INTRO TO DATA SCIENCE

II: POLYNOMIAL REGRESSION

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"Although polynomial regression fits a nonlinear model to the data, as a statistical estimation problem it is linear, in the sense that the regression function E(y|x) is linear in the unknown parameters that are estimated from the data. For this reason, polynomial regression is considered to be a special case of multiple linear regression." -- *Wikipedia*

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But there is one problem with the model we've written down so far.

Q: Does anyone know what it is?

A: This model violates one of the assumptions of linear regression!

This model displays **multicollinearity**, *which means the predictor variables are highly correlated with each other.*

$$y = \alpha + \beta_1 x + \beta_2 x^2 + \ldots + \beta_n x^n + \varepsilon$$

```
> x <- seq(1, 10, 0.1)
> cor(x^9, x^10)
[1] 0.9987608
```

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Multicollinearity causes the linear regression model to break down, because it can't tell the predictor variables apart.

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OPTIONAL NOTE

These polynomial functions form an *orthogonal basis* of the function space.

So far, we've seen how polynomial regression allows us to fit complex nonlinear relationships, and even to avoid multicollinearity (by using basis functions).

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Q: Can a regression model be too complex?

III: REGULARIZATION

Recall our earlier discussion of **overfitting**.

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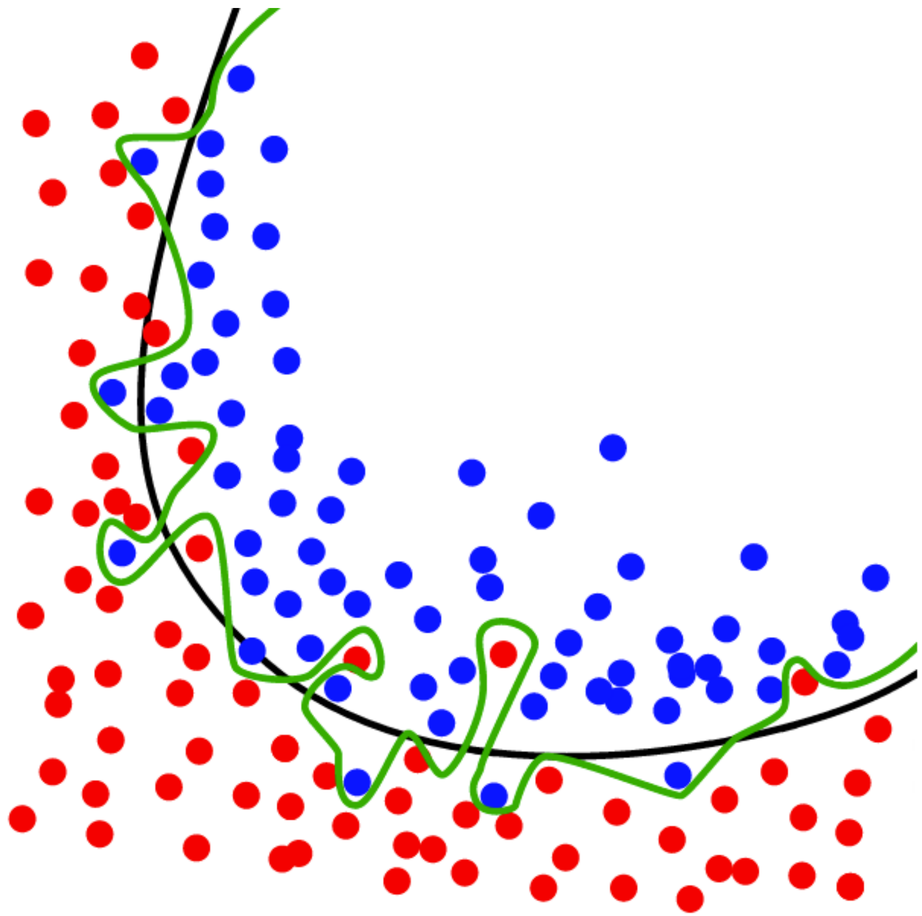
In other words, an overfit model matches the **noise** *in the dataset instead of the* **signal***.*

OVERFITTING EXAMPLE (CLASSIFICATION)



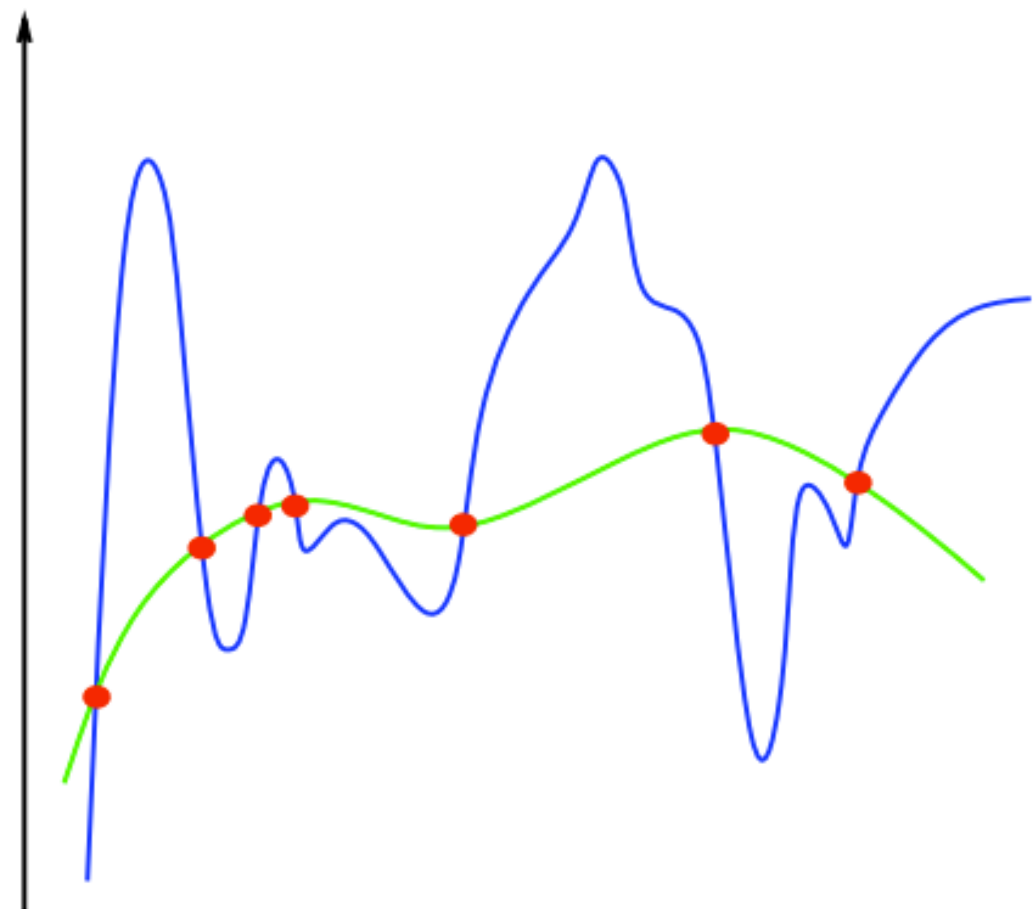
source: http://upload.wikimedia.org/wikipedia/commons/1/19/Overfitting.svg

The same thing can happen in regression.

It's possible to design a regression model that matches the noise in the data instead of the signal.

This happens when our model becomes too complex for the data to support.

OVERFITTING EXAMPLE (REGRESSION)



source: http://www.mit.edu/~9.520/spring12/slides/class02/class02.pdf

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Ex 1: $\Sigma |\beta_i|$

Ex 2: $\Sigma \beta_i^2$

Q: How do we define the **complexity** *of a regression model?*

A: One method is to define complexity as a function of the size of the coefficients.

Ex 1: $\Sigma |\beta_i|$ *this is called the* **L1-norm**

Ex 2: $\Sigma \beta_i^2$ *this is called the* **L2-norm**

These measures of complexity lead to the following **regularization** *techniques:*

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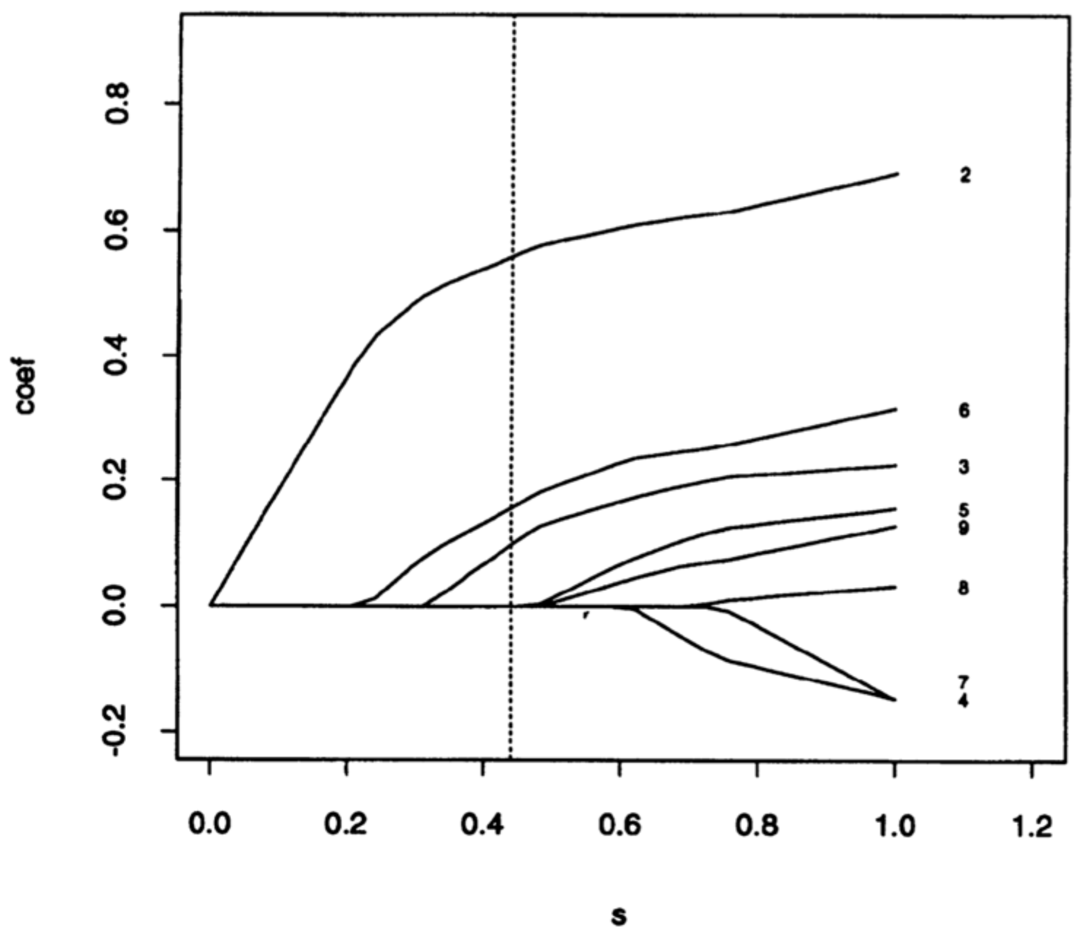
Regularization *refers to the method of preventing* **overfitting** *by explicitly controlling model* **complexity**.

These regularization problems can also be expressed as:

L1 regularization (Lasso): $min(\|y - x\beta\|^2 + \lambda\|x\|)$

L2 regularization (Ridge): $min(\|y - x\beta\|^2 + \lambda\|x\|^2)$

This (Lagrangian) formulation reflects the fact that there is a cost associated with regularization.



As the regularization parameter (s in this chart, lambda on the previous slide) goes to zero, so do the coefficients of the features

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BIAS AND VARIANCE

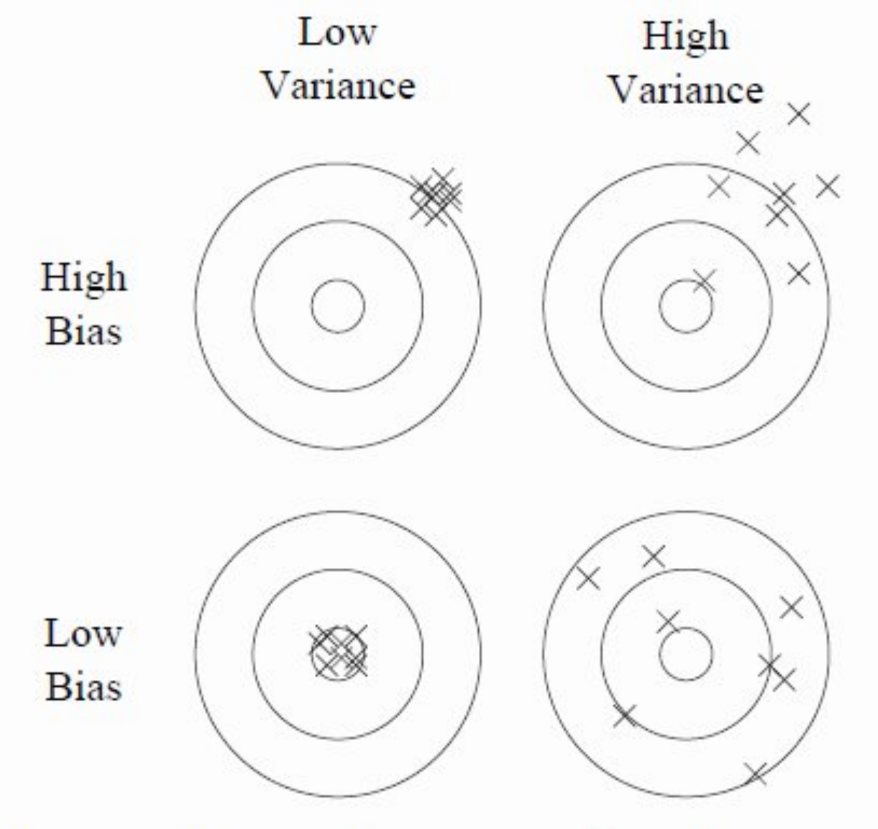


Figure 1: Bias and variance in dart-throwing.

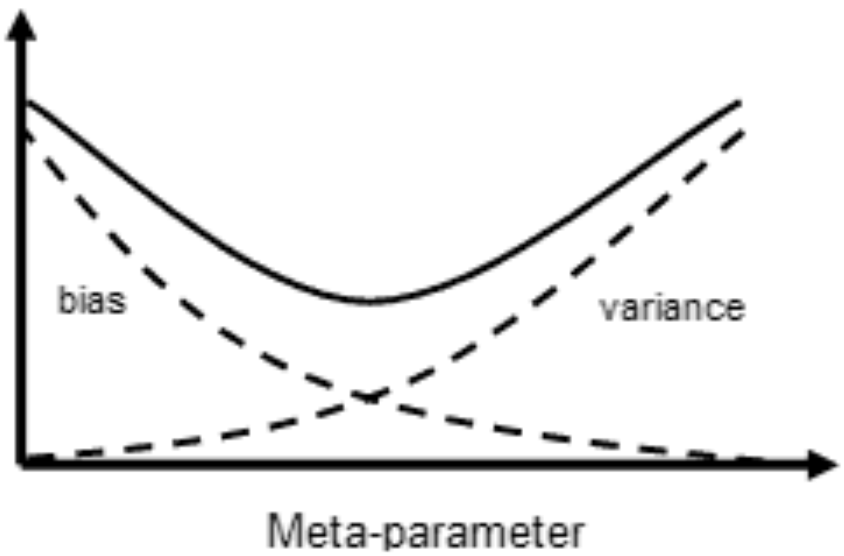
source: http://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf

Q: What are bias and variance?

A: Bias refers to predictions that are systematically inaccurate. Variance refers to predictions that are generally inaccurate.

It turns out (after some math) that the generalization error in our model can be decomposed into a bias component and variance component.

This is another example of the **bias-variance tradeoff**.



source: http://www.isu.edu/chem/images/kalivasmeta.gif

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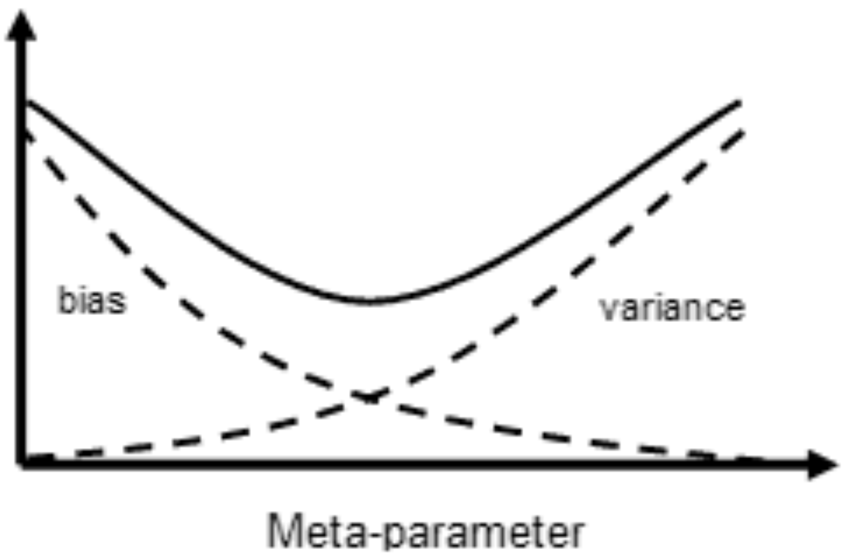

NOTE

The “meta-parameter” here is the lambda we saw above.

A more typical term is “hyperparameter”.

source: http://www.isu.edu/chem/images/kalivasmeta.gif

This tradeoff is regulated by a **hyperparameter** λ, *which we've already seen:*

L1 regularization: $y = \Sigma\, \beta_i x_i + \varepsilon \quad st. \quad \Sigma\, |\beta_i| < \lambda$

L2 regularization: $y = \Sigma\, \beta_i x_i + \varepsilon \quad st. \quad \Sigma\, \beta_i^2 < \lambda$

So regularization represents a method to trade away some variance for a little bias in our model, thus achieving a better overall fit.

KEY CONCEPTS

- *Linear regression*
- *Multiple regression*
- *Polynomial regression*
- *The concept of minimizing some error or “cost” function*
- *Regularization*

LAB: REGRESSION & REGULARIZATION