INTRO TO DATA SCIENCE REGRESSION & REGULARIZATION

I. INTRO TO REGRESSION
II. LINEAR AND POLYNOMIAL
III. REGULARIZATION

EXERCISES: III. IMPLEMENTING MULTIPLE REGRESSION AND POLYNOMIAL REGRESSION IN PYTHON

I. LINEAR REGRESSION

	continuous	categorical
supervised	???	???
unsupervised	???	???

REGRESSION PROBLEMS

supervised
unsupervisedregression
dimension reductionclassification
clustering

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The **simple linear regression** model captures a linear relationship between a single input variable x and a response variable y:

$$y = \beta_0 + \beta_1 x + \varepsilon$$

Q: What do the terms in this model mean?

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 ε = **residual** (the prediction error)

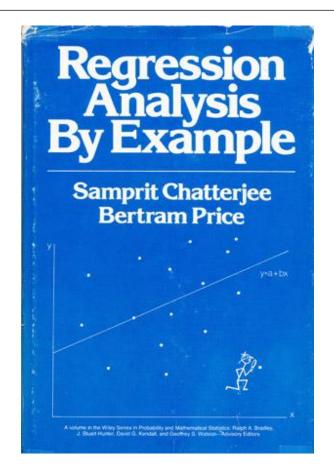
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$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_n x_n + \varepsilon$$

Linear regression involves several technical assumptions and is often presented with lots of mathematical formality.

The math is not very important for our purposes, but you should check it out if you get serious about solving regression problems.



Statistical Models Theory and Practice REVISED EDITION David A. Freedman

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In practice, any respectable piece of software will do this for you.

But again, if you get serious about regression, you should learn how this works!

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

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \dots + \beta_n x^n + \varepsilon$$

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

POLYNOMIAL REGRESSION



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

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

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

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This results in a singularity. We will see an example of this in just a minute!

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OPTIONAL NOTE

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

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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

OVERFITTING

Recall our earlier discussion of overfitting.

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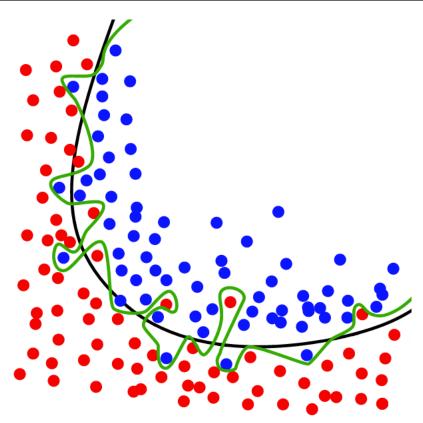
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When we talked about this in the context of classification, we said that it was a result of matching the training set too closely.

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

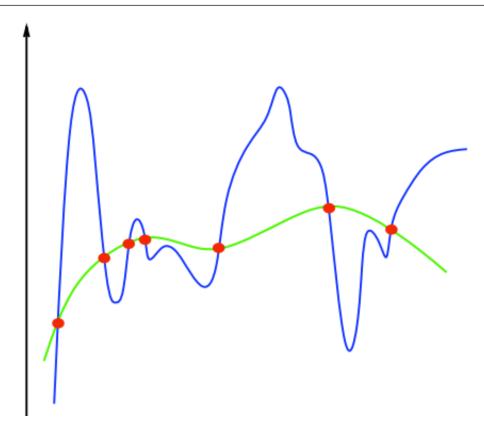
OVERFITTING EXAMPLE (CLASSIFICATION)



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.



MODEL COMPLEXITY

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Ex 2: $\sum \beta_i^2$

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

REGULARIZATION

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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: $min(||y - x \cdot \beta||^2 + \lambda ||\beta||)$

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

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

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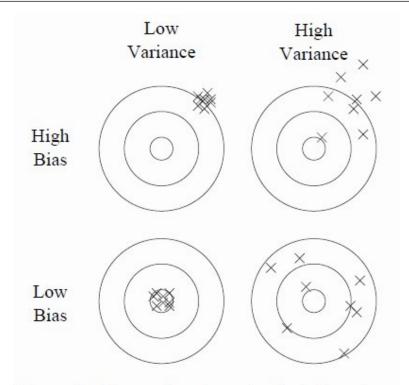


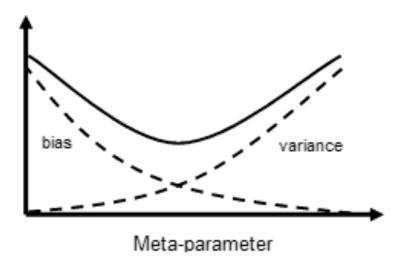
Figure 1: Bias and variance in dart-throwing.

Q: What are bias and variance?

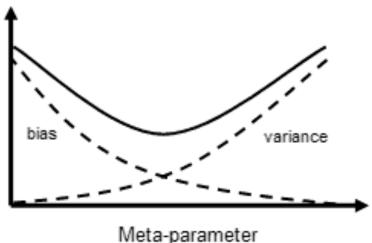
A: Bias refers to predictions that are *systematically* inaccurate. Variance refers to predictions that are *generally* inaccurate.

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

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NOTE

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

A more typical term is "hyperparameter".

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

L1 regularization:
$$y = \sum \beta_i x_i + \varepsilon$$
 st. $\sum |\beta_i| < \lambda$
L2 regularization: $y = \sum \beta_i x_i + \varepsilon$ st. $\sum \beta_i^2 < \lambda$

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

EX: POLYNOMIAL REGRESSION & REGULARIZATION