GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 3: SUPERVISED LEARNING

LAST TIME:

- GGPLOT
- INTRO TO MACHINE LEARNING & TYPICAL PROBLEMS
- KNN CLASSIFICATION

QUESTIONS?

I. CLASSIFICATION PROBLEMS
II. INTRODUCTION TO REGRESSION

I. CLASSIFICATION PROBLEMS

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

	continuous	*categorical*
supervised	regression	classification
unsupervised	dimension reduction	clustering

Here's (part of) an example dataset:

Fisher's *Iris* Data

Sepal length	Sepal width	Petal length	Petal width	Species
5.1	3.5	1.4	0.2	*I. setosa*
4.9	3.0	1.4	0.2	*I. setosa*
4.7	3.2	1.3	0.2	*I. setosa*
4.6	3.1	1.5	0.2	*I. setosa*
5.0	3.6	1.4	0.2	*I. setosa*
5.4	3.9	1.7	0.4	*I. setosa*
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independent variables

class labels *(qualitative)*

Q: What does “supervised” mean?

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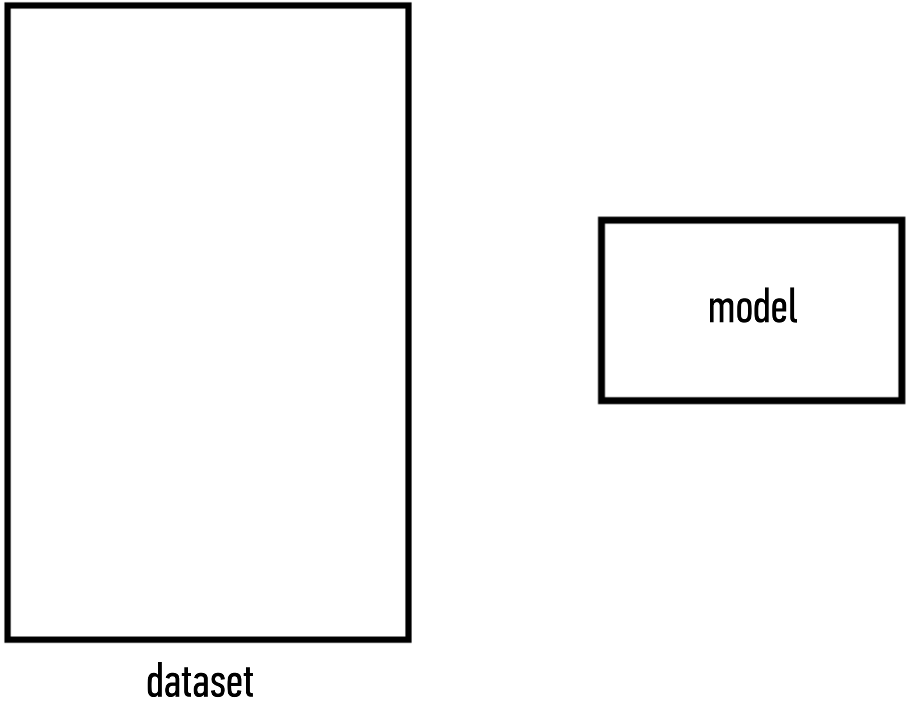
A: We know the labels.

```
Welcome to R! Thu Feb 28 13:07:25 2013
> summary(iris)
  Sepal.Length    Sepal.Width     Petal.Length    Petal.Width   
 Min.   :4.300   Min.   :2.000   Min.   :1.000   Min.   :0.100  
 1st Qu.:5.100   1st Qu.:2.800   1st Qu.:1.600   1st Qu.:0.300  
 Median :5.800   Median :3.000   Median :4.350   Median :1.300  
 Mean   :5.843   Mean   :3.057   Mean   :3.758   Mean   :1.199  
 3rd Qu.:6.400   3rd Qu.:3.300   3rd Qu.:5.100   3rd Qu.:1.800  
 Max.   :7.900   Max.   :4.400   Max.   :6.900   Max.   :2.500  
       Species  
 setosa    :50  
 versicolor:50  
 virginica :50  
```

Q: How does a classification problem work?

Q: What steps does a classification problem require?



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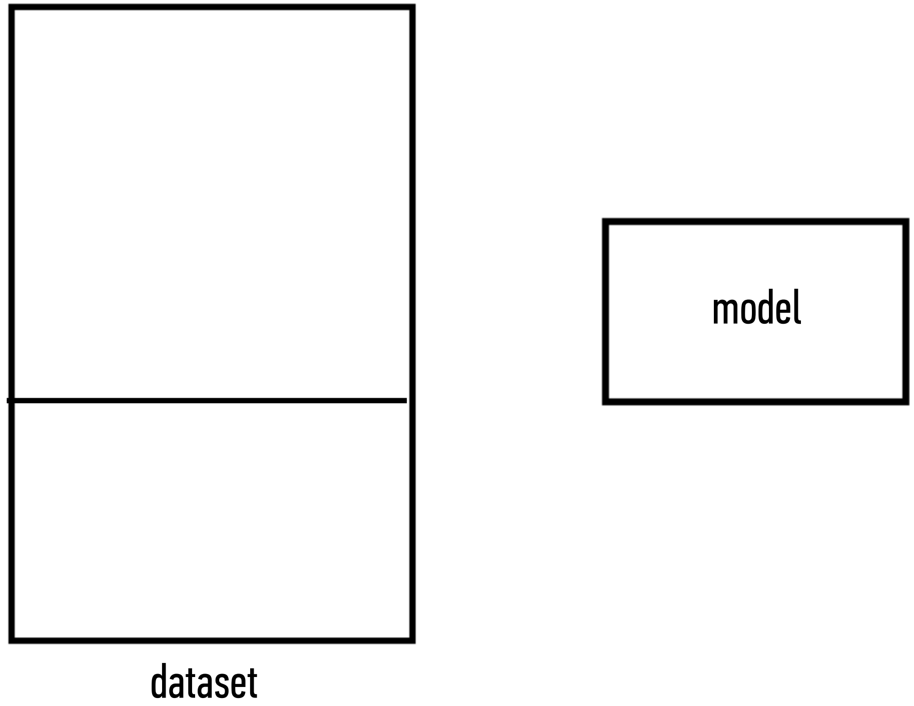
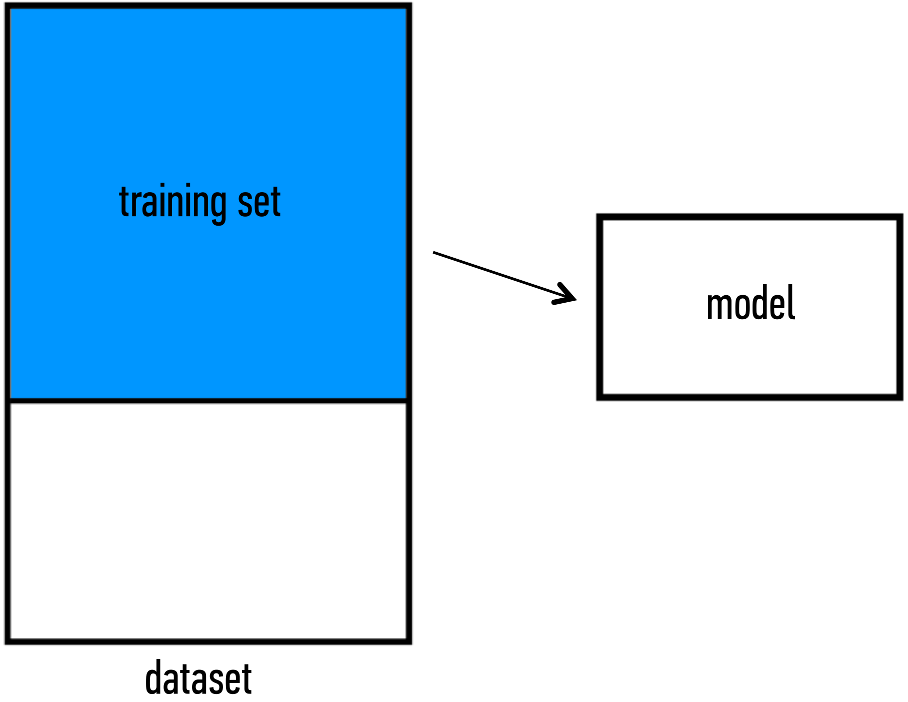
1) split dataset



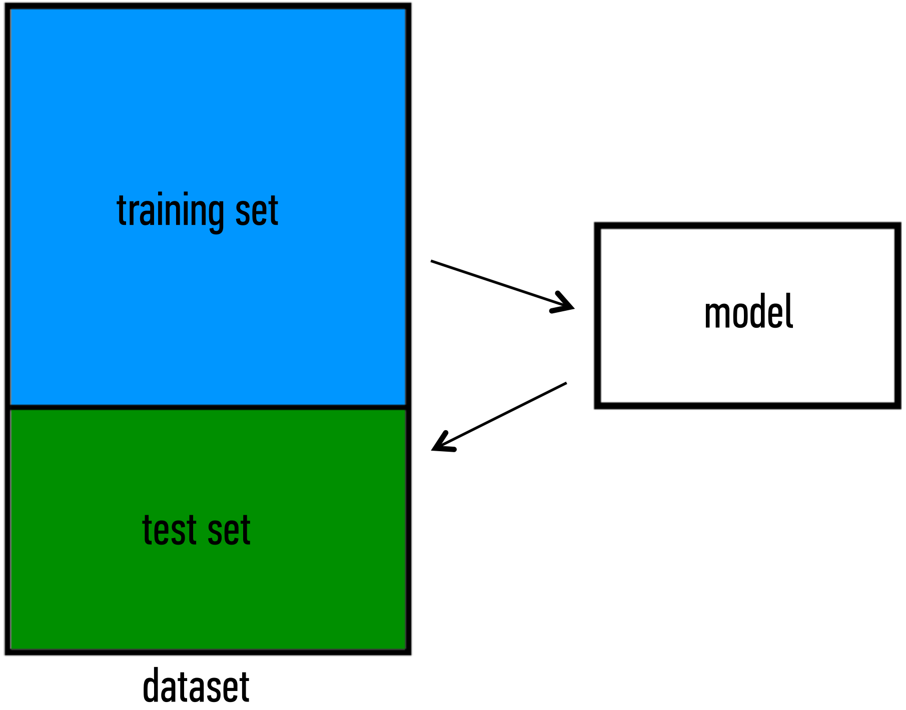
Q: What steps does a classification problem require?

1) split dataset
2) train model



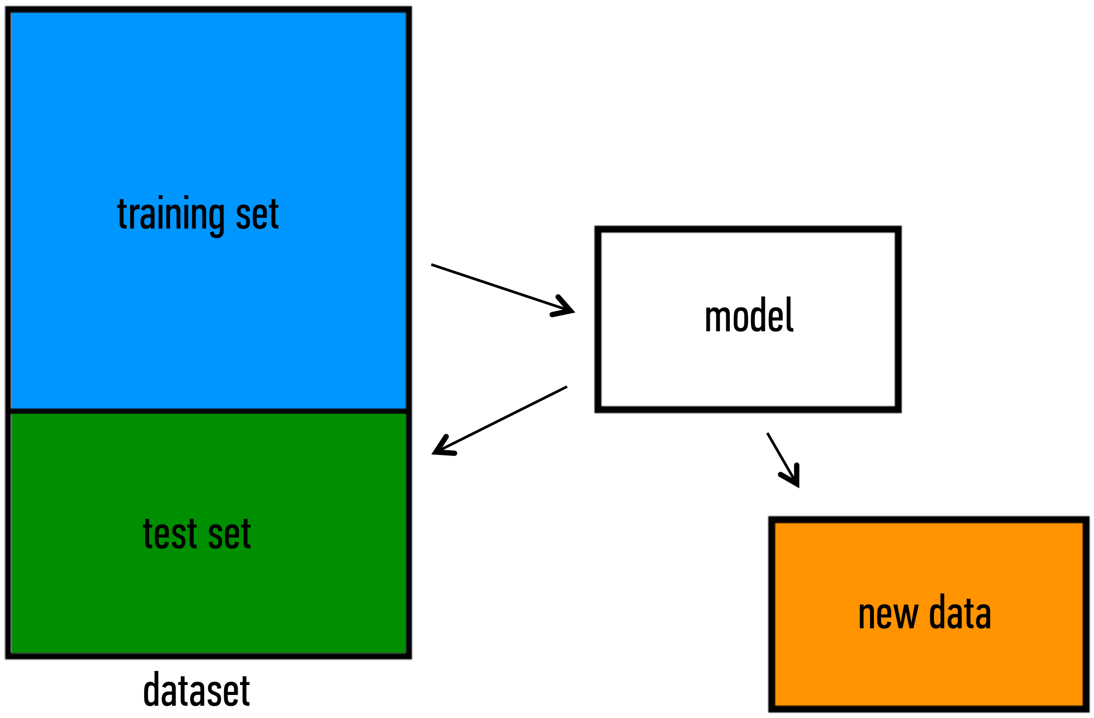
Q: What steps does a classification problem require?

1) split dataset
2) train model
3) test model



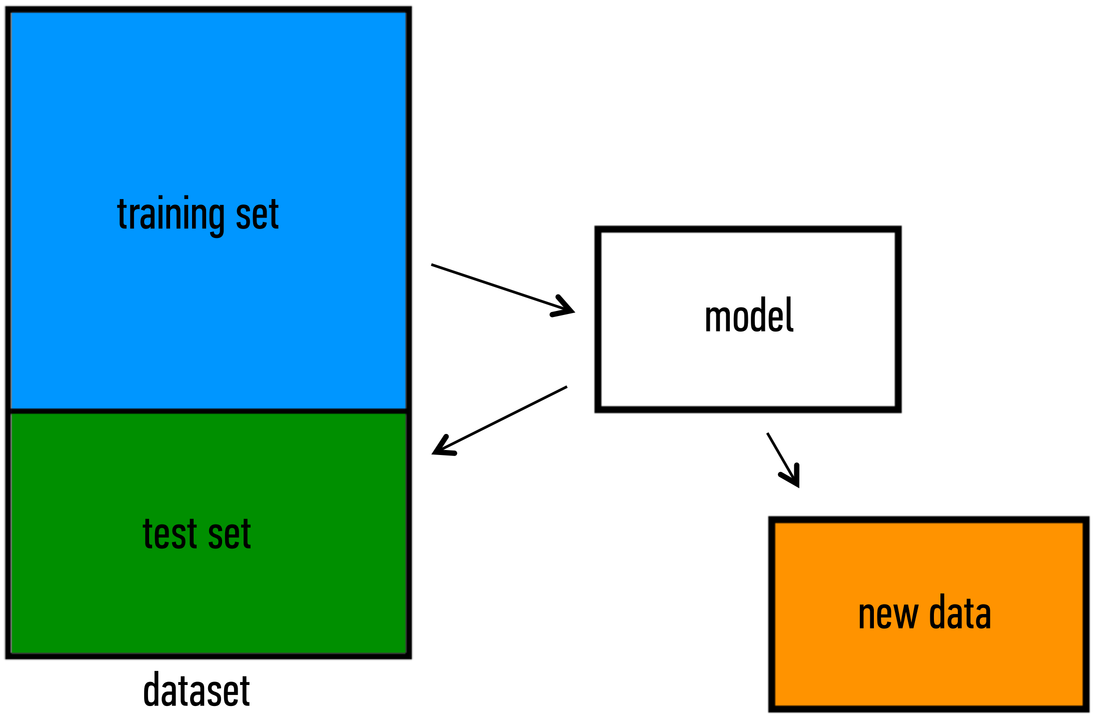
Q: What steps does a classification problem require?

1) split dataset
2) train model
3) test model
4) make predictions



II. BUILDING EFFECTIVE CLASSIFIERS

Q: What types of prediction error will we run into?



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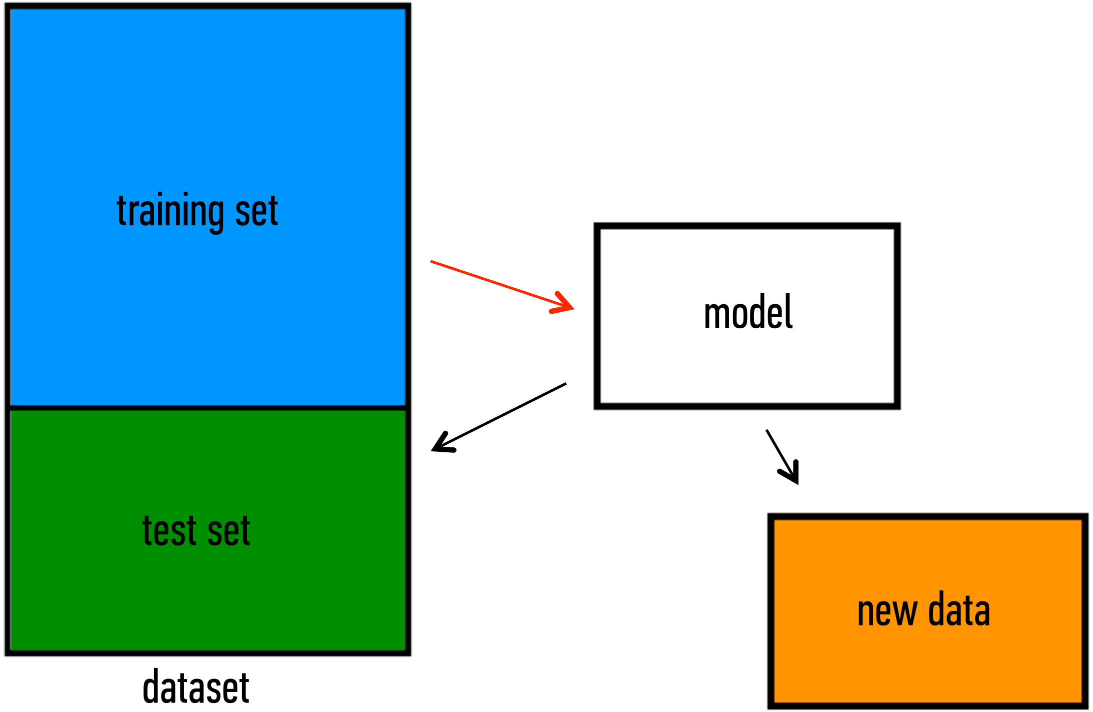

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1) training error
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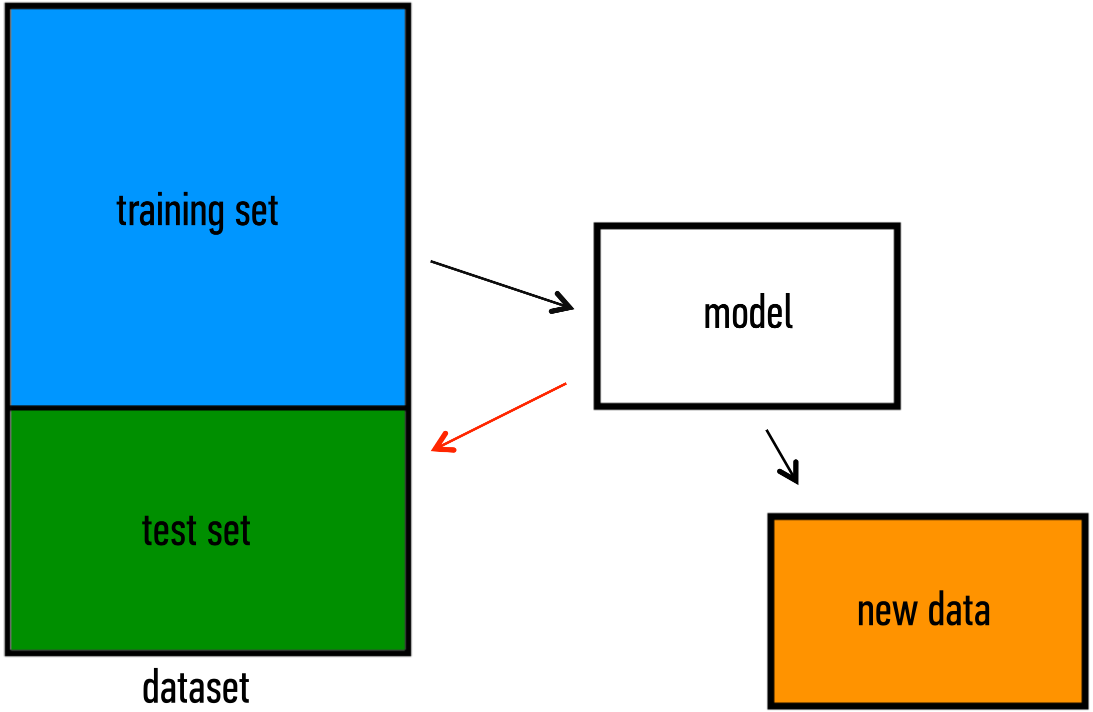
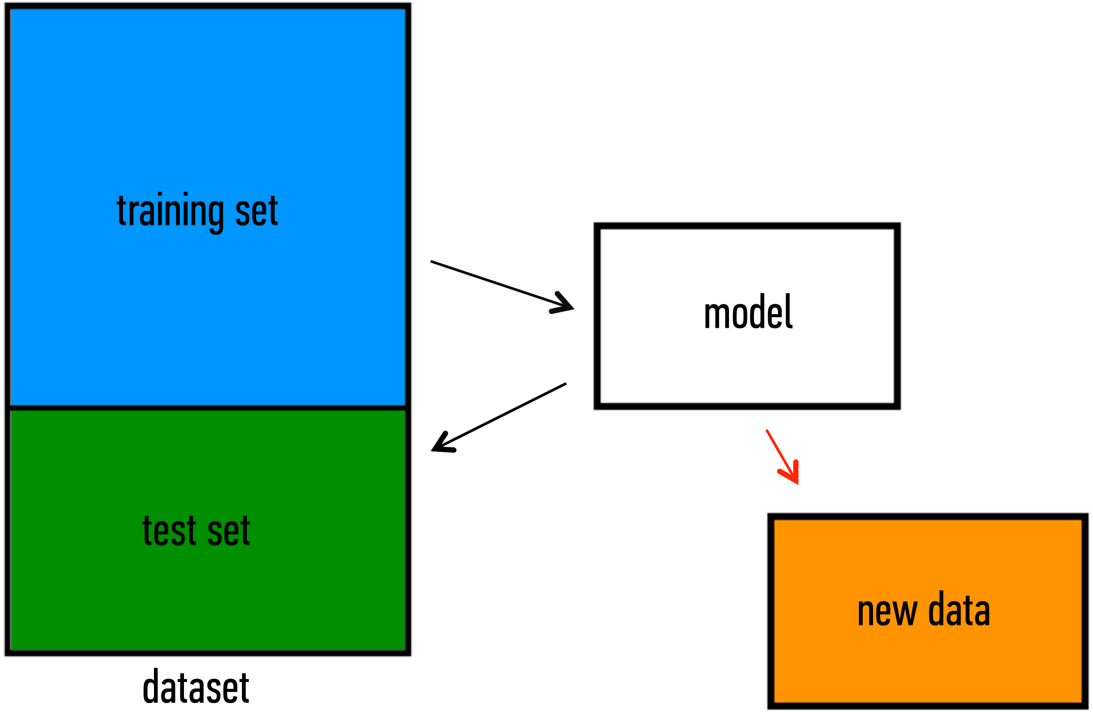


Q: What types of prediction error will we run into?

1) training error
2) generalization error
3) OOS error



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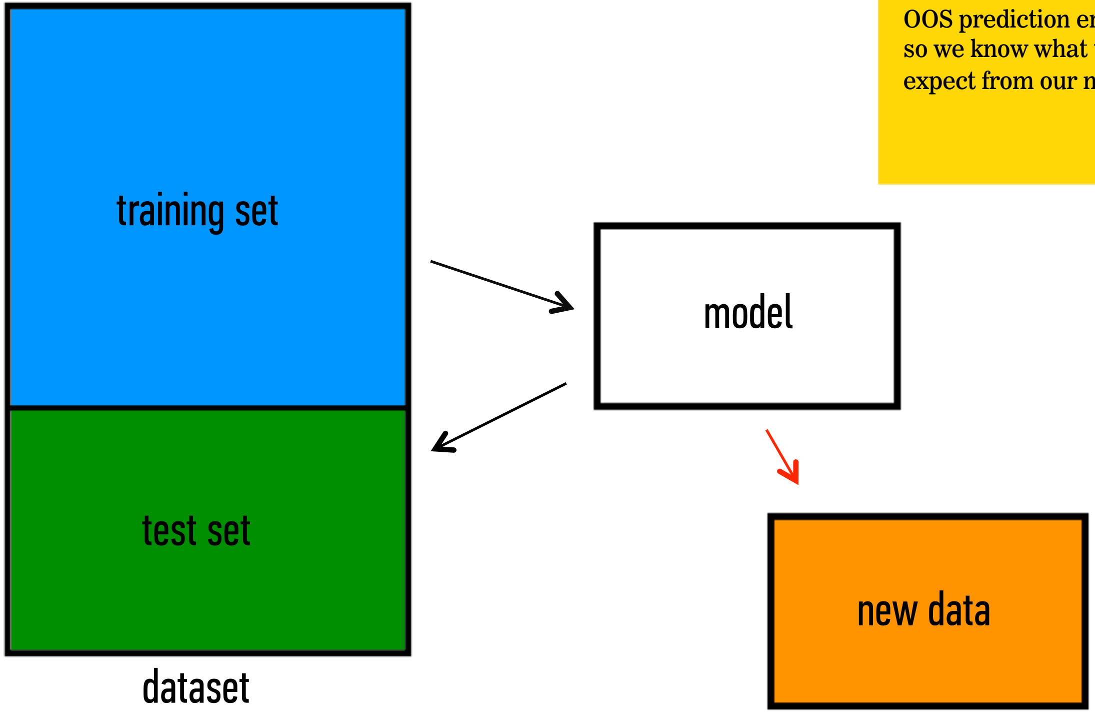

NOTE

We want to estimate OOS prediction error so we know what to expect from our model.

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NOTE

This phenomenon is called *overfitting*.

OVERFITTING

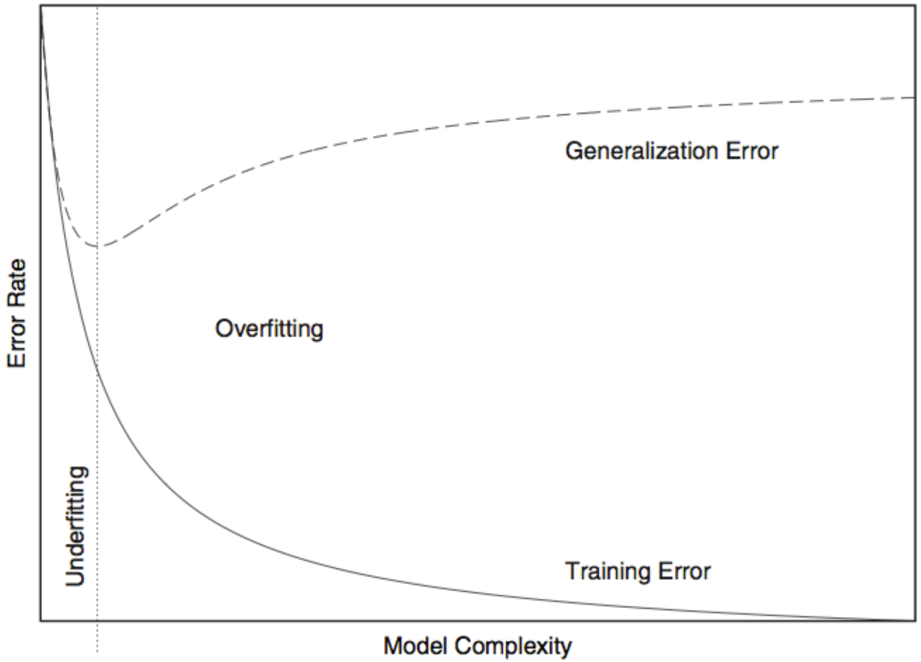
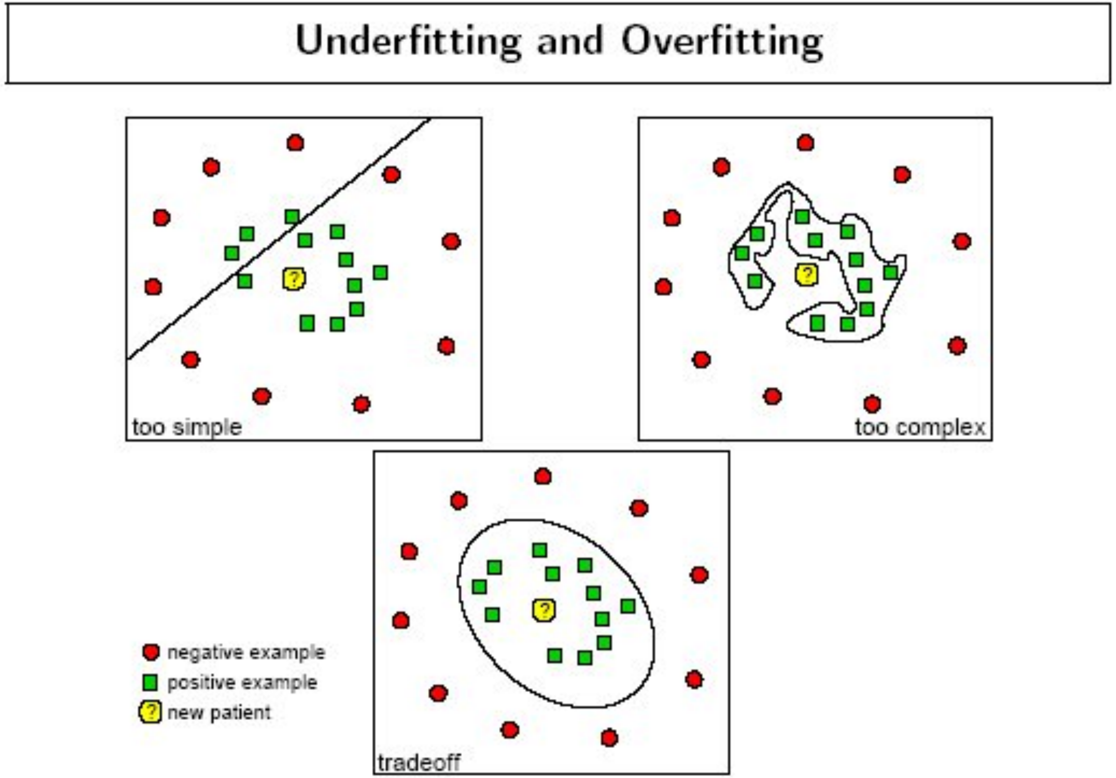


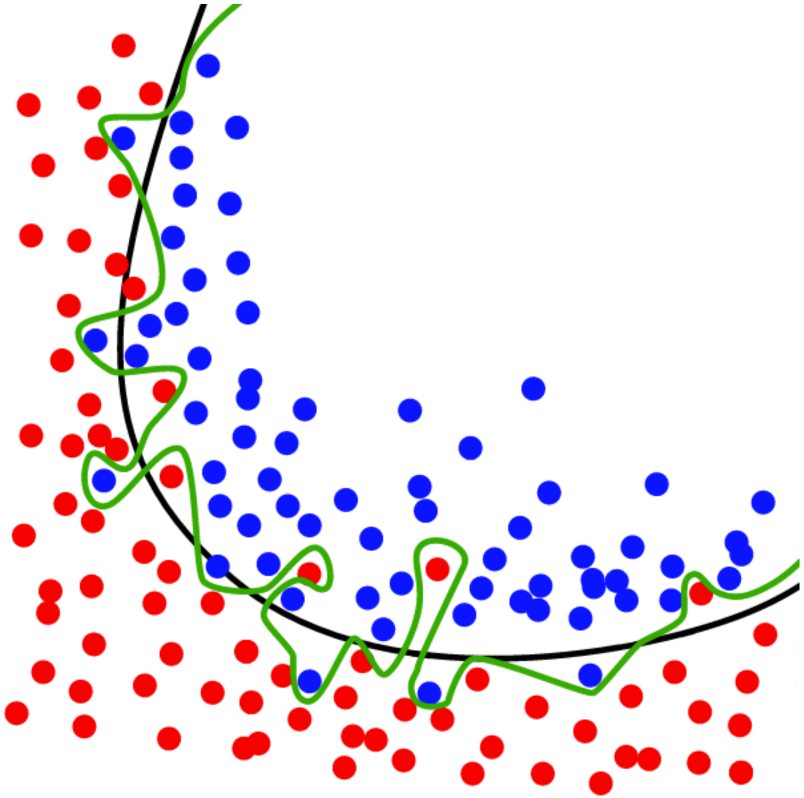
FIGURE 18-1. Overfitting: as a model becomes more complex, it becomes increasingly able to represent the training data. However, such a model is overfitted and will not generalize well to data that was not used during training.

source: Data Analysis with Open Source Tools, by Philipp K. Janert. O'Reilly Media, 2011.

OVERFITTING - EXAMPLE



source: http://www.dtreg.com



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A: Training error is not a good estimate of OOS accuracy.

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Thought experiment:

Suppose we had done a different train/test split.

Q: Would the generalization error remain the same?

A: Of course not!

A: On its own, not very well.

Something is still missing!

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Q: How can we do better?

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Different train/test splits will give us different generalization errors.

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A: Cross-validation.

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5) Take the average generalization error as the estimate of OOS accuracy.

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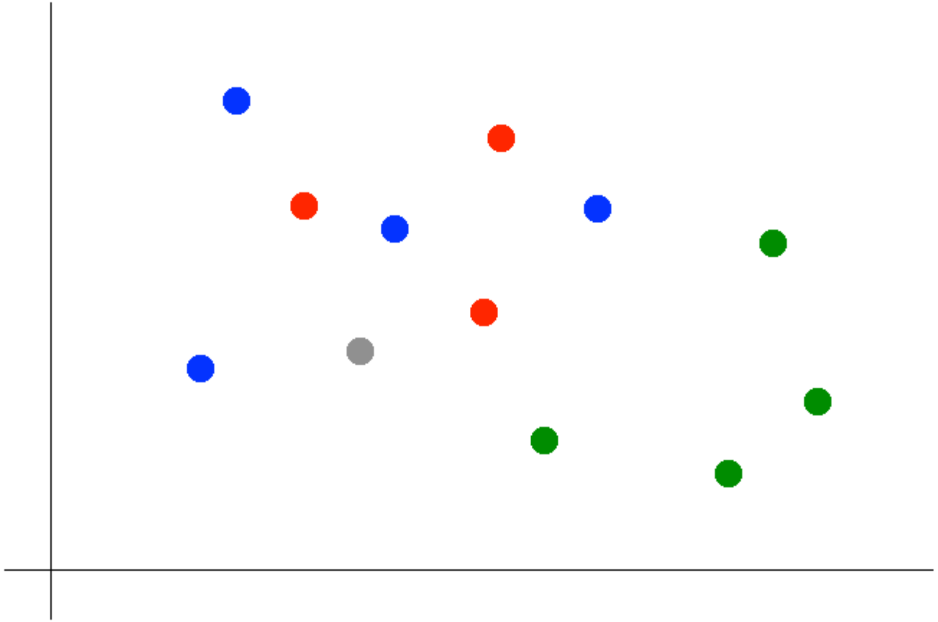
    - 10-fold CV is 10x more expensive than a single train/test split
4) Can be used for model selection.

III. KNN CLASSIFICATION

Suppose we want to predict the color of the grey dot.



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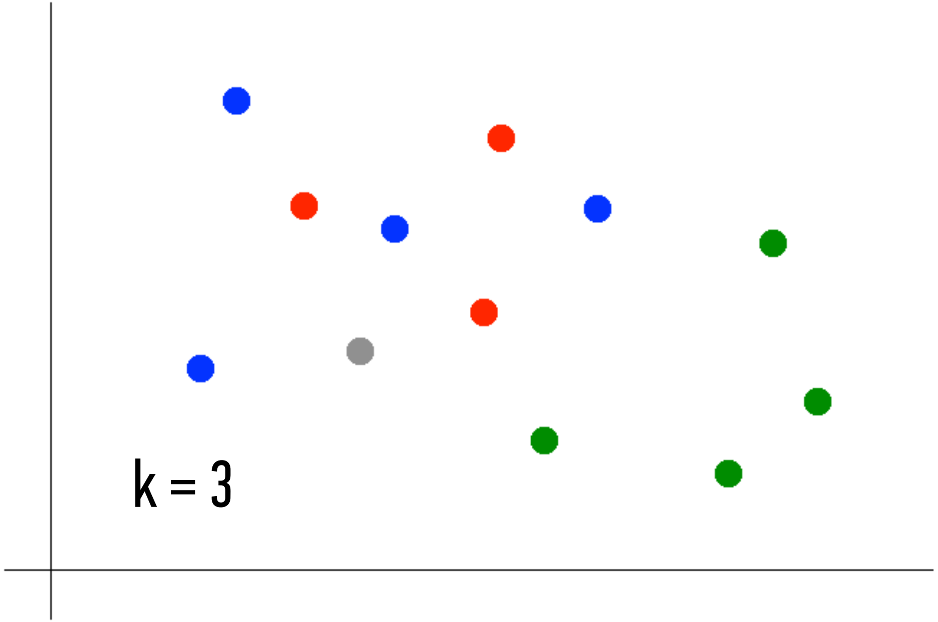
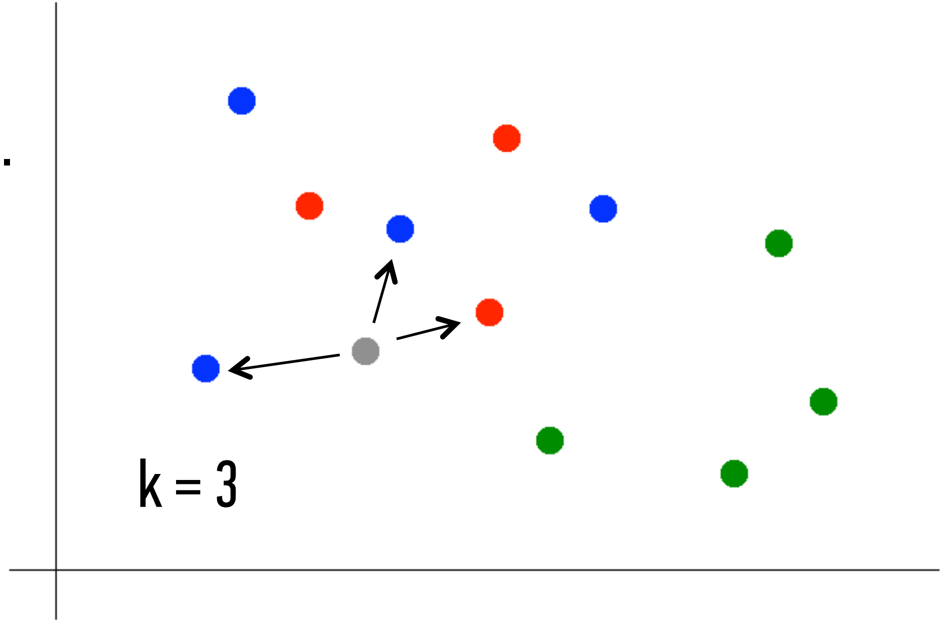
1) Pick a value for k.



Suppose we want to predict the color of the grey dot.

1) Pick a value for k.
2) Find colors of k nearest neighbors.



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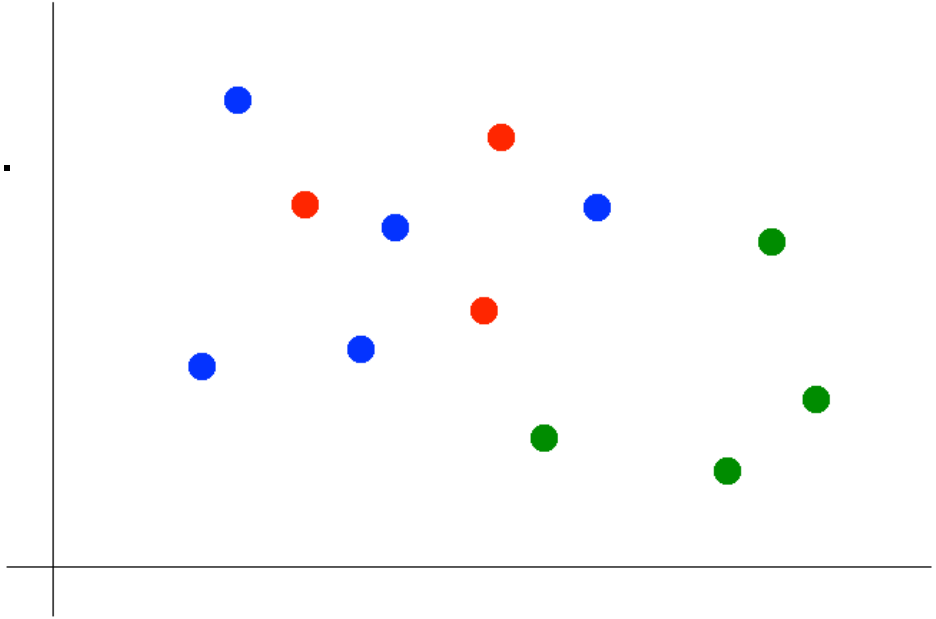
2) Find colors of k nearest neighbors.
3) Assign the most common color to the grey dot.



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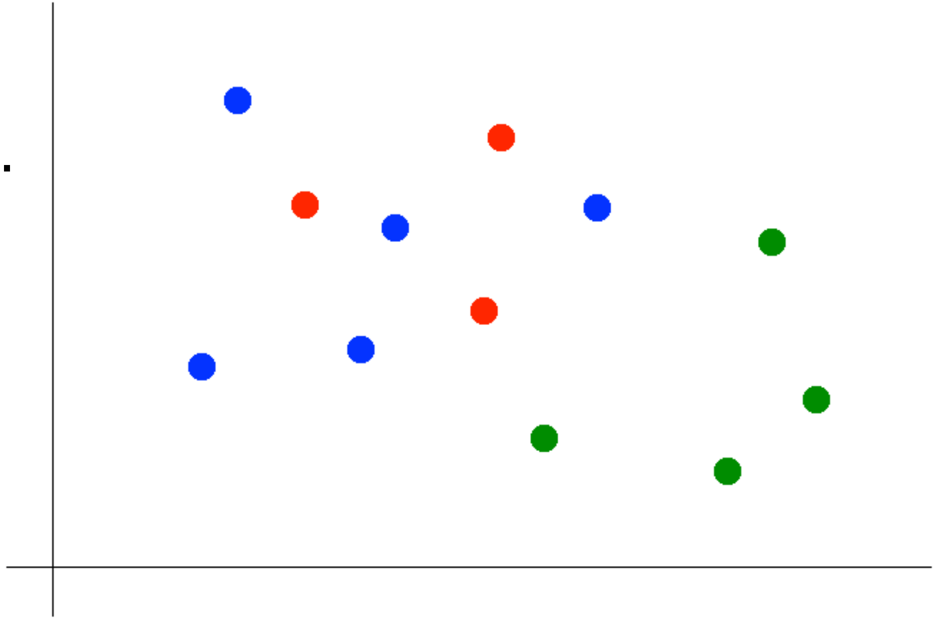

OPTIONAL NOTE

Our definition of "nearest" implicitly uses the *Euclidean distance function.*

IV. LINEAR REGRESSION

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

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supervised	regression	classification
unsupervised	dimension reduction	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:

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α = **intercept** (where the line crosses the y-axis)

β = **regression coefficient** (the model "parameter")

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

We can extend this model to several input variables, giving us the **multiple linear regression** model:

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$$y = \alpha + \beta_1 x_1 \; + \; \dots \; + \; \beta_n x_n + \varepsilon$$

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.

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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!

V. POLYNOMIAL REGRESSION

Consider the following **polynomial regression** model:

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

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Q: This represents a nonlinear relationship. Is it still a linear model?

A: Yes, because it's linear in the β's!

Polynomial regression allows us to fit very complex curves to data.

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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.

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

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

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

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

Q: What can we do about this?

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A: Replace the correlated predictors with uncorrelated predictors.

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$$y = \alpha + \beta_1 f_1(x) + \beta_2 f_2(x^2) + \ldots + \beta_n f_n(x^n) + \varepsilon$$

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?

V. REGULARIZATION

Recall our earlier discussion of **overfitting**.

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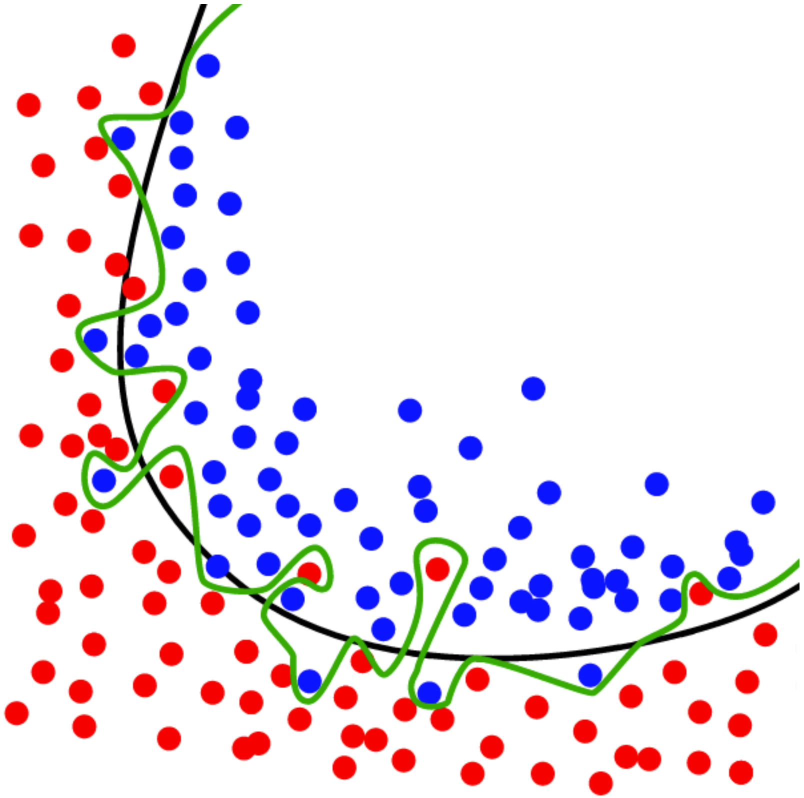
In other words, an overfit model matches the **noise** in the dataset instead of the **signal**.



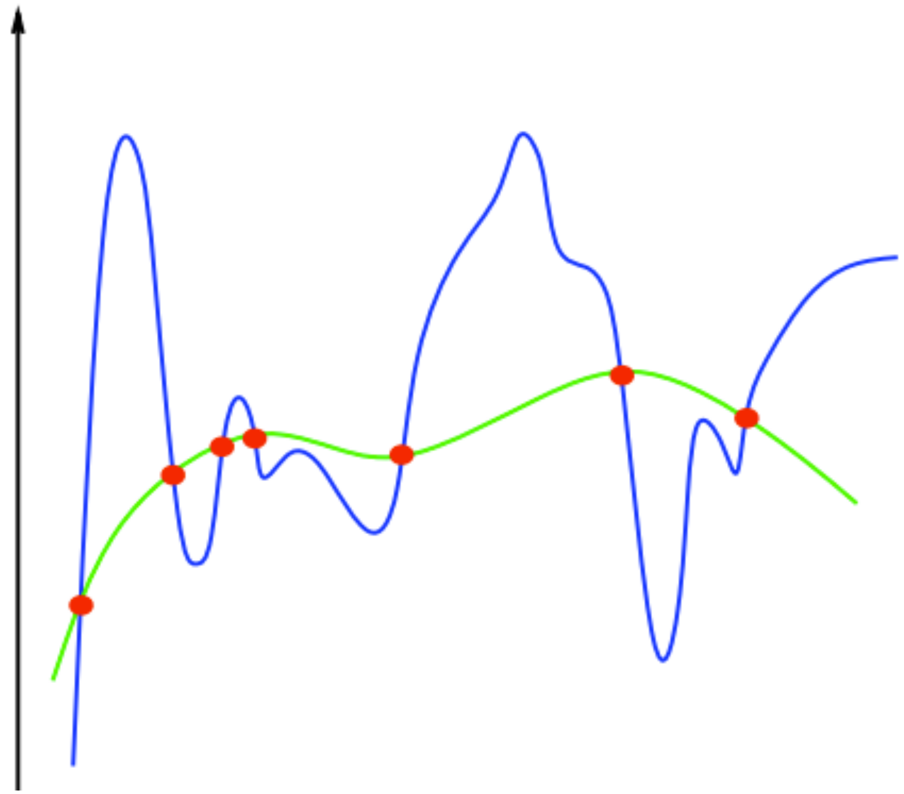
source: *http://upload.wikimedia.org/wikipedia/commons/1/19/Overfitting.svg*

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**

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

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***Lasso* regularization**: $y = \Sigma\, \beta_i x_i + \varepsilon \quad st. \quad \Sigma\, |\beta_i| < s$

***Ridge* regularization**: $y = \Sigma\, \beta_i x_i + \varepsilon \quad st. \quad \Sigma\, \beta_i^2 < s$

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

These regularization problems can also be expressed as:

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

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

These regularization problems can also be expressed as:

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

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

We are no longer just minimizing error but also an additional term.

DISCUSSION