Evaluating Predictive Models

36-350, Data Mining

20 October 2008

1 Errors, In and Out of Sample

So far in the course, we have largely been concerned with descriptive models, which try to summarize our data in compact and comprehensible ways, with information retrieval, etc. We have seen some predictive models, in three forms:

- simple classifier algorithms (nearest neighbors and the prototype method), which try to predict discrete class labels;
- regression models (linear, kernel, nearest neighbor, generalizations of linear) which try to predict the mean value of a quantitative response variable[1]
- factor analysis, which tries to predict the *distribution* of a set of correlated quantitative variables, and so lets us guess the values of some variables from knowing the values of others.

Now, in the second half of the course, we are going to focus exclusively on predictive models, i.e., ones which make some kind of assertion about what will happen with new data.

With any predictive model, we can gauge how well it works by looking at its **accuracy**, or equivalently at its **errors**. For classification, the usual measure of error is the fraction of cases mis-classified, called the **mis-classification rate** or just the **error rate**.[2] For linear regression, the usual measure of error is the sum of squared errors, or equivalently $1 - R^2$, and the corresponding measure of accuracy is R^2. In the method of maximum likelihood, the accuracy is just the likelihood value, and the error is conventionally the negative log-likelihood. When a model predicts a whole distribution (as factor analysis does), the negative log-likelihood is the usual measure of error, though sometimes one will use a direct measure of the distance between the predicted and the observed distribution.

[1] Incidentally, we have only looked at predicting a single response variable, but we could predict a vector of responses in the same way.

[2] With our information-retrieval examples, we had *two* accuracy measures, precision and recall. This gives us two error rates. The raw mis-classification rate would just be their sum; we could however also look at both type I and type II errors, and try to make some trade-off between them.

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

- 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 never quite the true values (almost surely). But we can hope to make this source of imperfection smaller and smaller as we get more data.

- Our models are always more or less **mis-specified**, or, in plain words, wrong. We never 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] 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.

- Things change, even as we try to model them. In many scientific areas, we can hope to find and model invariant relationships, aspects of how the universe is put together that change very slowly, or not at all. The areas where people use data mining are, for the most part, not like that at all. In commercial applications, in particular, ten years is a very long time; conditions ten years ago were very different, twenty years ago were extremely different, and thirty years ago can seem like another world. None of you were alive *alive* thirty years ago, but trust me.[4] Yet, collecting daily observations, ten years is only 3652 sample points, which is not a lot when trying to fit a complicated model. Extending the data by looking in parallel at many different individuals or other units helps, but does not eliminate the fundamental problem. By the time our model comes to the end of its path and has converged, the world has moved on, and the data we used at the beginning is simply no longer relevant.

- The world just really is a noisy and stochastic place, and this means even the true, ideal model has non-zero error.[5] If $Y = \beta X + \epsilon$, $\epsilon \sim \mathcal{N}(0, \sigma^2)$, then σ^2 sets a limit on how well Y can be predicted, and nothing will get us below that limit.

  Exercise: Express the R^2 of the true model as a function of σ^2 and $\mathrm{Var}[X]$.

So, because our models are flawed, and the world they are trying to model is both stochastic and changing, we can not expect even the best model to have

[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, and anyway the next point applies.

[4] Interestingly, the same statement could have been truthfully made at any point in the last 150 or even 200 years. So the fact of rapid change seems, itself, to be a constant of industrial society.

[5] 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 coarsens shows up as randomness. For details, if you care, take 36-462 next semester.

zero error all the time. Instead, we would like to minimize the **expected error**, or **risk**, on future data.

If we didn't care about *future* data specifically, minimizing expected error would be easy. We have various possible models, each with different parameter settings, conventionally written θ. We also have a collection of data $x_1, x_2, \ldots x_n \equiv \mathbf{x}$. For each possible model, then, we can compute the error on the data, $L(\mathbf{x}, \theta)$, called the **in-sample loss** or the **empirical risk**. The simplest strategy is then to pick the model, the value of θ, which minimizes the in-sample loss. This strategy is imaginatively called **empirical risk minimization**. This means picking the classifier with the lowest in-sample error rate, or the regression which minimizes the sum of squared errors, or the likelihood-maximizing parameter value — what you've usually done in statistics courses so far.

There is however a potential problem here, because $L(\mathbf{x}, \theta)$ is not what we *really* want to minimize. Past data is, after all, past, and "let the dead bury the data"; we care about what will happen in the future. That is, $\mathbb{E}[L(\mathbf{X}, \theta)]$, the *expected* loss on new data drawn from the same distribution. This is also called the risk, as I said, or the **out-of-sample loss**, or the **generalization error** (because it involves generalizing from the old data to new data). The in-sample loss equals the risk plus sampling noise:

$$L(\mathbf{x}, \theta) = \mathbb{E}[L(\mathbf{X}, \theta)] + \eta_n(\theta)$$

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 effected 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 ($\mathbb{E}[L(\mathbf{X}, \theta)]$ is small), or it could be one which got very lucky ($\eta_n(\theta)$ was large and negative).

We hope that $\eta_n(\theta) \to 0$ as $n \to \infty$. This hope rests on the law of large numbers, at least if the error measure L is not too complicated. This is not *quite* enough for empirical risk minimization to work, i.e., for the parameter value which minimizes the in-sample risk to converge on the one which minimizes the out-of-sample risk. The complication is that the *rate* at which $\eta_n(\theta)$ goes to zero can depend on θ. The faster the rate at which these fluctuations die away, the easier it is to estimate a model's generalization error. When the rates change with θ, it becomes unclear whether a model which did well in-sample is really good, or just from a part of the parameter space where performance is hard to discern. The main tools of statistical learning theory are therefore *uniform* laws of large numbers, which control the size of the fluctuations $\eta_n(\theta)$ for all θ simultaneously.

Learning theory is a beautiful, deep, and practically important subject, but also subtle and involved one.[6] Rather than try to explain Vapnik-Chervonenkis

[6] Some comparatively easy starting points are Kearns and Vazirani (1994) or Cristianini and Shawe-Taylor (2000). At a more advanced level, look at the review paper by Bousquet *et al.* (2004), or read the book by Vapnik (2000) (one of the founders), or take the class 36-712.

dimension and empirical process theory at this level, I will stick with some more-or-less heuristic methods, which are generally good enough for many purposes.

2 Some Examples: Over-Fitting and Under-Fitting

To see how these distinctions between in-sample and out-of-sample performance can matter, consider choosing among different classes of models — also called **model selection**. We are fortunate enough to have in our possession twenty labeled data points, with covariates and a response, and all we have to do is guess the response variable. We recognize this as a supervised learning problem, specifically regression, so we try different regression models. In fact, we try ten different polynomial regressions, running from a constant prediction through a linear model up to polynomials of order nine. Figure 1 shows the results.

Looking at the figure suggests that the higher-order polynomials give better fits. In fact, this has to be true, since we're (i) looking for the *best*-fitting polynomial of a given order, and (ii) every lower-order polynomial is a special case of the higher-order ones. We can confirm this by looking at the mean squared error (= residual sum of squares/n), as in Figure 2.

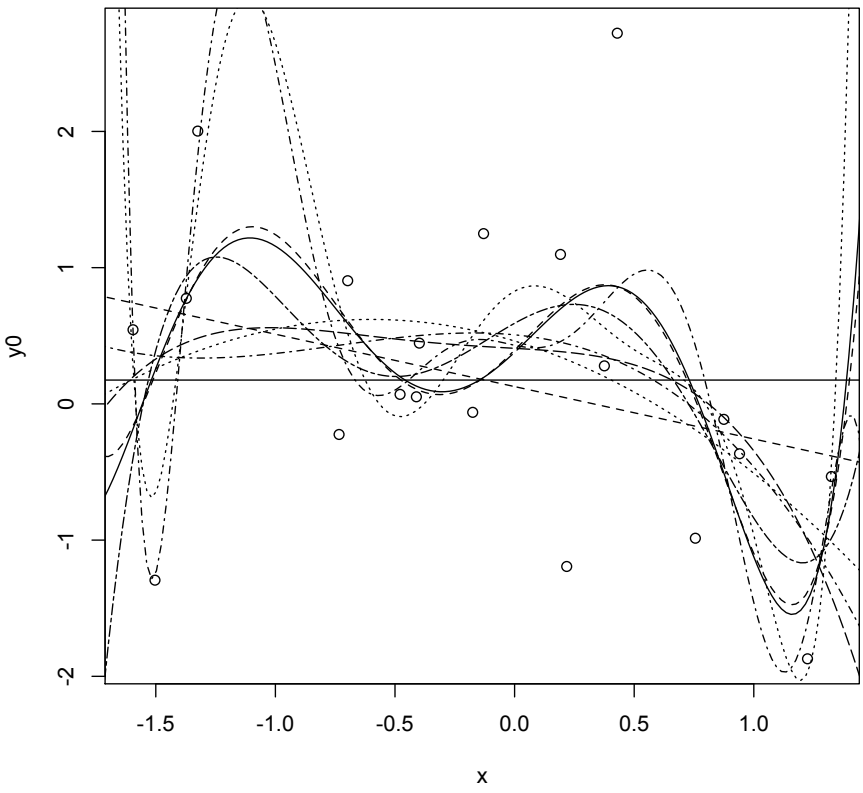
Since there are only twenty data points, if I continued this out to polynomials of degree twenty, I could get the mean squared error down to zero, apparently perfect prediction. That this is *not* a good idea becomes clear when we take these models and try to generalize to new data, such as an extra 200 data points drawn from exactly the same distribution. Let's begin by just adding the generalization error to the previous plot (Figure 3).

Since all o the error measurements don't fit on the same plot, we expand the vertical range... but they still don't fit (Figure 3). Switching to a logarithmically-scaled vertical axis (Figure 5), we see that the generalization error grows very rapidly indeed with the order of the polynomial — and it *only* grows. To get a sense of what's going wrong, let's go back to our scatterplot-plus-estimated-curves figure, and add the new data points (Figure 6).

Notice, first of all, that the fits now all look horrible. Some of the estimated curves come quite close to the training data (black circles), but none of them bear any particular relation to the testing data (blue triangles). Notice, second of all, that all of the curves zoom off to $\pm\infty$ as we go away from the center of the data, except for the flat line belonging to the constant, order-0 polynomial. This is part of why the higher order polynomials do so incredibly badly: they're blowing up outside the range of the original sample, which is to say where a non-trivial number of the new data are.

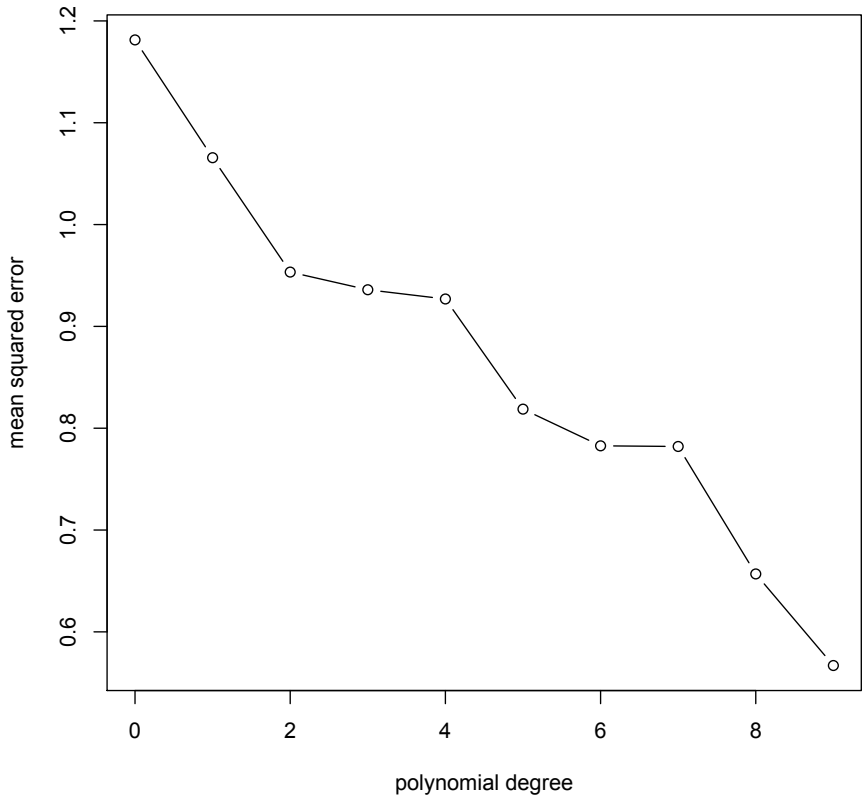
However, the blowing-up issue isn't the whole story. The next figure shows what happens when we only include testing data points that fall within the original range. (We don't usually have this kind of luxury in reality, of course.) The generalization error *still* climbs with the polynomial order, though less dizzyingly. Why?

What's going on here is that the more complicated models — the higher-order polynomials, with more terms and parameters — were not actually fitting




```
plot(x,y0)
y0.0 = lm(y0 ~ 1)
abline(h=y0.f0$coefficients[1])
d = seq(-2,2,length.out=200)
for (degree in 1:9) {
fm = lm(y0 ~ poly(x,degree))
assign(paste("y0",degree,sep="."), fm)
lines(d, predict(fm,data.frame(x=d)),lty=(degree+1))
}
```

Figure 1: 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 = vector(length=10)
for (degree in 0:9) {
fm = get(paste("y0",degree,sep="."))
mse[degree+1] = mean(summary(fm)$residuals^2)
}
plot(0:9,mse,type="b",xlab="polynomial degree",
     ylab="mean squared error")
```

Figure 2: In-sample mean squared error of the different polynomials on the data in Figure 1.

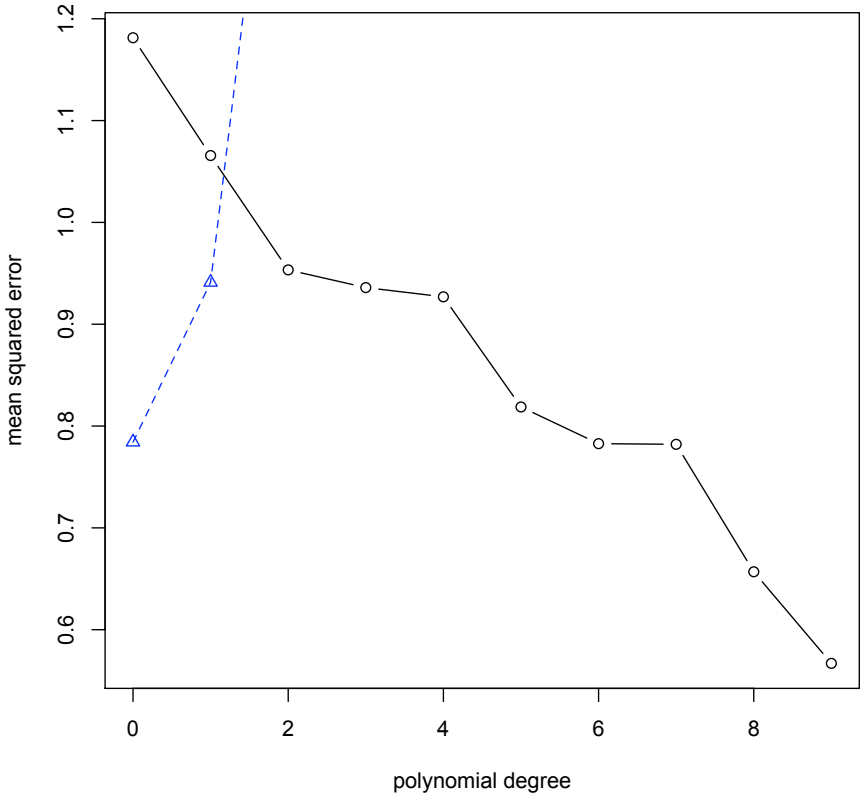


Figure 3: Mean-squared errors for the models in the previous figure, adding out-of-sample, generalization error in blue triangles.

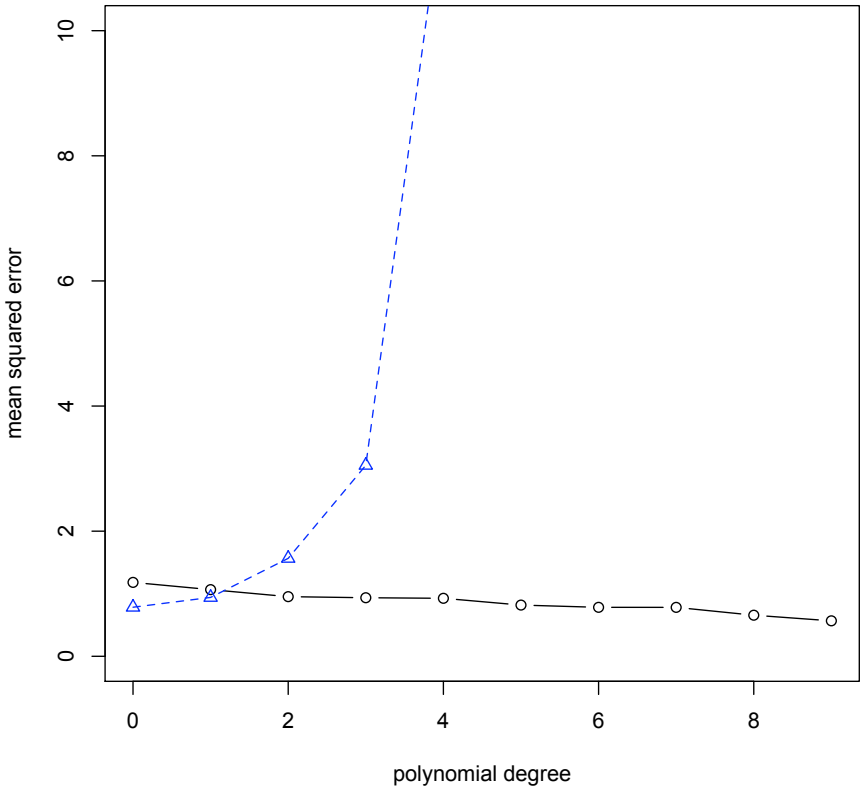


Figure 4: As in the previous figure, but with the vertical range expanded.

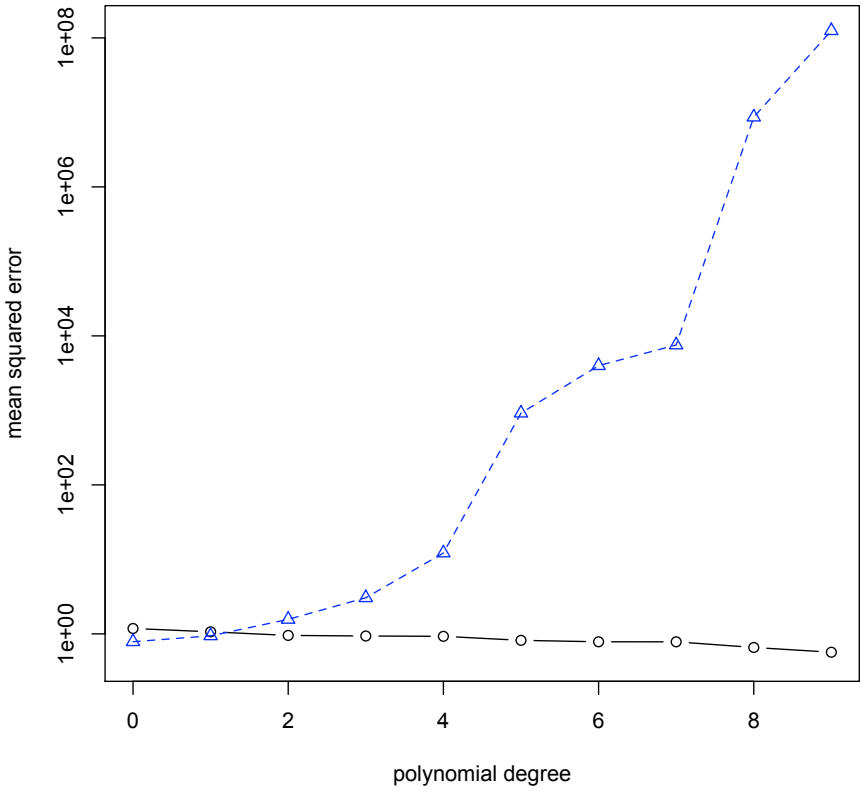


Figure 5: As in the previous figure, but with a log scale on the vertical axis.

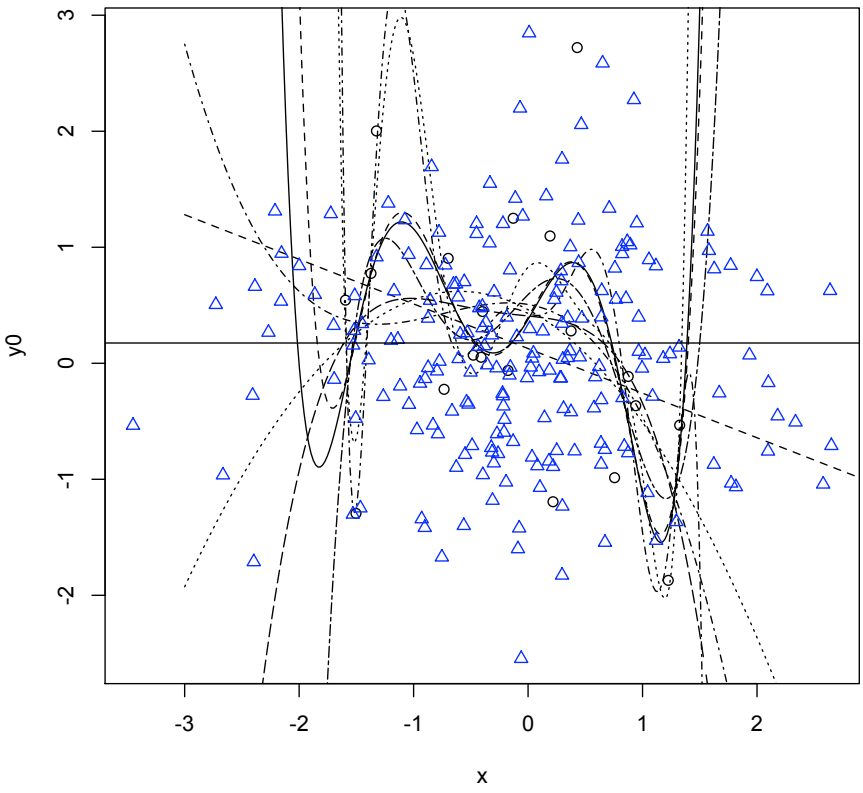


Figure 6: Data and polynomial curves from Figure 1, plus new data from the same source (blue triangles). Note the change in scale on both axes.

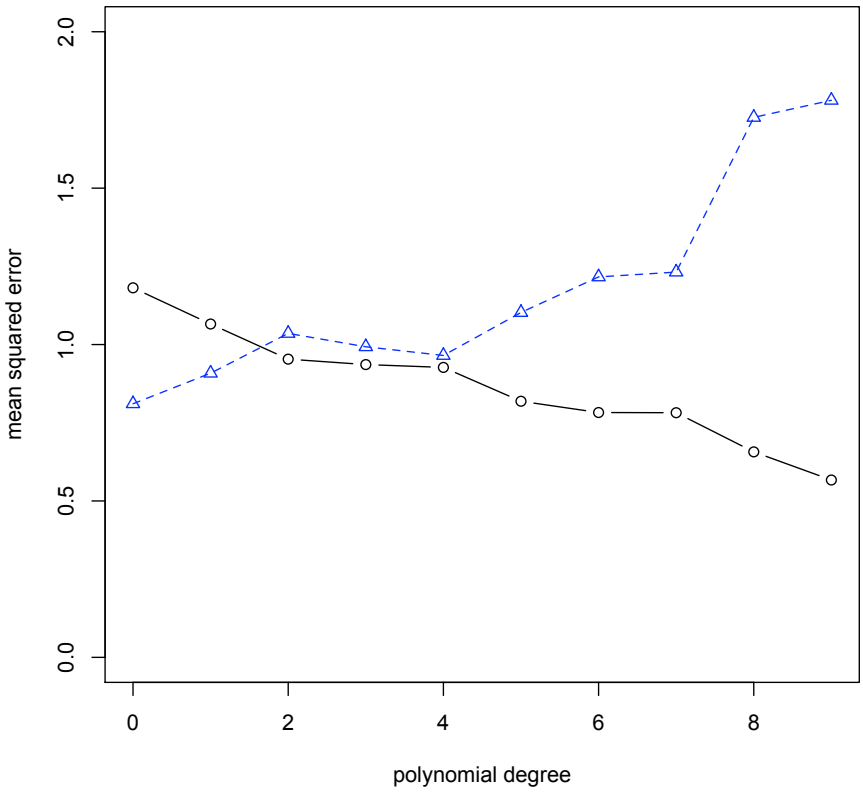


Figure 7: Generalization error, as in Figure 4, but only evaluated on points which fall within the same range as the training set.

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 flat-line, constant model, because the true regression function happens to be of that form — X and Y are independent standard Gaussians. 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. The dumber models lack the same ability to fit the data, but by the same token it's much harder for them to *over*-fit.

Does this mean that simpler is always best? No. Consider the data in Figure 8. This has the same X values as before, but now $Y = 7X^2 - 0.5X + \epsilon$, $\epsilon \sim \mathcal{N}(0,1)$. That is, the true regression curve is quadratic. We can repeat the same steps with the new data.

Looking at the plot of mean squared error versus polynomial degree, we see that much of it is similar to the same plot for the case where the right model is a zeroth-order polynomial: the in-sample error declines monotonically as the order of the model grows. That is, yet again, higher-order polynomials have more flexibility, and so more capacity to match the data. Out of sample, adding too much capacity leads to huge errors. The best generalization performance comes from using the right model class (here, second-order polynomials). The difference, now, is that it's possible to have too little capacity, as with zeroth- and first- order models. These also do badly on future data, because they are **under-fit**. This is the more usual case; when we can plot the generalization error versus model capacity, it usually has a minimum.

In these two cases, we get our best generalization performance by using the correct model class. This is possible because our models are well-specified. What if the true regression function does not belong to any class of model available to us? Then there is still generally a capacity/error minimum, but the location of the minimum, i.e., which model class generalizes best, can depend on the sample size.

To understand why, remember that we can always decompose the mean-squared error into bias (squared) plus variance. (Similar decompositions hold for other error measures.) If none of our model classes contain the truth, they are all more or less biased; the size of the bias does not, however, depend on n — it's basically the mis-match between the best model in that class and the truth. The variance term does depend on n — it's related to η_n. Since high-capacity models start with large values of η_n when n is small, their *total* generalization error can be larger than that of low-capacity models. As n grows, however, their variance penalty declines, and their superior flexibility (smaller bias) takes over. (If this isn't clear now, wait for the homework!)

Exercise: Why does the argument above break down when the true model *does* belong to one of our model classes?

There is nothing special about polynomials here. All of the same lessons apply to any other flexible family of models, such as k-nearest neighbors (where we need to choose k), or kernel regression (where we need to choose the bandwidth), or local linear regression (where we need to choose the smoothing range), or fac-

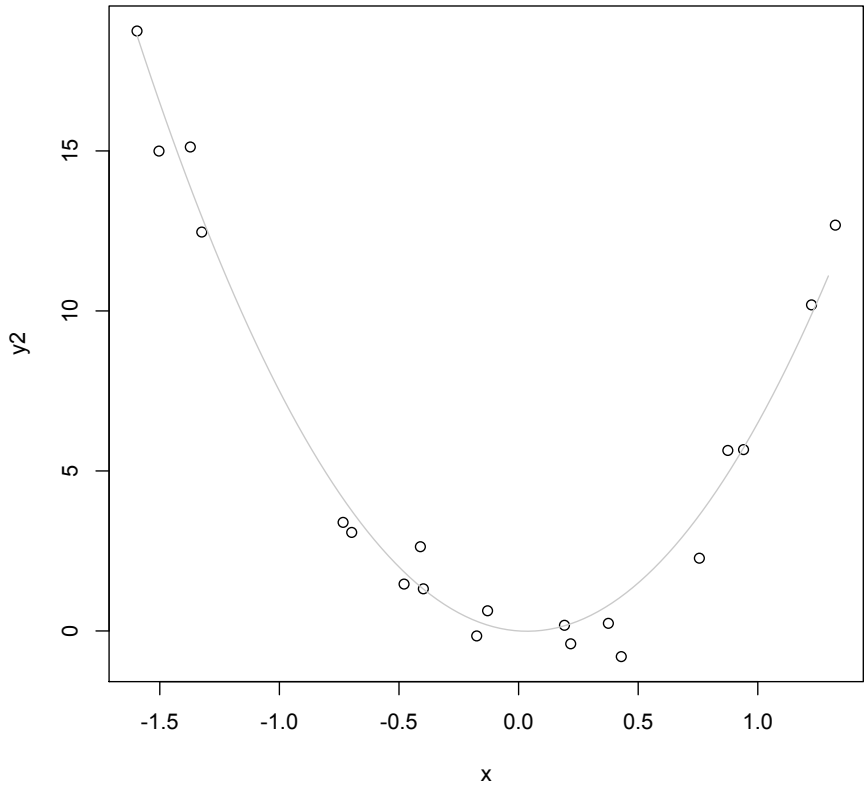


Figure 8: Scatter-plot showing sample data and the true, quadratic regression curve (grey parabola).

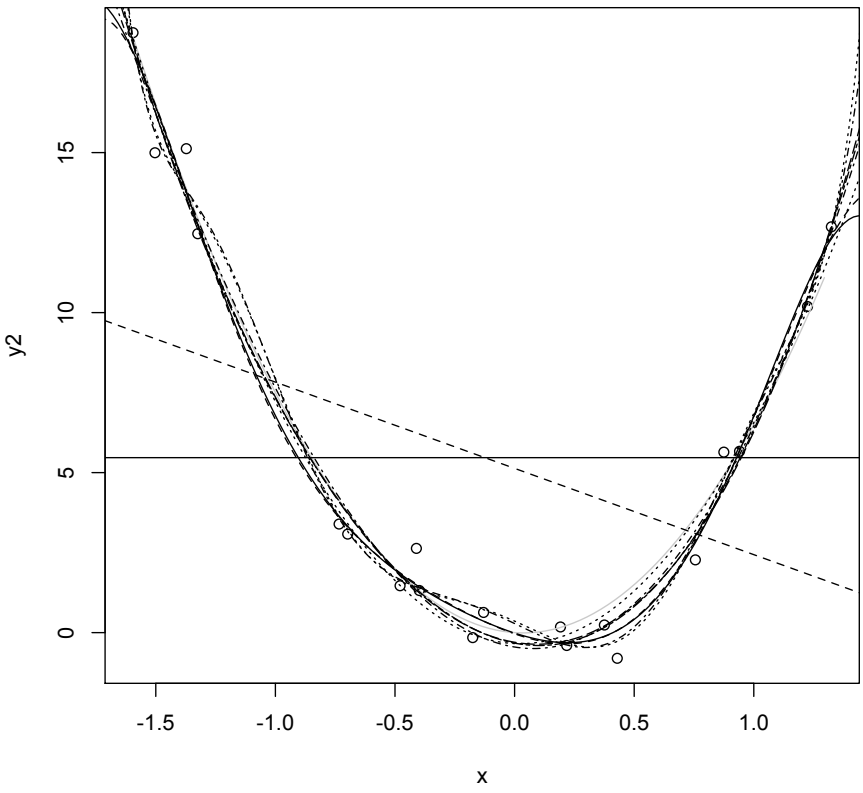


Figure 9: Polynomial fits to the data in the previous figure.

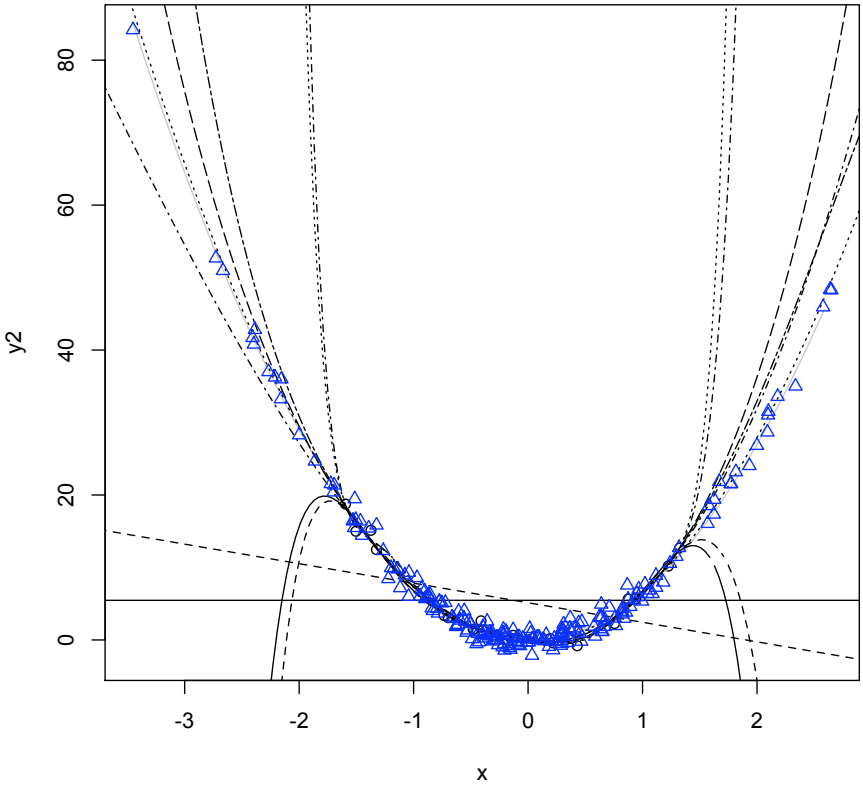


Figure 10: Previous figure, with addition of new data points (blue triangles). This figure has zoomed out to show the range of the new data, which helps distinguish the different regression curves.

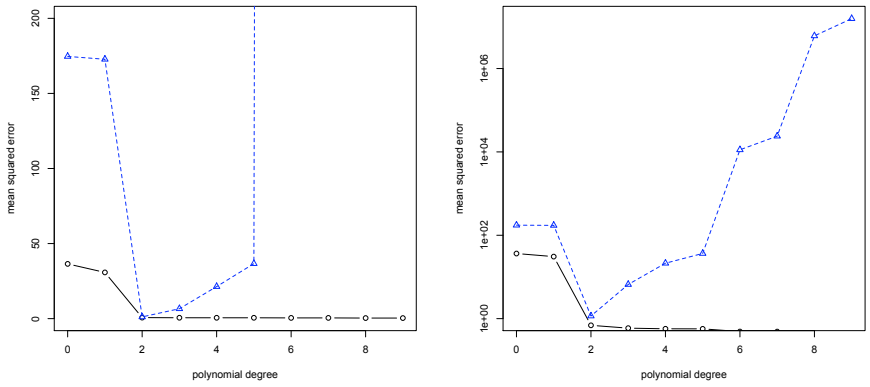


Figure 11: In-sample and generalization error for the quadratic case. The left-hand plot shows the mean squared error (black for in-sample, blue for generalization) on a linear scale; the right-hand plot uses a logarithmic scale.

tor analysis (where we need to choose the number of factors), or other methods we'll see later.

3 Model Selection and Capacity Control

The biggest single problem with making data mining work is bad data. The *second* biggest problem is controlling model capacity, making sure it's neither so small that we're missing useful and exploitable patterns, nor so large that we are confusing pattern and noise.

How can we do this?

3.1 Some Model Selection Methods

Big Data The simplest approach to dealing with over-fitting is to hope that it will go away. As we get more and more data, the law of large numbers (and other limit theorems) tell us that it should become more and more representative of the true data-generating distribution, *assuming there is one*. Thus, η, the difference between the empirical risk and the generalization risk, should grow smaller and smaller. If you are dealing with a *lot* of data, you can hope that η is very small, and that minimizing the in-sample loss will give you a model which generalizes *almost* as well as possible. Unfortunately, if your model is very flexible, "lots of data" can be exponentially large.

A slightly more subtle point is what happens in cases like the polynomials, where the larger-capacity models always have better fits. Then empirical risk minimization will always select the largest-capacity model class you let it. If that maximum capacity is fixed, this can be OK: suppose the real regression

function is quadratic, but we allow polynomials of up to order twenty. Empirical risk minimization will always pick the model of order 20, but as the data grows more and more of the terms in that model (20-3 = 17, to be precise) will be shrinking to zero, and we'll be getting a closer and closer approximation to the correct cubic. If we knew it was a cubic we could do better by setting those terms exactly to zero — they're adding variance without reducing bias — but, with enough data, this works OK.

This same idea can apply even when it seems like we're not doing model selection, as when we do a big linear regression of a response on a whole mess of variables. With enough data, the coefficients which should be zero will all become small, and have little influence on our predictions, *so long as new data has the same distribution as the old*.

This approach, however, will generally fail if we allow the classes of models to grow as we consider more data, or if we have an infinite collection of model classes to start with. We can always fit n data points exactly with an n^{th} order polynomial, so without a limit on the order we always select a curve which goes exactly through the training data and generalizes horribly.

Penalization The next bright idea is to say that if the problem is over-flexible models, we should penalize flexibility. That is, instead of minimizing $L(x, \theta)$, minimize $L(x, \theta) + \lambda g(\theta)$, where $g(\theta)$ is some kind of indication of the complexity or flexibility of θ, say the number of parameters, and λ is our trade-off factor. Standard linear regression packages implement a simple scheme like this in the form of "adjusted R^2."[7]

Two more refined ideas for regression are called **ridge regression**, where the penalized error measure is

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - x_i\theta))^2 + \lambda\sum_{j=1}^{p}\theta_j^2$$

and the **lasso**,

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - x_i\theta))^2 + \lambda\sum_{j=1}^{p}|\theta_j|$$

In both cases, the penalty "marks down" models which give lots of weight to many predictors, compared to those with smaller coefficients but similar errors. The lasso, in particular, tends to shrink regression coefficients to zero when it can. The trade-off here is controlled by λ, which becomes another adjustable

[7]The idea there is that adding an extra predictor variable can never increase the residual sum of squares. (We can always get our old solution back by setting the coefficient equal to zero.) So R^2, in sample, must be a non-increasing function of the number of independent variables. Assume that the real regression coefficient of the variable we're adding is zero, and a lot of extra assumptions like independent Gaussian noise, we can calculate the expected increase in R^2 when we go from p to $p+1$ independent variables, and the true regression coefficient on the $p+1^{\text{st}}$ variable is zero. This expected decrease in the RSS is what adjusted R^2 is adjusted by.

control setting, and so it needs to be picked by some other method; the usual approach is cross-validation.

Capacity Control Penalization can work very well, but the trick is in choosing the penalty term; the number of parameters is often used but *not* always appropriate, though it is in the polynomial example. The real issue is what I have already referred to a few times as **capacity**. Roughly speaking, the idea is that a class of models has high capacity if changing the data a little bit gives rise to a very different model, i.e., one which makes very different predictions. A more exact view is to look at *how many* distinct models we can get by changing the data, where "distinct" involves setting some threshold on how different the models' predictions must be. Low-capacity model classes are insensitive to the data, and the number of distinct models grows only slowly with the number of data points. High-capacity model classes are very sensitive to the data.[8] The trade-off, again, is between have a (potentially) high bias, and having a high variance — between under-fitting and over-fitting.

Capacity, in this sense, is *often* related to the number of parameters, but not always. There are examples (not crazy ones, even) of model classes with one adjustable parameter whose capacity is, in fact, infinite, making generalization very difficult indeed.[9] In the case of things like kernel regression or nearest neighbors, choosing a large neighborhood (high k or high bandwidth) reduces the capacity, by making the model less sensitive to the data.

All of this suggests that a reasonable kind of penalty to apply would be an estimate of how big $\eta_n(\theta)$ can get. All else being equal, this will be large for high-capacity model classes, and it will shrink as n grows. Statistical learning theory provides tools for estimating those penalties, and the resulting strategy is called **structural risk minimization**. However, computing capacity-based penalties is hard, because one needs to know the capacities of different model classes, which are generally quite difficult to compute. (Trust me, or read the references, or take 36-712.)

Cross-Validation Since we often aren't in a position to use real capacity-based penalties, what shall we do instead? A short-cut trick, which is often reliable and in some ways is the industry standard, is to simulate the process of fitting to different data sets and seeing how different the predictions can be.

Divide your data at random into two parts. Call the first part the **training** set, and use it to fit your models. Then evaluate their performance on the other part, the **testing** set. Because you divided the data up randomly, the performance on the test data should be an *unbiased* estimate of the generalization performance. (But, unbiased doesn't necessarily mean "close".) In

[8] To be really precise, we need to consider not just the scaling with the number of data points but also the scaling with the cut-off for being distinct models, except in the case of classification where the outputs are discrete. See Vapnik (2000) for details.

[9] The canonical example is to take classifiers which output 1 if $\sin ax$ is positive and 0 otherwise. That is, the classes correspond to two halves of a periodic cycle. By adjusting a, one can always match the classes on *any* collection of binary-labeled data.

fact, you can do this multiple times, say selecting 90% of the data at random to be the training set, testing on the remaining 10%, and then repeating this ten times, with different choices of training and test sets, and picking the model which comes out best when averaged over these ten trials; this is called **ten-fold cross-validation**. (There is nothing magic about ten, it's just large enough to get a bit of averaging but small enough to usually run in decent time.)

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.

(Of course, all of this assumes that the original data is in fact a representative sample of the data we will be applying our models to in the future — that our data-generating process isn't biased, that there isn't too much dependence between data points, etc.)

Why Chose? Alternately, we can refuse to pick *a* model at all, and simply average all the ones we feel like fitting. We'll say more about this later.

3.2 Warnings

Two 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.

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. (This relates to the first problem, of course.)

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