The problem with parameters: using information theory to evaluate models

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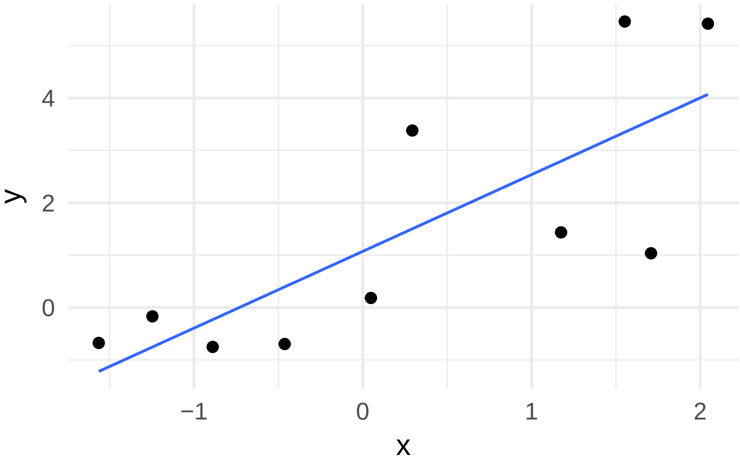
March 16, 2017

$$\hat{y} = \beta_0 + \beta_1 x$$



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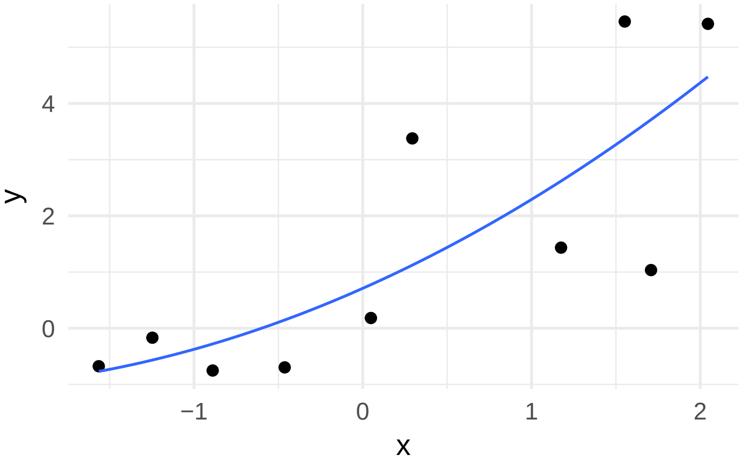

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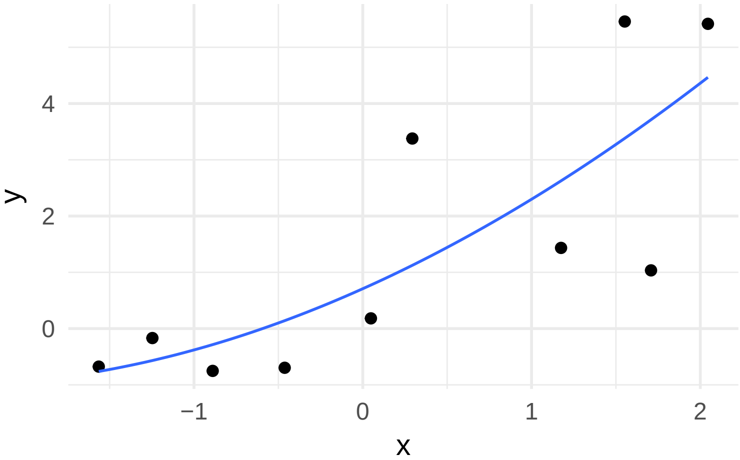

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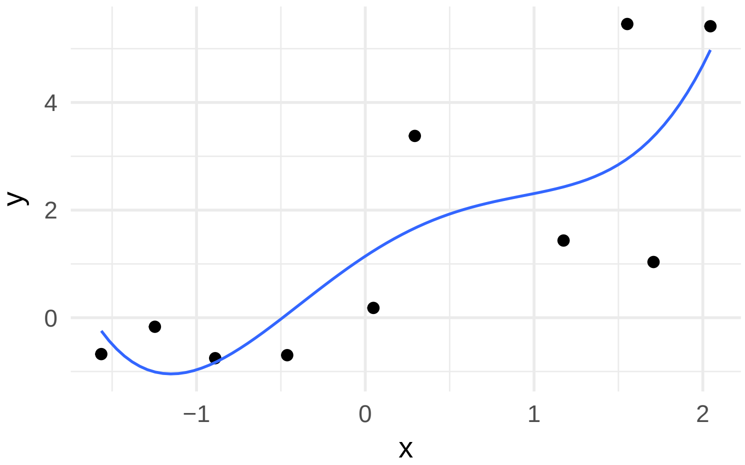

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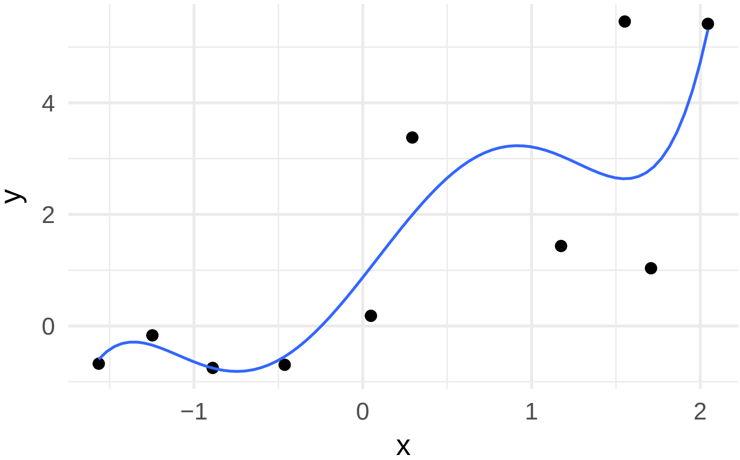

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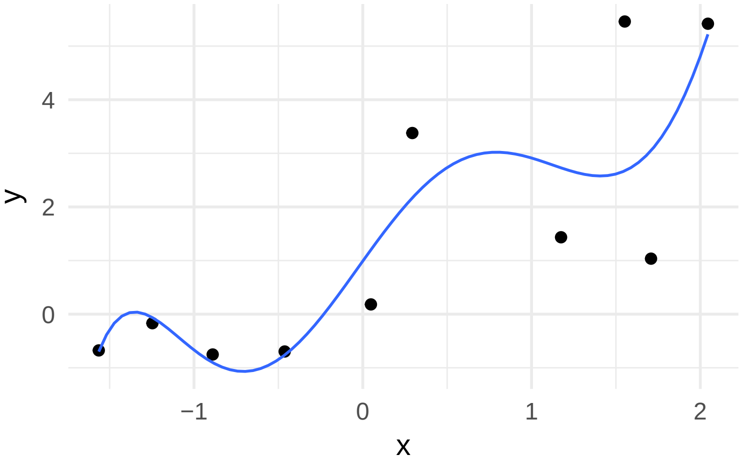

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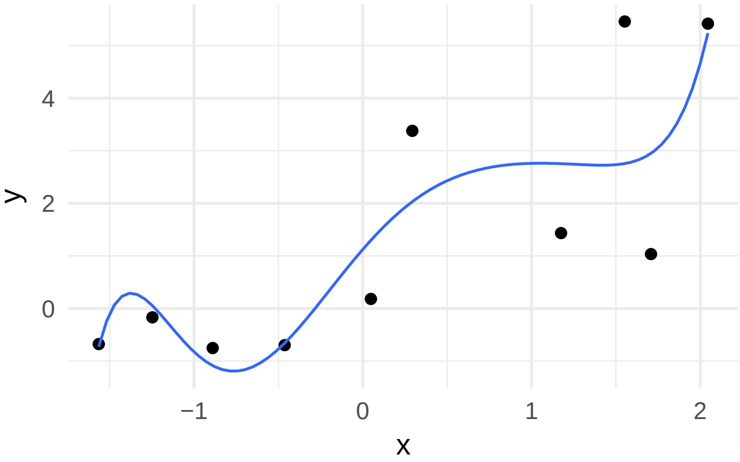

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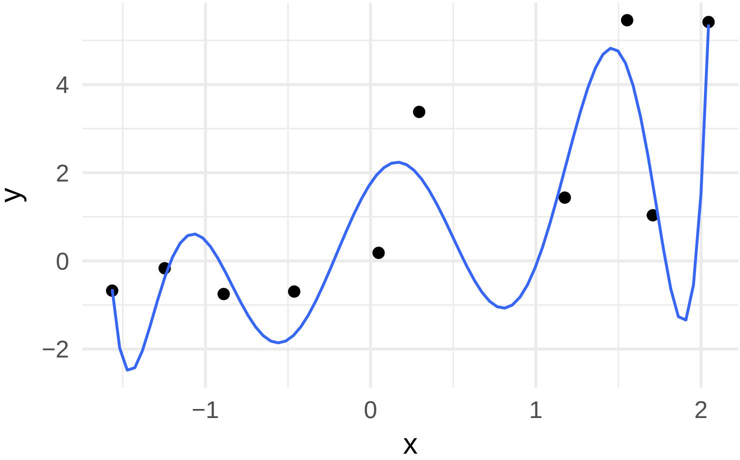

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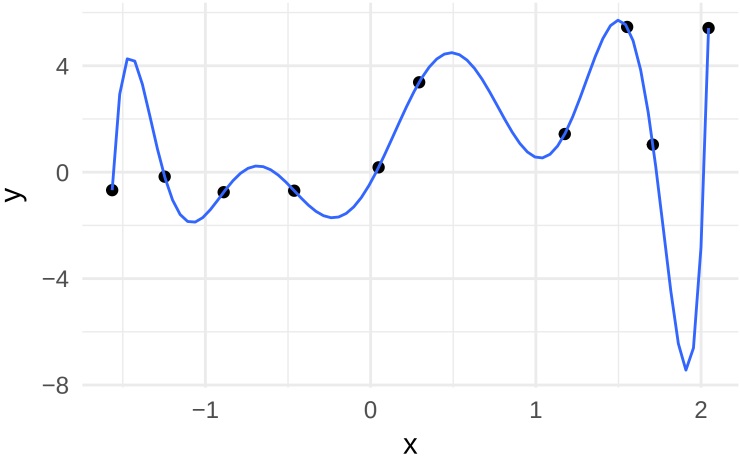
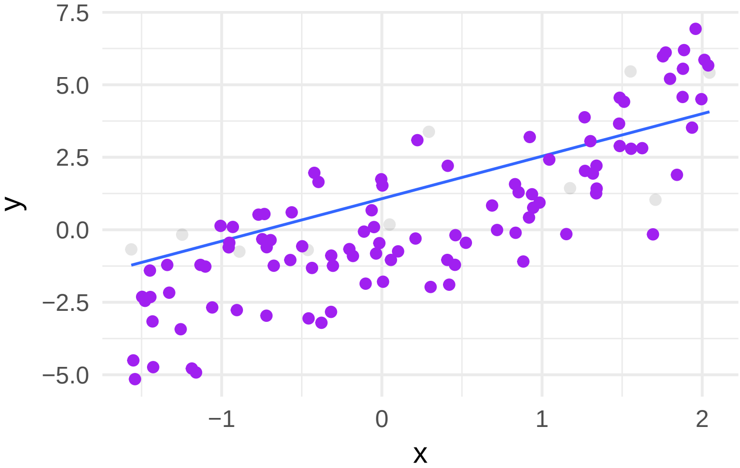


Overfitting

Parameters begin to fit to **noise**

- good fit to **training data**
- bad predictions for out of sample data

$$\hat{y} = \beta_0 + \beta_1 x$$



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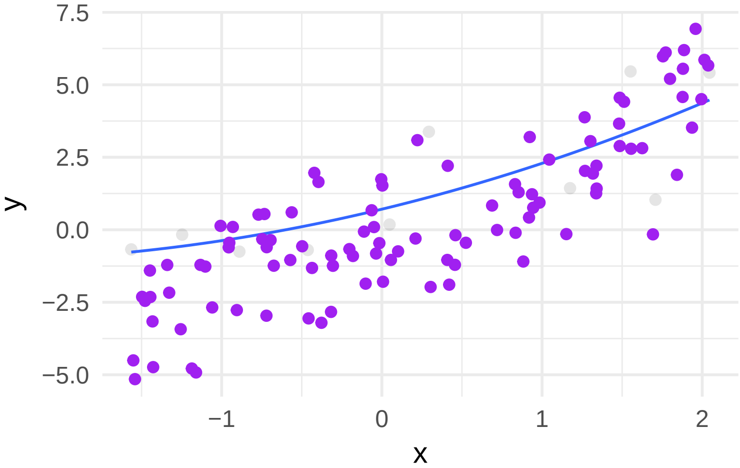

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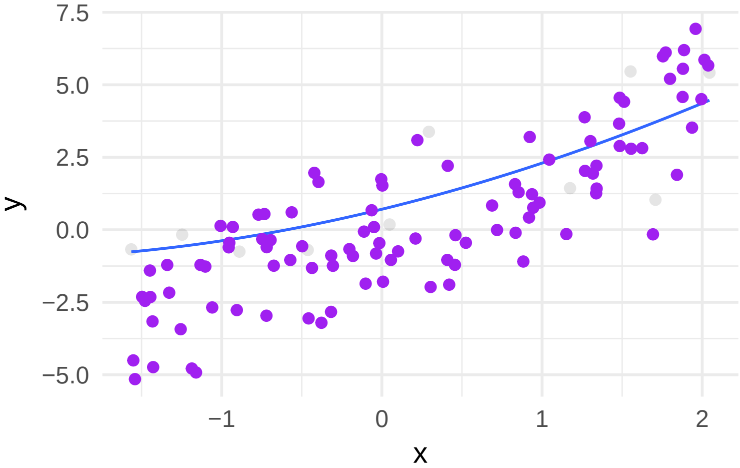

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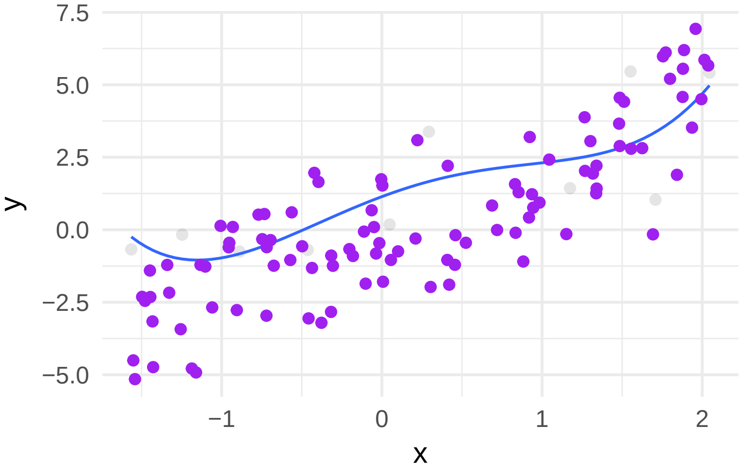

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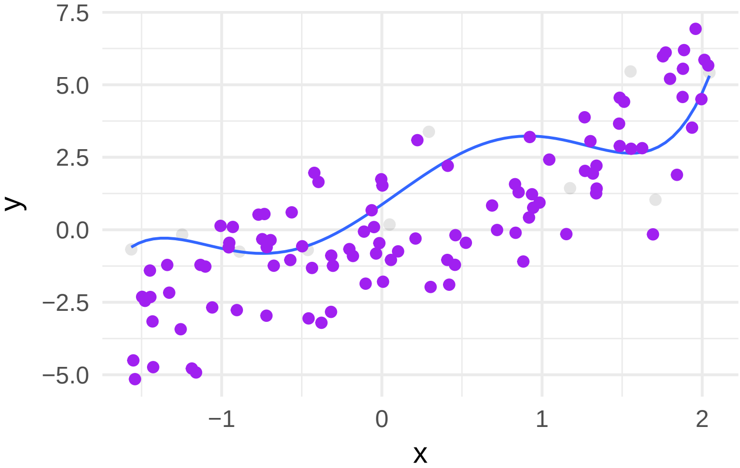

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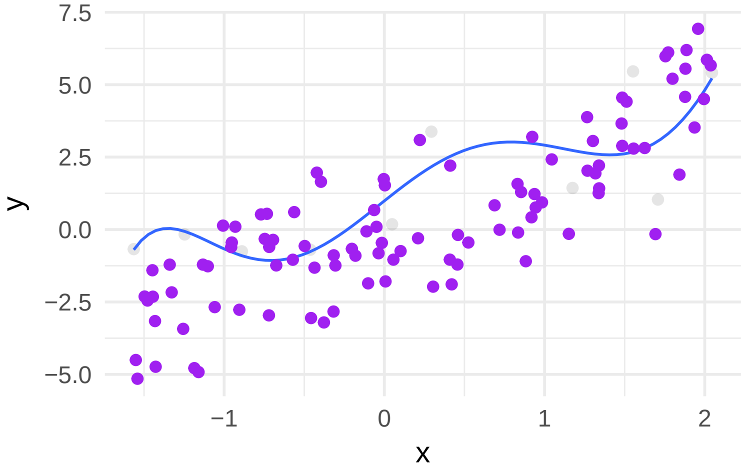

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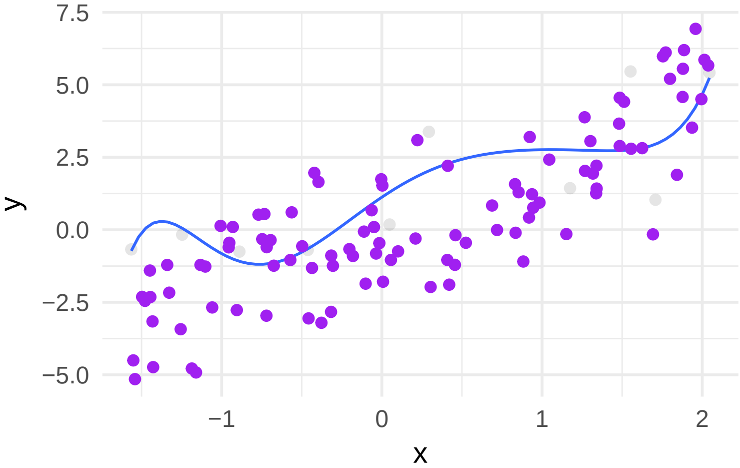

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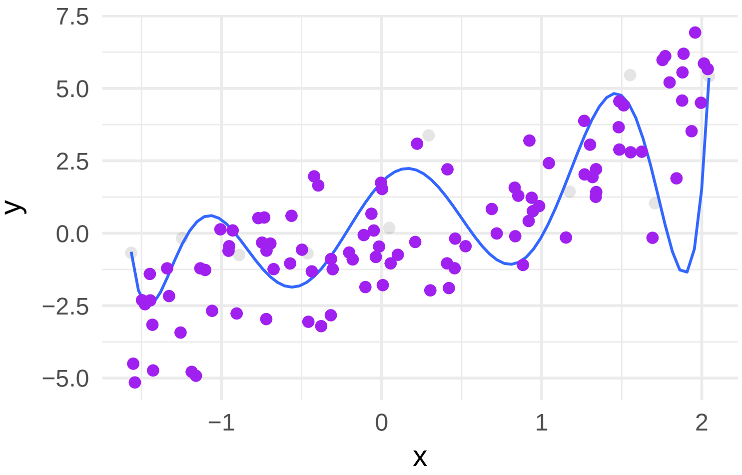

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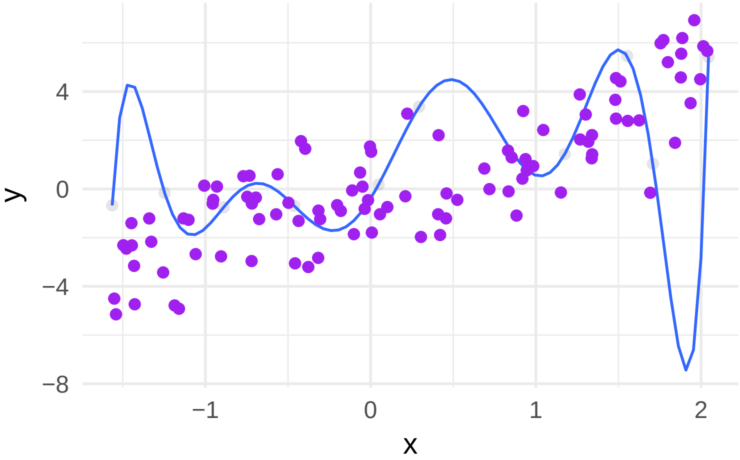
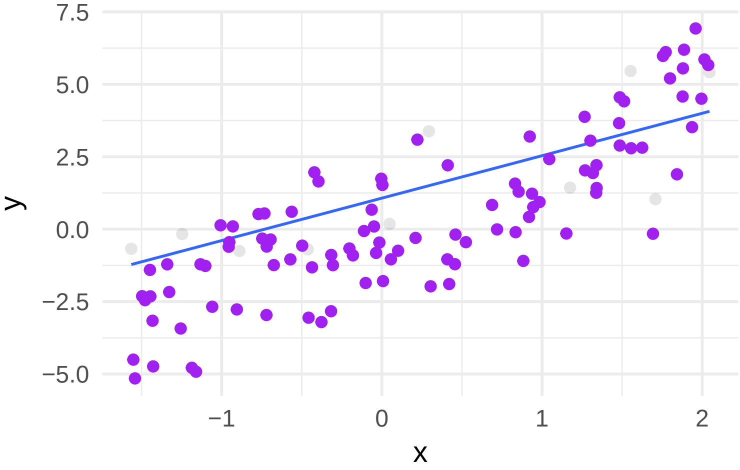


Underfitting

Model is too simplistic to capture signal



Today

Working toward **information criteria** to balance:

- model complexity
- out of sample predictive power

Roadmap

1. Information entropy
2. Kullback-Leiber divergence
3. Deviance
4. Akaike's information criterion

Information entropy

Uncertainty contained in a probability distribution

$$H(p) = -\sum_{i=1}^{n} p_i \log(p_i)$$

- $H(p)$: information entropy of a distribution p
- n: the number of possible outcomes
- p_i: the probability of outcome i

Activity

Compute the information entropy for your die!

$$H(p) = -\sum_{i=1}^{n} p_i \log(p_i)$$

What if we didn't know anything about dice?

Find an estimate of information entropy:

1. Estimate $p_1, p_2, p_3, \ldots$
2. Compute information entropy of your estimated distribution:

$$H(\hat{p}) = -\sum_{i=1}^{n} \hat{p}_i \log(\hat{p}_i)$$

Divergence

How far off is our model from the true distribution?

Example

We used $\hat{p}$ to estimate p

- What's the "divergence" between $\hat{p}$ and p?

Kullback-Leibler divergence

How far off is our model q from the true distribution p?

$$D_{\mathrm{KL}} = \sum_{i=1}^{n} p_i \log\left(\frac{p_i}{q_i}\right)$$

Activity

Calculate KL divergence for the following sample sizes:

- 5
- 10
- 20

$$D_{\mathrm{KL}} = \sum_{i=1}^{n} p_i(\log(p_i) - \log(q_i))$$

- Average difference in log probability between p and q

Bonus

- What happens when you draw 1000 samples?
- What happens when our approximation q is exactly the same as p?

The problem with reality

We almost never know the true probability of events!

What *do* we have

Typically we have data $y_1, y_2, ..., y_n$

and some models (let's say two)

$$q, r$$

So we can ask

Which model seems closer to the true distribution p?

$$D_{\mathrm{KL}}(p, q) - D_{\mathrm{KL}}(p, r) = -(E \log(q_i) - E \log(r_i))$$

Comparing models q and r

$$D_{\mathrm{KL}}(p, q) - D_{\mathrm{KL}}(p, r) = -(E \log(q_i) - E \log(r_i))$$

Notice that we don't need p to compute this difference!

Deviance

$$D_{\mathrm{KL}}(p, q) - D_{\mathrm{KL}}(p, r) = -(E \log(q_i) - E \log(r_i))$$

We can plug in something proportional to the expected log likelihood:

$$E \log(q_i) \propto$$

$$D(q) = -2 \sum_{i=1}^{n} log(q_i)$$

where $D(q)$ is the **Deviance**

Deviance in plain english

$$D(q) = -2 \sum_{i=1}^{n} log(q_i)$$

A relative measure of divergence from the true distribution p

- one deviance value is useless
- multiple values allow us to compare models

How to calculate deviance

$$D(q) = -2\sum_{i=1}^{n} log(q_i)$$

Log likelihood: $\sum_{i=1}^{n} log(q_i)$

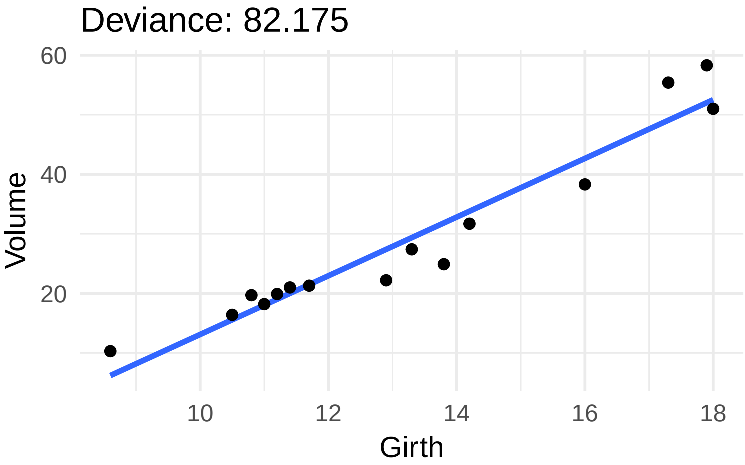
$\rightarrow$ multiply log likelihood by -2.

*demo

The problem with Deviance

New predictors improve (reduce) deviance

- same problem as R^2



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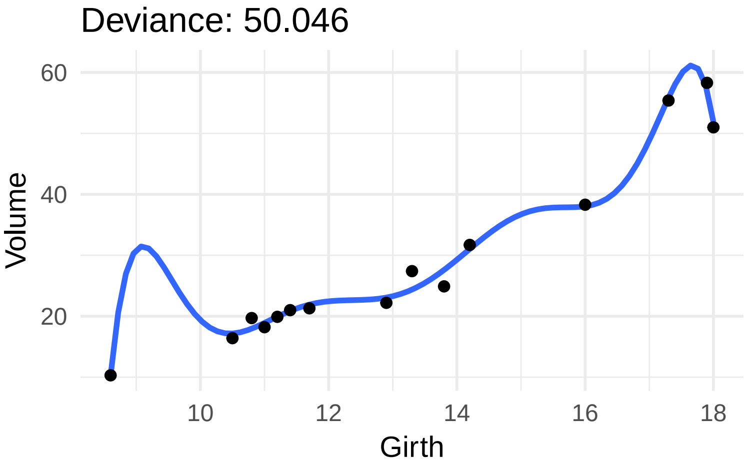


At the end of the day

We want to be close to the **truth** but not too close to our training **data**

We want to make good predictions

In other words, we'd like low deviance for **new** observations

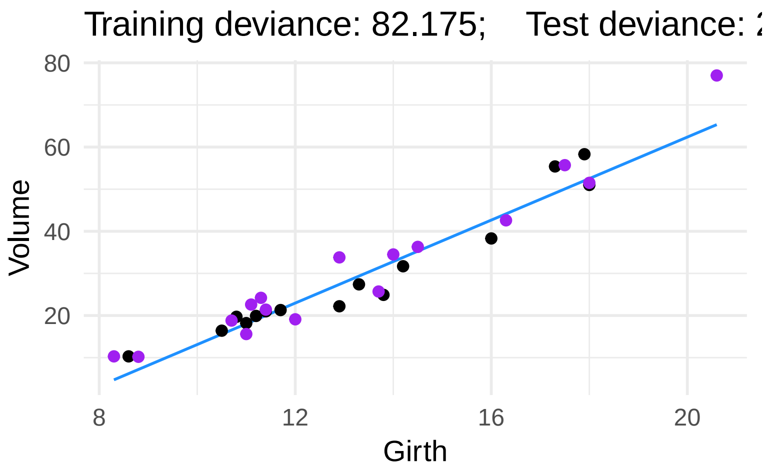
Deviance of training data $(q_1, q_2, ...)$:

$$D_{\text{train}}(q) = -2 \sum_i log(q_i)$$

Deviance of future data $(\tilde{q}_1, \tilde{q}_2, ...)$:

$$D_{\text{test}}(q) = -2 \sum_i log(\tilde{q}_i)$$

Evaluating deviance of the training and test set



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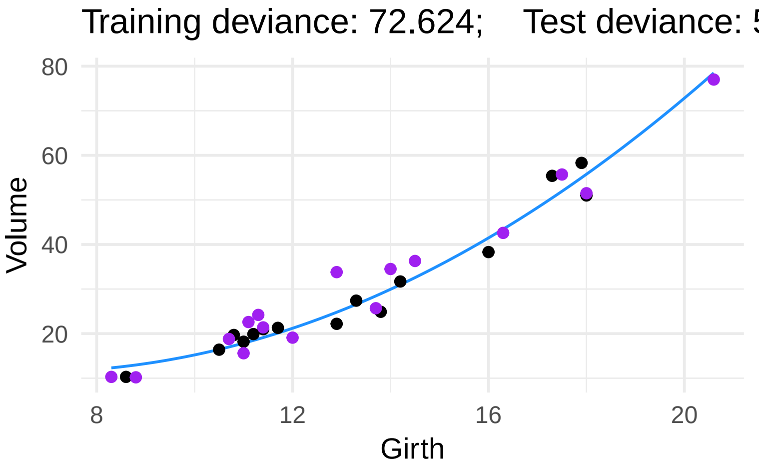

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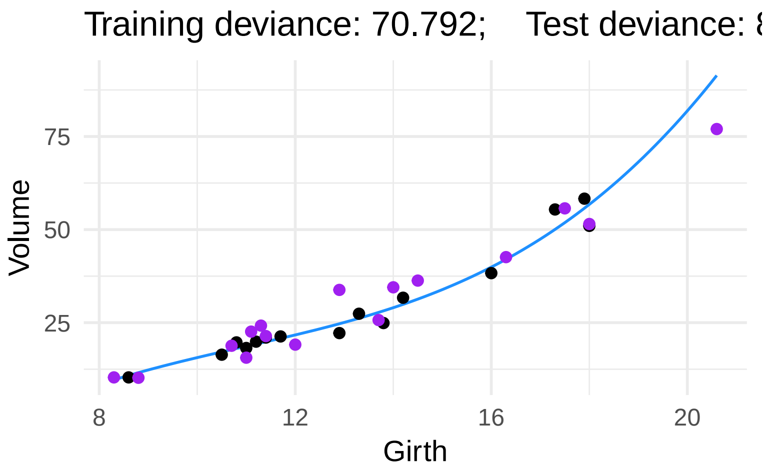

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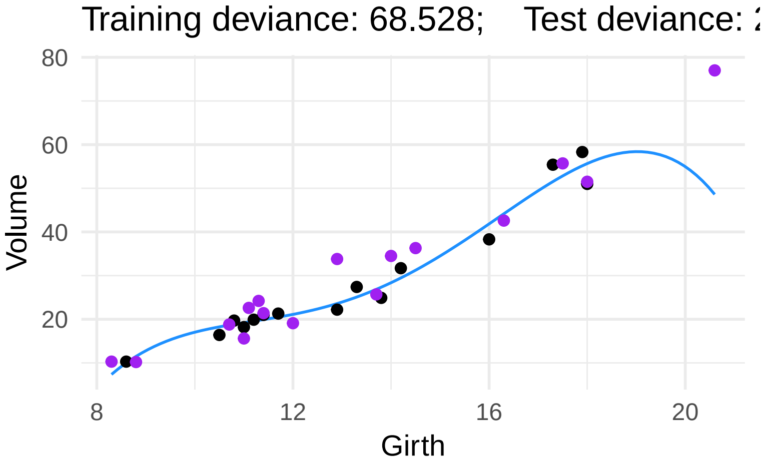

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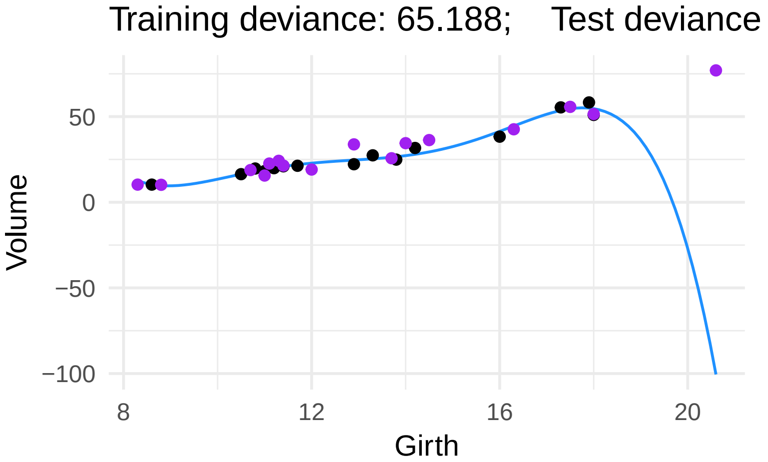
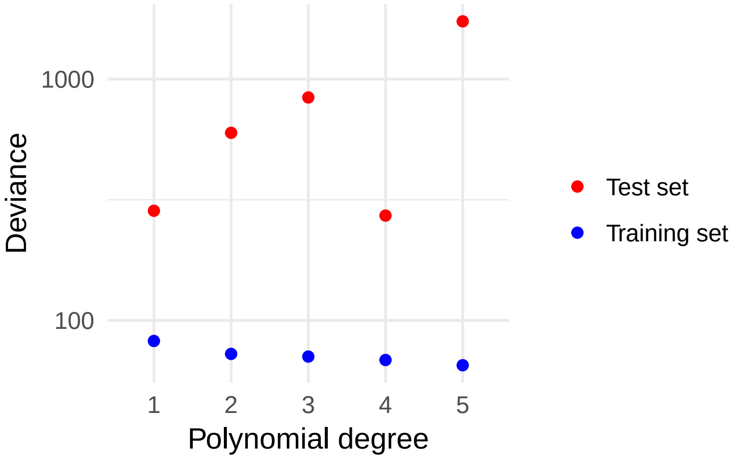


Training and test deviance across a range of model complexity



Some problems with training vs. test splits

1. How to decide what goes where?
2. What if you have a small dataset?
3. What is your data are structured (e.g., by spatial location)

Enter AIC

Instead of computing D_{test}, approximate with

Akaike's information criterion

$$AIC = D_{\text{train}} + 2p$$

- D_{train} is your training set deviance
- p is the number of parameters in your model

"Better" models have lower AIC

Recap:

1. Over vs. underfitting
2. Measured how close a model q is to truth p (KL divergence)
3. Realized that since we don't know truth, we need a **relative** measure
4. Learned that AIC is that relative measure

- how well can a model predict new data?

$$AIC = D_{\text{train}} + 2p$$