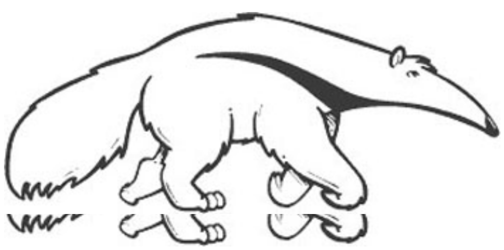
Machine Learning and Data Mining

Introduction

Prof. Alexander Ihler



BREN:ICS
INFORMATION AND COMPUTER SCIENCES
UNIVERSITY of CALIFORNIA IRVINE

Artificial Intelligence (AI)

- Building “intelligent systems”
- Lots of parts to intelligent behavior

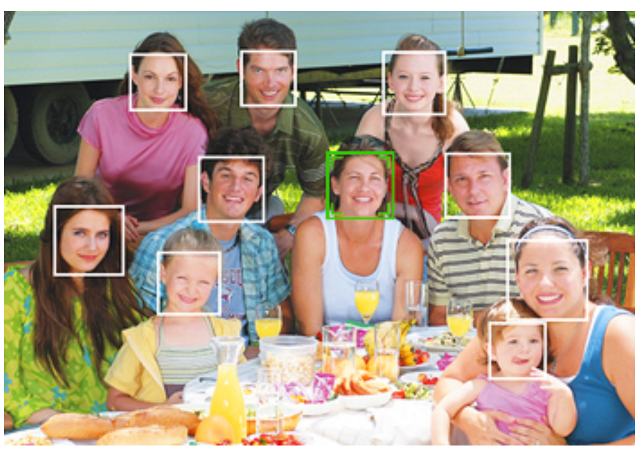
Darpa GC (Stanley)

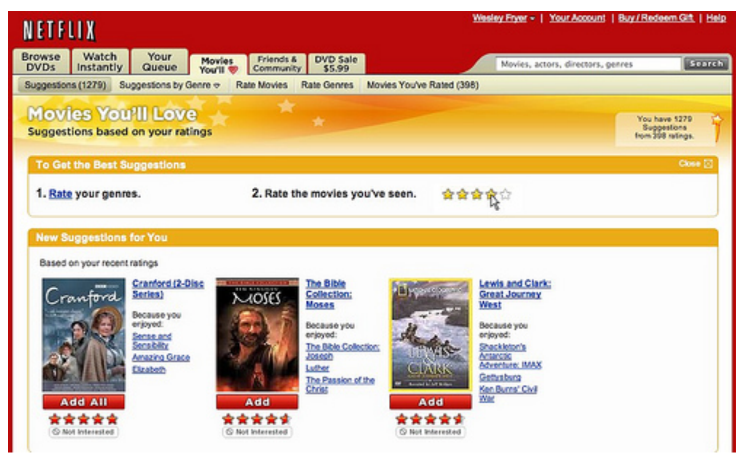
RoboCup

Chess (Deep Blue v. Kasparov)

Machine learning (ML)

- One (important) part of AI
- Making predictions (or decisions)
- Getting better with experience (data)
- Problems whose solutions are “hard to describe”

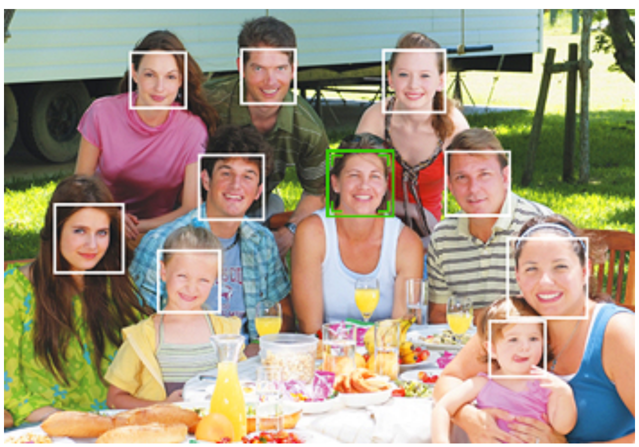


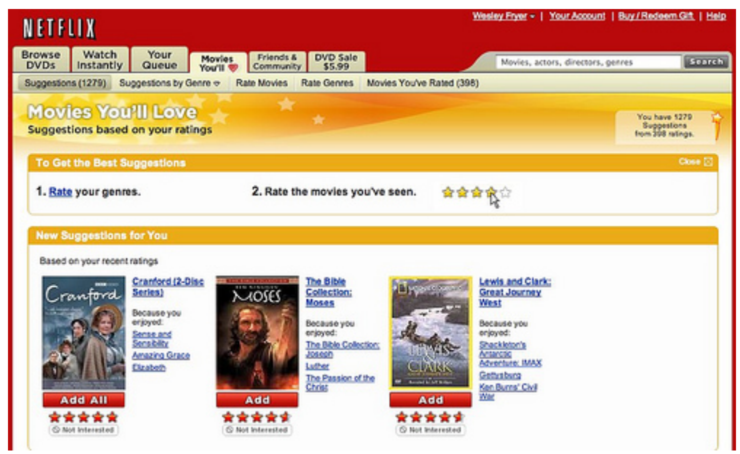


Types of prediction problems

- Supervised learning
  - "Labeled" training data
  - Every example has a desired target value (a "best answer")
  - Reward prediction being close to target

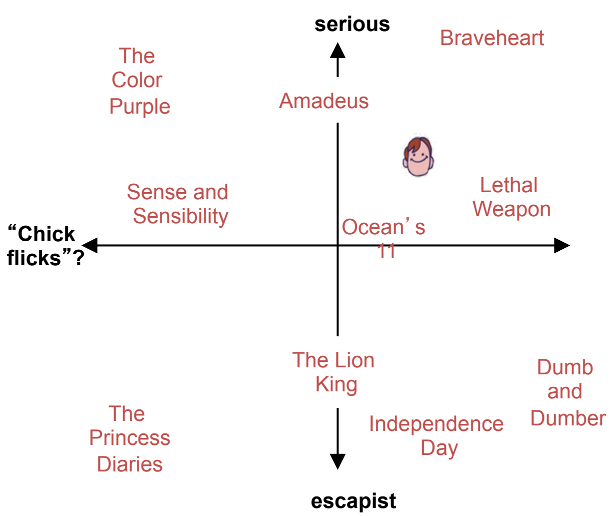
  - Classification: a discrete-valued prediction (often: action / decision)
  - Regression: a continuous-valued prediction

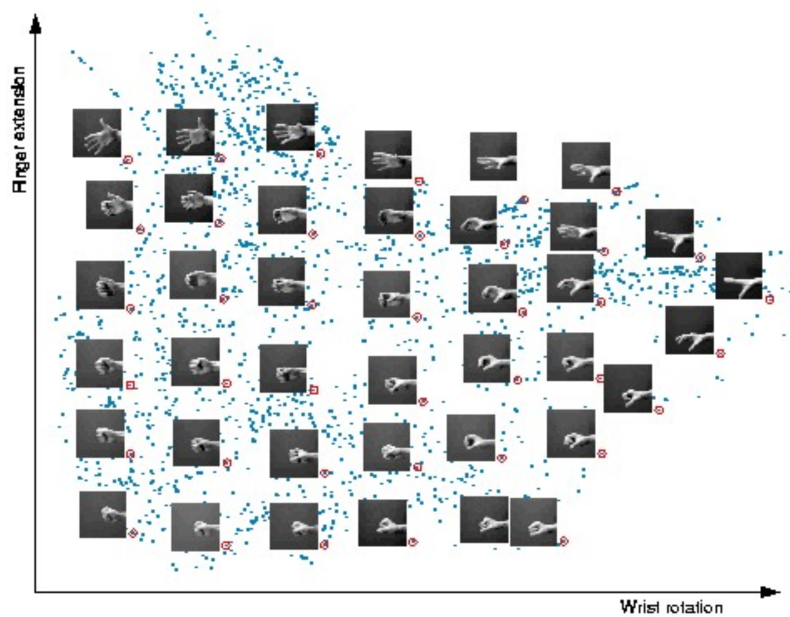




Types of prediction problems

- Supervised learning
- Unsupervised learning
  - No known target values
  - No targets = nothing to predict?
  - Reward "patterns" or "explaining features"
  - Often, data mining





Types of prediction problems

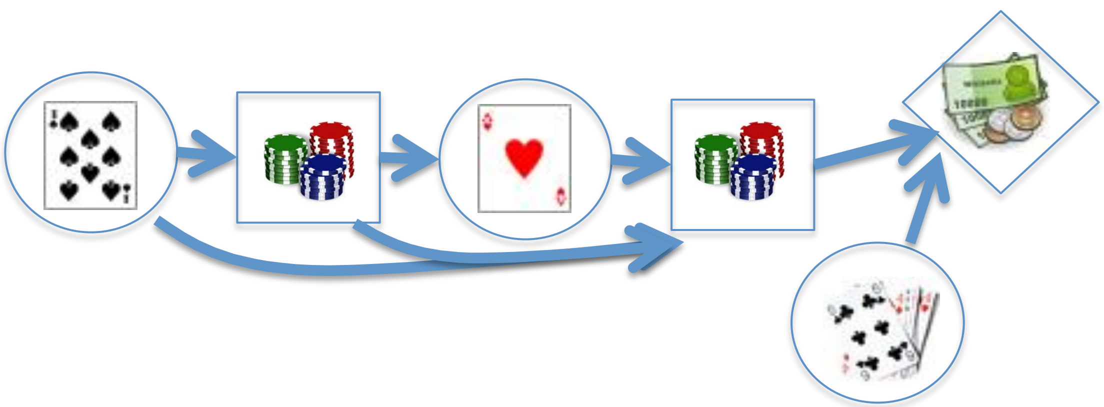
- Supervised learning
- Unsupervised learning
- Semi-supervised learning
  - Similar to supervised
  - some data have unknown target values

- Ex: medical data
  - Lots of patient data, few known outcomes
- Ex: image tagging
  - Lots of images on Flikr, but only some of them tagged

Types of prediction problems

- Supervised learning
- Unsupervised learning
- Semi-supervised learning
- Reinforcement learning

- "Indirect" feedback on quality
  - No answers, just "better" or "worse"
  - Feedback may be delayed



Logistics

- Course webpage for assignments & other info (?)
- EEE for homework submission & return
- Piazza for questions & discussions

- No required textbook
  - Recommended: Murphy, "Machine Learning...", 2012.
  - Also
    - Duda, Hart & Stork, "Pattern classification"
    - Hastie, Tibshirani & Friedman, "Elements of Statistical Learning"
- But
  - I'll try to cover everything needed in lectures and notes
  - All textbooks mainly for reference purposes

Logistics

- Grading (may be subject to change)
  - 25% homework (6+?   >5: drop 1)
  - 15% project (Kaggle)
  - 25% midterm, 35% final
  - Due 11:59pm listed day, EEE or my office
  - Late homework:
    - 10% off per day or part
    - No credit after solutions posted: turn in what you have
- Collaboration
  - Study groups, discussion, assistance encouraged
    - Whiteboards, etc.
  - Do your homework yourself
    - Don't exchange solutions or HW code

Data exploration

- Machine learning is a data science
  - Look at the data; get a “feel” for what might work

- What types of data do we have?
  - Binary values? (spam; gender; …)
  - Categories? (home state; labels; …)
  - Integer values? (1..5 stars; age brackets; …)
  - (nearly) real values? (pixel intensity; prices; …)

- Are there missing data?

- “Shape” of the data? Outliers?

Scientific software

- **Python**
  - **Numpy, MatPlotLib, SciPy…**
- Matlab
  - Octave (free)
- R
  - Used mainly in statistics
- C++
  - For performance, not prototyping
- And other, more specialized languages for modeling…

Representing data

- Example: Fisher's "Iris" data
  http://en.wikipedia.org/wiki/Iris_flower_data_set

- Three different types of iris
  - "Class", y

- Four "features", $x_1,\ldots,x_4$
  - Length & width of
    sepals & petals

- 150 examples (data points)

Representing the data (Matlab)

- Have m observations (data points)

$$\left\{x^{(1)} \ldots, x^{(m)}\right\}$$

- Each observation is a vector consisting of n features

$$x^{(j)} = [x_1^{(j)} x_2^{(j)} \ldots x_n^{(j)}]$$

- Often, represent this as a "data matrix"

$$\underline{X} = \begin{bmatrix} x_1^{(1)} & \ldots & x_n^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(m)} & \ldots & x_n^{(m)} \end{bmatrix}$$

```
import numpy as np    # import numpy
iris = np.genfromtxt("data/iris.txt",delimiter=None)
X = iris[:,0:4]           # load data and split into features, targets
Y = iris[:,4]
print X.shape             # 150 data points; 4 features each
   (150, 4)
```

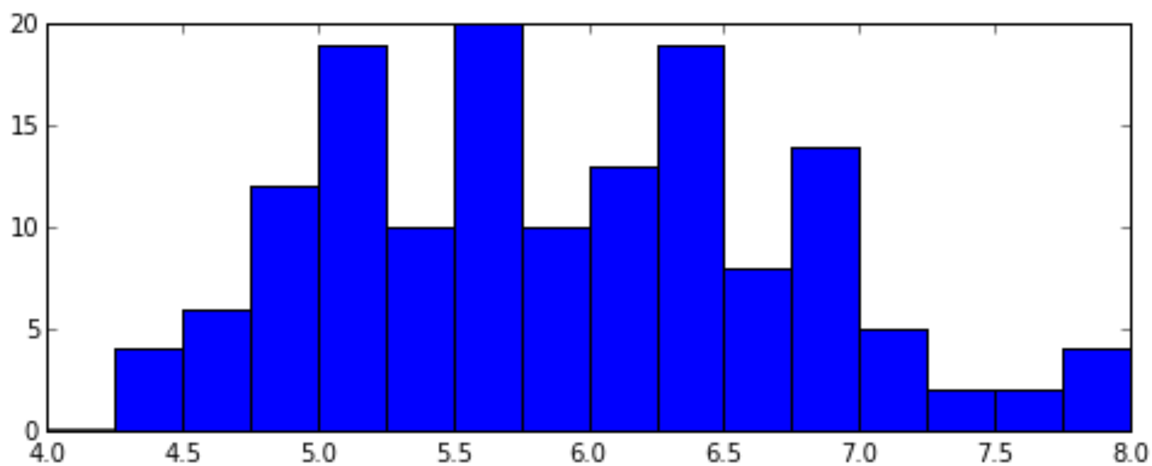
Basic statistics

- Look at basic information about features
  - Average value? (mean, median, etc.)
  - "Spread"?   (standard deviation, etc.)
  - Maximum / Minimum values?

```
print np.mean(X, axis=0)          # compute mean of each feature
 [ 5.8433    3.0573    3.7580    1.1993 ]
print np.std(X, axis=0)           #compute standard deviation of each feature
 [ 0.8281    0.4359    1.7653    0.7622 ]
print np.max(X, axis=0)           # largest value per feature
 [  7.9411    4.3632    6.8606    2.5236 ]
print np.min(X, axis=0)           # smallest value per feature
 [  4.2985    1.9708    1.0331    0.0536  ]
```

Histograms

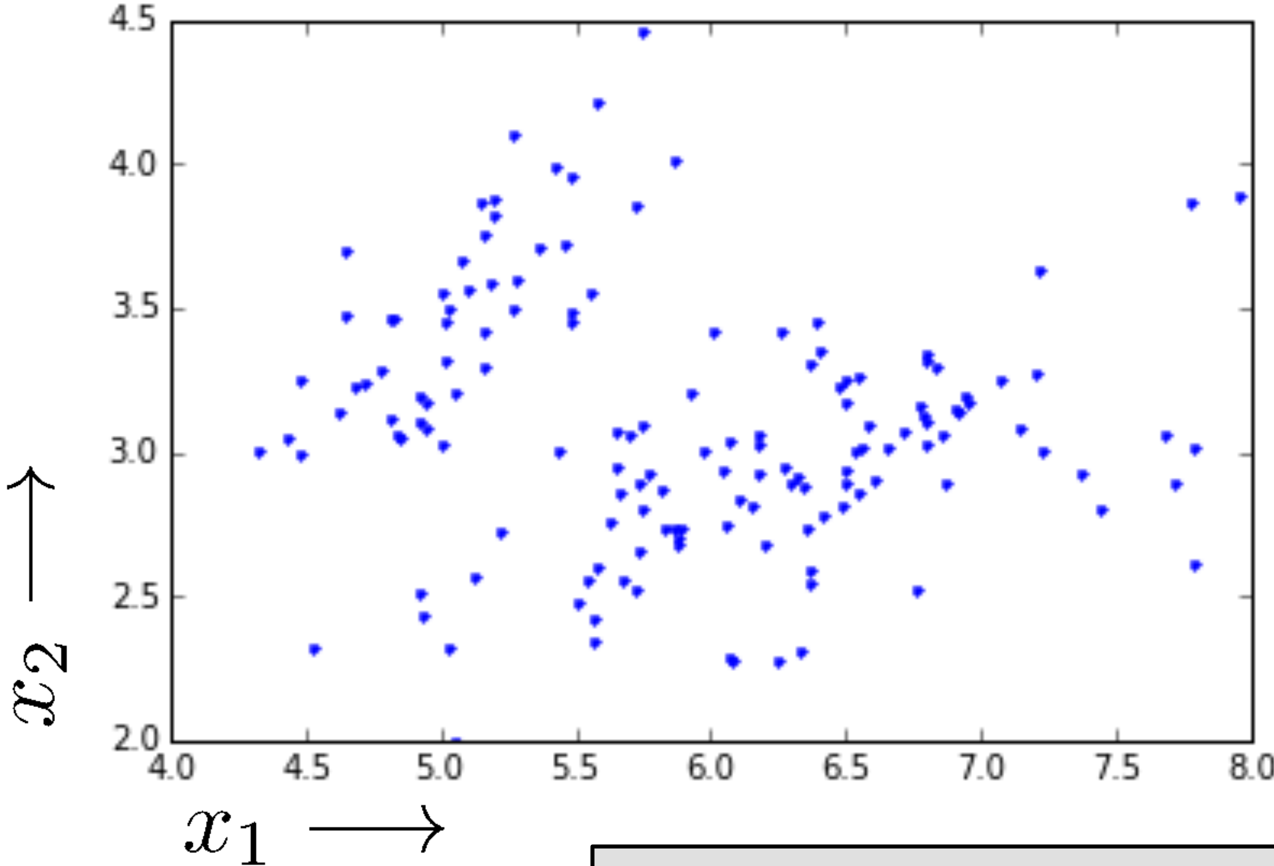
- Count the data falling in each of K bins
  - "Summarize" data as a length-K vector of counts (& plot)
  - Value of K determines "summarization"; depends on # of data
    - K too big: every data point falls in its own bin; just "memorizes"
    - K too small: all data in one or two bins; oversimplifies




```
% Histograms in MatPlotLib
import matplotlib.pyplot as plt
X1 = X[:,0]                      # extract first feature
Bins = np.linspace(4,8,17)       # use explicit bin locations
plt.hist( X1, bins=Bins )        # generate the plot
```

Scatterplots

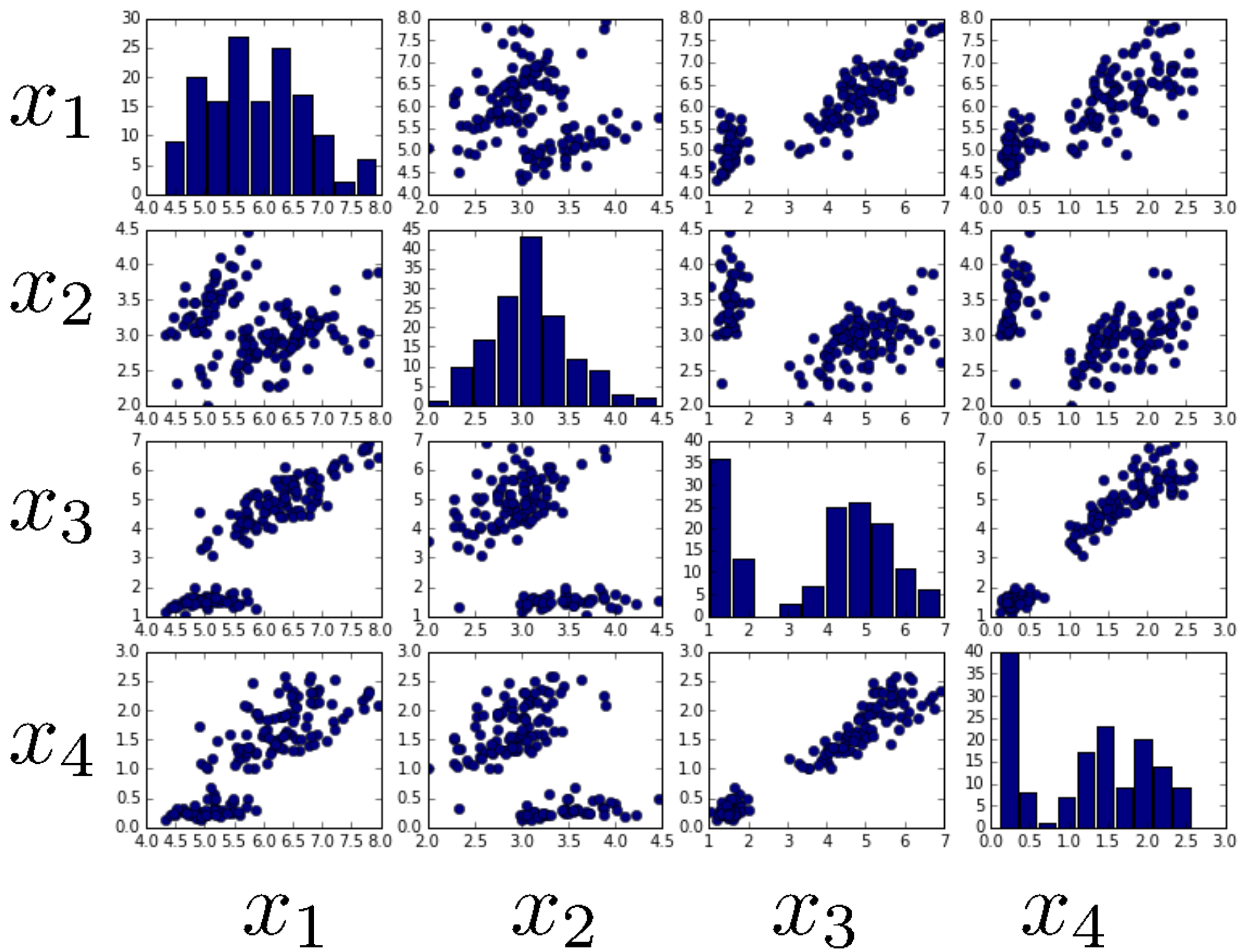
- Illustrate the relationship between two features




```
% Plotting in MatPlotLib
plt.plot(X[:,0], X[:,1], 'b.');   % plot data points as blue dots
```

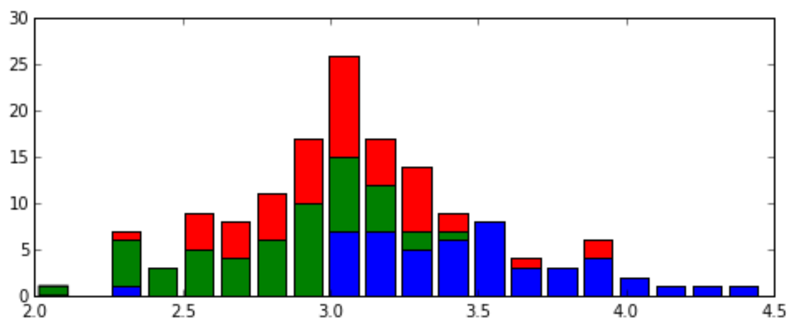
Scatterplots

- For more than two features we can use a pair plot:

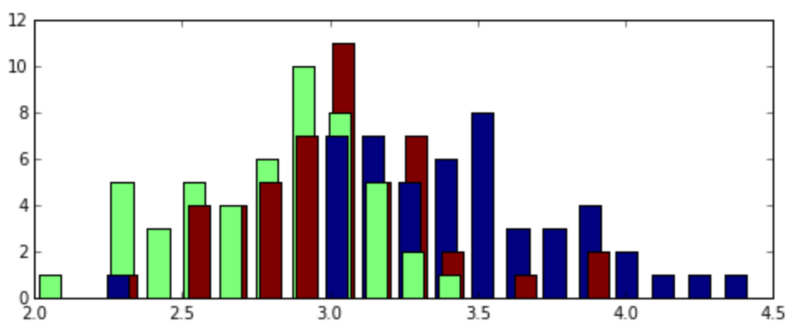


Supervised learning and targets

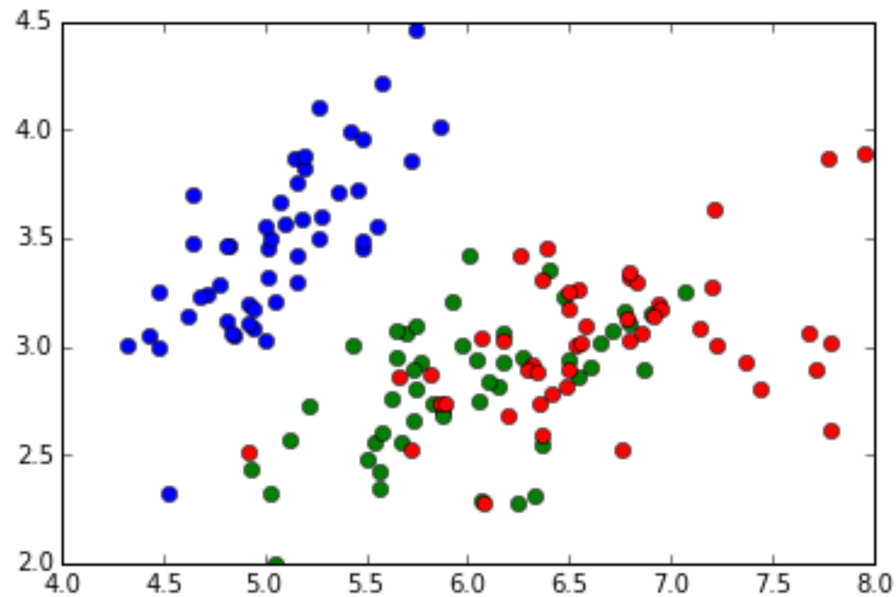
- Supervised learning: predict target values
- For discrete targets, often visualize with color




```
plt.hist( [X[Y==c,1] for c in np.unique(Y)] ,
          bins=20, histtype='barstacked')
```



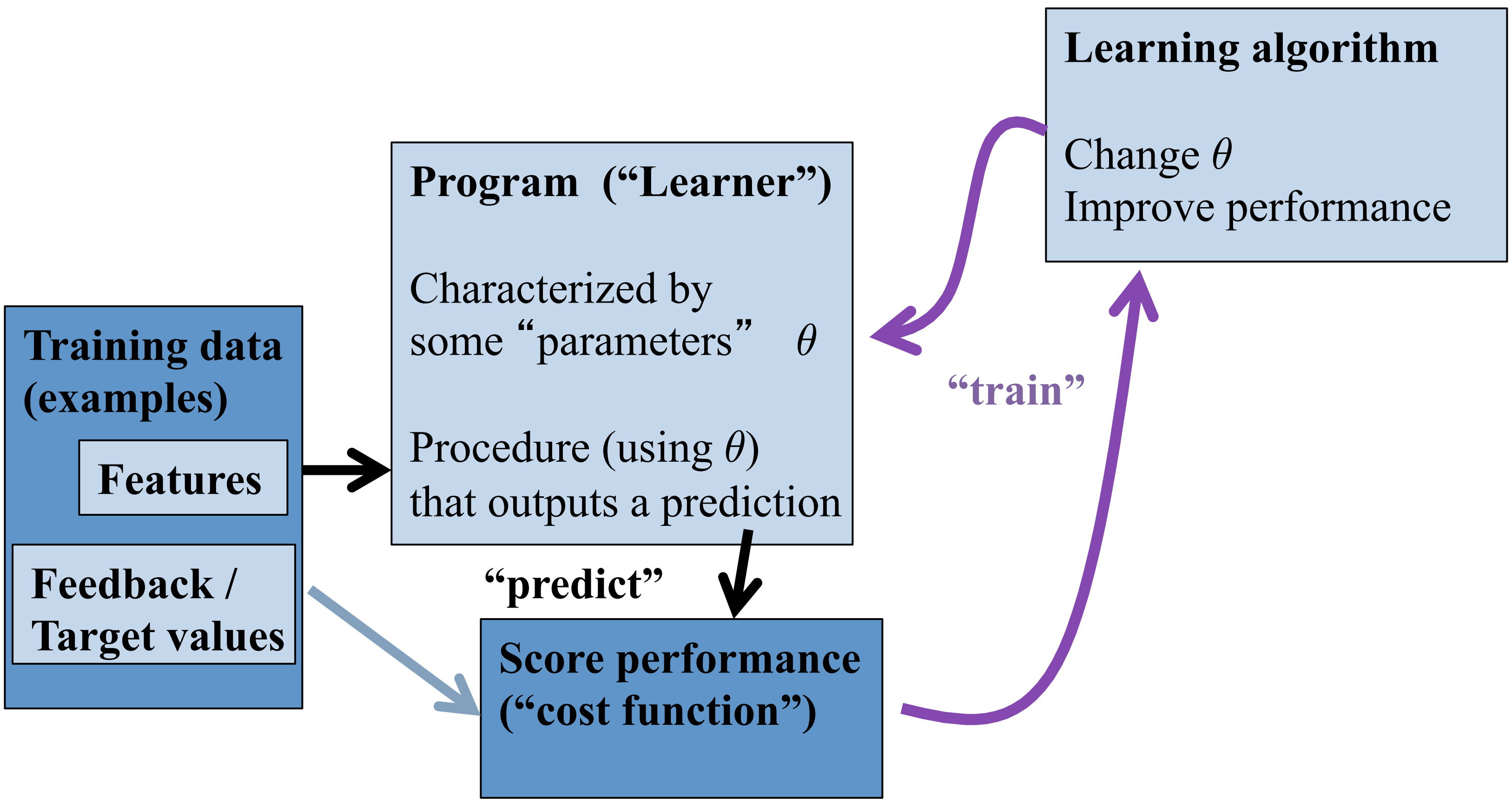

```
ml.histy(X[:,1], Y, bins=20)
```




```
colors = ['b','g','r']
for c in np.unique(Y):
    plt.plot( X[Y==c,0], X[Y==c,1], 'o',
              color=colors[int(c)] )
```

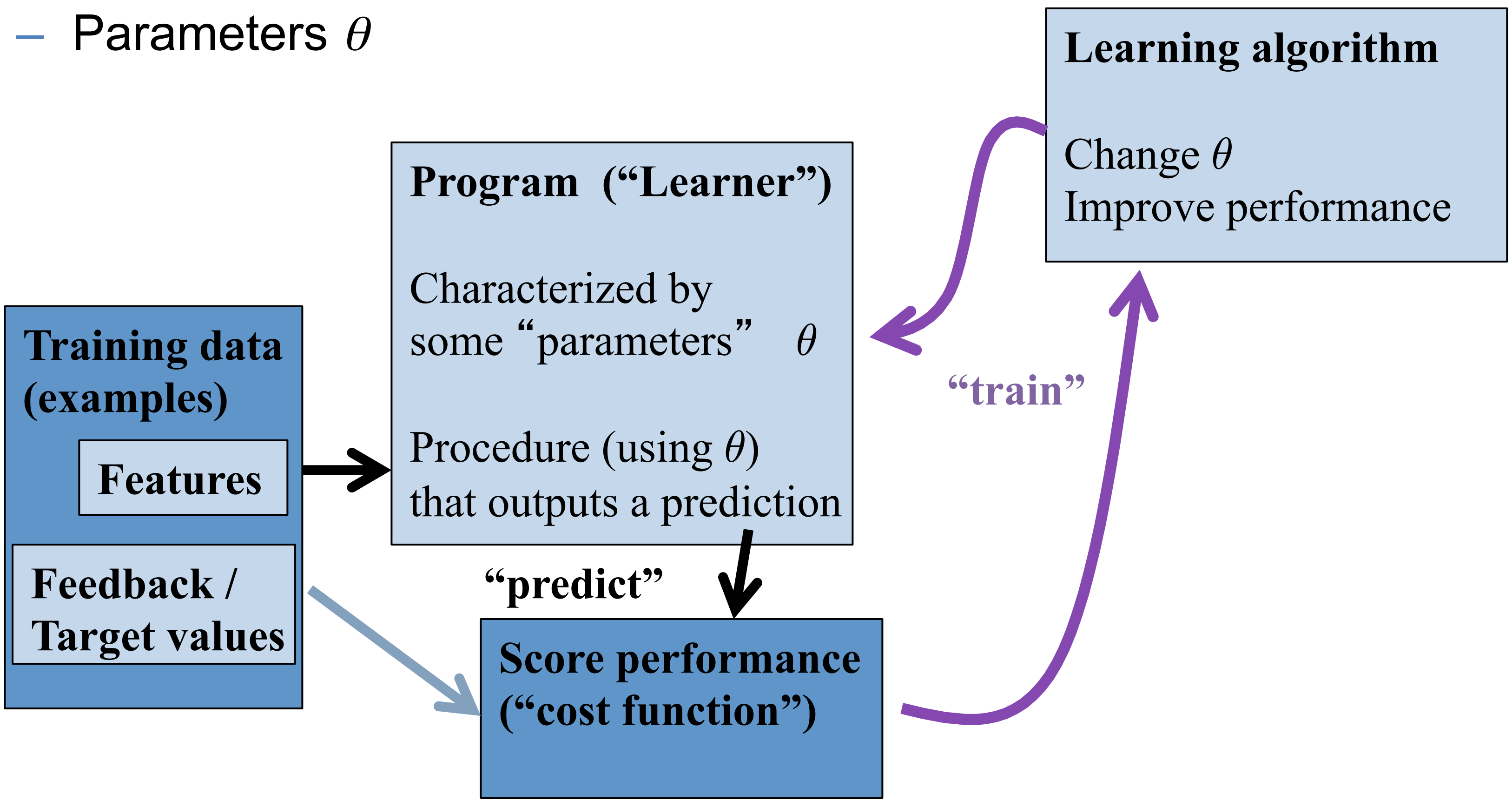
How does machine learning work?

- "Meta-programming"
  - Predict – apply rules to examples
  - Score – get feedback on performance
  - Learn – change predictor to do better

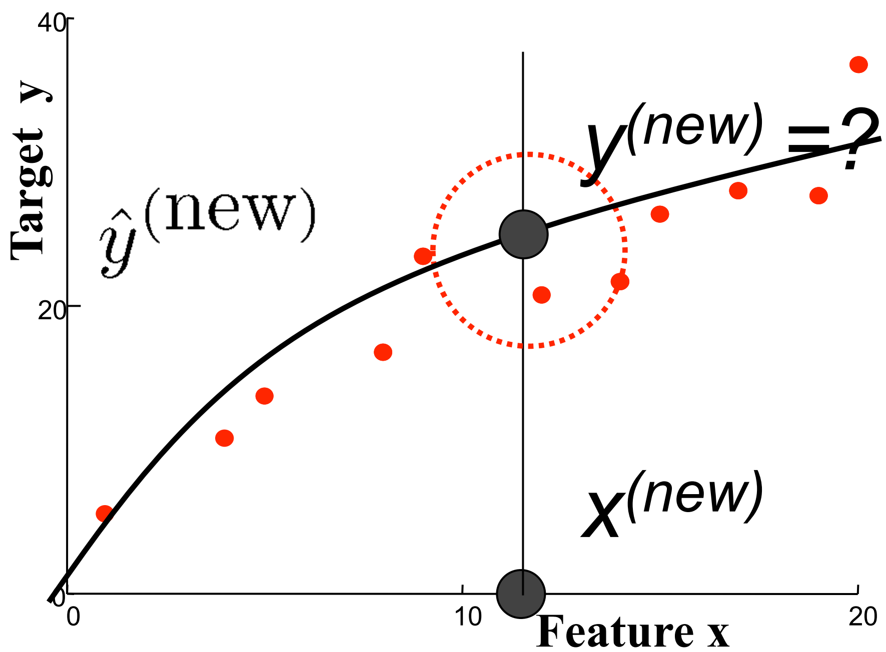


Supervised learning

- Notation
  - Features x
  - Targets y
  - Predictions $\hat{y} = f(x\ ;\ \theta)$
  - Parameters θ

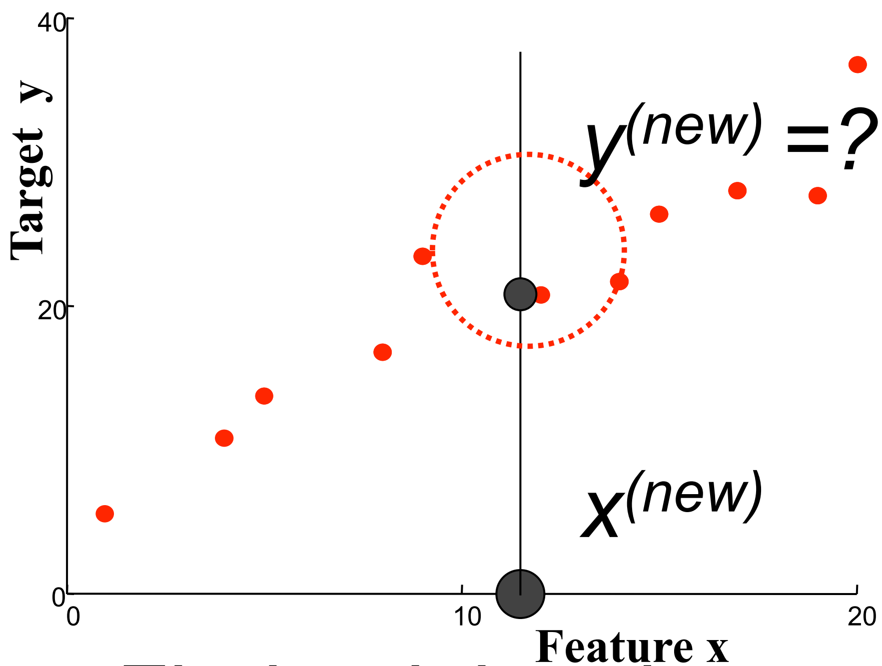


Regression; Scatter plots



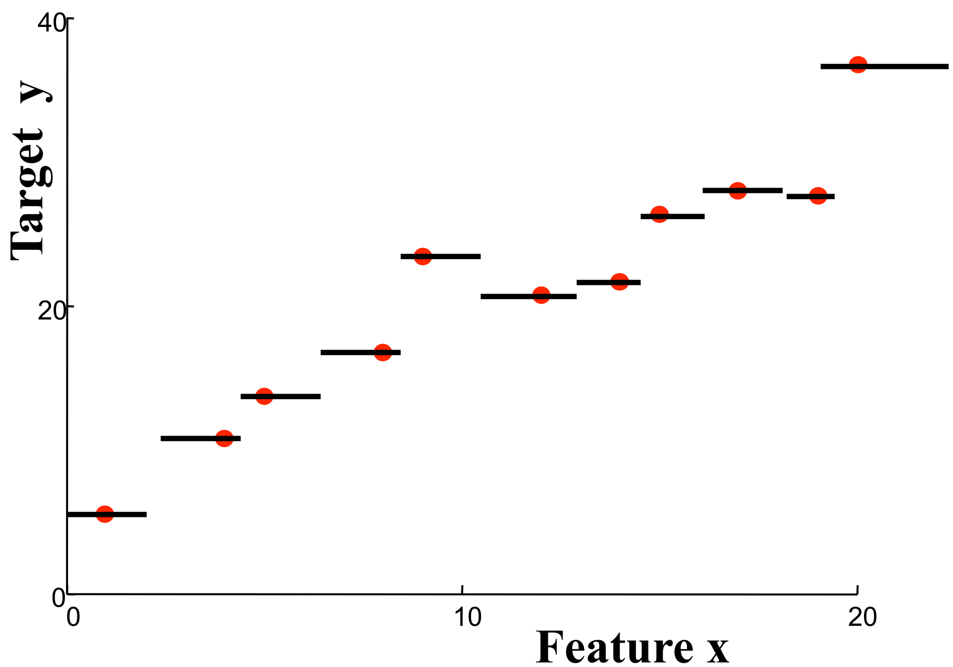
- Suggests a relationship between x and y
- *Prediction*: new x, what is y?

Nearest neighbor regression



- Find training datum $x^{(i)}$ closest to $x^{(new)}$
  Predict $y^{(i)}$

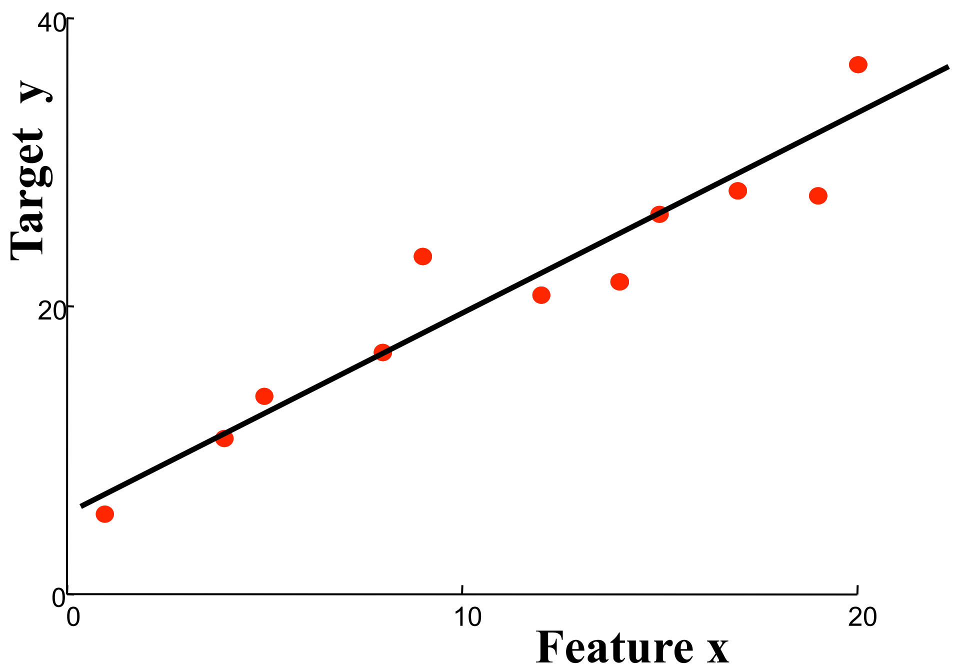
Nearest neighbor regression



"Predictor":
Given new features:
  Find nearest example
  Return its value

- Defines a function f(x) implicitly
- "Form" is piecewise constant

Linear regression



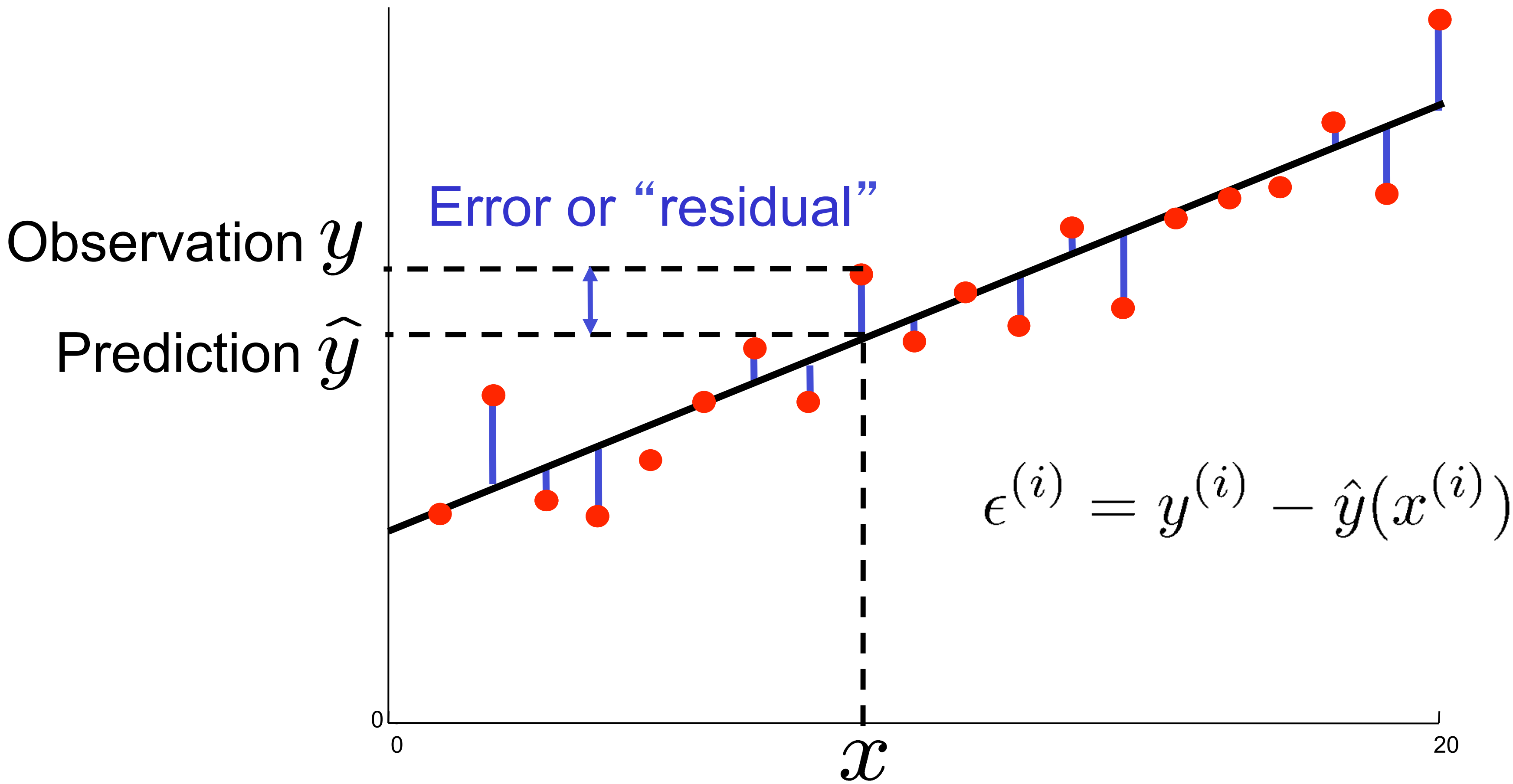
"Predictor":
Evaluate line:

$$r = \theta_0 + \theta_1 x_1$$

return r

- Define form of function f(x) explicitly
- Find a good f(x) within that family

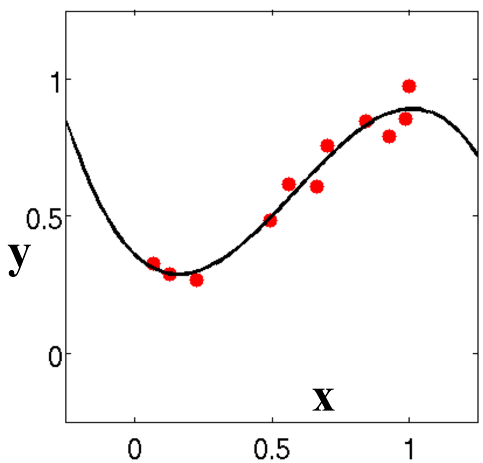
Measuring error



$$\mathrm{MSE} = \frac{1}{m} \sum_i \left(y^{(i)} - \hat{y}(x^{(i)}) \right)^2$$

Regression vs. Classification

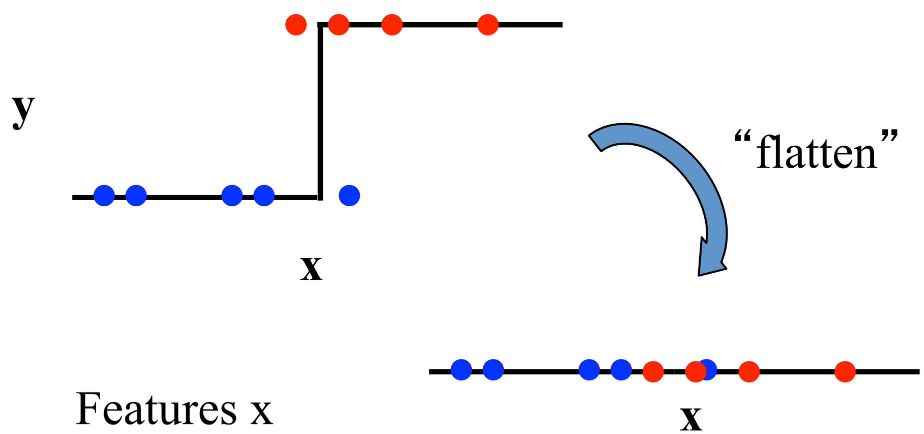
Regression



Features x
Real-valued target y

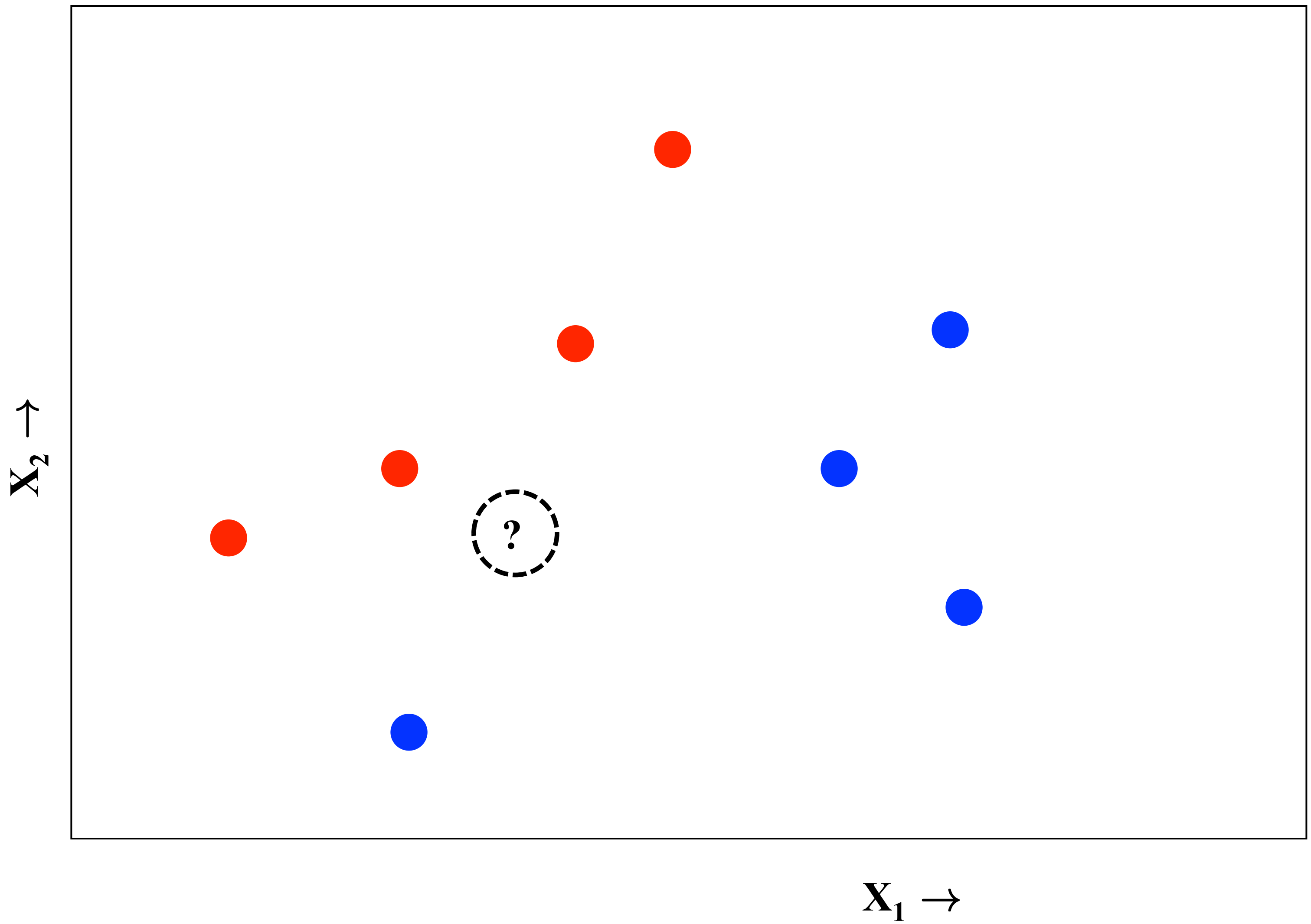
Predict continuous function ŷ(x)

Classification

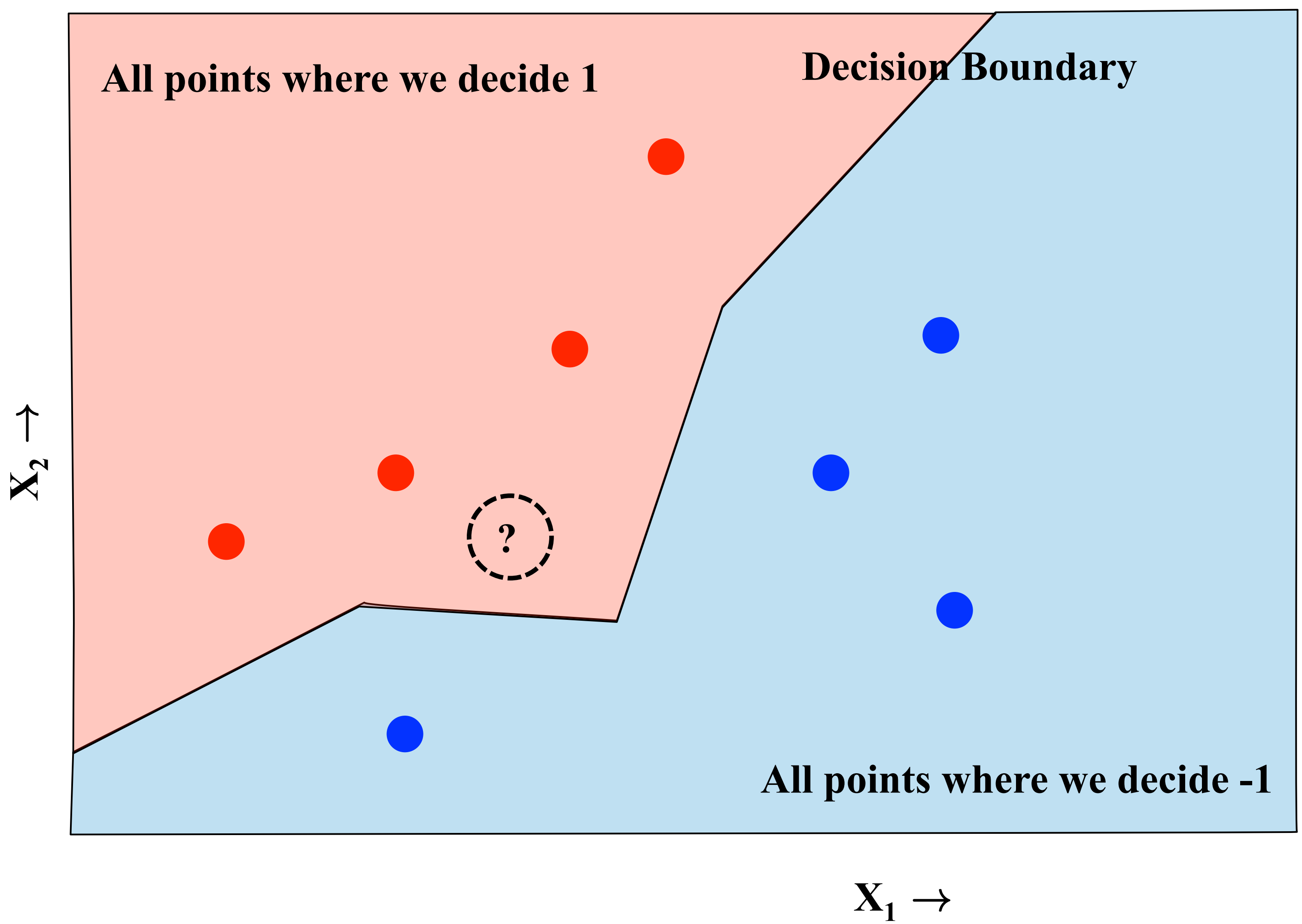


Features x
Discrete class c
(usually 0/1 or +1/-1)
Predict discrete function ŷ(x)

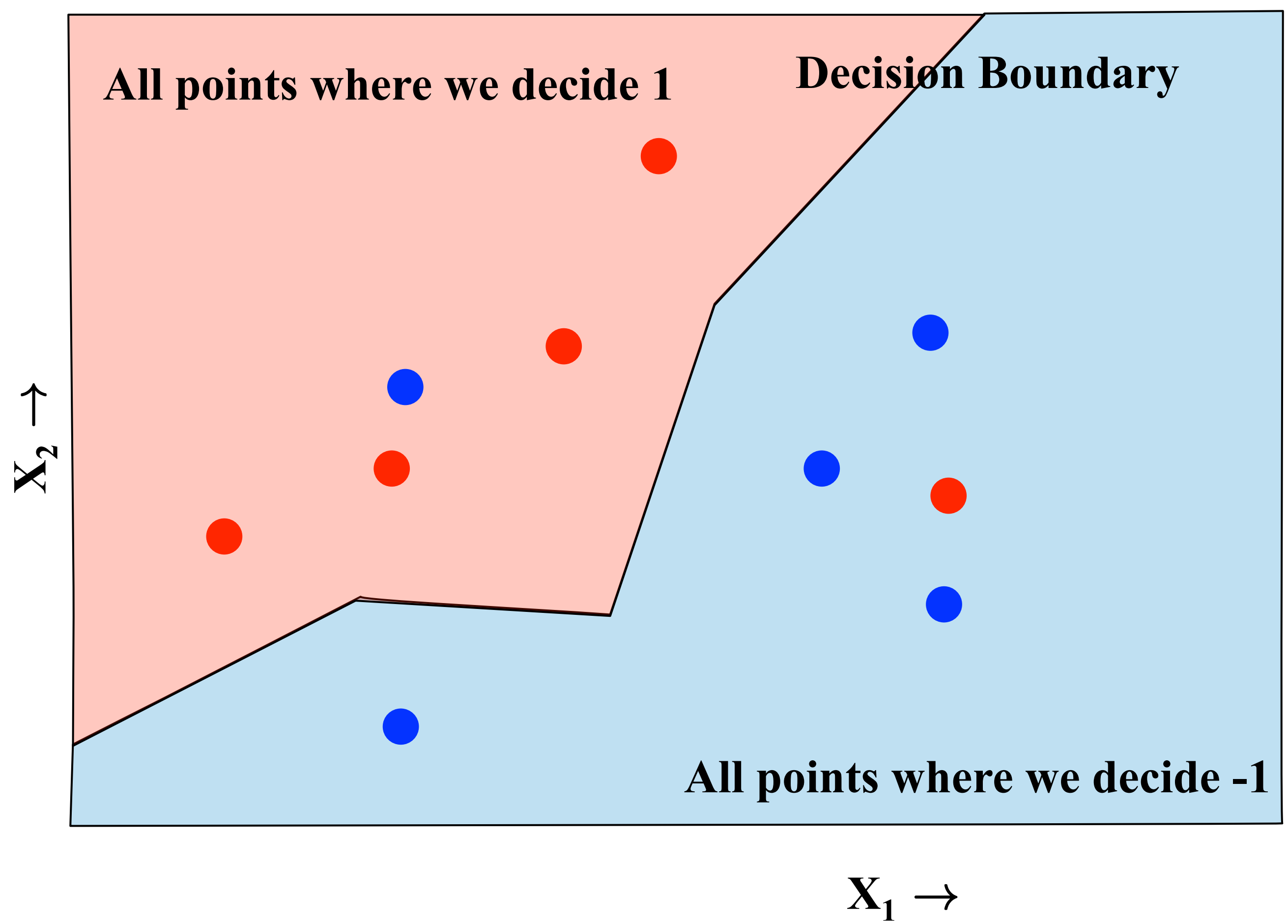
Classification



Classification



Measuring error



$$\mathrm{ERR} = \frac{1}{m} \sum_i \left[y^{(i)} \neq \hat{y}(x^{(i)}) \right]$$

A simple, optimal classifier

- Classifier f(x ; θ)
  - maps observations x to predicted target values
- Simple example
  - Discrete feature x: f(x ; θ) is a contingency table
  - Ex: spam filtering: observe just X_1 = in contact list?
- Suppose we knew the true conditional probabilities:
- Best prediction is the most likely target!

Feature	spam	keep
X=0	0.6	0.4
X=1	0.1	0.9

"Bayes error rate"

Pr[X=0] * Pr[wrong | X=0] + Pr[X=1] * Pr[wrong | X=1]

= Pr[X=0] * (1- Pr[Y=S | X=0]) + Pr[X=1] * (1-Pr[Y=K | X=1])

Optimal least-squares regression

- Suppose that we know true p(X,Y)
- Prediction f(x): *arbitrary* function
  - Focus on some specific x: f(x) = v
- Expected squared error loss is

$$\mathbb{E}_{Y|X=x}\left[(Y-v)^2\right] = \int p(Y|X=x)(Y-v)^2 \; dY$$

- Minimum: take derivitave & set to zero

$$\frac{\partial}{\partial v} \int p(Y|X=x)(Y-v)^2 \; dY = \int p(Y|X=x) 2(Y-v) = 0$$

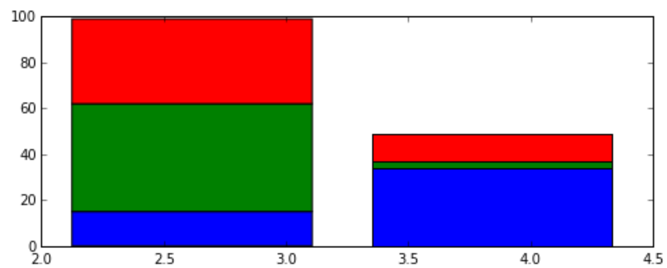
$$\Rightarrow \qquad 2\int p(Y|X=x) Y = 2\Big(\int p(Y|X=x)\Big) v$$

$$\Rightarrow \qquad v = \int p(Y|X=x) Y = \mathbb{E}_{Y|X=x}[Y]$$

Optimal estimate of Y: conditinal expectation given X

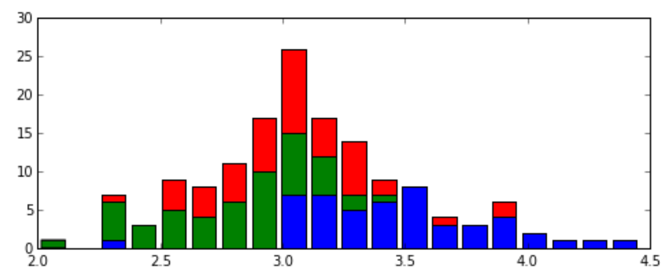
Bayes classifier, estimated

- Now, let's see what happens with "real" data
  - Use empirically estimated probability **model** for p(x,y)
- Iris data set, first feature only (real-valued)
  - We can estimate the probabilities (e.g., with a histogram)

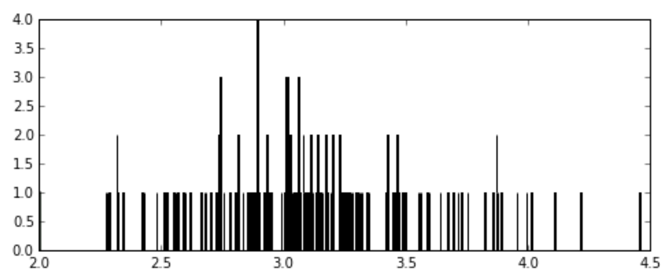


2 Bins:
Predict "green" if X < 3.25, else "blue"

Model is "too simple"



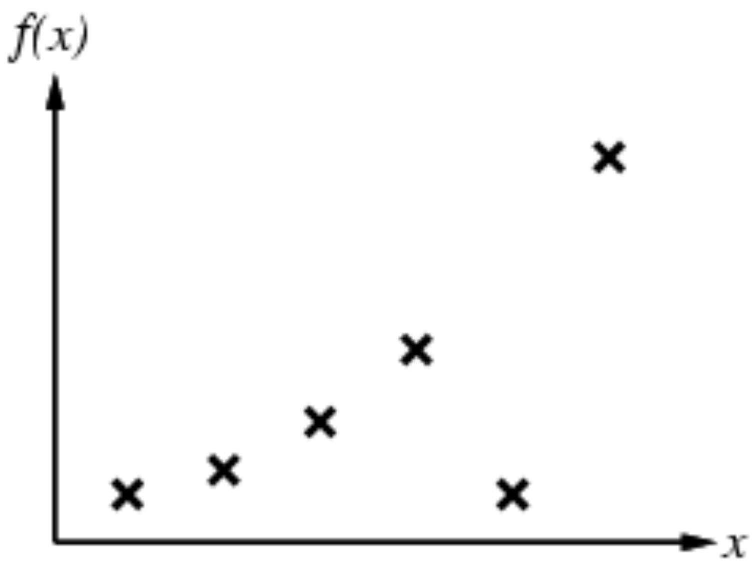
20 Bins:
Predict by majority color in each bin

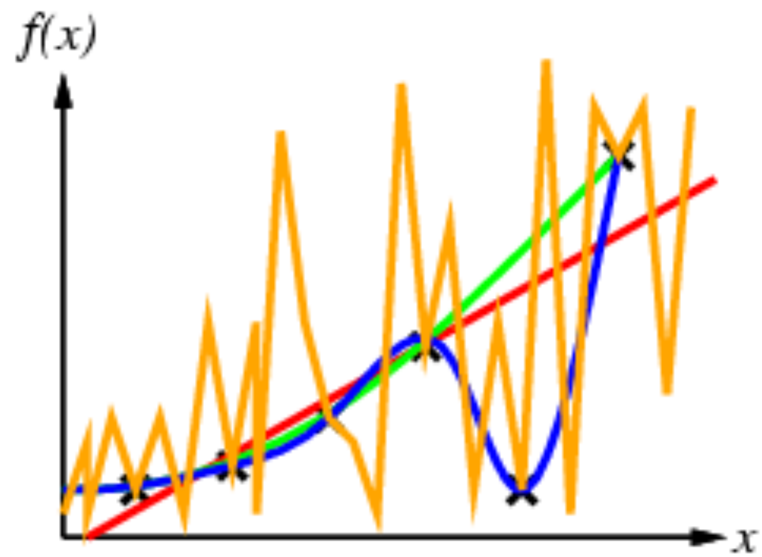


500 Bins:
Each bin has ~ 1 data point!
What about bins with 0 data?
Model is "too complex"

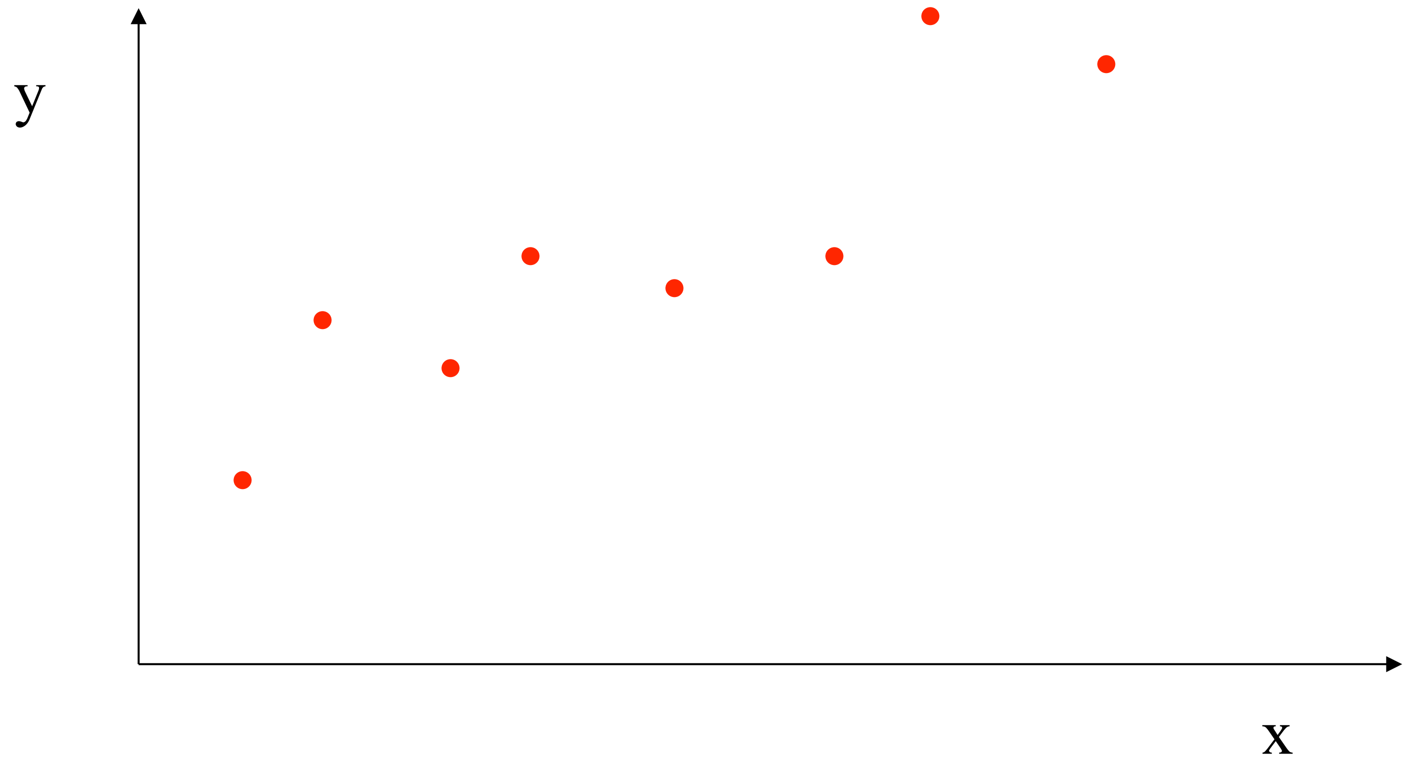
Inductive bias

- “Extend” observed data to unobserved examples
  - “Interpolate” / “extrapolate”
- What kinds of functions to expect? Prefer these (“bias”)
  - Usually, let data pull us away from assumptions only with evidence!



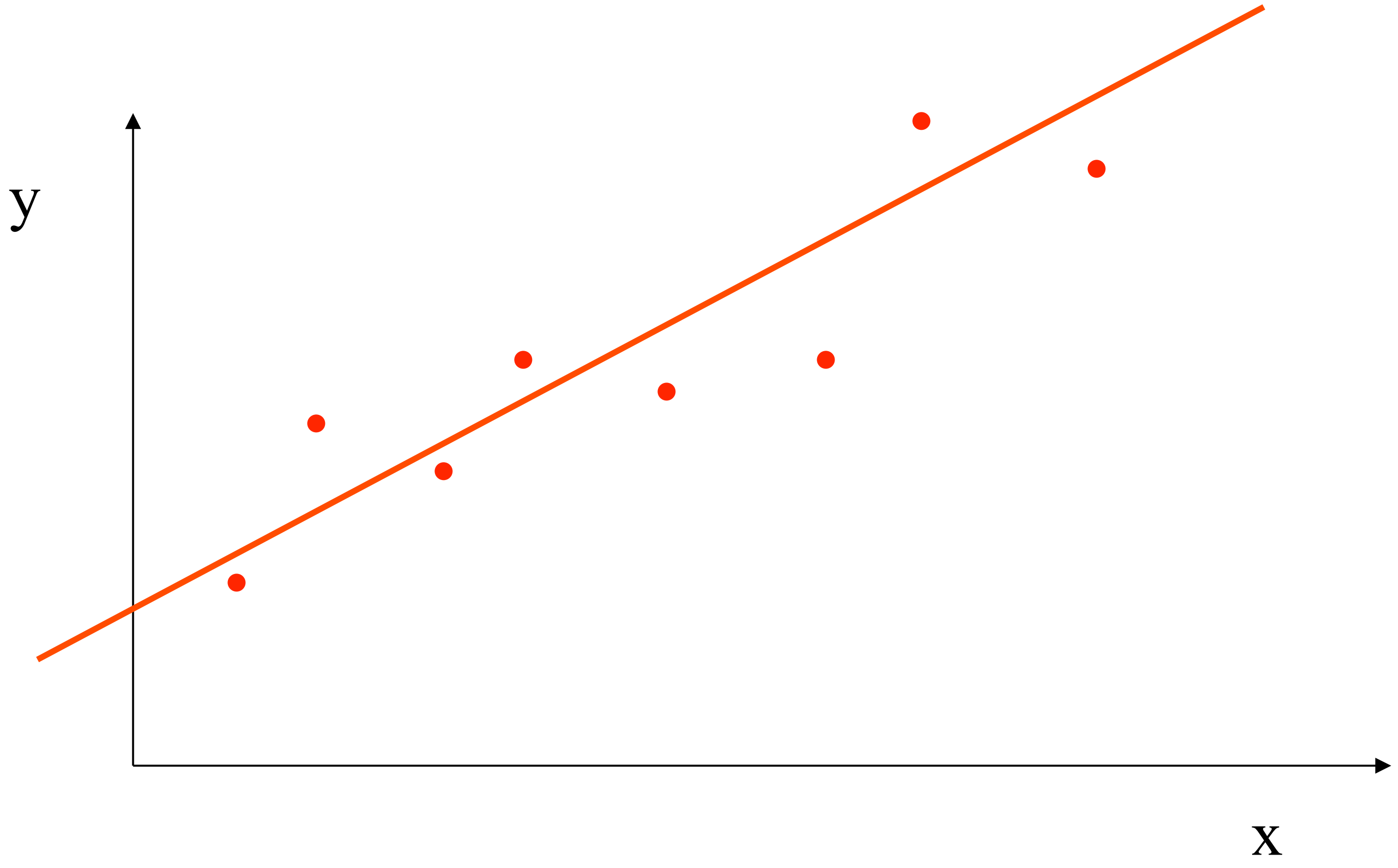


Overfitting and complexity

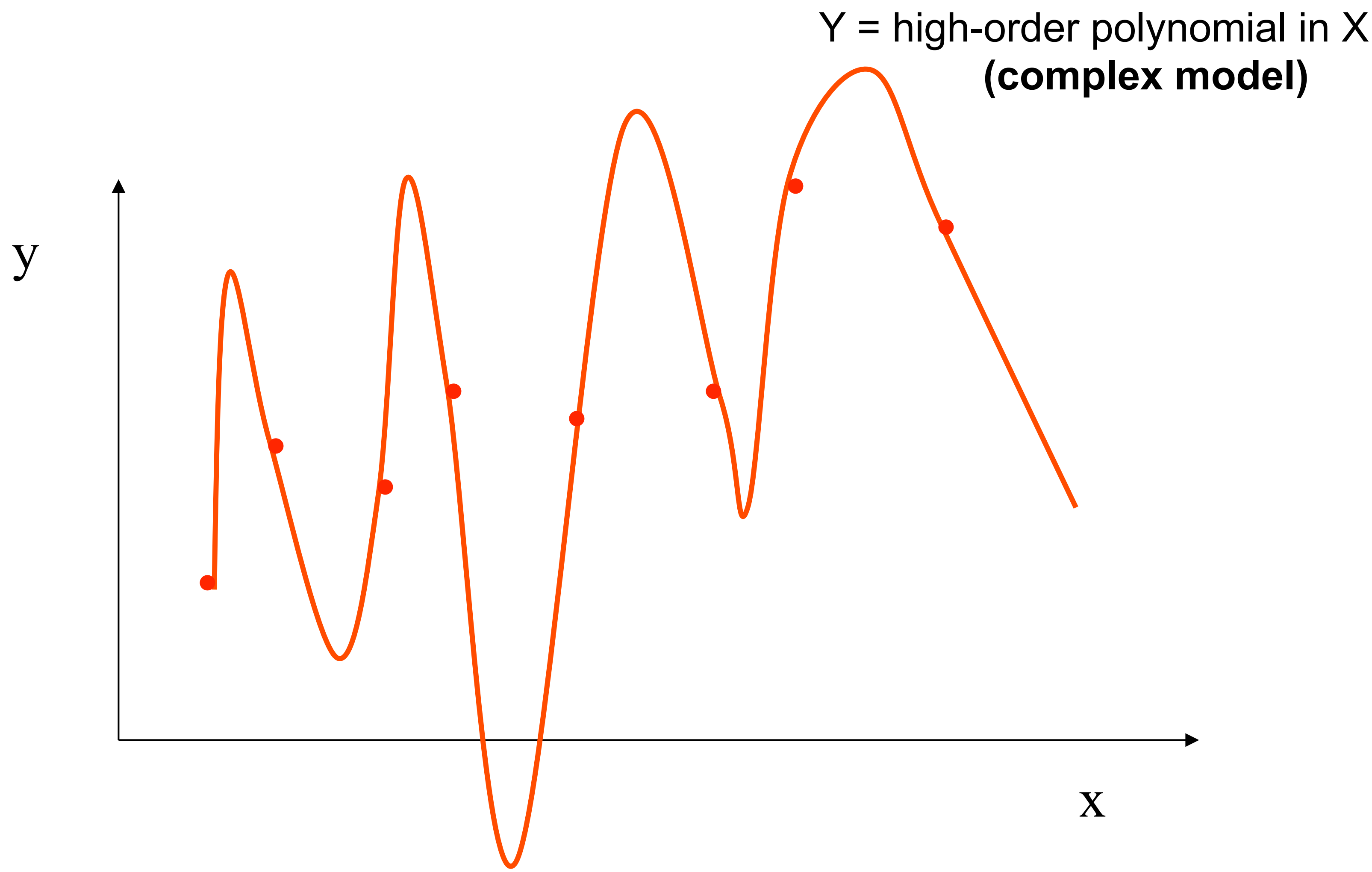


Overfitting and complexity

Simple model: Y= aX + b + e

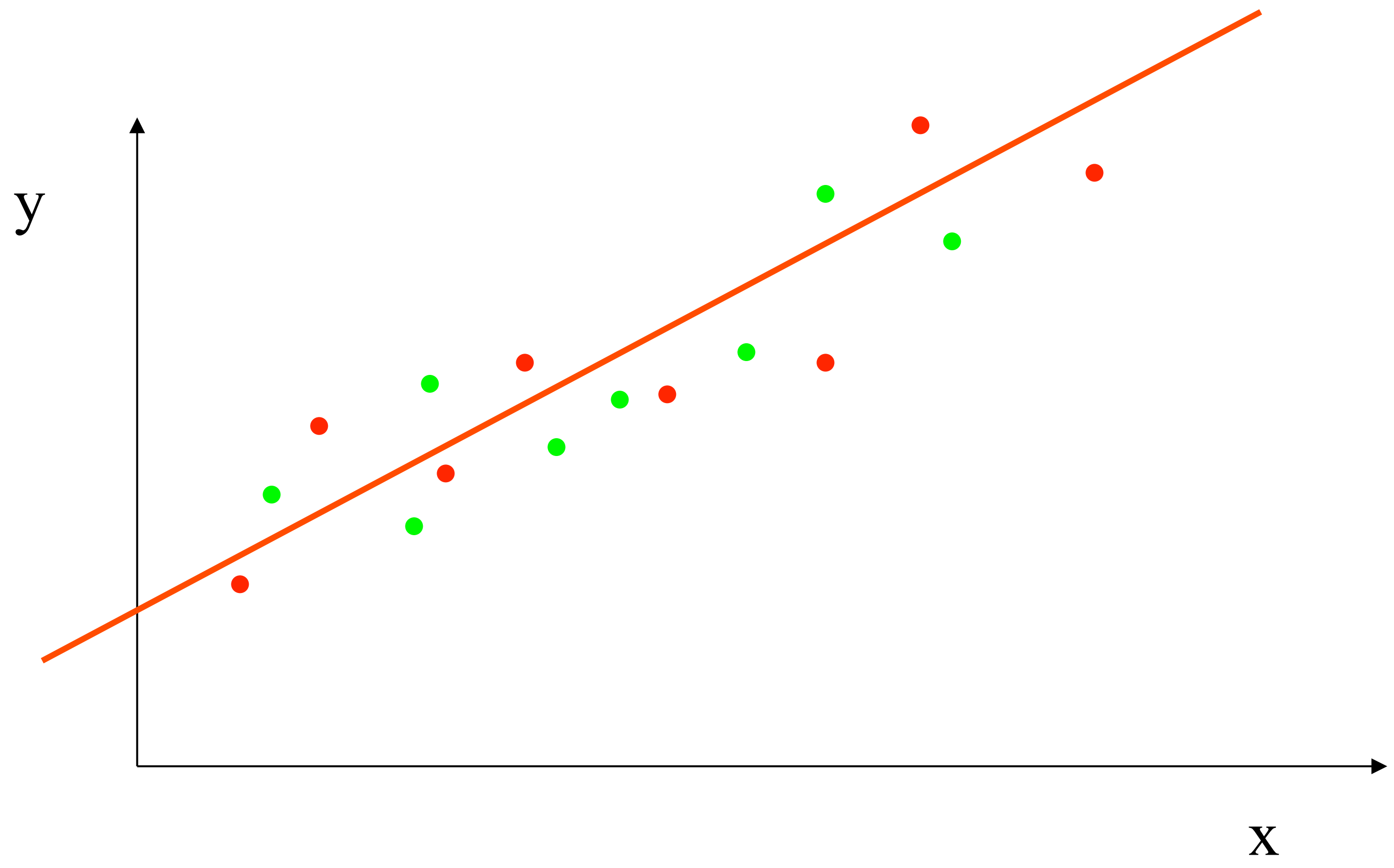


Overfitting and complexity

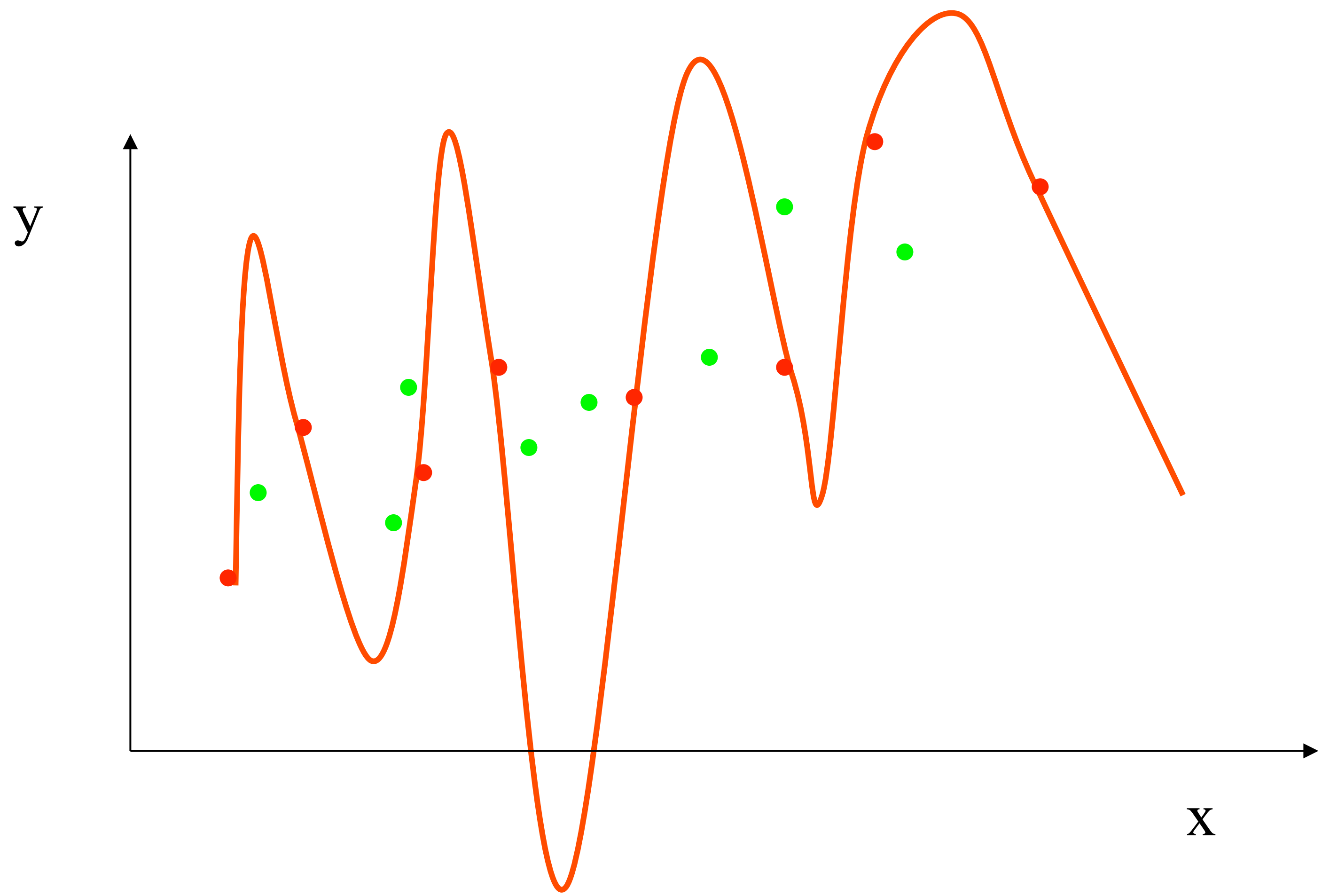


Overfitting and complexity

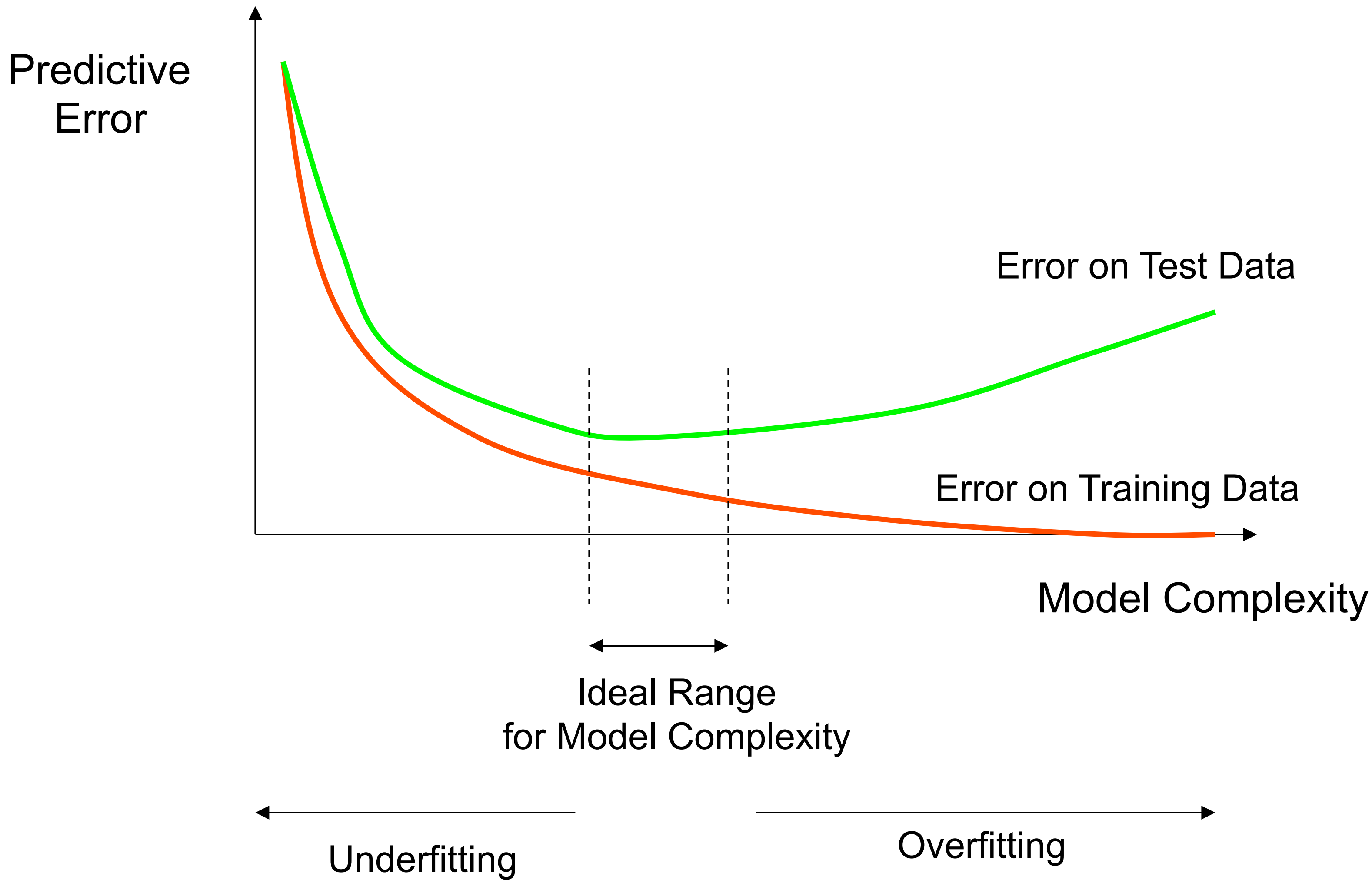
Simple model: Y= aX + b + e



Overfitting and complexity



How Overfitting affects Prediction



Competitions

- Training data
  - Used to build your model(s)
- Validation data
  - Used to assess, select among, or combine models
  - Personal validation; leaderboard; …
- Test data
  - Used to estimate "real world" performance

#	Δ1w	Team Name * in the money	Score	Entries	Last Submission UT
1	-	BrickMover *	1.21251	40	Sat, 31 Aug 2013 23:
2	new	vsu *	1.21552	13	Sat, 31 Aug 2013 20:
3	↑2	Merlion	1.22724	29	Sat, 31 Aug 2013 23:
4	↓2	Sergey	1.22856	15	Sat, 31 Aug 2013 23:
5	new	liuyongqi	1.22980	13	Sat, 31 Aug 2013 13:

Summary

- What is machine learning?
  - Types of machine learning
  - How machine learning works
- Supervised learning
  - Training data: features x, targets y
- Regression
  - (x,y) scatterplots; predictor outputs f(x); optimal MSE predictor
- Classification
  - (x,x) scatterplots
  - Decision boundaries, colors & symbols; Bayes optimal classifier
- Complexity
  - Training vs test error
  - Under- & over-fitting