general, and derived from a *likelihood* approach. (More on that later.)

AIC, BIC

Note that:

- AIC is the same (up to scaling) as C_p in the linear population model with normal ε.
- BIC penalizes model complexity more heavily than AIC.

AIC, BIC in software [$*$]

In practice, there can be significant differences between the actual values of C_p, AIC, and BIC depending on software; but these don't affect model selection.

- The estimate of sample variance $\hat{\sigma}^2$ for C_p will usually be computed using the full fitted model (i.e., with all p covariates), while the estimate of sample variance for AIC and BIC will usually be computed using just the fitted model being evaluated (i.e., with just $|S|$ covariates). This typically has no substantive effect on model selection.
- In addition, sometimes AIC and BIC are reported as the *negation* of the expressions on the previous slide, so that larger values are better; or without the scaling coefficient in front. Again, none of these changes affect model selectin.

Cross validation

Cross validation

Accuracy of C_p, AIC, and BIC depends on some knowledge of population model (in general, though they are often used even without this).

What general tools are avialable that don't depend on such knowledge?

Cross validation is a simple, widely used technique for estimating prediction error of a model, when data is (relatively) limited.

K-fold cross validation

K-fold cross validation (CV) works as follows:

- Divide data (randomly) into K equal groups, called *folds*. Let A_k denote the set of data points $(Y_i, \mathbf{X}_i)$ placed into the k'th fold.[3]
- For $k = 1, \ldots, K$, train model on all except k'th fold. Let $\hat{f}^{-k}$ denote the resulting fitted model.
- Estimate prediction error as:

$$\text{Err}_{\text{CV}} = \frac{1}{K} \sum_{k=1}^{K} \left(\frac{1}{n/K} \sum_{i \in A_k} (Y_i - \hat{f}^{-k}(\mathbf{X}_i))^2 \right).$$

In words: for the k'th model, the k'th fold acts as a *validation set*. The estimated prediction error from CV Err_{CV} is the average of the test set prediction errors of each model.

[3] For simplicity assume n/K is an integer.

K-fold cross validation

A picture:

Using CV

After running K-fold CV, what do we do?

- We then build a model from *all* the training data. Call this $\hat{f}$.
- The idea is that Err_{CV} should be a good estimate of Err, the generalization error of $\hat{f}$.[4]

So with that in mind, how to choose K?

- If $K = N$, the resulting method is called *leave-one-out* (LOO) cross validation.
- If $K = 1$, then there is no cross validation at all.
- In practice, in part due to computational considerations, often use $K = 5$ to 10.

[4] Recall generalization error is the expected prediction error of $\hat{f}$ on new samples.

How to choose K?

Bias and variance play a role in choosing K.

Let's start with *bias*: *How well does* Err_{CV} *approximate* Err*?*

- When $K = N$, the training set for each $\hat{f}^{-k}$ is nearly the entire training data.
  Therefore Err_{CV} will be nearly unbiased as an estimate of Err.
- When $K \ll N$, since the models use much less data than the entire training set, each model $\hat{f}^{-k}$ has higher generalization error; therefore Err_{CV} will tend to *overestimate* Err.

How to choose K?

Bias and variance play a role in choosing K.

Now let's look at variance: *How much does* Err_{CV} *vary if the training data is changed?*

- When $K = N$, because the training sets are very similar across all the models $\hat{f}^{-k}$, they will tend to have strong positive correlation in their predictions.
  This contributes to higher variance.
- When $K \ll N$, the models $\hat{f}^{-k}$ are less correlated with each other, reducing variance. On the other hand, each model is trained on significantly less data, increasing variance (e.g., for linear regression, the variance term increases if n decreases).

The overall effect depends on the population model and the model class being used.

Leave-one-out CV and linear regression

Leave-one-out CV is particularly straightforward for linear models fitted by OLS: there is no need to refit the model at all. This is a useful computational trick for linear models.

Theorem

Given training data $\mathbf{X}$ *and* $\mathbf{Y}$, *let* $\mathbf{H} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1}\mathbf{X}^\top$ *be the* hat matrix, *and let* $\hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y}$ *be the fitted values under OLS with the full training data.*
Then for leave-one-out cross validation:[5]

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

Interpretation: Observations with H_{ii} close to 1 are very "influential" in the fit, and therefore have a big effect on generalization error.

[5] It can be shown that $H_{ii} < 1$ for all i.

LOO CV and OLS: Proof sketch [$*$]

- Let $\hat{f}^{-i}$ be the fitted model from OLS when observation i is left out.
- Define $Z_j = Y_j$ if $j \neq i$, and $Z_i = \hat{f}^{-i}(\mathbf{X}_i)$.
- Show that OLS with training data $\mathbf{X}$ and $\mathbf{Z}$ has $\hat{f}^{-i}$ as solution.
- Therefore $\hat{f}^{-i}(\mathbf{X}_i) = (\mathbf{HZ})_i$.
- Now use the fact that:

$$(\mathbf{HZ})_i = \sum_j H_{ij} Z_j = (\mathbf{HY})_i - H_{ii} Y_i + H_{ii} \hat{f}^{-i}(\mathbf{X}_i).$$

A hypothetical example

- You are given a large dataset with many covariates. You carry out a variety of visualizations and explorations to conclude that you only want to use p of the covariates.
- You then use cross validation to pick the best model using these covariates.
- Question: is Err_{CV} a good estimate of Err in this case?

A hypothetical example (continued)

No – You already used the data to choose your p covariates!

The covariates were chosen because they looked favorable on the training data; this makes it more likely that they will lead to low cross validation error.

Thus in this approach, Err_{CV} will typically be *lower* than true generalization error Err.[6]

MORAL: To get unbiased results, any model selection must be carried out without the holdout data included!

[6] Analogous to our discussion of validation and test sets in the train-validate-test approach.

Cross validation in R

In R, cross validation can be carried out using the `cvTools` package.

```
> library(cvTools)
> cv.folds = cvFolds(n, K)
> cv.out = cvFit(lm, formula =  ...,
                 folds = cv.folds, cost = mspe)
```

When done, `cv.out$cv` contains Err_{CV}. Can be used more generally with other model fitting methods.

Simulation: Comparing C_p, AIC, BIC, CV

Repeat the following steps 10 times:

- For $1 \leq i \leq 100$, generate $X_i \sim$ uniform$[-3, 3]$.
- For $1 \leq i \leq 100$, generate Y_i as:

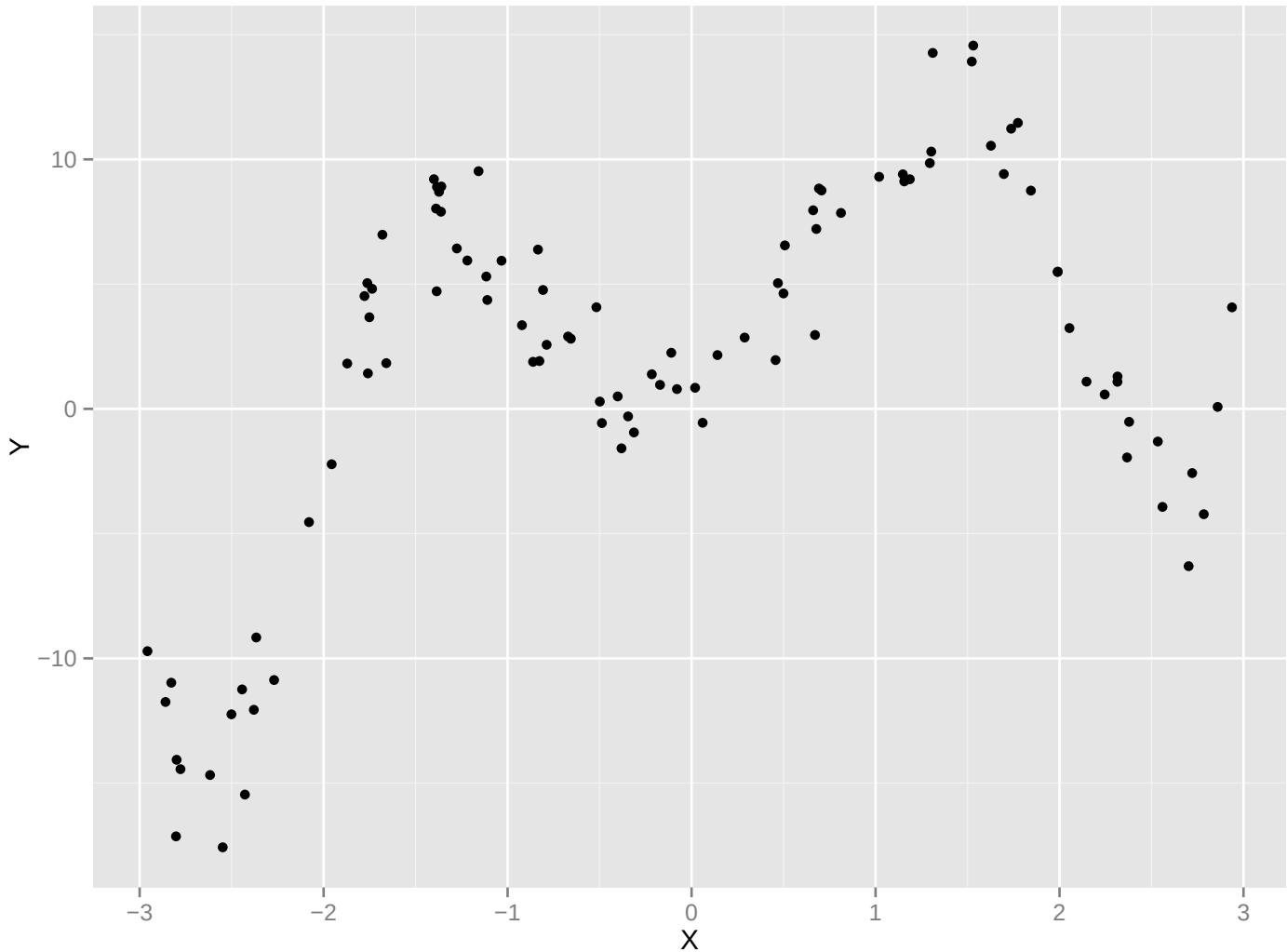
$$Y_i = \alpha_1 X_i + \alpha_2 X_i^2 - \alpha_3 X_i^3 + \alpha_4 X_i^4 - \alpha_5 X_i^5 + \alpha_6 X_i^6 + \varepsilon_i,$$

  where $\varepsilon_i \sim$ uniform$[-3, 3]$.
- For $p = 1, \ldots, 20$, we evaluate the model `Y ~ 0 + X + I(X^2) + ... + I(X^p)` using C_p, BIC, and 10-fold cross validation.[7]

How do these methods compare?

[7] We leave out AIC since it is exactly a scaled version of C_p.

Simulation: Visualizing the data



Simulation: Comparing C_p, AIC, BIC, CV