Evaluating Statistical Models

36-402, Data Analysis

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Optional Readings: Berk, chapter 2.

Contents

1 What Are Statistical Models For? Summaries, Forecasts, Simulators

There are (at least) three levels at which we can use statistical models in data analysis: as summaries of the data, as predictors, and as simulators.

The lowest and least demanding level is just to use the model as a summary of the data — to use it for **data reduction**, or **compression**. Just as one can use the sample mean or sample quantiles as descriptive statistics, recording some features of the data and saying nothing about a population or a generative process, we could use estimates of a model's parameters as descriptive summaries. Rather than remembering all the points on a scatter-plot, say, we'd just remember what the OLS regression surface was.

It's hard to be wrong about a summary, unless we just make a mistake. (It may or may not be *helpful* for us later, but that's different.) When we say "the slope which best fit the training data was $\hat{b} = 4.02$", we make no claims about anything *but* the training data. It relies on no assumptions, beyond our doing the calculations right. But it also asserts nothing about the rest of the world. As soon as we try to connect our training data to the rest of the world, we start relying on assumptions, and we run the risk of being wrong.

Probably the most common connection to want to make is to say what *other* data will look like — to make predictions. In a statistical model, with random noise terms, we do not anticipate that our predictions will ever be *exactly* right, but we also anticipate that our mistakes will show stable probabilistic patterns. We can evaluate predictions based on those patterns of error — how big is our typical mistake? are we biased in a particular direction? do we make a lot of little errors or a few huge ones?

Statistical inference about model parameters — estimation and hypothesis testing — can be seen as a kind of prediction, extrapolating from what we saw in a small piece of data to what we would see in the whole population, or whole process. When we *estimate* the regression coefficient $\hat{b} = 4.02$, that involves predicting new values of the dependent variable, but also predicting that if we repeated the experiment and re-estimated $\hat{b}$, we'd get a value close to 4.02.

Using a model to summarize old data, or to predict new data, doesn't commit us to assuming that the model describes the process which generates the data. But we often want to do that, because we want to interpret parts of the model as aspects of the real world. We think that in neighborhoods where people have more money, they spend more on houses — perhaps each extra \$1000 in income translates into an extra \$4020 in house prices. Used this way, statistical models become stories about how the data were generated. If they are accurate, we should be able to use them to *simulate* that process, to step through it and produce something that looks, probabilistically, just like the actual data. This is often what people have in mind when they talk about *scientific* models, rather than just statistical ones.

An example: if you want to predict where in the night sky the planets will be, you can actually do very well with a model where the Earth is at the center of the universe, and the Sun and everything else revolve around it. You can even estimate, from data, how fast Mars (for example) goes around the Earth, or where, in this model, it should be tonight. But, since the Earth is *not* at the center of the solar system, those parameters don't actually refer to anything in reality. They are just mathematical fictions. On the other hand, we can also predict where the planets will appear in the sky using models where all the planets orbit the Sun, and the parameters of the orbit of Mars in that model *do* refer to reality.[1]

We are going to focus today on evaluating predictions, for three reasons. First, often we just want prediction. Second, if a model can't even predict well, it's hard to see how it could be right scientifically. Third, often the best way of checking a scientific model is to turn some of its implications into statistical

[1] We can be pretty confident of this, because we use our parameter estimates to send our robots to Mars, and they get there.

predictions.

2 Errors, In and Out of Sample

With any predictive model, we can gauge how well it works by looking at its errors. We want these to be small; if they can't be small all the time we'd like them to be small on average. We may also want them to be patternless or unsystematic (because if there was a pattern to them, why not adjust for that, and make smaller mistakes). We'll come back to patterns in errors later, when we look at specification testing. For now, we'll concentrate on how big the errors are.

To be a little more mathematical, we have a data set with points $\mathbf{z}_n = z_1, z_2, \ldots z_n$. (For regression problems, think of each data point as the pair of input and output values, so $z_i = (x_i, y_i)$, with x_i possibly a vector.) We also have various possible models, each with different parameter settings, conventionally written θ. For regression, θ tells us which regression function to use, so $m_\theta(x)$ or $m(x;\theta)$ is the prediction we make at point x with parameters set to θ. Finally, we have a **loss function** L which tells us how big the error is when we use a certain θ on a certain data point, $L(z, \theta)$. For mean-squared error, this would just be

$$L(z, \theta) = (y - m_\theta(x))^2$$

But we could also use the mean absolute error

$$L(z, \theta) = |y - m_\theta(x)|$$

or many other loss functions. Sometimes we will actually be able to measure how costly our mistakes are, in dollars or harm to patients. If we had a model which gave us a distribution for the data, then $p_\theta(z)$ would a probability density at z, and a typical loss function would be the negative log-likelihood, $-\log m_\theta(z)$. No matter what the loss function is, I'll abbreviate the sample average of the loss over the whole data set by $L(\mathbf{z}_n, \theta)$.

What we would like, ideally, is a predictive model which has zero error on future data. We basically never achieve this:

- The world just really is a noisy and stochastic place, and this means even the true, ideal model has non-zero error.[2] If, in the usual linear regression assumptions, $Y = \beta X + \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma^2)$, then σ^2 sets a limit on how well Y can be predicted, and nothing will truly get the mean-squared error below that limit.

- Our models are never perfectly estimated. Even if our data come from a perfect IID source, we only ever have a finite sample, and so our parameter estimates are (almost) never quite the true, infinite-limit values. This is

[2]This is so even if you believe in some kind of ultimate determinism, because the variables we plug in to our predictive models are not complete descriptions of the physical state of the universe, but rather immensely coarser, and this coarseness shows up as randomness.

the origin of the variance term in the bias-variance decomposition. But as we get more and more data, the sample should become more and more representative of the whole process, and estimates should converge too.

- Our models are usually more or less **mis-specified**, or, in plain words, wrong. We hardly ever get the functional form of the regression, the distribution of the exogenous noise, the form of the causal dependence between two factors, etc., *exactly* right.[3] This is the origin of the bias term in the bias-variance decomposition. Of course we can get any of the details in the model specification *more or less* wrong, and we'd prefer to be less wrong.

So, because our models are flawed, we have limited data and the world is stochastic, we cannot expect even the best model to have zero error. Instead, we would like to minimize the **expected error**, or **risk**, or **generalization error**, on new data.

What we would like to do is to minimize the risk or expected loss

$$\mathbb{E}\left[L(Z,\theta)\right] = \int dz p(z) L(z,\theta)$$

To do this, however, we'd have to be able to calculate that expectation. Doing that would mean knowing the distribution of Z — the joint distribution of X and Y, for the regression problem. Since we don't know the true joint distribution, we need to approximate it somehow.

A natural approximation is to use our training data $\mathbf{z}_n$. For each possible model θ, we can could calculate the error on the data, $L(\mathbf{z}_n, \theta)$, called the **in-sample loss** or the **empirical risk**. The simplest strategy for estimation is then to pick the model, the value of θ, which minimizes the in-sample loss. This strategy is imaginatively called **empirical risk minimization**. Formally,

$$\widehat{\theta_n} \equiv \operatorname*{argmin}_{\theta \in \Theta} L(\mathbf{z}_n, \theta)$$

This means picking the regression which minimizes the sum of squared errors, or the density with the highest likelihood[4]. This what you've usually done in statistics courses so far, and it's very natural, but it does have some issues, notably optimism and over-fitting.

The problem of optimism comes from the fact that our training data isn't perfectly representative. The in-sample loss is a sample average. By the law of large numbers, then, we anticipate that, for each θ,

$$L(\mathbf{z}_n, \theta) \rightarrow \mathbb{E}\left[L(Z,\theta)\right]$$

[3]Except maybe in fundamental physics, and even there our predictions are about our fundamental theories *in the context of experimental set-ups*, which we never model in complete detail.

[4]Remember, maximizing the likelihood is the same as maximizing the log-likelihood, because log is an increasing function. Therefore maximizing the likelihood is the same as *minimizing* the negative log-likelihood.

as $n \to \infty$. This means that, with enough data, the in-sample error is a good approximation to the generalization error of any given model θ. (Big samples are representative of the underlying population or process.) But this does *not* mean that the in-sample performance of $\hat{\theta}$ tells us how well it will generalize, because we purposely picked it to match the training data $\mathbf{z}_n$. To see this, notice that the in-sample loss equals the risk plus sampling noise:

$$L(\mathbf{z}_n, \theta) = \mathbb{E}\left[L(\mathbf{Z}, \theta)\right] + \eta_n(\theta) \tag{1}$$

Here $\eta(\theta)$ is a random term which has mean zero, and represents the effects of having only a finite quantity of data, of size n, rather than the complete probability distribution. (I write it $\eta_n(\theta)$ as a reminder that different models are going to be affected differently by the same sampling fluctuations.) The problem, then, is that the model which minimizes the in-sample loss could be one with good generalization performance ($\mathbb{E}\left[L(\mathbf{Z}, \theta)\right]$ is small), or it could be one which got very lucky ($\eta_n(\theta)$ was large and negative):

$$\widehat{\theta_n} = \operatorname*{argmin}_{\theta \in \Theta} \left(\mathbb{E}\left[L(Z, \theta)\right] + \eta_n(\theta)\right) \tag{2}$$

We only want to minimize $\mathbb{E}\left[L(Z, \theta)\right]$, but we can't separate it from $\eta_n(\theta)$, so we're almost surely going to end up picking a $\widehat{\theta_n}$ which was more or less lucky ($\eta_n < 0$) as well as good ($\mathbb{E}\left[L(Z, \theta)\right]$ small). This is the reason why picking the model which best fits the data tends to exaggerate how well it will do in the future.

Again, by the law of large numbers $\eta_n(\theta) \to 0$ for each θ, but now we need to worry about how fast it's going to zero, and whether that rate depends on θ. Suppose we knew that $\min_\theta \eta_n(\theta) \to 0$, or $\max_\theta |\eta_n(\theta)| \to 0$. Then it would follow that $\eta_n(\widehat{\theta_n}) \to 0$, and the over-optimism in using the in-sample error to approximate the generalization error would at least be shrinking. If we knew how fast $\max_\theta |\eta_n(\theta)|$ was going to zero, we could even say something about how much bigger the true risk was likely to be. A lot of more advanced statistics and machine learning theory is thus about uniform laws of large numbers (showing $\max_\theta |\eta_n(\theta)| \to 0$) and rates of convergence.

Learning theory is a beautiful, deep, and practically important subject, but also subtle and involved one.[5] To stick closer to analyzing real data, and to not turn this into an advanced probability class, I will only talk about some more-or-less heuristic methods, which are good enough for many purposes.

3 Over-Fitting and Model Selection

The big problem with using the in-sample error is related to over-optimism, but at once trickier to grasp and more important. This is the problem of **over-fitting**. To illustrate it, let's start with Figure 1. This has the twenty X values

[5]Some comparatively easy starting points are Kearns and Vazirani (1994) or Cristianini and Shawe-Taylor (2000). At a more advanced level, look at the tutorial papers by Bousquet *et al.* (2004); von Luxburg and Schölkopf (2008), or the textbook by Vidyasagar (2003), or read the book by Vapnik (2000) (one of the founders), or take the class 10-702.

from a Gaussian distribution, and $Y = 7X^2 - 0.5X + \epsilon$, $\epsilon \sim \mathcal{N}(0,1)$. That is, the true regression curve is a parabola, with additive and independent Gaussian noise. Let's try fitting this — but pretend that we didn't know that the curve was a parabola. We'll try fitting polynomials of different orders in x — order 0 (a flat line), order 1 (a linear regression), order 2 (quadratic regression), up through order 9. Figure 3 shows the data with the polynomial curves, and Figure 3 shows the in-sample mean squared error as a function of the order of the polynomial.

Notice that the in-sample error goes down as the order of the polynomial increases; it has to. Every polynomial of order p is also a polynomial of order $p+1$, so going to a higher-order model can only reduce the in-sample error. Quite generally, in fact, as one uses more and more complex and flexible models, the in-sample error will get smaller and smaller.[6]

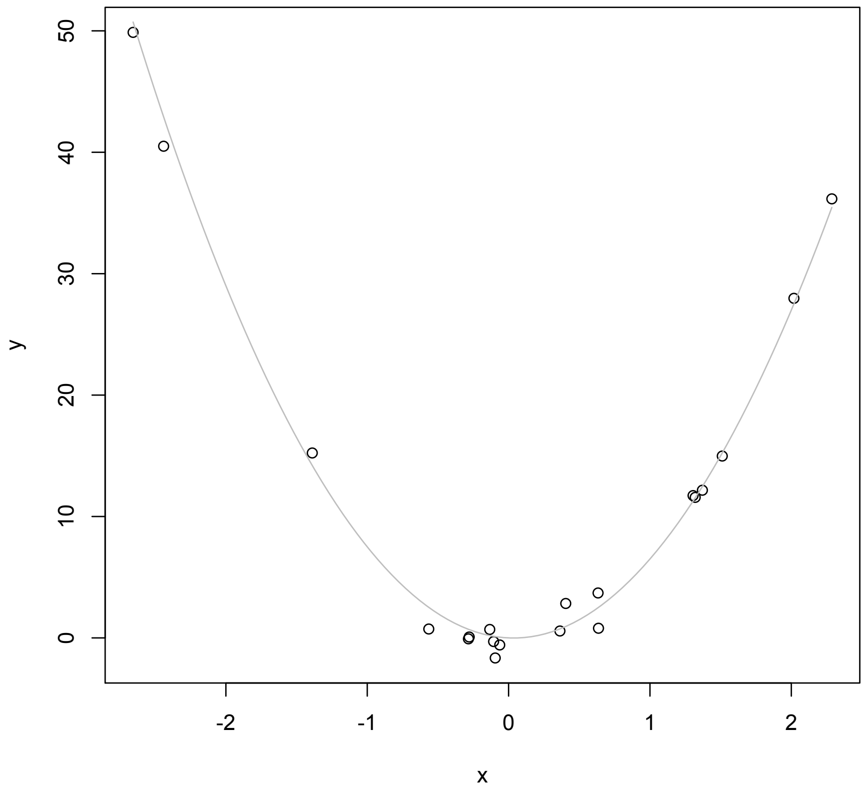
Things are quite different if we turn to the generalization error. In principle, I could calculate that for any of the models, since I know the true distribution, but it would involve calculating things like $\mathbb{E}\left[X^{18}\right]$, which won't be very illuminating. Instead, I will just draw a lot more data from the same source, twenty thousand data points in fact, and use the error of the old models on the new data as their generalization error. The results are in Figure 4.

What is happening here is that the higher-order polynomials — beyond order 2 — are not just a bit optimistic about how well they fit, they are *wildly* over-optimistic. The models which seemed to do notably better than a quadratic actually do much, much worse. If we picked a polynomial regression model based on in-sample fit, we'd chose the highest-order polynomial available, and suffer for it.

What's going on here is that the more complicated models — the higher-order polynomials, with more terms and parameters — were not actually fitting the *generalizable* features of the data. Instead, they were fitting the sampling noise, the accidents which don't repeat. That is, the more complicated models **over-fit** the data. In terms of our earlier notation, η is bigger for the more flexible models. The model which does best here is the quadratic, because the true regression function happens to be of that form. The more powerful, more flexible, higher-order polynomials were able to get closer to the training data, but that just meant matching the noise better. In terms of the bias-variance decomposition, the bias shrinks with the model order, but the variance of estimation grows.

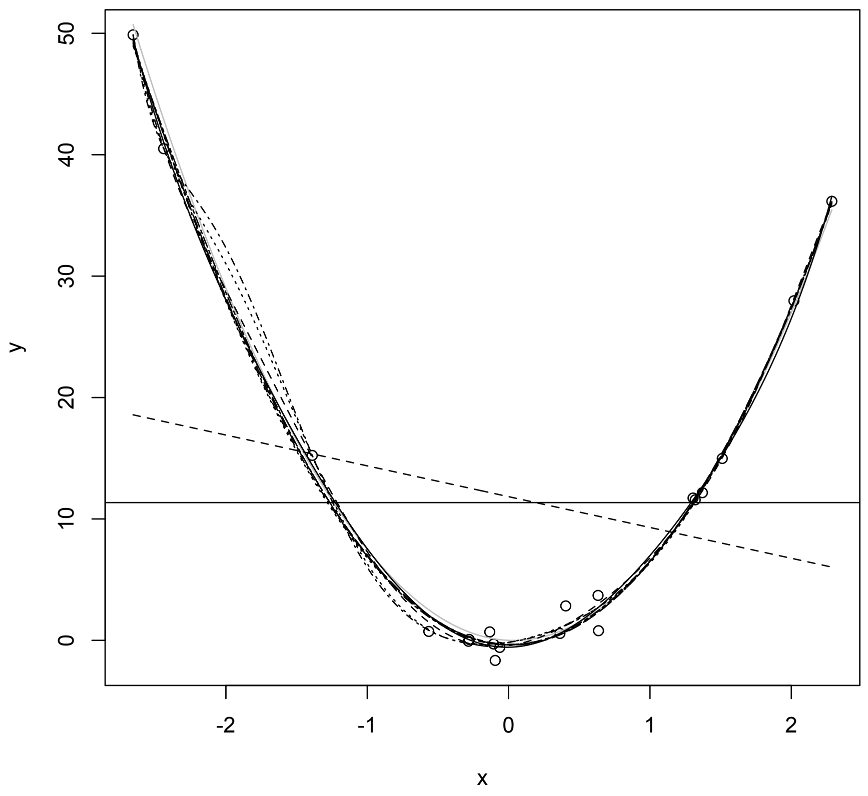
Notice that the models of order 0 and order 1 also do worse than the quadratic model — their problem is not over-fitting but *under*-fitting; they would do better if they were more flexible. Plots of generalization error like this usually have a minimum. If we have a choice of models — if we need to do **model selection** — we would like to find the minimum. Even if we do not have a *choice* of models, we might like to know how big the gap between our in-sample error and our generalization error is likely to be.

[6]In fact, since there are only 20 data points, they could all be fit exactly if the order of the polynomials went up to 19. (Remember that any two points define a line, any three points a parabola, etc. — $p+1$ points define a polynomial of order p which passes through them.)



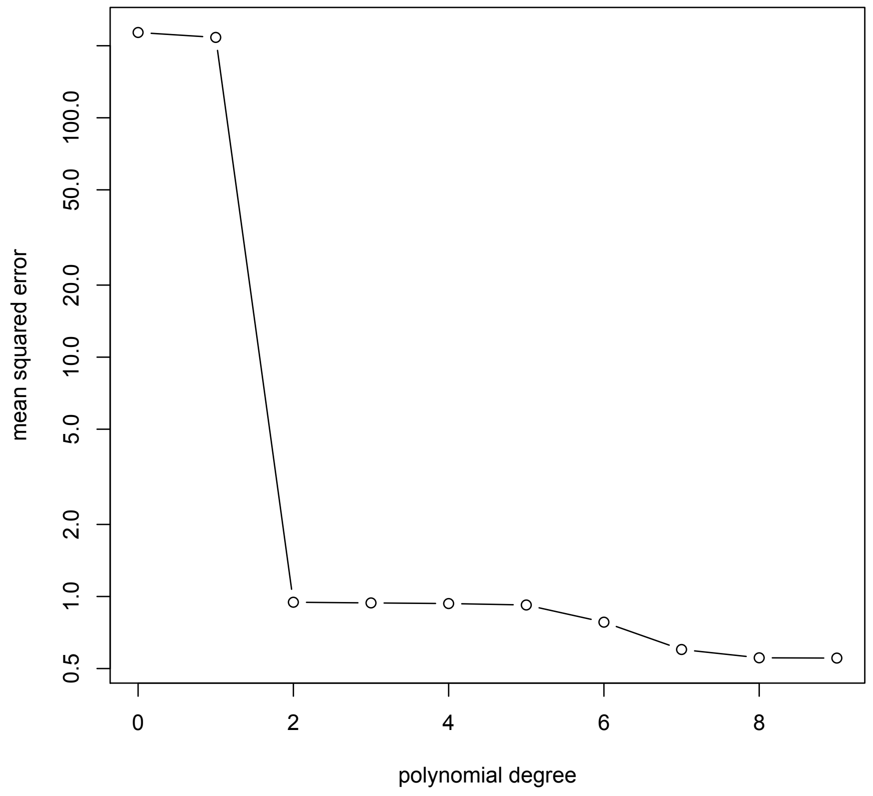
```
plot(x,y2)
curve(7*x^2-0.5*x,add=TRUE,col="grey")
```

Figure 1: Scatter-plot showing sample data and the true, quadratic regression curve (grey parabola).



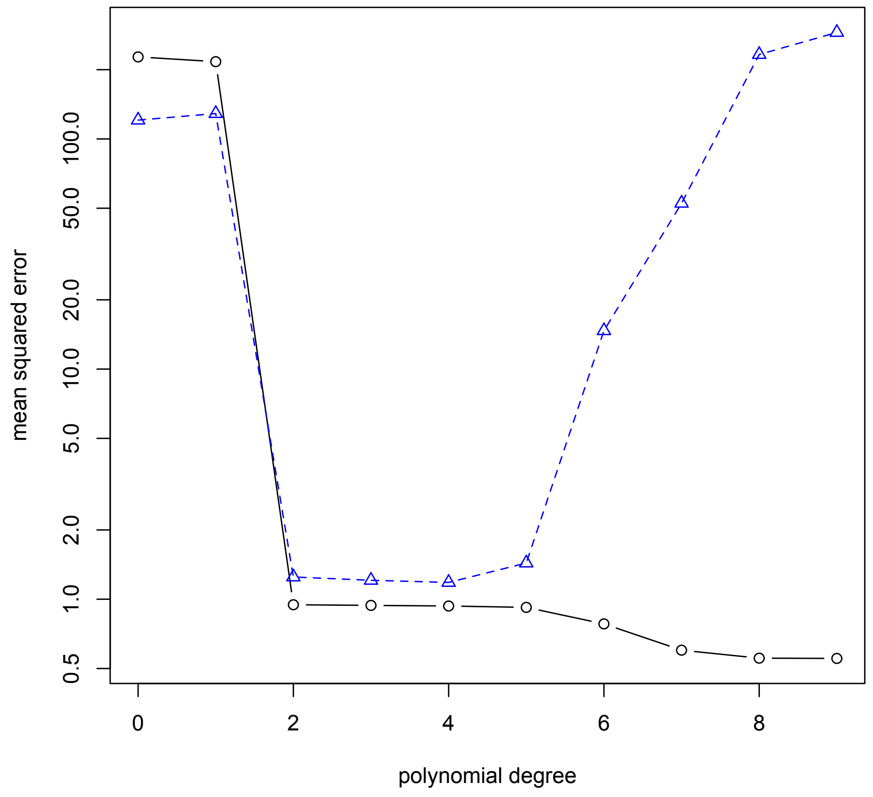
```
y2.0 = lm(y2 ~ 1)
abline(h=y2.0$coefficients[1])
d = seq(-2,2,length.out=200)
for (degree in 1:9) {
  fm = lm(y2 ~ poly(x,degree))
  assign(paste("y2",degree,sep="."), fm)
  lines(d, predict(fm,data.frame(x=d)),lty=(degree+1))
}
```

Figure 2: Twenty training data points (dots), and ten different fitted regression lines (polynomials of order 0 to 9, indicated by different line types). R NOTES: The `poly` command constructs orthogonal (uncorrelated) polynomials of the specified degree from its first argument; regressing on them is conceptually equivalent to regressing on $1, x, x^2, \ldots x^{\text{degree}}$, but more numerically stable. (See `help(poly)`.) This use of the `assign` and `paste` functions together is helpful for storing results which don't fit well into arrays.



```
mse.q = vector(length=10)
for (degree in 0:9) {
  # The get() function is the inverse to assign()
  fm = get(paste("y",degree,sep="."))
  mse.q[degree+1] = mean(residuals(fm)^2)
}
plot(0:9,mse.q,type="b",xlab="polynomial degree",ylab="mean squared error",
     log="y")
```

Figure 3: Degree of polynomial vs. its in-sample mean-squared error on the data from the previous figure. Note the logarithmic scale for the vertical axis.



```
gmse.q = vector(length=10)
for (degree in 0:9) {
  fm = get(paste("y",degree,sep="."))
  predictions = predict(fm,data.frame(x=x.new))
  resids = y.new - predictions
  gmse.q[degree+1] = mean(resids^2)
}
plot(0:9,mse.q,type="b",xlab="polynomial degree",
     ylab="mean squared error",log="y",ylim=c(min(mse.q),max(gmse.q)))
lines(0:9,gmse.q,lty=2,col="blue")
points(0:9,gmse.q,pch=24,col="blue")
```

Figure 4: In-sample error (black dots) compared to generalization error (blue triangles). Note the logarithmic scale for the vertical axis.

There is nothing special about polynomials here. All of the same lessons apply to variable selection in linear regression, to k-nearest neighbors (where we need to choose k), to kernel regression (where we need to choose the bandwidth), and to other methods we'll see later. In every case, there is going to be a minimum for the generalization error curve, which we'd like to find.

(A minimum with respect to what, though? In Figure 4, the horizontal axis is the model order, which here is the number of parameters (minus one). More generally, however, what we care about is some measure of how complex the model space is, which is not necessarily the same thing as the number of parameters. What's more relevant is how flexible the class of models is, how many different functions it can approximate. Linear polynomials can approximate a smaller set of functions than quadratics can, so the latter are more complex, or have higher **capacity**. More advanced learning theory has a number of ways of quantifying this, but the details are pretty arcane, so we will just use the concept of complexity or capacity informally.)

4 Cross-Validation

The most straightforward way to find the generalization error would be to do what I did above, and to use fresh, independent data from the same source — a **testing** or **validation** data-set. Call this $\mathbf{z}'_m$, as opposed to our training data $\mathbf{z}_n$. We fit our model to $\mathbf{z}_n$, and get $\widehat{\theta_n}$. The loss of this on the validation data is

$$\mathbb{E}\left[L(Z, \widehat{\theta_n})\right] + \eta'_m(\widehat{\theta_n})$$

where now the sampling noise on the *validation* set, η'_m, is independent of $\widehat{\theta_m}$. So this gives us an unbiased estimate of the generalization error, and, if m is large, a precise one. If we need to select one model from among many, we can pick the one which does best on the validation data, with confidence that we are not just over-fitting.

The problem with this approach is that we absolutely, positively, cannot use any of the validation data in estimating the model. Since collecting data is expensive — it takes time, effort, and usually money, organization and skill — this means getting a validation data set is expensive, and we often won't have that luxury.

4.1 Data-set Splitting

The next logical step, however, is to realize that we don't strictly need a separate validation set. We can just take our data and *split* it ourselves into training and testing sets. If we divide the data into two parts at random, we ensure that they have (as much as possible) the same distribution, and that they are independent of each other. Then we can act just as though we had a real validation set. Fitting to one part of the data, and evaluating on the other, gives us an unbiased estimate of generalization error.

4.2 Cross-Validation (CV)

The problem with data-set splitting is that, while it's an unbiased estimate of the risk, it is often a very noisy one. If we split the data evenly, then the test set has $n/2$ data points — we've cut in half the number of sample points we're averaging over. It would be nice if we could reduce that noise somewhat, especially if we are going to use this for model selection.

One solution to this, which is pretty much the industry standard, is what's called **k-fold cross-validation**. Pick a small integer k, usually 5 or 10, and divide the data at random into k equally-sized subsets. (The subsets are sometimes called "folds".) Take the first subset and make it the test set; fit the models to the rest of the data, and evaluate their predictions on the test set. Now make the second subset the test set and the rest of the training sets. Repeat until each subset has been the test set. At the end, average the performance across test sets. This is the cross-validated estimate of generalization error for each model. Model selection then picks the model with the smallest estimated risk.[7]

The reason cross-validation works is that it uses the existing data to simulate the process of generalizing to new data. If the full sample is large, then even the smaller portion of it in the training data is, with high probability, fairly representative of the data-generating process. *Randomly* dividing the data into training and test sets makes it very unlikely that the division is rigged to favor any one model class, over and above what it would do on real new data. Of course the original data set is never *perfectly* representative of the full data, and a smaller testing set is even less representative, so this isn't ideal, but the approximation is often quite good.

Cross-validation is probably the most widely-used method for model selection, and for picking control settings, in modern statistics. There are circumstances where it can fail — especially if you give it *too many* models to pick among — but it's the first thought of seasoned practitioners, and it should be your first thought, too. The homework to come will make you *very* familiar with it.

4.3 Leave-one-out Cross-Validation

Suppose we did k-fold cross-validation, but with $k = n$. Our testing sets would then consist of single points, and each point would be used in testing once. This is called **leave-one-out cross-validation**. It actually came before k-fold cross-validation, and has two advantages. First, it doesn't require any random number generation, or keeping track of which data point is in which subset. Second, and more importantly, because we are only testing on *one* data point, it's often possible to find what the prediction on the left-out point would be by

[7]A closely related procedure, sometimes also called "k-fold CV", is to pick $1/k$ of the data points at random to be the test set (using the rest as a training set), and then pick an *independent* $1/k$ of the data points as the test set, etc., repeating k times and averaging. The differences are subtle, but what's described in the main text makes sure that each point is used in the test set just once.

doing calculations on a model fit to the *whole* data. This means that we only have to fit each model once, rather than k times, which can be a big savings of computing time.

The drawback to leave-one-out CV is subtle but often decisive. Since each training set has $n-1$ points, any two training sets must share $n-2$ points. The models fit to those training sets tend to be strongly correlated with each other. Even though we are averaging n out-of-sample forecasts, those are correlated forecasts, so we are not really averaging away all that much noise. With k-fold CV, on the other hand, the fraction of data shared between any two training sets is just $\frac{k-2}{k-1}$, not $\frac{n-2}{n-1}$, so even though the number of terms being averaged is smaller, they are less correlated.

There are situations where this issue doesn't really matter, or where it's overwhelmed by leave-one-out's advantages in speed and simplicity, so there is certainly still a place for it, but one subordinate to k-fold CV.

5 Warnings

Some caveats are in order.

1. All the model selection methods we have discussed aim at getting models which *predict well*. This is not necessarily the same as getting the *true theory of the world*. Presumably the true theory will also predict well, but the converse does not necessarily follow. We will see examples later where false but low-capacity models, because they have such low variance of estimation, actually out-predict correctly specified models.

2. All of these model selection methods aim at getting models which will generalize well to new data, *if it follows the same distribution* as old data. Generalizing well even when distributions change is a much harder and much less well-understood problem (Quiñonero-Candela *et al.*, 2009). It is particularly troublesome for a lot of applications involving large numbers of human beings, because society keeps changing all the time — it's natural for the variables to vary, but the *relationships* between variables also changes. (That's history.)

6 Exercises

To think through, not to hand in.

1. Suppose that one of our model classes contains the true and correct model, but we also consider more complicated and flexible model classes. Does the bias-variance trade-off mean that we will over-shoot the true model, and always go for something more flexible, when we have enough data? (This would mean there was such a thing as *too much* data to be reliable.)

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