Chapter 14

Optimization and Complexity

We start this chapter by taking up our hamster population model from earlier and reconsidering it. As you recall, your friend requested our help in constructing a model to simulate the population of the endangered Aquatic Hamsters. There are many ways to exploit valuable empirical data to improve your models. For instance, if we had data on hamster fecundity, we might be able to plug that information in directly as a parameter in our hamster population model.

One of the most useful kinds of empirical data is historical time series. Some of these time series might represent data and factors that feed into the model, but are not directly modeled. For example, we might have historical temperature data. The temperature could be an important thing to include in the model, as it would affect hamster survival however it is not something we directly model. By this we mean that we do not expect our hamsters to have any effect on the temperature in the region but we do expect the temperature to have an effect on the hamsters. Thus, we can feed the temperature data into the model. We can do this by importing this historical temperature data and including it in the model using a converter primitive.

In other cases, the historical data may represent factors you are directly trying to model. For example, we have a data series of biannual hamster population surveys going back 20 years. This data series lets us know roughly how many hamsters there were over time. Because we are trying to model this data, it is not something plug directly into our model as we could with the temperature, but it is something we can use to calibrate and assess the accuracy of our model.

How do we do this and what will be the results?

Assessing Model Accuracy

We first import our historical data into a converter primitive. We then assess the accuracy of the model in two ways: qualitatively and quantitatively. To assess how well our model fits the historical data qualitatively we plot the simulated and historical data series next to each other. Ideally, they will match up closely but if they do not we should pay close attention to how they differ.

If they have the same general shape (except for a vertical or horizontal displacement) that is good news, as it indicates that you may have gotten the general dynamics of your model correct and that you may just need to fine-tune the relationships and parameter values. If the results look considerably different you may have more work to do in improving the model.

You can also assess the accuracy of models quantitatively. One standard tool people use to assess the accuracy of a model is the R^2 metric[1]. R^2 is the fraction of the squared error explained by the model compared to the "null" model. It ranges from 0 (the model basically provides no predictive power), to 1 (the model predicts perfectly). Mathematically, R^2 is calculated like so:

$$R^2 = \sum_t \frac{(\overline{\text{Truth}} - \text{Truth})^2 - (\text{Model} - \text{Truth})^2}{(\overline{\text{Truth}} - \text{Truth})^2}$$

Naively used, R^2 has a number of issues that we will discuss later in this chapter. However, it is still a useful tool that many people use and with which they are familiar. It is also relatively straightforward to calculate. The following code calculates an R^2 for a model fit. This is code written in JavaScript and can be placed as the **Action** for a button primitive in Insight Maker. The code is written assuming two primitives: a converter [**Historical Hamsters**] containing historical population sizes and a stock [**Hamsters**] containing simulated population sizes. You can edit the code to reference the actual names of the primitives in your model.

```
var simulated = findName("Hamsters"); // Replace with your primitive name
var historical = findName("Historical Hamsters"); // Replace with your primitive name

var results = runModel({silent: true});

var sum = 0;
for(var t = 0; t < results.periods; t++){
    sum += results.value(historical)[t];
}

var average = sum/results.periods;

var nullError = 0;
var simulatedError = 0;
for(var t = 0; t < results.periods; t++){
```

[1]Though this metric is not often used in systems dynamics or agent-based models, it is widely used for statistical models such as linear regressions.

```
    nullError += Math.pow(results.value(historical)[t] - average, 2);
    simulatedError += Math.pow(results.value(historical)[t] - results.value(simulated)[t], 2)
}

showMessage("Pseudo R^2: "+((nullError-simulatedError)/nullError));
```

Calibrating the Model

In addition to using historical data to assess the model fit, you can also use historical data to calibrate model parameters. Depending on the model, you may have many parameters for which you do not have a good way to determine their values. Earlier, we discussed how to use sensitivity testing to assess whether our results are resilient to this uncertainty and to build confidence in the model. Another way to build confidence in your parameter values is, instead of guessing the values of these uncertain parameters, to choose the set of values that results in the best fit between simulated and historical data. This is a semi-objective criterion that helps to remove personal biases you might have from the modeling process.

Goodness of Fit

The first step to using historical data to calibrate the model parameters is to understand what is meant by "the best fit" between historical and simulated data. Conceptually, the idea of a "good fit" seems obvious. A good fit is one where the historical and simulated results are very close together (a *perfect* fit is when they are the same, but that is generally more than we can hope for). However, putting a precise mathematical definition on the concept is not trivial.

Many commonly used goodness of fit measures exist, and below we list some key ones.

Squared Error

Squared error is probably the most widely used of all measures of fit[2]. To calculate the squared error we carry out the following procedure. For each time period we take the difference between the historical data value and the simulated value and then we square that difference. We then sum up all these differences to obtain the total error for the fit. Higher totals indicate worse fits, and lower totals indicate better fits.

The following equation could be placed in a variable to calculate the squared error between a primitive named [**Simulated**] and one named [**Historical**]:

```
([Simulated]-[Historical])^2
```

[2]The key reason for this is that regular linear regression (ordinary least squares, the most widely used modeling tool) uses squared error as its measure of goodness of fit. Doing so simplifies the mathematics of the regression problem greatly in the linear case.

Please note that maximizing the R^2 measure we described earlier is equivalent to minimizing the squared error.

Absolute Value Error

A characteristic of squared error is that outliers have high penalties compared to other data points. Outliers are points in time where the fit is unusually bad. Since the squared error metric squares the differences between simulated and historical data, large differences can cause even larger amounts of error when they are squared. This can sometimes be a negative feature of squared error if you do not want to outliers to have special prominence and weight in the analysis.

An alternative to squared error that treats all types of differences the same is the absolute value error. Here, the absolute value of the difference between the simulated and historical data series is taken. The following equation could be placed in a variable to calculate the absolute value error between a primitive named [**Simulated**] and one named [**Historical**]:

```
Abs([Simulated]-[Historical])
```

Other Approaches

Many other techniques are available for measuring error or assessing goodness of fit. Most statistical approaches function by specifying a full probability model for the data and then taking the goodness of fit not as a measure of error, but rather as the *likelihood*[3] of observing the results we saw given the parameter values. To be clear the issue of optimizing parameter values for models is one that is more complex than what we have presented here. Many sources of error exist in time series and analyzing them is a very complex, statistical challenge. The basic techniques we have presented are, however, useful tools that serve as gateways towards further analytical work.

Finding the Best Fit

After choosing how to measure the quality of a fit quantitatively, we need to find the set of parameter values that maximize the fit and minimize the error. To do this we use a computer algorithm called an optimizer that automatically experiments with many different combinations of parameter values to find the set of parameters that has the best fit.

Many optimizers basically work by starting with an initial combination of parameter values and measuring the error for that combination. The optimizer then slightly changes the parameter values in order to check the error at nearby combinations of parameter values. For instance, if you are optimizing one

[3]Likelihood is a technical statistical term. It can be roughly thought of as equivalent to "probability", though it is not precisely that.

parameter, say the hamster birth rate, and your initial starting value is a birth rate of 20% per year; the optimizer will first measure the error at 20% and then measure the errors at 19% and 21%.

If one of the neighbors has a lower error than the initial starting point, the optimizer will keep testing additional values in that direction. It will steadily "move" towards the combination of parameters that results in the lowest error, one step at a time. If, however, the optimizer does not find any nearby combination of parameter values with a lower error than its current combination of parameter values, it will assume it has found the optimal combination of parameter values and stop searching for anything better.

The precise details of optimization algorithms are not important. You need to be aware of one key thing however: these algorithms are not perfect and they sometimes make mistakes. The root cause of these mistakes are so-called "local minimums". An optimizer works by searching through combinations of different parameter values trying to find the combination that minimizes the error of the fit. The combination that has the smallest error out of all possible combinations is known as the true minimum or the "global" minimum.

A local minimum is a combination of parameter values that are not the global minimum, yet whose nearby neighbors all have higher errors. Figure 1 illustrates the problem of local minimum. If the optimizer starts near the first minimum in this figure it might head towards that minimum without ever realizing that another, improved minimum exists. Thus, if you are not careful, you may think you have found the optimal set of parameters when in fact you have only found a local minimum that might have much worse error than the true minimum.

! Figure 1. An illustration of local and global minimum for an optimization problem involving a single parameter.

There is no foolproof way to deal with local minimums and no guarantee that you have found the true minimum[4]. The primary method for attempting to prevent an optimization from settling in on a local minimum is to introduce stochasticity into the optimization algorithm. Optimization techniques such as *Simulated Annealing* or *Genetic Algorithms* will sometimes choose combinations of parameter values at random that are actually *worse* than what the optimizer has already found. By occasionally moving in the "wrong" direction, away from the nearest local minimum, these optimization algorithms are more resilient and less likely to become stuck on a local minimum and more likely to keep searching for the global minimum.

Unfortunately, in our experience we have not been satisfied by the performance of these types of stochastic optimization algorithms. They are generally very slow and without fine-tuning by an expert can still easily become stuck in a

[4]This is true for the type of optimization problems you will generally be dealing with. Other types of optimization problems are much easier than the ones you may be encountering, as they are what are known as *convex* optimization problems and are guaranteed not to have any local minimums.

local minimum. We prefer to use non-stochastic deterministic methods as the core of our optimizations. We then introduce stochasticity into the algorithm by using multiple random starting sets of parameter values. For instance, instead of carrying out a single optimization we will do 10 different optimizations each starting at a different set of parameter values. If all 10 optimizations arrive at the same final minimum that is strong evidence we have found the global minimum. If they all arrive at different minima, then there is a good chance we have not found the global minimum.

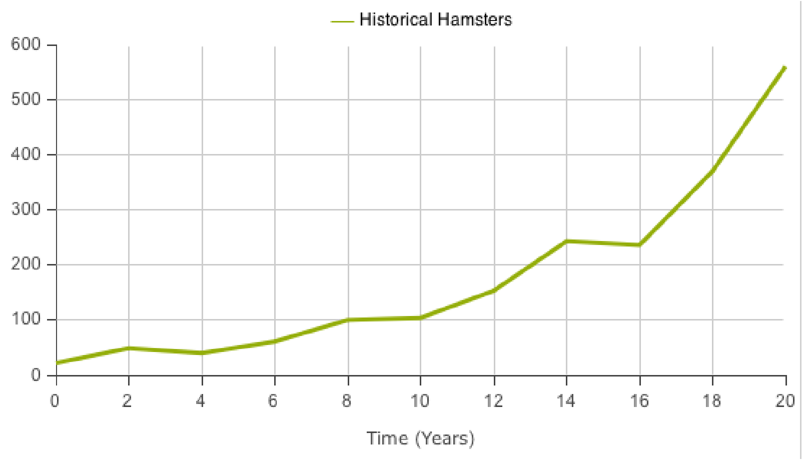
Optimizing Parameter Values

This model illustrates the use of optimization and historical data to select the growth rate for a simulated population of hamsters.

1. Create a new **Converter** named [**Historical Hamsters**].
2. Change the **Data** property of the primitive [**Historical Hamsters**] to `0, 22; 2, 49; 4, 40; 6, 61; 8, 100; 10, 104; 12, 153; 14, 243; 16, 236; 18, 370; 20, 560`.
3. The model diagram should now look something like this:

Historical Hamsters

4. We start by importing our historical population data into a converter primitive. In this illustrative example we have twenty years of data with a census of the hamster population being carried out every two years. We run the model to see what this historical data looks like.
5. Run the model. Here are sample results:



6. There is a lot of variability and the population even declines some years. However, it looks like in general the rate of growth increases as the population size increases. This is what we would expect to see with exponential growth. Let's build a simple exponential growth model to attempt to replicate what we see with the historical data.

7. Create a new **Stock** named [**Hamsters**].

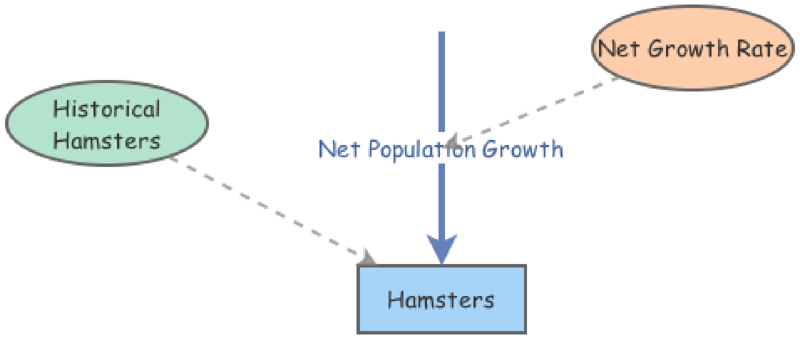
8. Create a new **Flow** going from empty space to the primitive [**Hamsters**]. Name that flow [**Net Population Growth**].

9. Create a new **Variable** named [**Net Growth Rate**].

10. Create a new **Link** going from the primitive [**Net Growth Rate**] to the primitive [**Net Population Growth**].

11. Create a new **Link** going from the primitive [**Historical Hamsters**] to the primitive [**Hamsters**].

12. The model diagram should now look something like this:



13. That's the structure of our model. Now we can fill in the equations. We'll set the initial population size for our simulated hamster population to be the same as for the historical data.

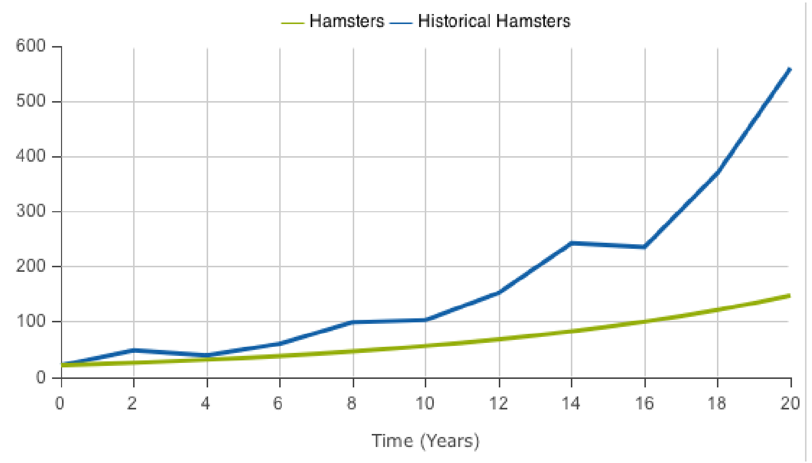
14. Change the **Initial Value** property of the primitive [**Hamsters**] to `[Historical Hamsters]`.

15. Change the **Flow Rate** property of the primitive [**Net Population Growth**] to `[Hamsters]*[Net Growth Rate]`.

16. What growth rate should we begin with? We do not have any data on this. Let's experiment by starting with 10% per year and see what we end up.

17. Change the **Equation** property of the primitive [**Net Growth Rate**] to `0.1`.

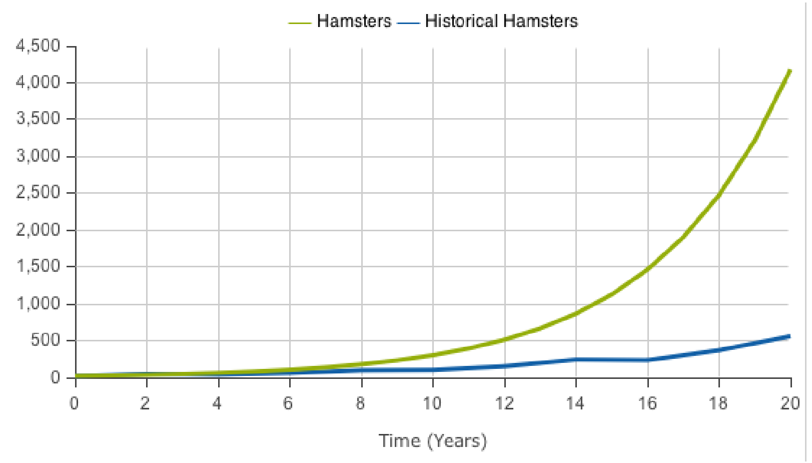
18. Run the model. Here are sample results:



19. That does not look too great. Our simulated population is much smaller than the historical values. Let's try a larger growth rate, say 30%.

20. Change the **Equation** property of the primitive [**Net Growth Rate**] to `0.3`.

21. Run the model. Here are sample results:



22. That's not good either, now our population is too large! We could keep experimenting with different growth rates to find a good one, but that might take a while. Let's just let the optimizer do the work for us. First we need to create a primitive to hold the error. We will use the squared error measure we discussed earlier.

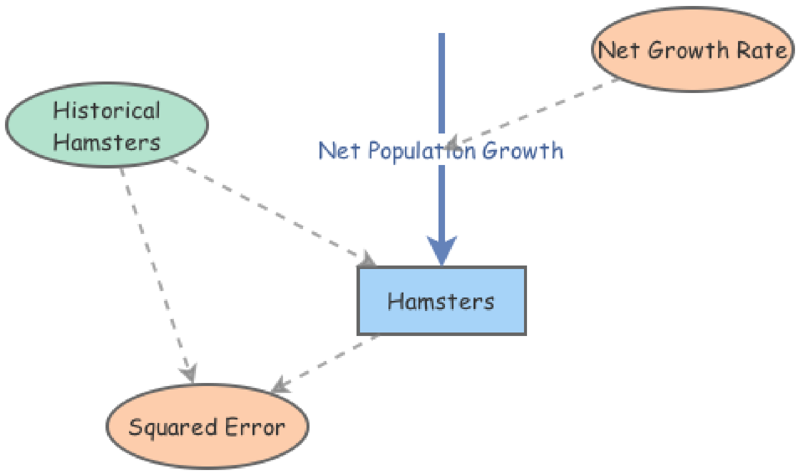
23. Create a new **Variable** named [**Squared Error**].

24. Create a new **Link** going from the primitive [**Hamsters**] to the primitive [**Squared Error**].

25. Create a new **Link** going from the primitive [**Historical Hamsters**] to the primitive [**Squared Error**].

26. Change the **Equation** property of the primitive [**Squared Error**] to `([Hamsters]-[Historical Hamsters])^2`.

27. The model diagram should now look something like this:

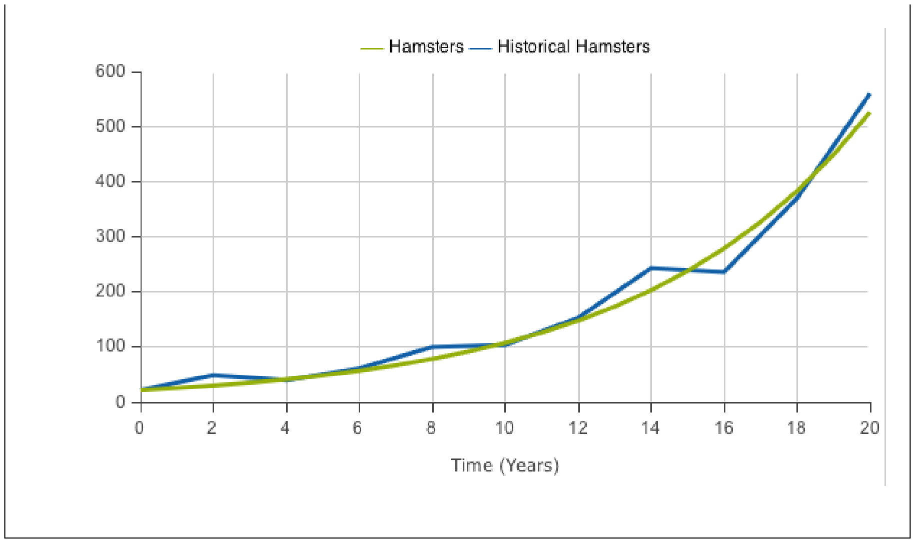


28. There, we have set up what we need for the optimizer to work. Now we can run the optimizer. We set the **Goal Primitive** to [**Squared Error**] and the **Primitive to Change** to [**Net Growth Rate**]. We tell the optimizer to minimize the integral of the error and set the optimizer to work.

29. The optimizer gets our results almost instantly: 0.172 or 17.2% is the optimal growth rate. When we run the model with this value the results look great. It's an almost perfect match between the historical and simulated data.

30. Change the **Equation** property of the primitive [**Net Growth Rate**] to `0.172`.

31. Run the model. Here are sample results:



Exercises

Calculate the pseudo R^2 for [**Growth Rate**] = `0.1`, `0.3`, and `0.172`.

The Cost of Complexity

After a good deal of work and many sleepless nights you have completed the first draft of your Aquatic Hamster population model. The results are looking great and your friend is really impressed. When he runs it by some colleagues however, they point out that your model does not account for the effects of the annual Pink Spotted Blue Jay migration.

Pink Spotted Blue Jays (PSBJ) are a species of bird that migrates every fall from northern Canada to Florida. In the spring they return from Florida to Canada. Along the way, they usually spend a few days by the lake where the Aquatic Hamsters have their last colony. During this time they eat the same Orange Hippo Toads the hamsters themselves depend upon as food. By reducing the Hippo Toad population, the PSBJ negatively affect the hamsters, at least for this period of time when there is less food available to support them.

The timing of the PSBJ migration can vary by several weeks each year no one knows precisely when the PSBJ's will arrive at the lake or even how long they will stay there. Further, the population of migrating birds can fluctuate significantly with maybe 100 birds arriving one year and 10,000 another year. The amount of toads they eat is proportional to the number of birds. Not much data exist quantifying the birds' effects on the hamsters, but it is a well-established fact that they eat the Hippo Toads the hamsters rely upon for their survival and many conservationists are concerned about the migration.

Your friend's colleagues wonder why you have decided to not include the PSBJ migration in your model. They want to know how they can trust a model that does not include this factor that clearly has an effect on the hamster population.

In response, you may point out that though the migration clearly has an impact, it appears to be a small one that is not as important as the other factors in the model. You add that there are no scientific studies or theoretical basis to define exactly how the migration functions or how it affects the hamster population. Given this, you think it is probably best to leave it out.

You say all this, but they remain unconvinced. "If there is a known process that affects the hamster population, it should be included in the model," they persist. "How can you tell us we shouldn't use what we know to be true in the model? We know the migration matters, and so it needs to be in there."

The Argument for Complexity

Your friend's colleagues have a point. If you intentionally leave out known true mechanisms from the model, how can you ask others to have confidence that the model is accurate? Put another way, by leaving out these mechanisms you ensure the model is wrong. Wouldn't the model *have* to be better if you included them?

This argument is, on the surface, quite persuasive. It is an argument that innately makes sense and appeals to our basic understanding of the world: Really it seems to be "common sense".

It is also an argument that is wrong and very dangerous.

Before we take apart this common sense argument piece by piece, let us talk about when complexity is a good thing. As we will show, complexity is not good from a modeling standpoint, but it can sometimes be a very good tool to help build confidence in your model and to gain support for the model.

Take the case of the PSBJ migration. It might be that adding a migration component to the model ends up *not* improving the predictive accuracy of the model. However, if other people view this migration as important, you may want to include the migration in the model if for no other reason than to get them on board. Yes, from a purely "prediction" standpoint it might be a waste of time and resources to augment the model with this component, but this is sometimes the cost of gaining support for a model. A "big tent" type model that brings lots of people on board might not be as objectively good as a tightly focused model, but if it can gain more support and adoption it might be able to effect greater positive change.

The Argument Against Complexity

Generally speaking, the costs of complexity to modeling are threefold. Two of them are self evident: there are computational costs to complex models as they take longer to simulate and there are also cognitive costs to complex models in that they are harder to understand. There is, however, a third cost to complexity that most people do not initially consider: complexity often leads to less accurate models compared to simpler models.

In the following sections we detail each of these three costs.

Computational Performance Costs

As a model becomes more complex, it takes longer to simulate. When you start building a model it may take less than a second to complete a simulation. As the model's complexity grows, the time required to complete a simulation may grow to a few seconds to a few minutes and then to even a few hours or more.

Lengthy simulation times can significantly impede model construction and validation. The agile approach to model development we recommend is predicated on rapid iteration and experimentation. As your simulation times cross beyond even something as small as 30 seconds, model results will no longer be effectively immediate and your ability to rapidly iterate and experiment will be diminished.

Furthermore, when working with an optimizer or sensitivity-testing tool, performance impacts can have an even larger effect. An optimization or sensitivity testing tool may run the model thousands of times or more in its analysis so even a small increase in the computation time for a single simulation may have a dramatic impact when using these tools.

Optimizations themselves are not only affected by the length of a simulation, they are also highly sensitive to the *number* of parameters being optimized. You should be extremely careful about increasing model complexity if this requires the optimizer to adjust additional parameter values. A simplistic, but useful, rule of thumb is that for every parameter you add for an optimizer to optimize, the optimization will take 10 times as long[5].

Thus if it takes one minute to find the optimal value for one parameter, then it takes 10 minutes to find the optimal values for two parameters and 100 minutes to find the optimal values for three parameters. Imagine we had built a model and optimized five parameters at once. We then increased the model complexity so we now had to optimize ten parameters. Our intuition would be that the optimization would now take twice as long. This is wrong. Using our power of ten rule we know that the time needed will be closer to 10^5 or 100,000 times as long!

That is a huge difference and highlights how important it is to keep model complexity at a manageable level. In practice, a rule of thumb is that you should

[5]In practice an optimizer should ideally perform a bit better than this, but this provides us a useful guideline to understand optimizations. Also it should be noted that the optimizations we are talking about here are for non-linear optimization problems for which gradients (derivatives) cannot be directly calculated. For other types of optimization problems, such as linear problems, much faster optimization techniques are available.

have no difficulty optimizing one or two parameters at a time. As you add more parameters that optimization task becomes rapidly more difficult. At five or so parameters you have a very difficult but generally tractable optimization challenge. Above five parameters you may be lucky to obtain good results.

Cognitive Costs

In addition to the computational cost of complexity, there is also a cognitive cost. As humans we have a finite ability to understand systems and complexity. This is partly why we model in the first place: to help us simplify and understand a world that is beyond our cognitive capacity.

Returning to our hamster population model, including the bird migration could create a confounding factor in the model that makes it more difficult to interpret the effects of the different components of the model and extract insights from them. If we observe an interesting behavior in the expanded model we will have to do extra work to determine if it is due to the migration or some other part of the model. Furthermore, the migration may obscure interesting dynamics in the model making it more difficult for us to understand the key dynamics in the hamster system and extract insights from the model.

We can describe this phenomenon using a simple conceptual model defined by three equations. The number of available insights in a model is directly proportional to model complexity. As the model complexity increases, the number of insights available in the model also grows.

$$\text{Available Insights} \propto \text{Complexity}$$

Conversely, our ability to understand the model and extract insights from it is inversely proportional to model complexity:

$$\text{Understandibility} \propto \frac{1}{\text{Complexity}}$$

The number of insights we actually obtain from a model is the product of the number of available insights and our ability to understand the model:

$$\text{Insights} = \text{Available Insights} \times \text{Understandability}$$

Thus when the model complexity is 0 – in effect basically no model – we gain no insights from the model. As the model complexity starts to rise, we begin to gain additional insights. After a certain point however, the added model complexity actually inhibits additional understanding. As complexity rises our insights will fall back down towards 0. This phenomenon is illustrated in Figure 2.

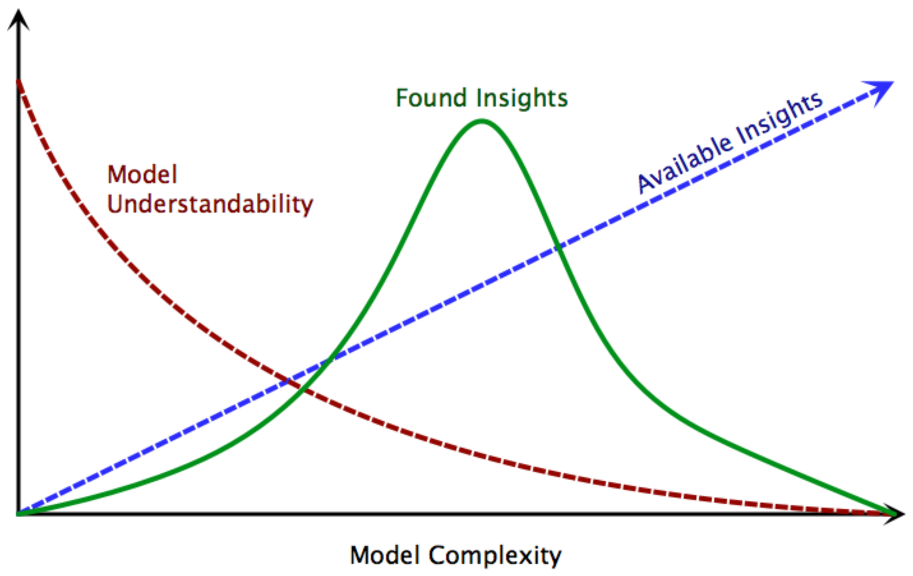


Figure 2. Expected discoveries of insights as model complexity increases.

Accuracy Costs

The negative effects of complexity on computational performance and our cognitive capacity should not be a surprise. What may be surprising on the other hand, is the fact that complex models are in fact often *less accurate* than simpler alternatives.

To illustrate this phenomenon, let us imagine that for part of our hamster population model we wanted to predict the size of the hamsters after a year[6]. The hamsters go through two distinct life stages in their first year: an infant life stage that lasts 3 months and a juvenile life stage that lasts 9 months. The hamsters' growth patterns are different during each of these periods.

Say a scientific study was conducted measuring the sizes of 10 hamsters at birth, at 3 months and at 12 months. The measurements at birth and 12 months are known to be very accurate (with just a small amount of error due to the highly accurate scale used to weigh the hamsters). Unfortunately, the accurate scale was broken when the hamsters were weighed at 3 months and a less accurate scale was used instead for that period. The data we obtain from this study are tabulated below and plotted in Figure 3:

Hamster	Birth	3 Months	12 Months

[6]Size could affect hamster survival and fecundity so it could be an important variable to model.

1	9.0	23.2	44.4
2	9.7	19.8	44.0
3	10.2	23.5	44.7
4	8.8	32.2	43.3
5	10.1	31.3	44.5
6	10.0	27.2	44.2
7	10.0	21.4	46.1
8	11.1	24.1	46.0
9	8.7	41.0	44.9
10	11.2	31.7	43.8

Now, unbeknownst to us, there are a pair of very simple equations that govern Aquatic Hamster growth. During the infant stage they gain 200% of their birth weight in that three-month period. Their growth rate slows down once they reach the juvenile stage such that at the end of the juvenile stage their weight is 50% greater than it was when they completed the infant stage. Figure 3 plots this true (albeit unknown) size trajectory compared to the measured values. The higher inaccuracy of the measurements at 3 months compared to 0 and 12 months is readily visible in this figure by the greater spread of measurements around the 3 month period.

We can summarize this relationship mathematically:

$$\text{Size}_{t=3\text{ months}} = 3.00 * \text{Size}_{t=0\text{ months}}$$
$$\text{Size}_{t=12\text{ months}} = 1.50 * \text{Size}_{t=3\text{ months}}$$

Naturally, we can combine these equations to directly calculate the weight of the hamsters at 12 months from their weight at birth:

$$\text{Size}_{t=12\text{ months}} = 4.50 * \text{Size}_{t=0\text{ months}}$$

Again, we don't know this is the relationship, so we need to estimate it from the data. All we care about is the size of hamsters at 12 months given their birth size. The simplest way to estimate this relationship is to do a linear regression estimating the final size as a function of the initial size. This regression would result in the following relationship:

$$\text{Size}_{t=12\text{ months}} = 4.65 * \text{Size}_{t=0\text{ months}}$$

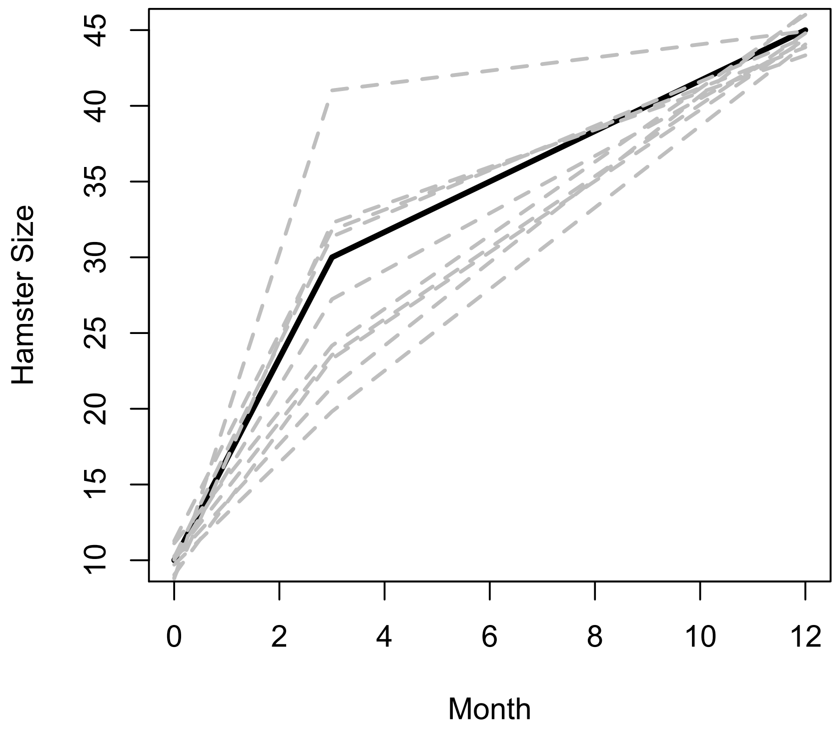


Figure 3. Recorded hamster sizes (dashed grey lines) and the unknown true size trajectory for a hamster starting with size 10 (solid black line).

This result is quite good. The linear coefficient we estimate of 4.65 is very close to the true value of 4.50. Our model so far is doing pretty well.

However, like with the bird migration, someone might point out that this model is too crude. “We know that the hamster go through an infant and juvenile stage”, they might say, “we should model these stages separately so the model is more accurate.”

This viewpoint moreover has actually been held to be the case in the law. For instance, there have been judicial decisions that “life-cycle” models, those that model each stage of an animal’s life are the only valid ones[7]. If we were

[7]Technically the determination is that life-cycle models are the “best available science”. These decisions are misguided and frankly wrong, but that is what occurs when judges are

presenting this model in to an audience that believed that, we would have to create two regressions: one for the infant stage and one for the juvenile stage.

Using the data we have, we would obtain these two regressions:

$$\text{Size}_{t=3\text{ months}} = 2.74 * \text{Size}_{t=0\text{ months}}$$
$$\text{Size}_{t=12\text{ months}} = 1.54 * \text{Size}_{t=3\text{ months}}$$

Combining these regression to get the overall size change for the 12 months we obtain the following:

$$\text{Size}_{t=12\text{ months}} = 4.22 * \text{Size}_{t=0\text{ months}}$$

Now, in this illustrative example we are fortunate to know that the true growth multiplier should be 4.50 so we can test how well our regression actually were. The error for this relatively detailed life-cycle model is $(4.50 - 4.22)/4.50$ or 6.2%. For the "cruder" model where we did not attempt to model the individual stages, the overall error is $(4.50 - 4.65)/4.50$ or 3.3%.

So by trying to be more accurate and detailed, we built a more complex model that has almost twice the error of our simpler model! Let's repeat that: The more complex model is significantly worse in accuracy than the simpler model.

Why is that? We can trace the key issue back to the problem that our data for the 3 month period are significantly worse than our data for 0 months or 12 months. By introducing it into the model, we bring down the overall quality of the model by injecting more error into it. When someone comes to you asking you to add a feature to a model you have to consider if this feature may actually introduce more error into the model as it did in this example.

We can think of life-cycle and many other kinds of models as a chain. Each link of the chain is a sub-model that takes data from the previous link, transforms them and feeds them into the next link. Like a chain, models may only be as good as their weakest link. It is often better to build a small model where all the links are strong, than a more complex model with many weak links.

Overfitting The act of building models that are too complex for the data you have is known as "overfitting" the data[8]. In the model of hamster sizes, the model where we look at each life stage separately is an overfit model; We do not have the data to justify this complex of a model. The simpler model (ignoring the different stages) is superior.

Overfitting is unfortunately too common in model construction. Part of the reason is that the techniques people use to assess the accuracy of a model are

put in the position of making highly technical scientific decisions.

[8]The reverse – building models that are too simple – is called "underfitting". In practice, underfitting will be less of a problem as our natural tendency is to overfit.

often incorrect and inherently biased to cause overfitting. To see this, let's explore a simple example. Say we want to create a model to predict the heights of students in high schools (this is seemingly trivial, but bear with us). To build the model we have data from five hundred students at one high school.

We begin by averaging the heights of all the students in our data set and we find that the average student height is 5 feet 7 inches. That number by itself is a valid model for student height. It is a very simple model[9], but it is a model nonetheless: Simply predict 5 feet 7 inches for the height of any student.

We know we can make this model more accurate. To start, we decide to create a regression for height where gender is a variable. This gives us a new model which predicts women high-school students have a height of 5 feet 5 inches on average, while men have a height of 5 feet 9 inches on average. We calculated the R^2 for the model to be 0.21.

That's not bad, but for prediction purposes we can do better. We decide to include students' race as a predictor as we think that on average there might be differences in heights for different ethnicities. We complete this extended model including ethnic status as a predictor alongside gender and the R^2 fit of our model increases to 0.33.

We still think we can do better though, so we add age as a third predictor: We hypothesize that the older the students are, the taller they will be. The model including age as an additional linear variable is significantly improved with an R^2 of 0.56.

Once we have built this model, we realize that maybe we should not just have a linear relationship with age because as students grow older, their rate of growth will probably slow down. To account for this we decide to also include the square of age in our regression. With this added variable our fit improves to an R^2 of 0.59.

This is going pretty well, we might be on to something. But why stop with the square; what happens if we add higher order polynomial terms based on age? Why not go further and use the cube of age. The fit improves slightly again. We think we are on a roll and so we keep going. We add age taken to the fourth power, and then to the fifth power, and then to the sixth, and so on.

We get a little carried away and end up including 100 different powers of age and each time we add and new power our R^2 gets slightly better. We could keep going, but it's time to do a reality check.

Do really we think that including AGE^{100} made our model any better than when we only had 99 terms based on age? According to the R^2 metric it did (if only by a very small amount). However, we know intuitively it did not. Maybe the first few age variables helped, but once we get past a quadratic

[9]Statisticians would call this the "null" model, the simplest model possible.

$(\mathrm{AGE} + \mathrm{AGE}^2)$ or cubic $(\mathrm{AGE} + \mathrm{AGE}^2 + \mathrm{AGE}^3)$ relationship, we probably are not capturing any more real characteristics of how age affects a person's size.

Variables	R^2
Gender	0.21
Gender, Race	0.33
Gender, Race, Age	0.56
Gender, Race, Age^2	0.59
Gender, Race, Age^2, . . . , Age^{100}	0.63
Gender, Race, Age^2, . . . , Age^{500}	1.00

So why does our reported model accuracy – R^2 – keep getting better and better as we add these higher order power terms based on age to our regression?

This question is at the heart of overfitting. Let's imagine taking our exploitation of age to its logical conclusion. We could build a model with 500 different terms based on age ($\text{AGE} + \text{AGE}^2 + \text{AGE}^3 + ... + \text{AGE}^{500}$). The result of this regression would go through every single point in our population of five hundred students[10].This model would have a perfect R^2 of one (as it matches each point perfectly) but we know intuitively that it would be a horrible model.

Why is this model so bad? Imagine two students born a day apart one with a height of 6 feet 2 inches the other with a height of 5 feet 5 inches. Our model would indicate that a single day caused a 7-inch difference in height. Even more ridiculous, the model would predict a roller coaster ride for students as they aged. They would gain inches one day (according to the model) and lose them the next. Clearly this model is nonsensical. However, this nonsensical model has a perfect R^2, it is a paradox!

The key to unlocking the solution to the paradox and overcoming overfitting turns out to be surprisingly simple: *assess the accuracy of a model using data that were not used to build the model.*

The reason our overfit model for students looks so good using the R^2 error metric is that we measured the R^2 using the same data that we just used to build the model. This is an issue as we can force an arbitrarily high R^2 simply by continually increasing the complexity of our model. In this context the R^2 we are calculating turns out to be meaningless.

What we need to do is to find new data – new students – to test our model on. That will be a more reliable test of its accuracy. If we first built our model and then took it and applied it to a different high school and calculated the R^2

[10]Remember a polynomial equation with two terms can perfectly pass through two data points, an equation with three terms can perfectly pass through three points, and so on.

using this new data, we would obtain a truer measure of how good our model actually was.

Figure 4 illustrates the effect of overfitting using observation from 9 students. The top three graphs show plots of the heights and ages for these nine students. We fit three models to these data: a simple linear one, a quadratic polynomial, and an equation with nine terms so that it goes through each point exactly.

Below the three graphs we show the regular R^2 that most people use when fitting models, and also what the true R^2[11] would be if we applied the resulting model to new data. The regular R^2 always increases so if we used this naive metric we would always end up choosing the most complex model. As we can see, the true accuracy of the model decreases after we reach a certain complexity. Therefore the middle model is really the better model in this case. When illustrated like this, this concept of overfitting should make a lot of sense; but, surprisingly, it is often overlooked in practice even by modeling experts.

In general, overfitting should be watched for carefully. If you do not have a good metric of model error, the inclination to add complexity to your model will be validated by misleadingly optimistic measures of error that make you think your model is getting better when it is actually getting worse. The optimization techniques we described earlier in this chapter are also susceptible to these problems as every time you add a new variable to be optimized the optimization error will always go down further (assuming the true optimal parameter configuration can be found). The more parameters you add the worse this effect will be.

How do we estimate the true error of the model fit? The simplest approach is to take your dataset and split it into two parts. Build the model with one half of the data and then measure the accuracy using the other half. So with our high-school students we would randomly assign each one to be used either to build the model or to assess the model's error. Advanced statistical techniques such as *cross-validation* or *bootstrapping* are other approaches and can be more effective given a finite amount of data. Unfortunately, we do not have space to discuss them here, but we would recommend the reader explore them on their own if they are interested in this topic.

No one ever got fired for saying, "Let's make this model more complex." After this chapter, we hope you understand why this advice, though safe to say, is often exactly the wrong advice.

[11] You might have heard of R^2 variants such as the Adjusted R^2. The Adjusted R^2 is better than the regular R^2; however it is important to note that it is not the true R^2. Adjusted R^2 also has some issues with overfitting.

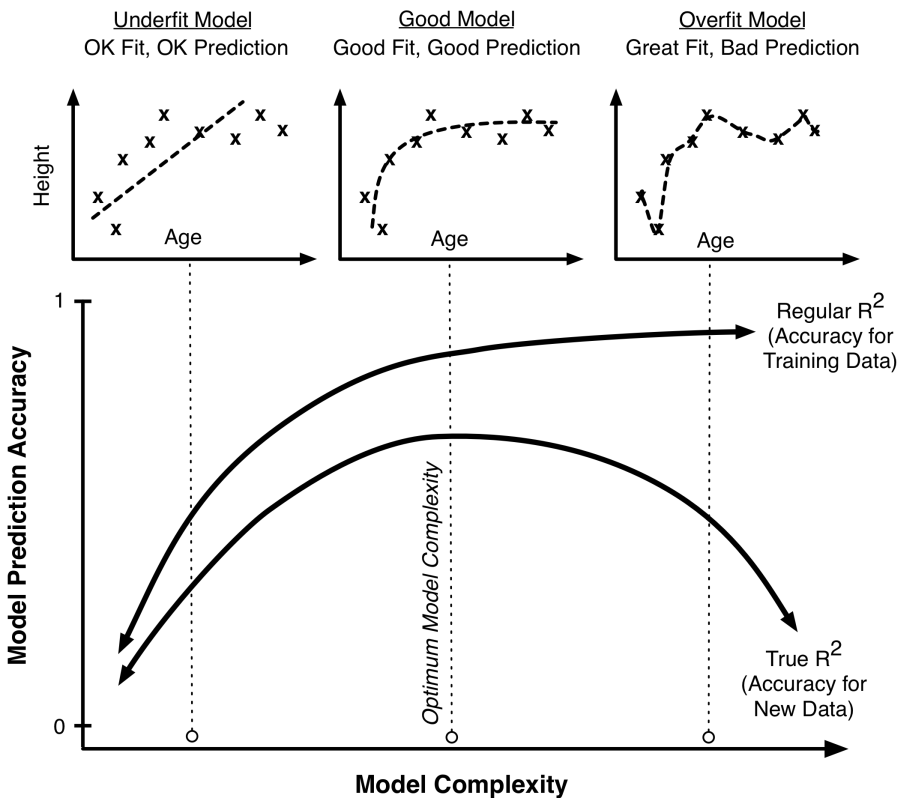

Underfit Model
OK Fit, OK Prediction
Good Model
Good Fit, Good Prediction
Overfit Model
Great Fit, Bad Prediction
Height
Age
Age
Age
1
0
Model Prediction Accuracy
Regular R2 (Accuracy for Training Data)
True R2 (Accuracy for New Data)
Optimum Model Complexity
Model Complexity

Figure 4. Illustration of overfitting. The best model is not necessarily the one that fits the data the closest.