Supervised Learning II

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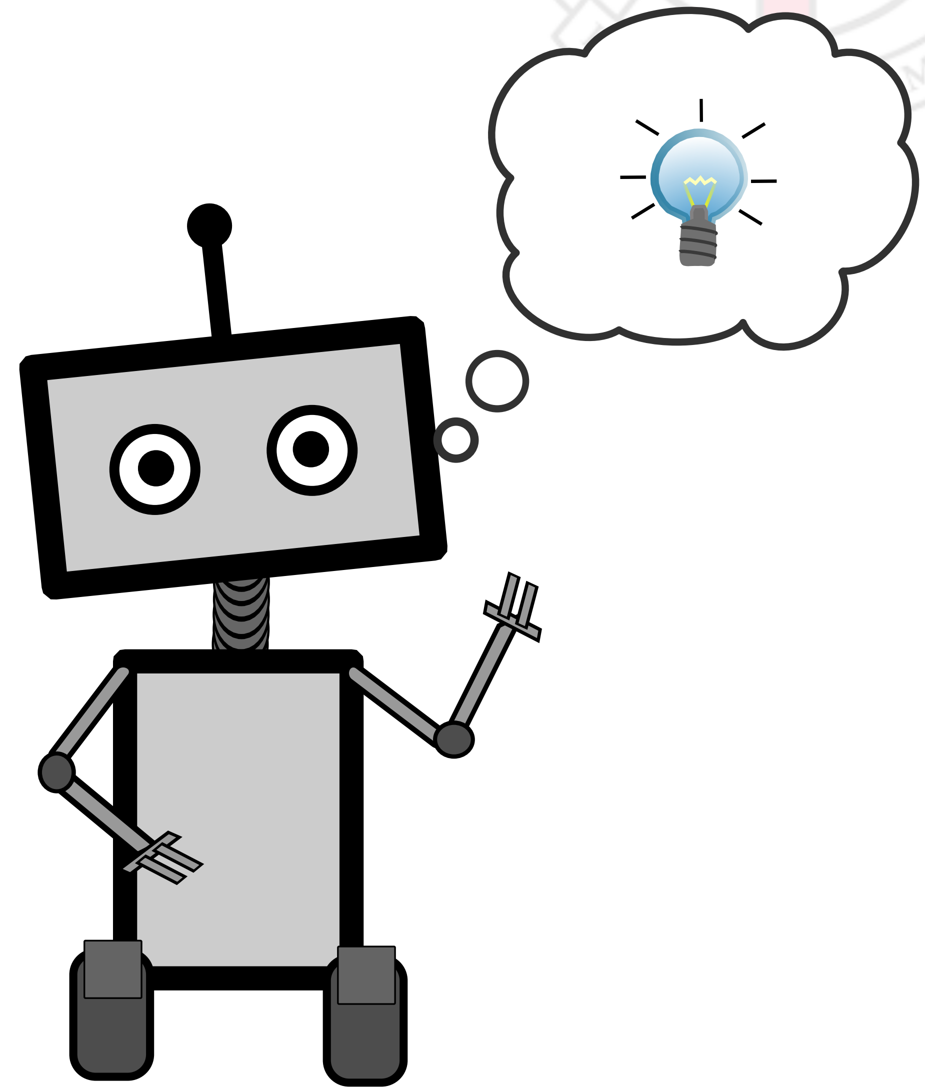
Machine Learning

Subfield of AI concerned with *learning from data*.

Broadly, using:

- ***Experience***
- To Improve ***Performance***
- On Some ***Task***

(Tom Mitchell, 1997)



Supervised Learning

Input:

$X = \{x_1, \ldots, x_n\}$ inputs

$Y = \{y_1, \ldots, y_n\}$ labels

training data

Learn to *predict new labels.*

Given x: y?

Supervised Learning

Formal definition:

Given training data:

$X = \{x_1, \ldots, x_n\}$ inputs

$Y = \{y_1, \ldots, y_n\}$ labels

Produce:

Decision function $f : X \to Y$

That minimizes error:

$$\sum_i err(f(x_i), y_i)$$

Nonparametric Methods

Most ML methods are parametric:

- Characterized by setting a few parameters.
- $y = f(x, w)$

Alternative approach:

- Let the data speak for itself.
- No finite-sized parameter vector.
- Usually more interesting decision boundaries.

K-Nearest Neighbors

Given training data:

$X = \{x_1, \ldots, x_n\}$

$Y = \{y_1, \ldots, y_n\}$

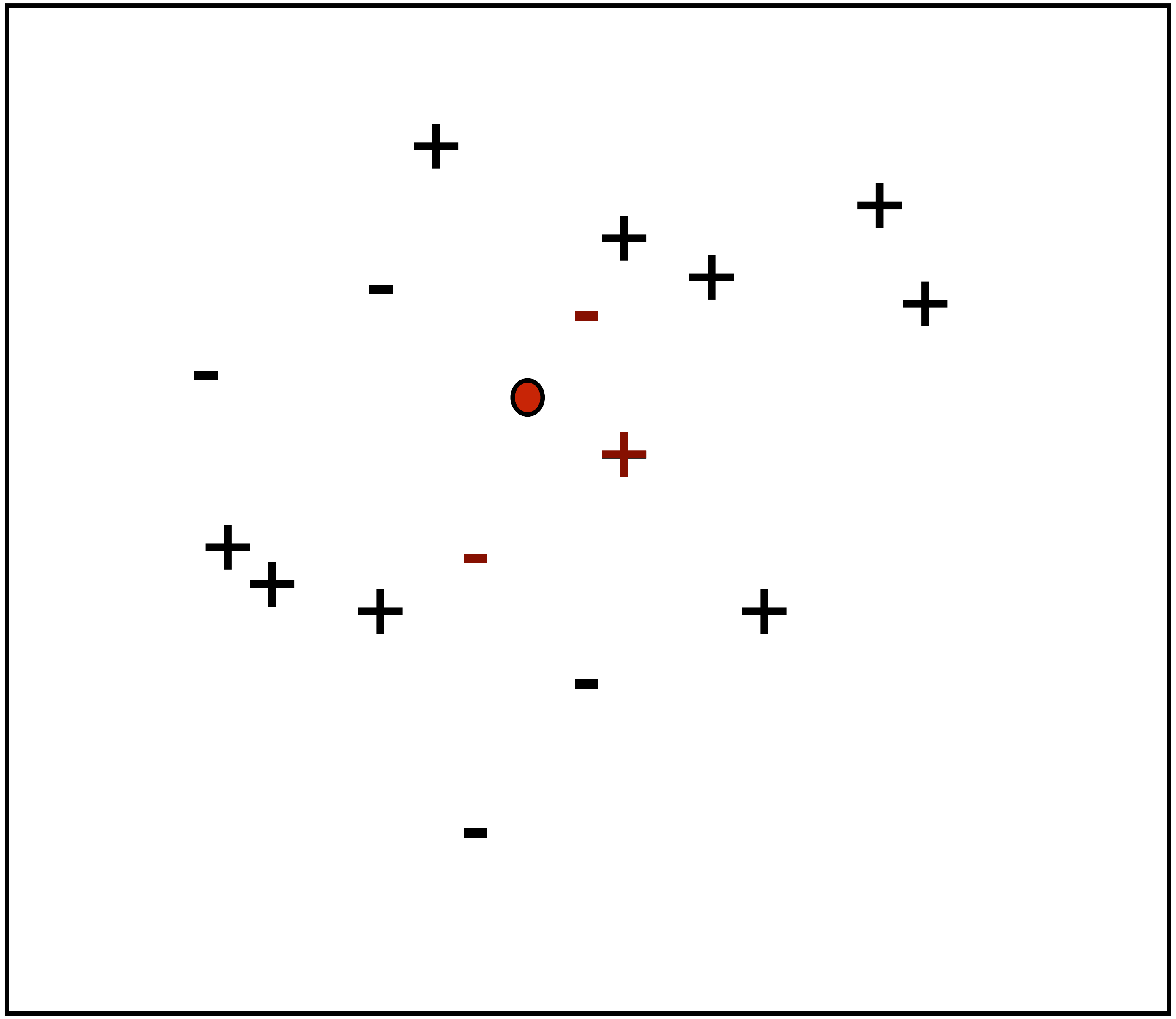
Distance metric $D(x_i, x_j)$

For a new data point x_{new}:

find k nearest points in X (measured via D)

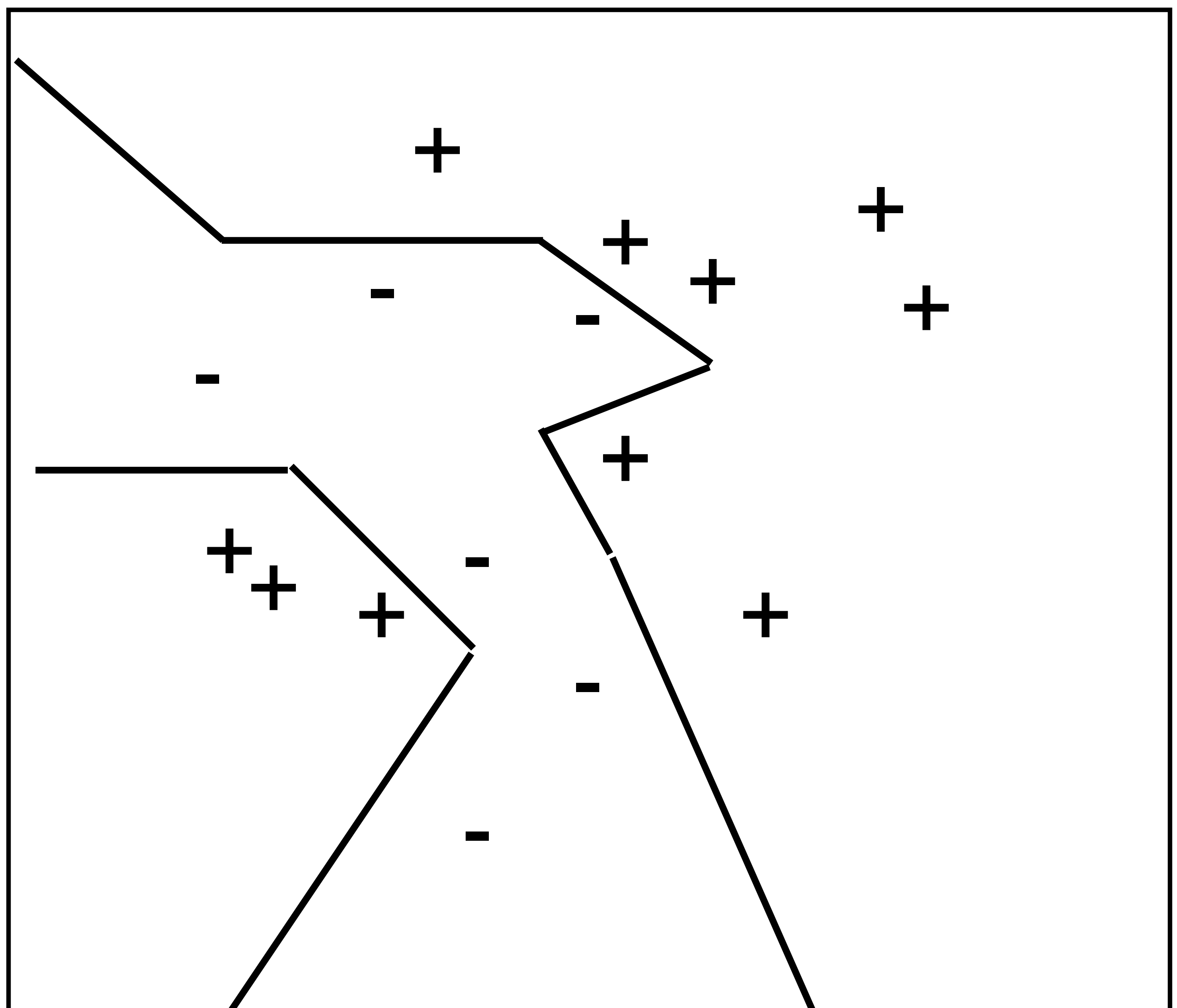
set y_{new} to the majority label

K-Nearest Neighbors



K-Nearest Neighbors

Decision boundary … what if k=1?



K-Nearest Neighbors

Properties:

- No learning phase.
- Must store all the data.
- *log(n)* computation per sample - *grows with data*.

Decision boundary:

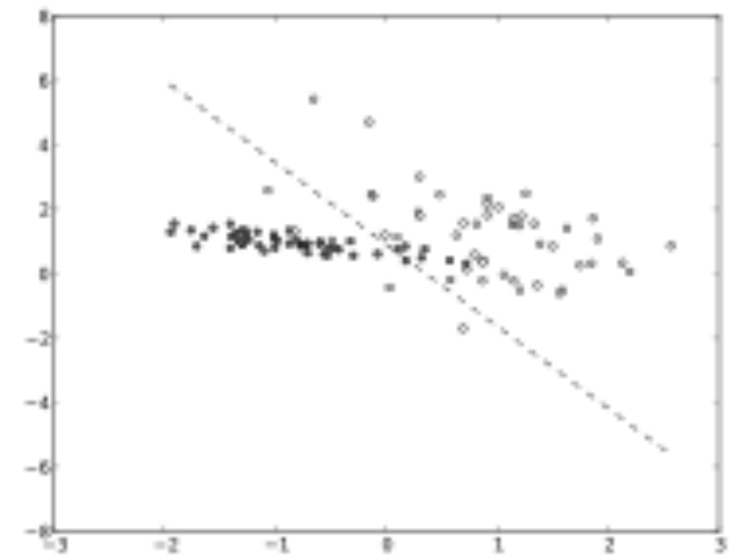
- ***any function, given enough data.***

Classic trade-off: memory and compute time for flexibility.

Classification vs. Regression

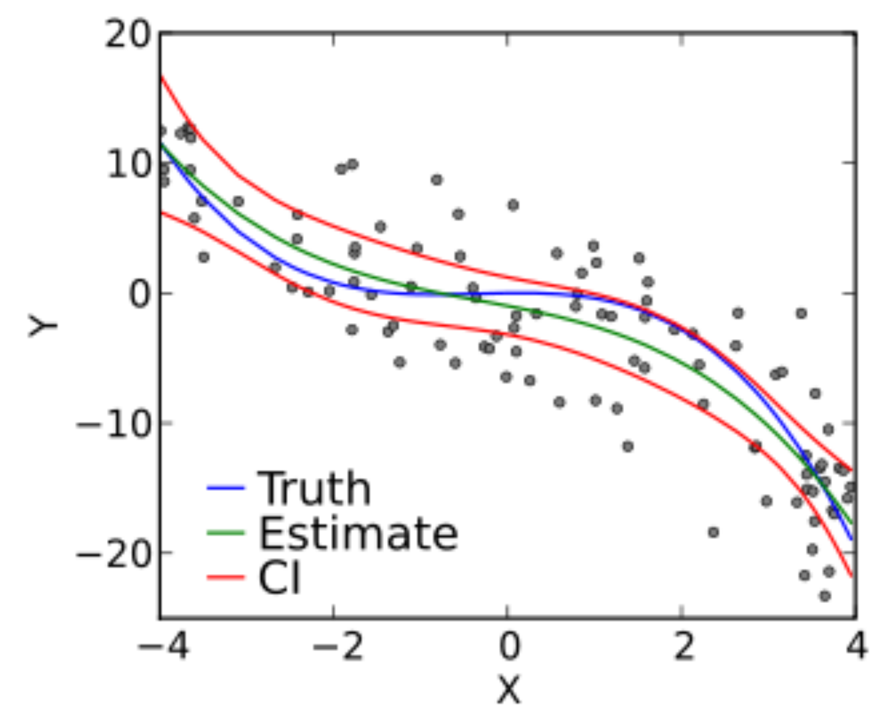
If the set of labels Y is discrete:

- Classification
- Minimize number of errors



If Y is real-valued:

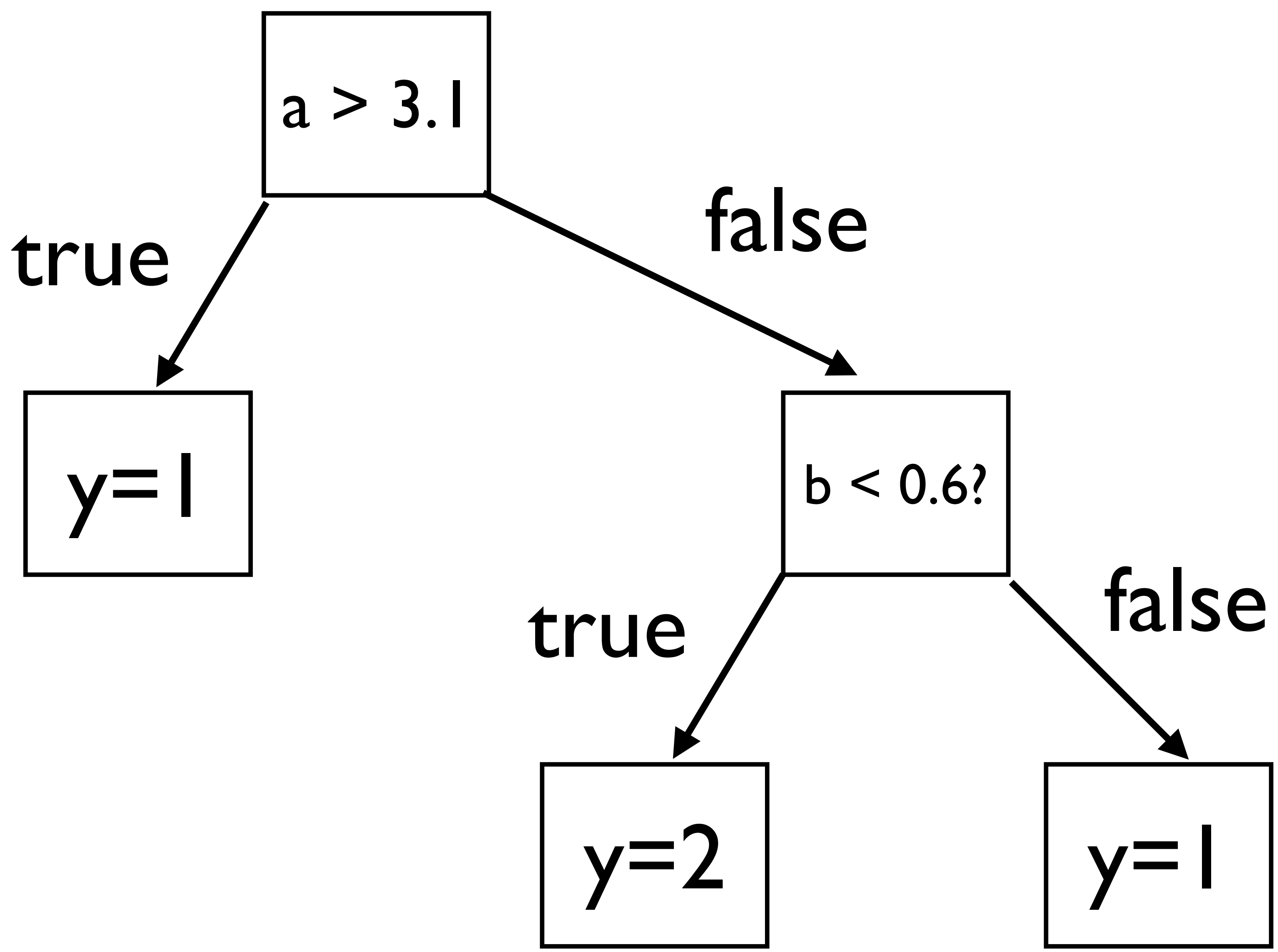
- Regression
- Minimize sum squared error



Let’s look at regression.

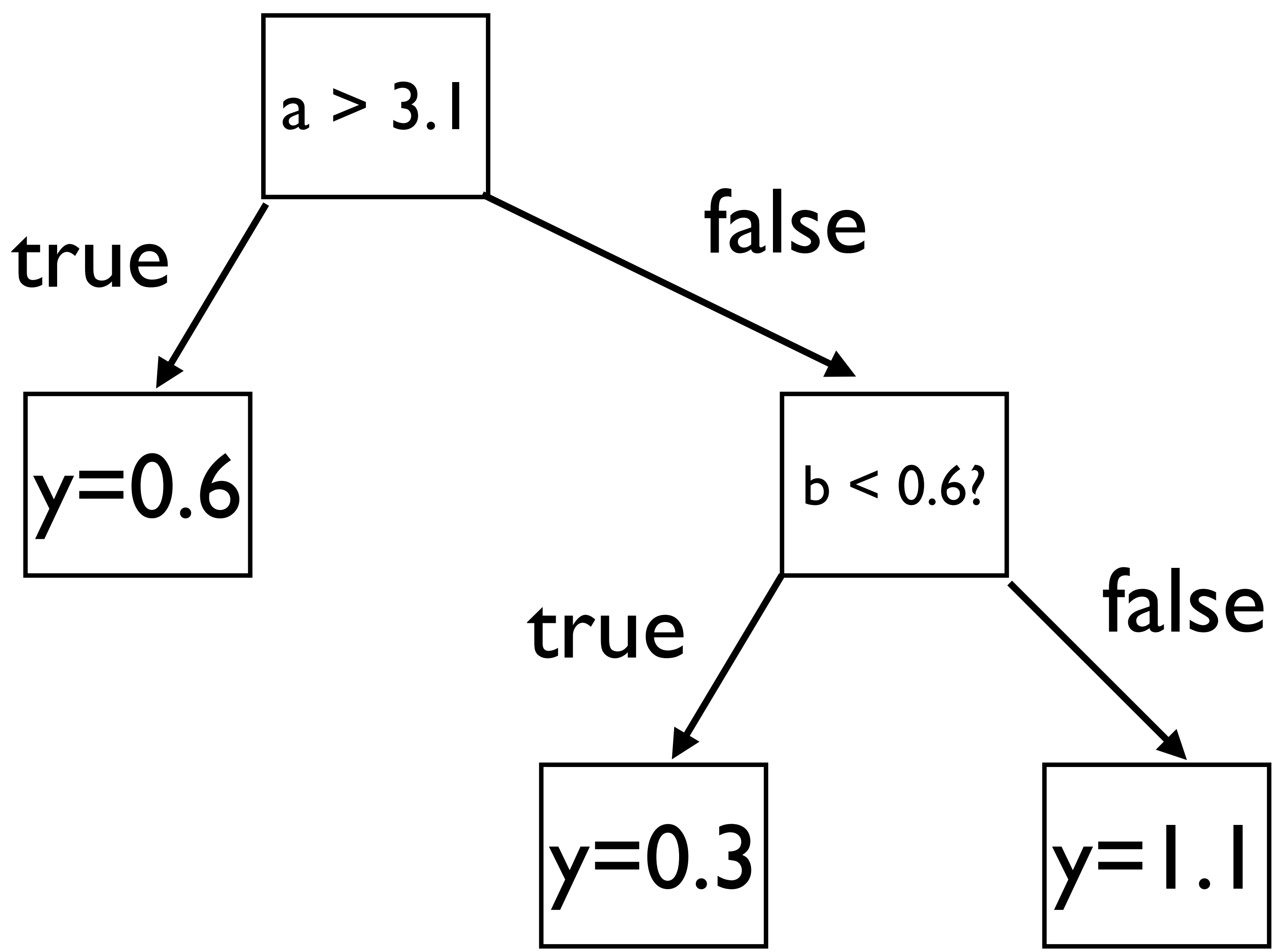
Regression with Decision Trees

Start with decision trees with real-valued inputs.



Regression with Decision Trees

… now real-valued outputs.



Regression with Decision Trees

Training procedure - fix a depth, *k*.

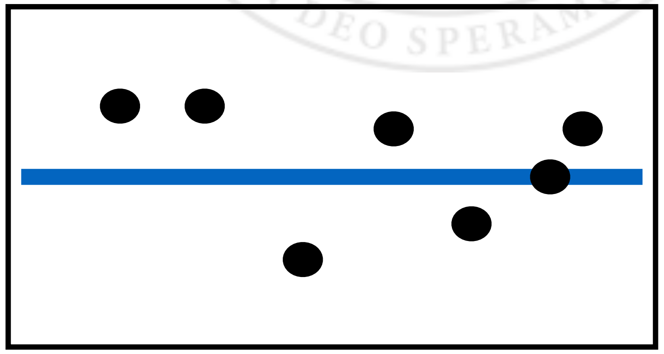
If you have k=1, fit the average.

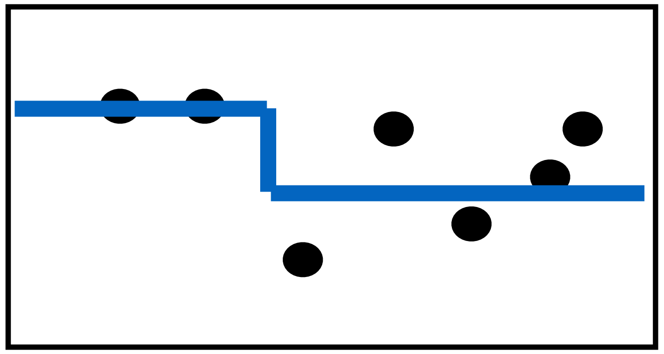
If k > 1:

Consider all variables to split on

Find the one that minimizes SSE

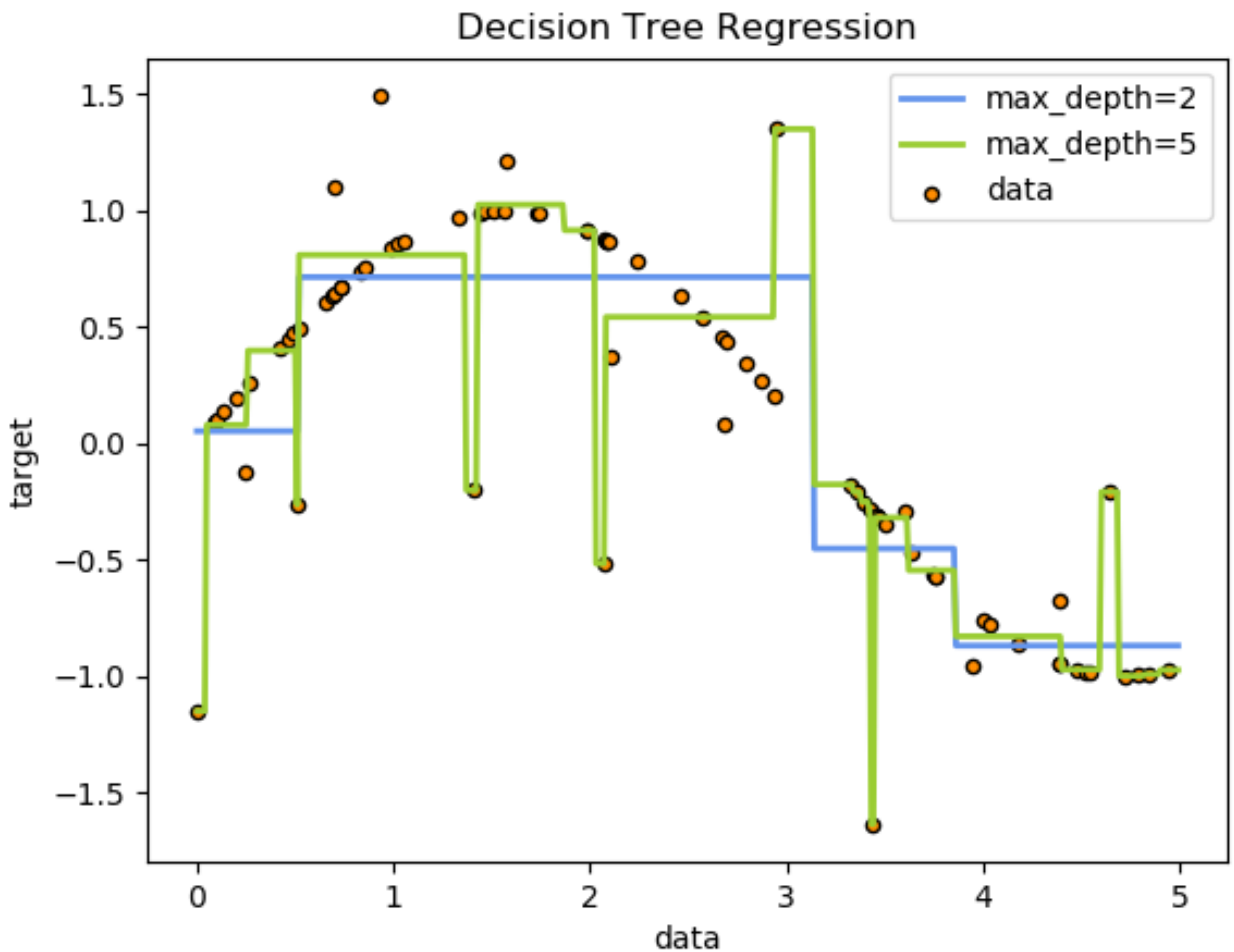
Recurse (*k-1*)





Choice of *k* prevents overfitting.

Regression with Decision Trees



(via scikit-learn docs)

Linear Regression

Alternatively, explicit equation for prediction.

Recall the Perceptron.

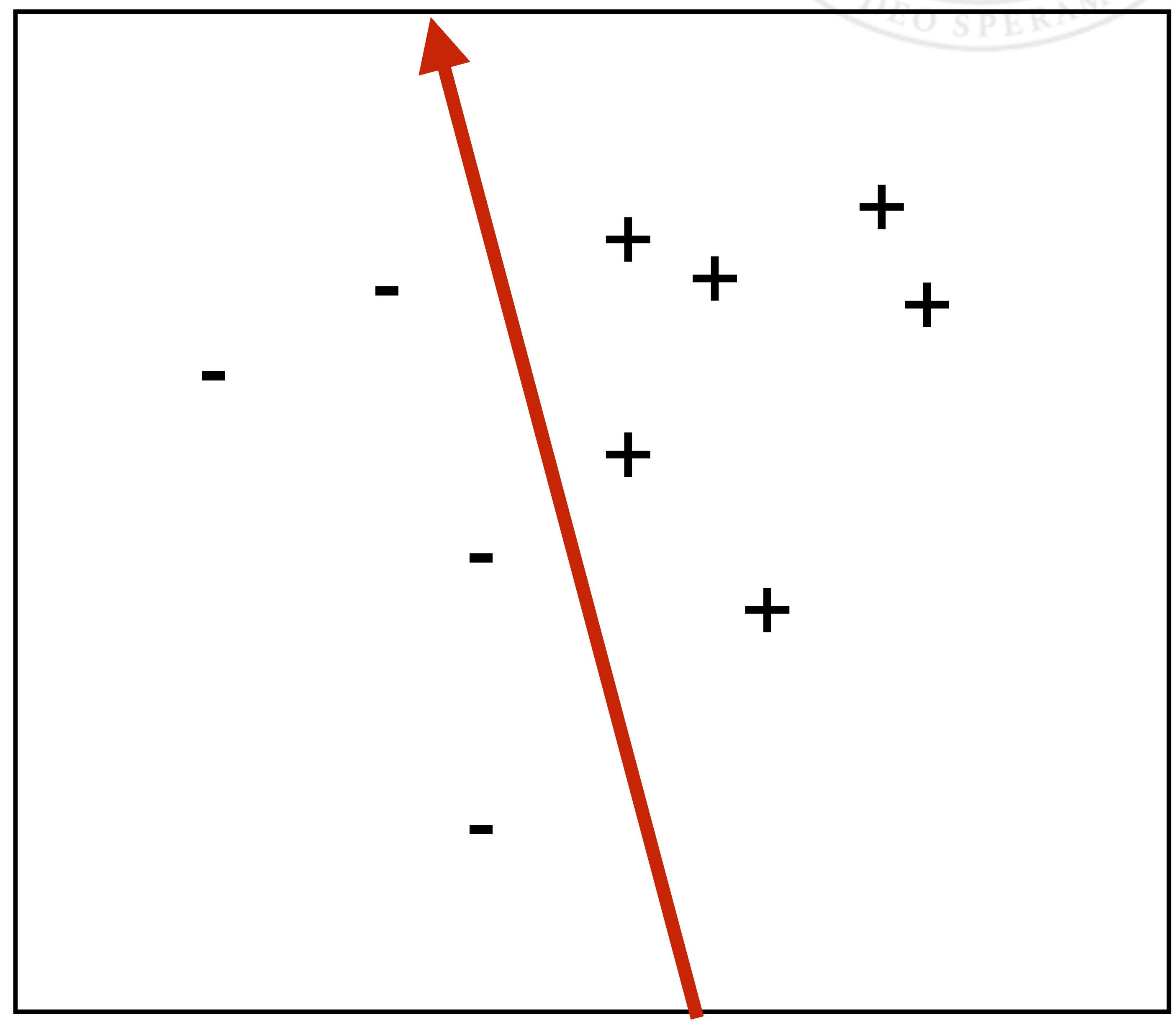
If x = [$x(1), \ldots, x(n)$]:

- Create an *n*-d line
- Slope for each $x(i)$
- Constant offset

$$f(x) = \texttt{sign}(w \cdot x + c)$$

gradient

offset

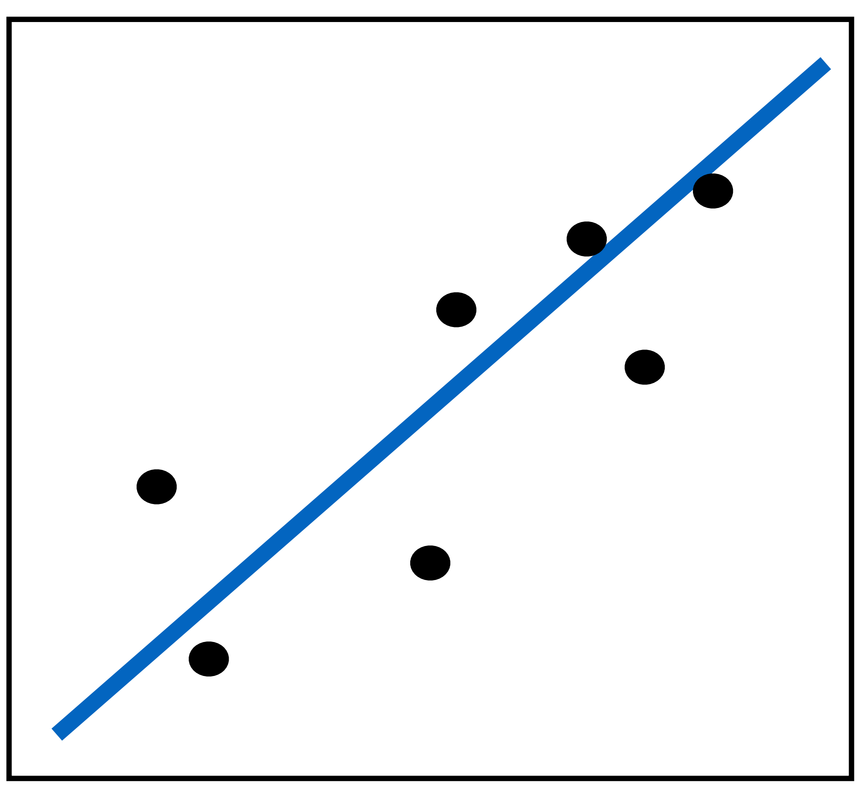


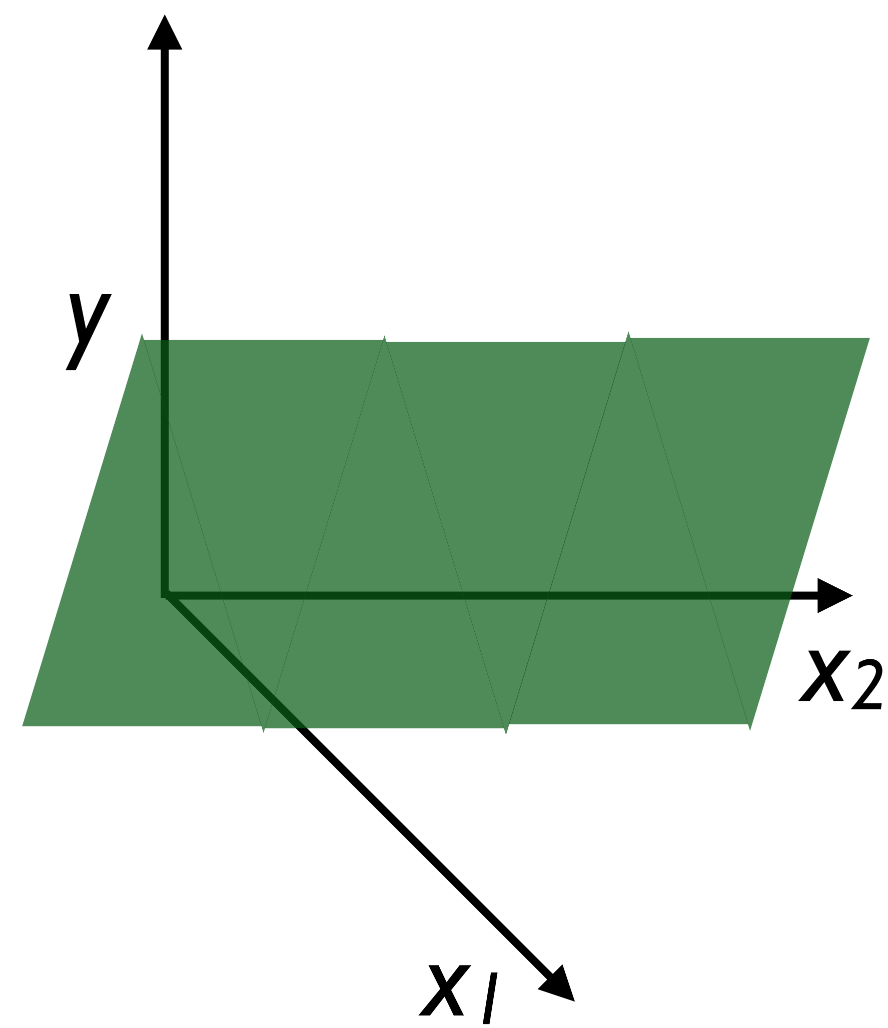
Linear Regression

Directly represent *f* as a linear function:

- $f(x, w) = w \cdot x + c$

What can be represented this way?





Linear Regression

How to train?

Given inputs:

- $x = [x_1, \ldots, x_n]$ (each x_i is a vector, first element = 1)
- $y = [y_1, \ldots, y_n]$ (each y_i is a real number)

Define error function:

Minimize summed squared error

$$\sum_{i=1}^{n} (w \cdot x_i - y_i)^2$$

Linear Regression

The usual story:

- Set derivative of error function to zero.

$$\frac{d}{dw}\sum_{i=1}^{n}(w \cdot x_i - y_i)^2 = 0$$

$$2\sum_{i=1}^{n}(w \cdot x_i - y_i)x_i^T = 0$$

$$\left(\sum_{i=1}^{n} x_i^T x_i\right) w = \sum_{i=1}^{n} x_i^T y_i$$

$$A = \left(\sum_{i=1}^{n} x_i^T x_i\right)$$

matrix

$$b = \sum_{i=1}^{n} x_i^T y_i$$

vector

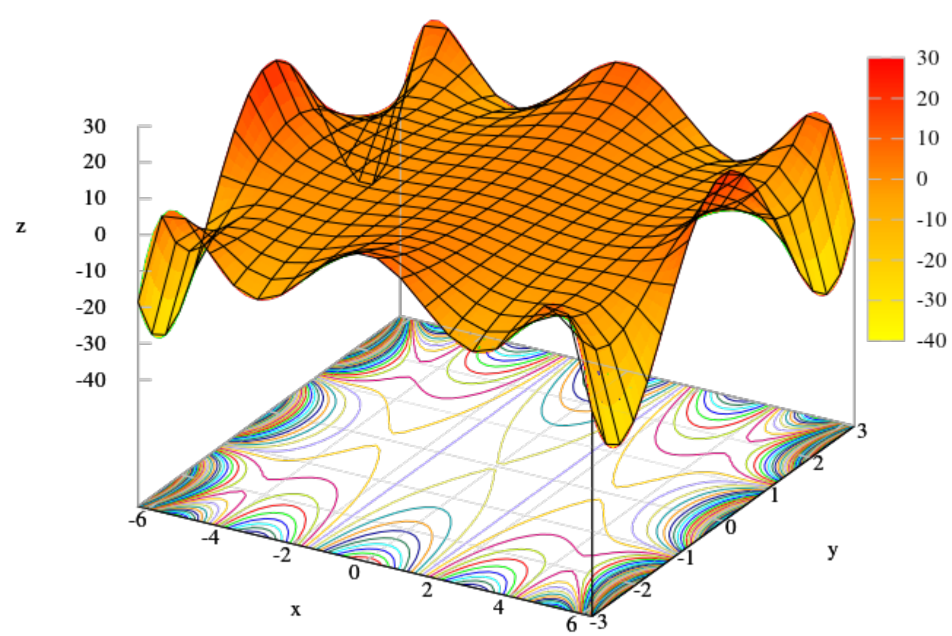
$$w = A^{-1} b$$

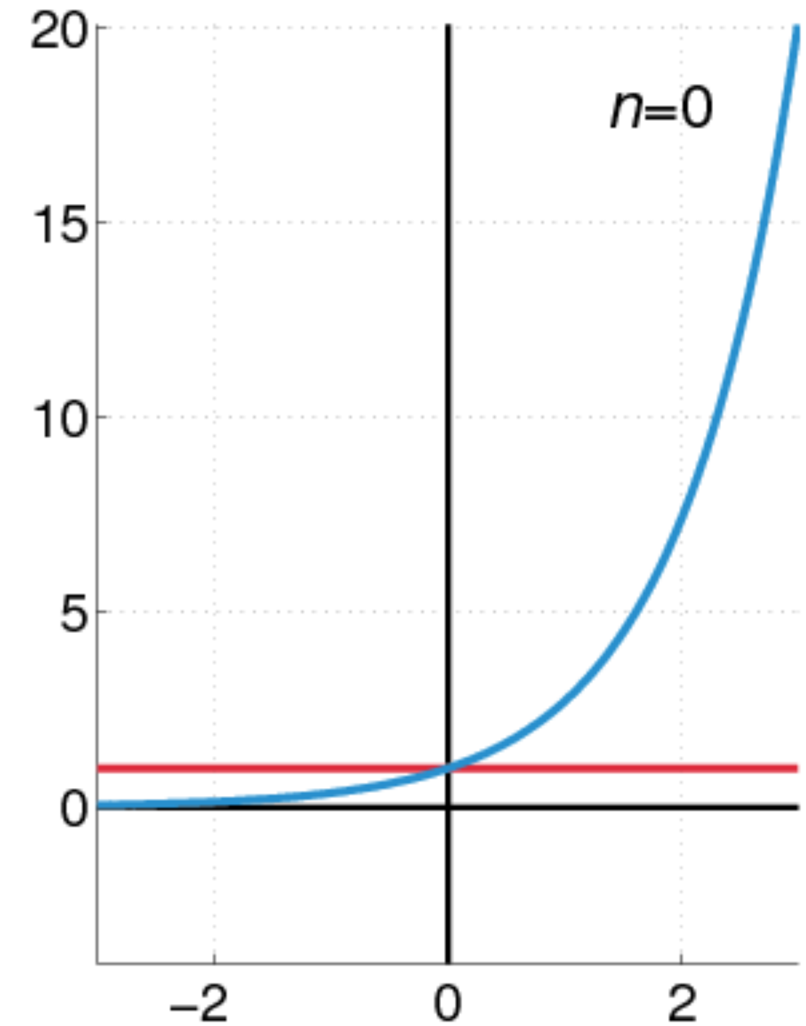
Polynomial Regression

More powerful:

- Polynomials in state variables.
  - 1st order: $[1, x, y, xy]$
  - 2nd order: $[1, x, y, xy, x^2, y^2, x^2y, y^2x, x^2y^2]$
- $y_i = w \cdot \Phi(x_i)$

What can be represented?





Polynomial Regression

As before …

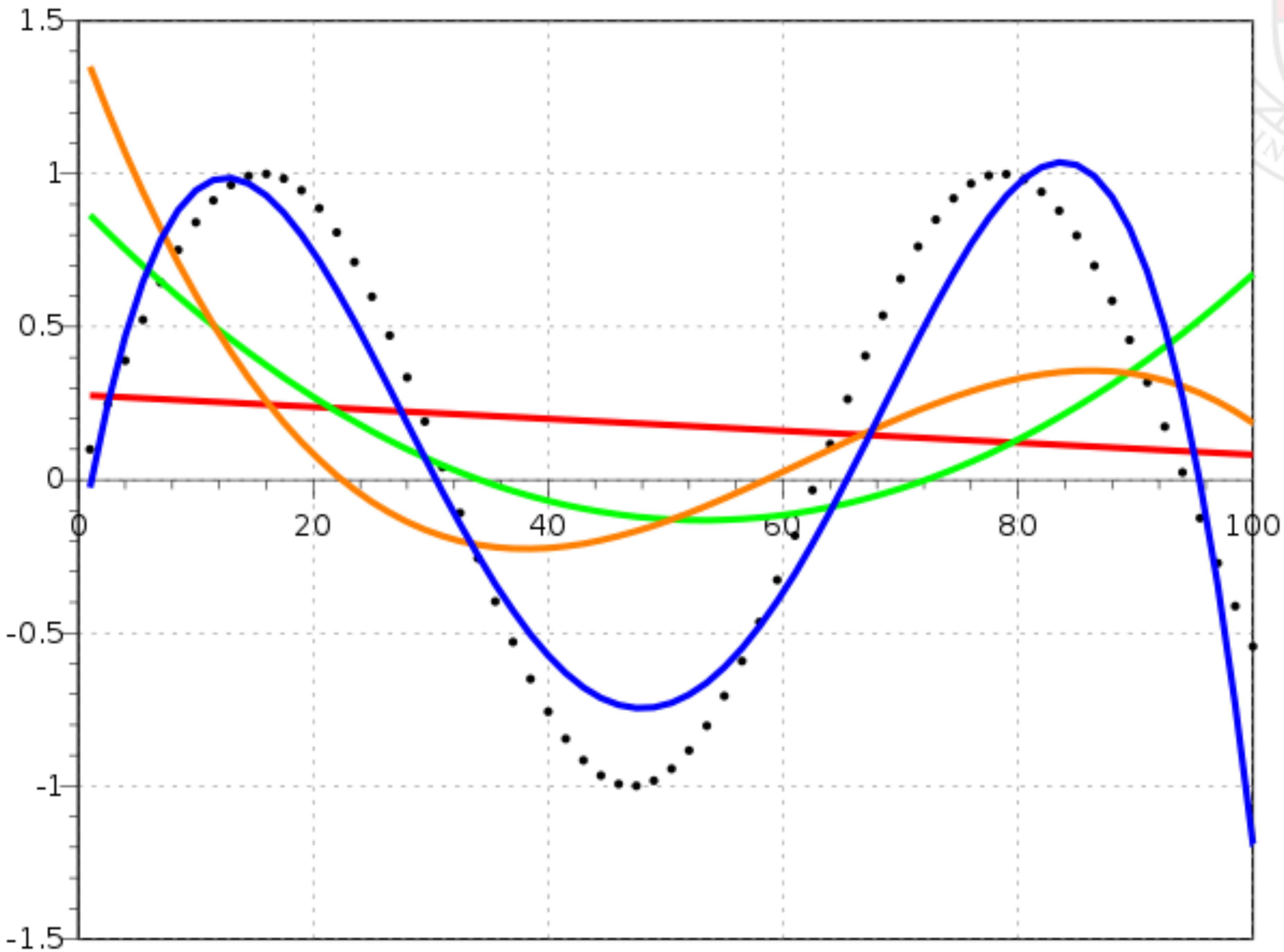
$$\frac{d}{dw}\sum_{i=1}^{n}(w \cdot \Phi(x_i) - y_i)^2$$

$$A = \sum_{i=1}^{n}\Phi^T(x_i)\Phi(x_i)$$

$$w = A^{-1}b$$

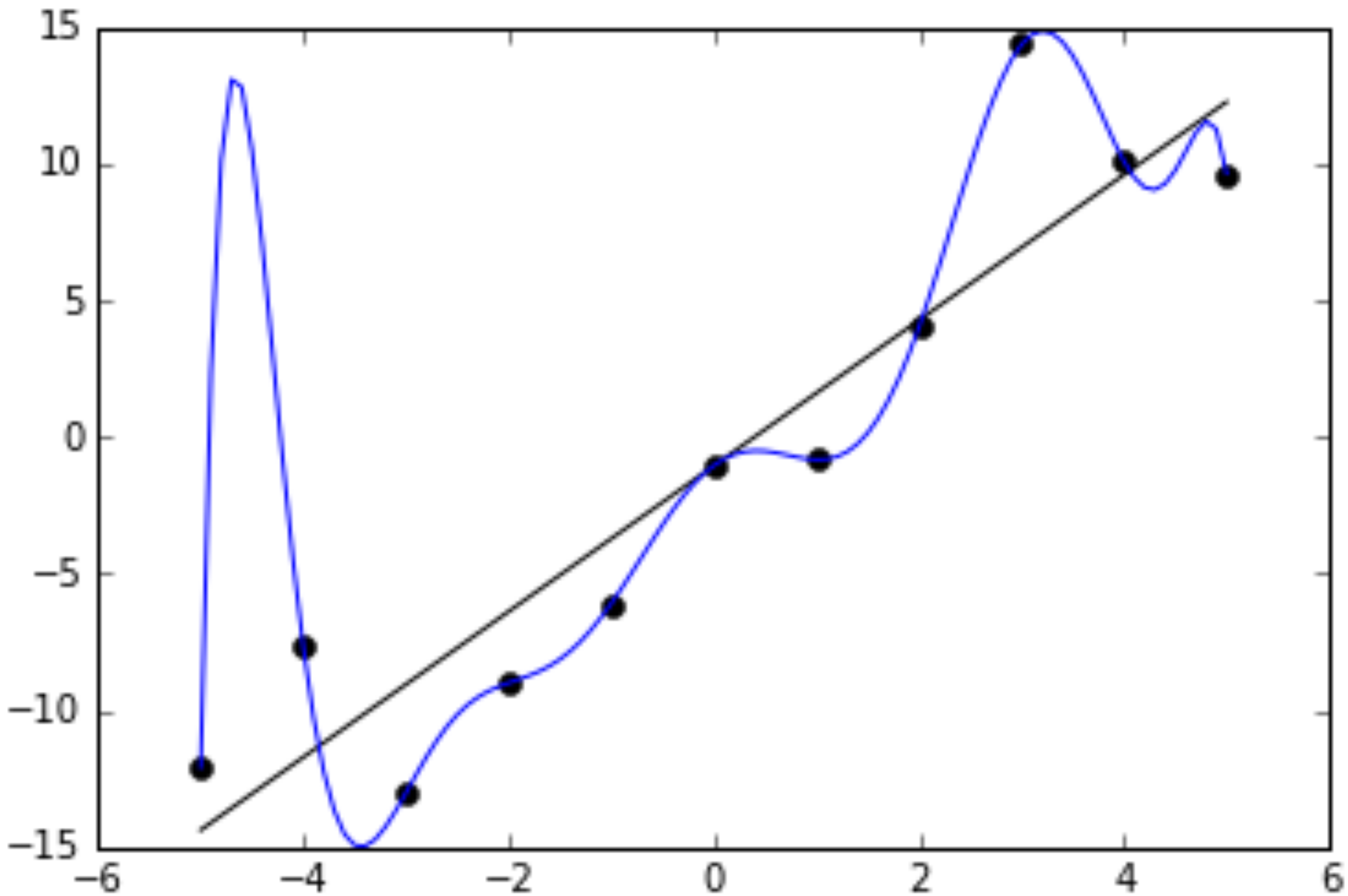
$$b = \sum_{i=1}^{n}\Phi^T(x_i)y_i$$

Polynomial Regression

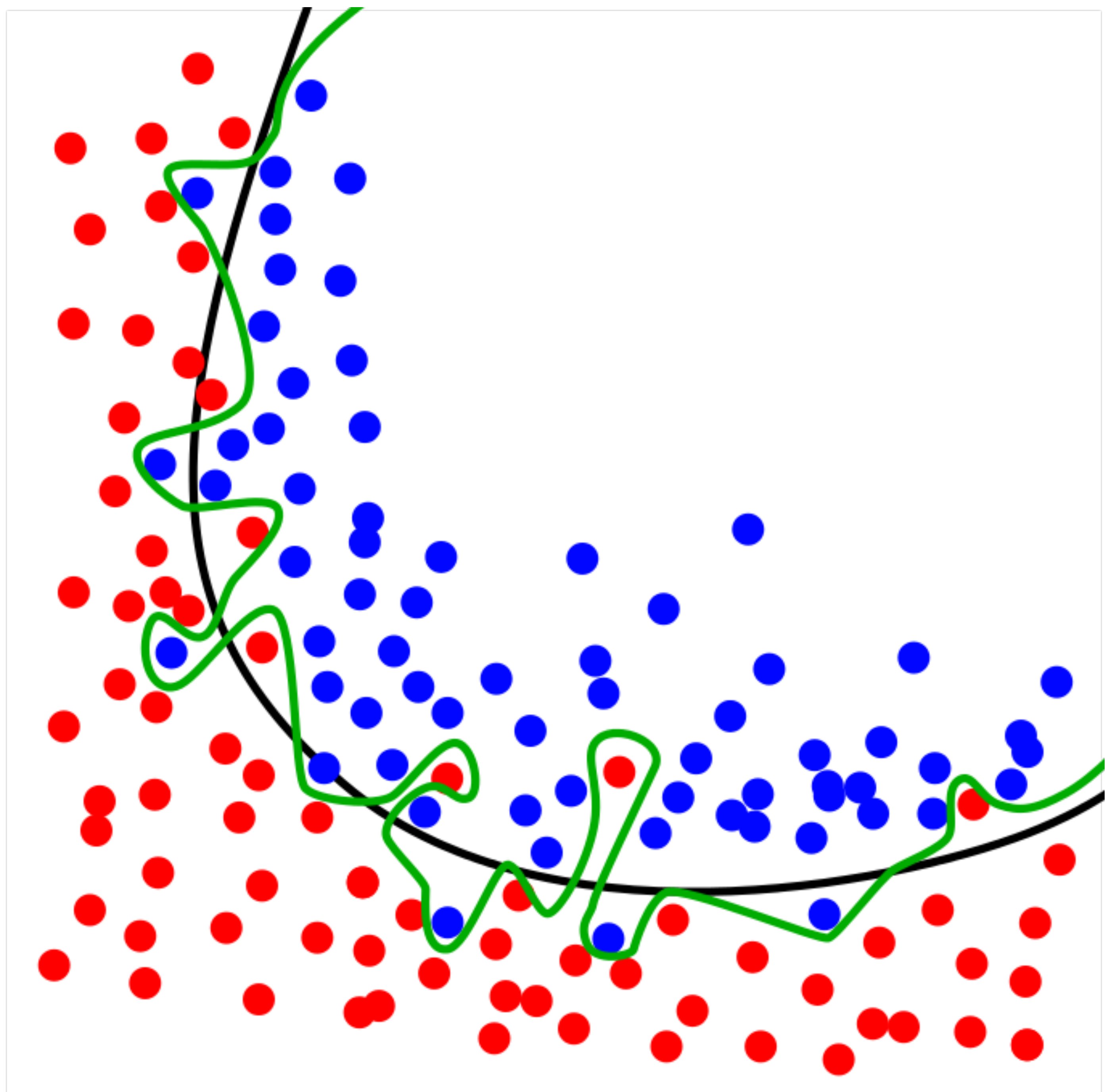


(wikipedia)

Overfitting



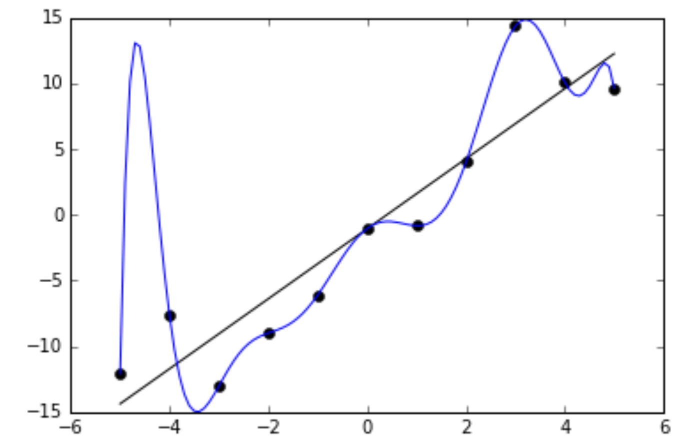
Overfitting



Ridge Regression

A characteristic of overfitting:

- Very large weights.

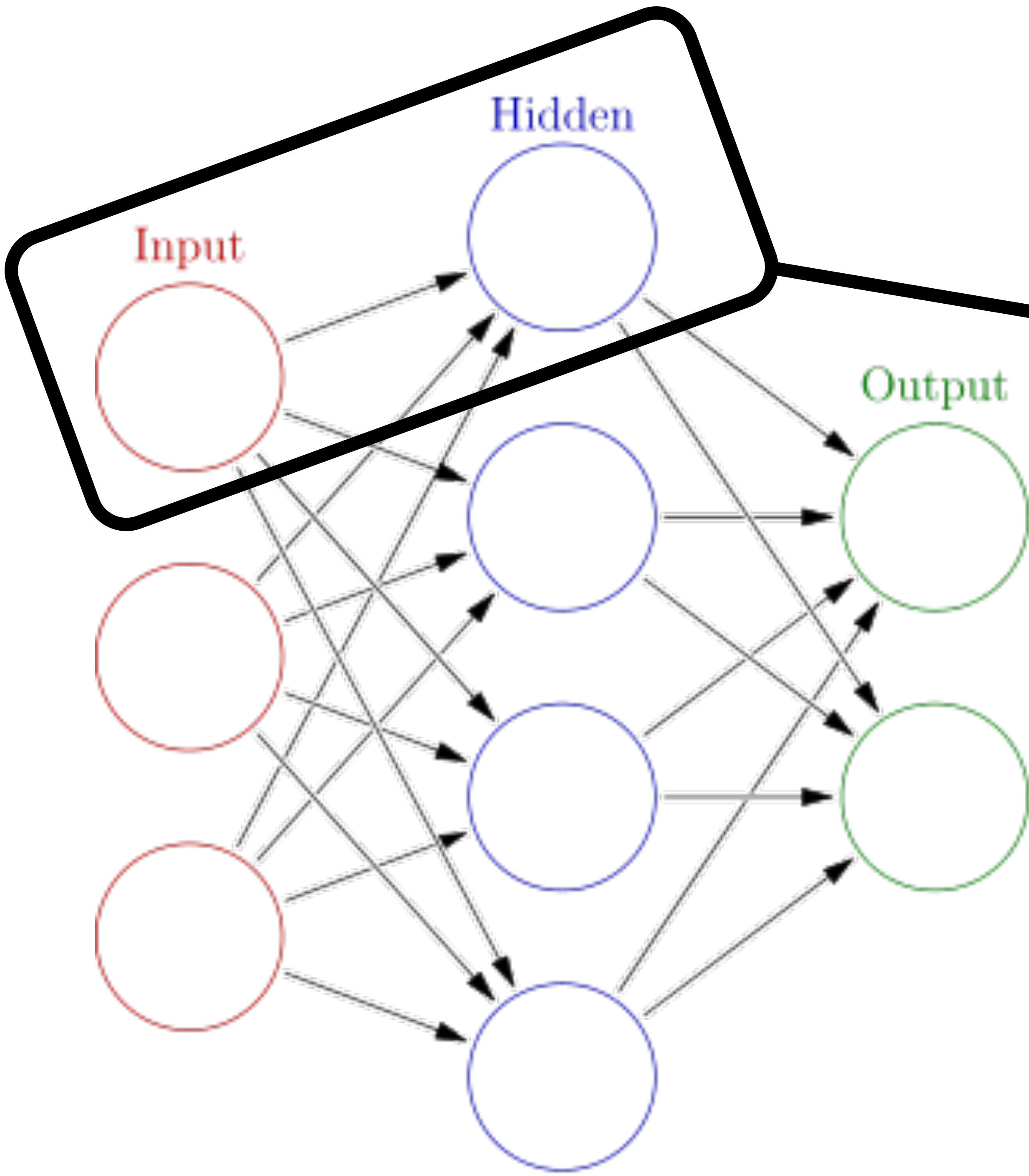


Modify the objective function to discourage this:

$$\min \underbrace{\sum_{i=1}^{n} (w \cdot x_i - y_i)^2}_{\text{error term}} + \underbrace{\lambda ||w||}_{\text{regularization term}}$$

$$w = (A^T A + \Lambda^T \Lambda)^{-1} A^T b$$

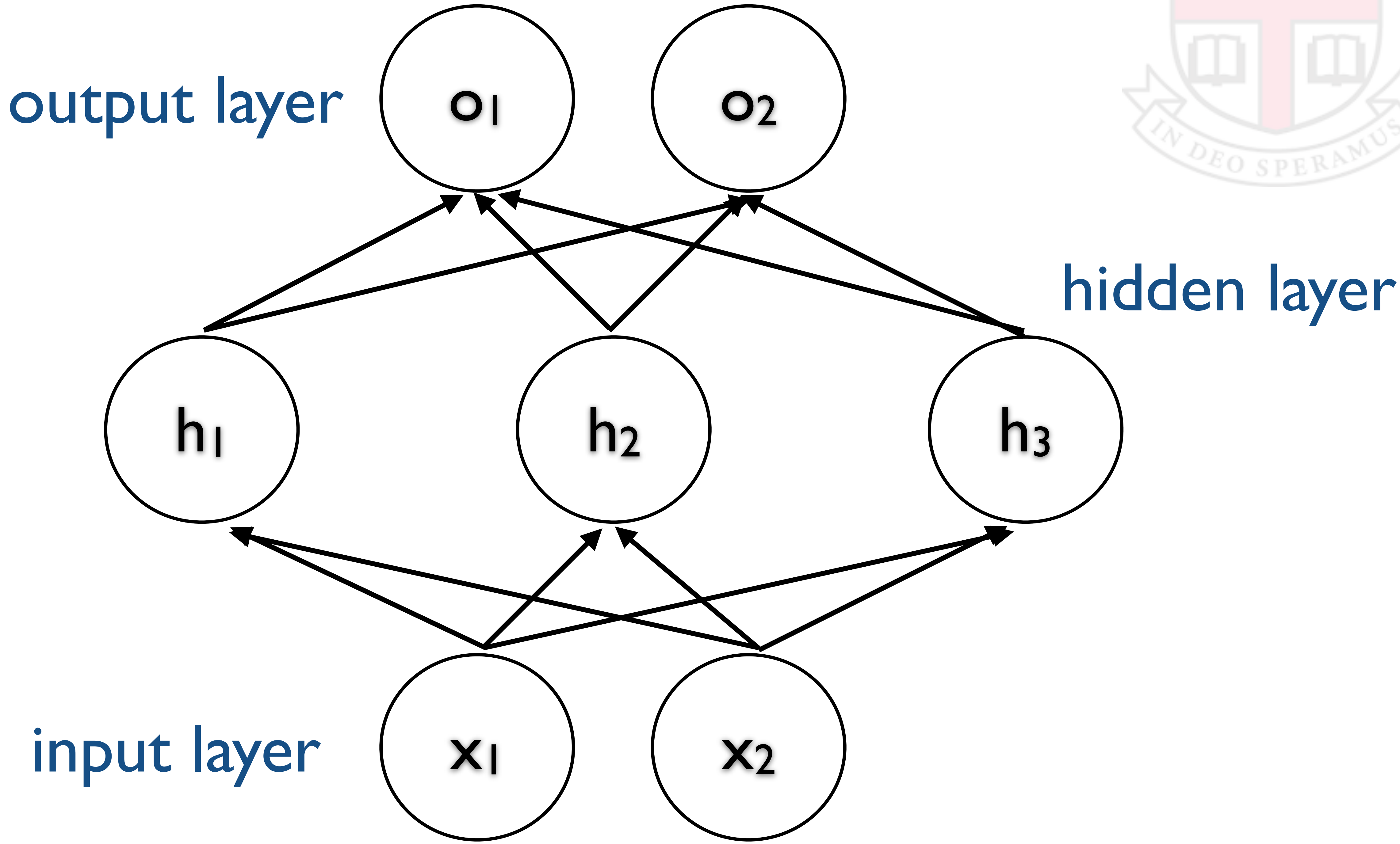
Neural Network Regression



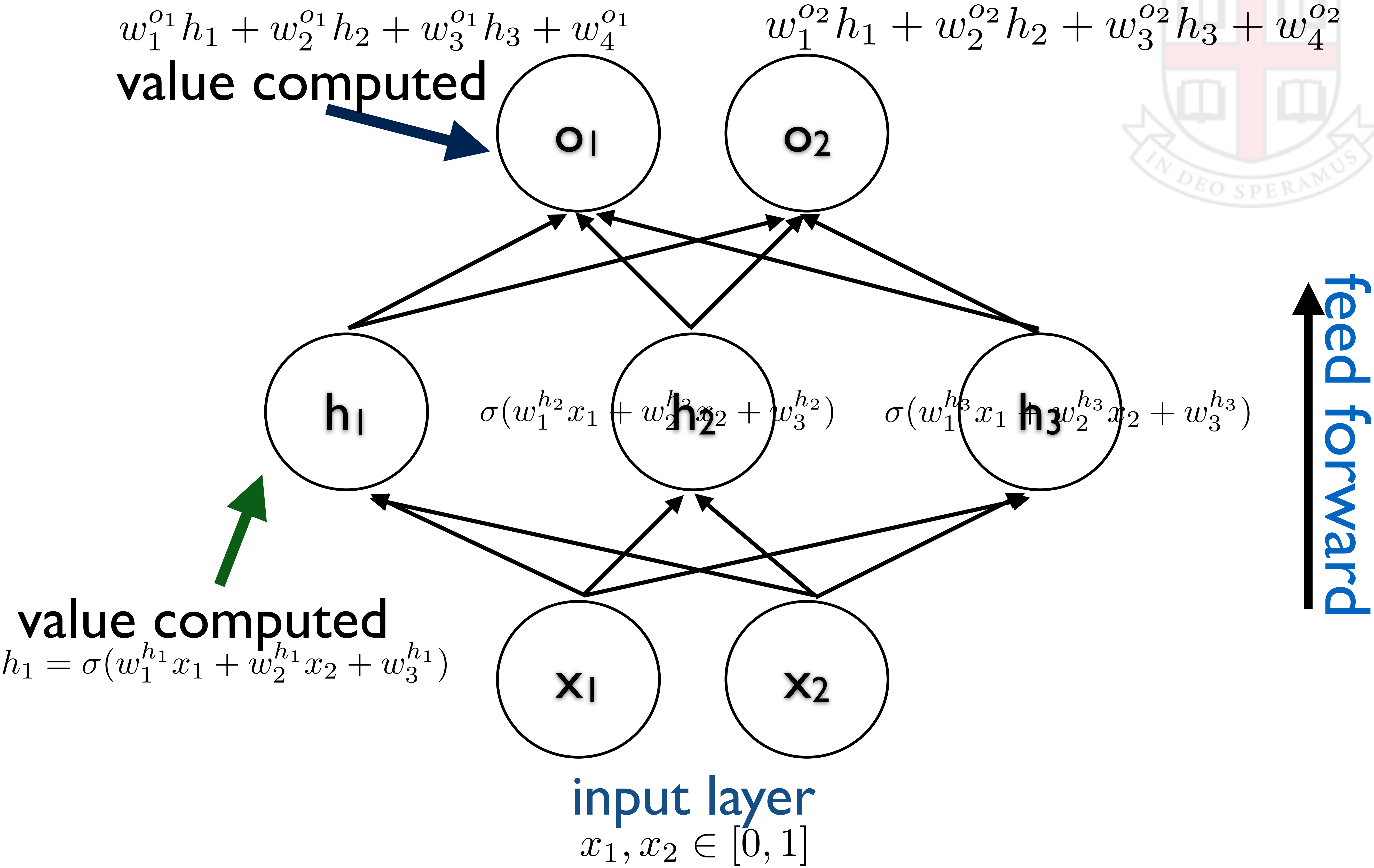
$$\sigma(w \cdot x + c)$$

classification

Neural Network Regression



Neural Network Regression



Neural Network Regression

A neural network is just a parametrized function: $y = f(x, w)$

How to *train* it?

Write down an error function:

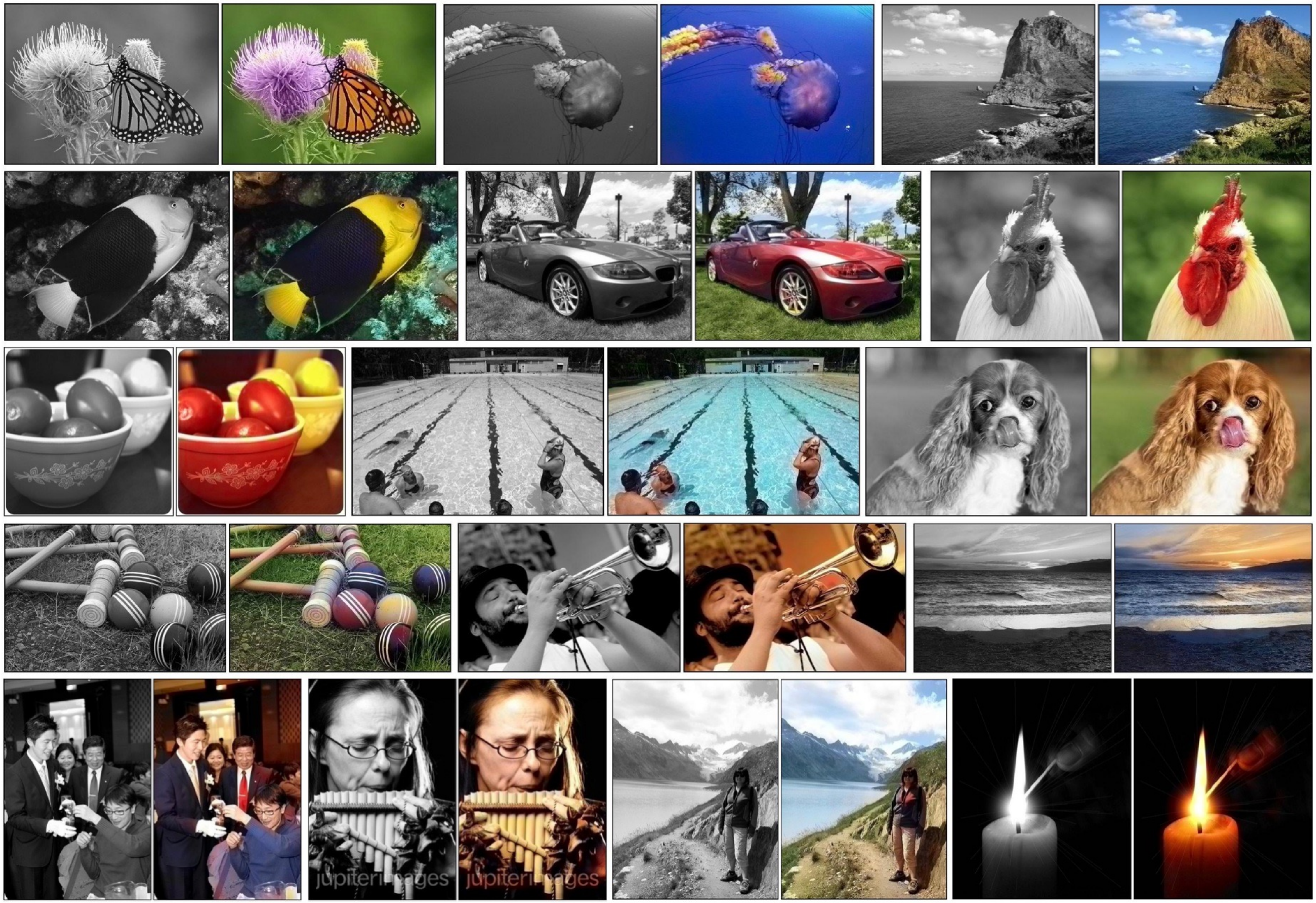
$$(y_i - f(x_i, w))^2$$

Minimize it! (w.r.t. *w*)

No closed form solution to gradient = 0.
Hence, stochastic gradient descent:

- Compute $\frac{d}{dw}(y_i - f(x_i, w))^2$
- Descend

Image Colorization



(Zhang, Isola, Efros, 2016)

Nonparametric Regression

Most ML methods are parametric:

- Characterized by setting a few parameters.
- $y = f(x, w)$

Alternative approach:

- Let the data speak for itself.
- No finite-sized parameter vector.
- Usually more interesting decision boundaries.

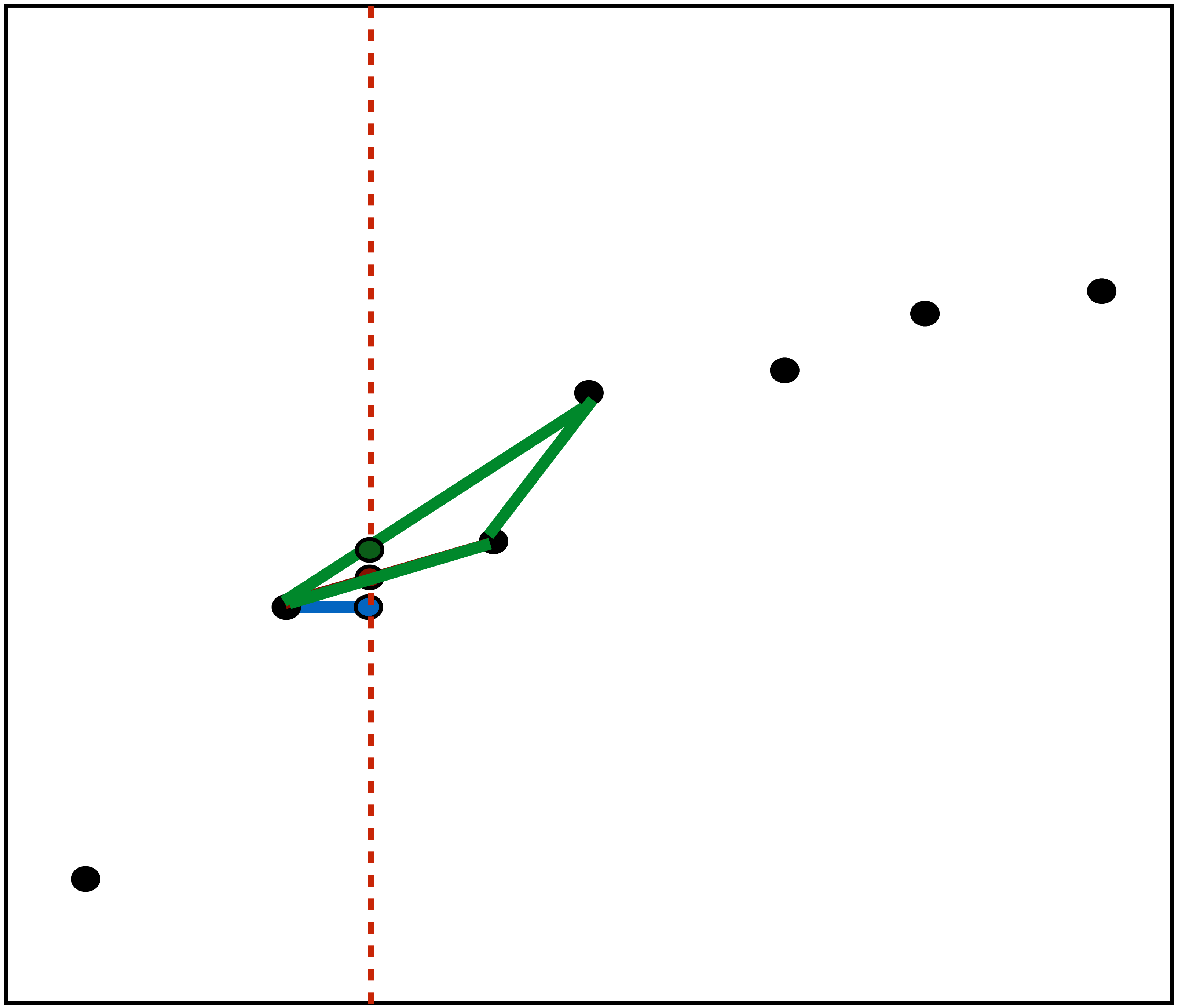
Nonparametric Regression

What's the regression equivalent of *k*-means?

<u>Given</u> training data:
$X = \{x_1, \ldots, x_n\}$
$Y = \{y_1, \ldots, y_n\}$
Distance metric $D(x_i, x_j)$

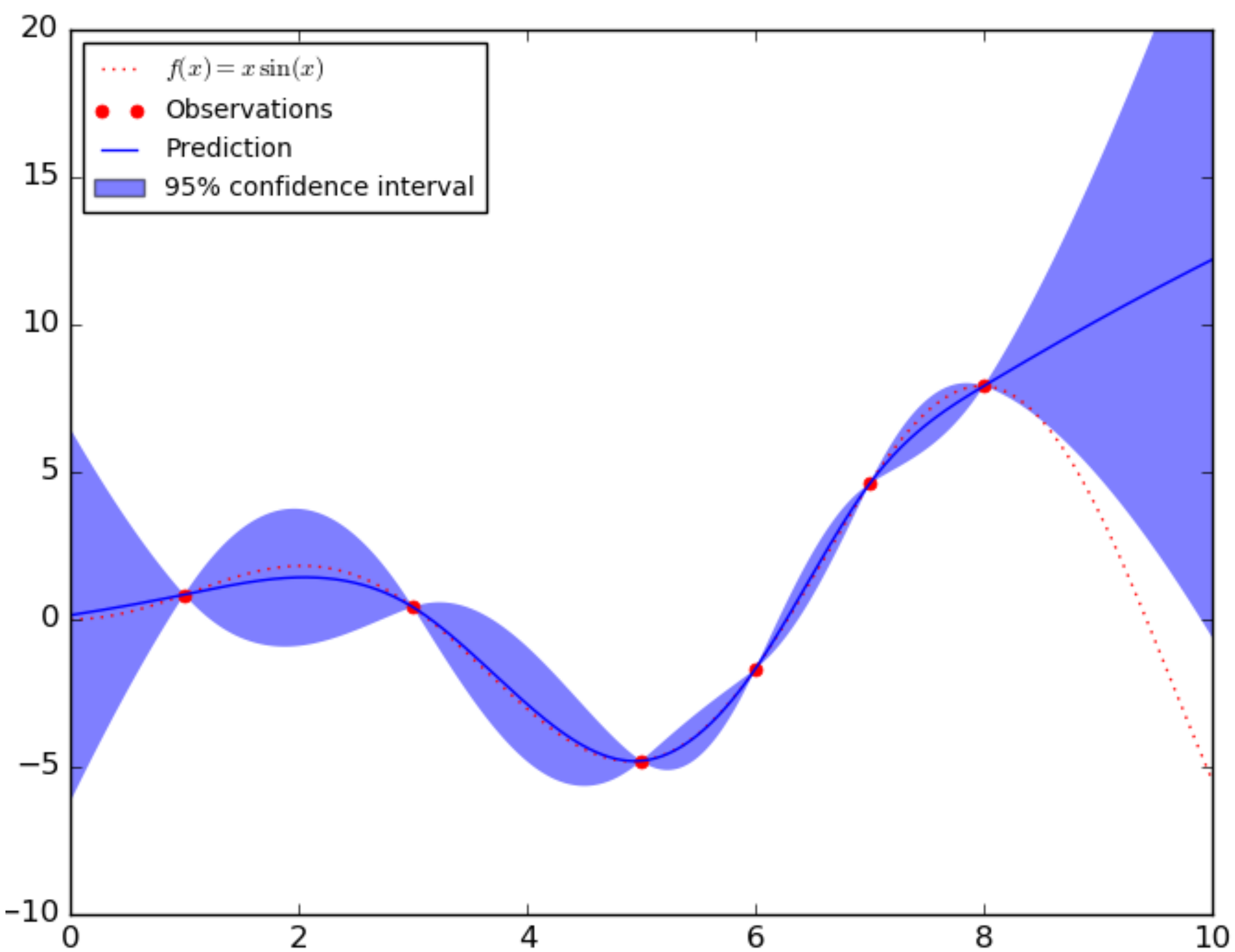
For a new data point x_{new}:
find *k* nearest points in X (measured via D)
set y_{new} to the (weighted by D) average y_i labels

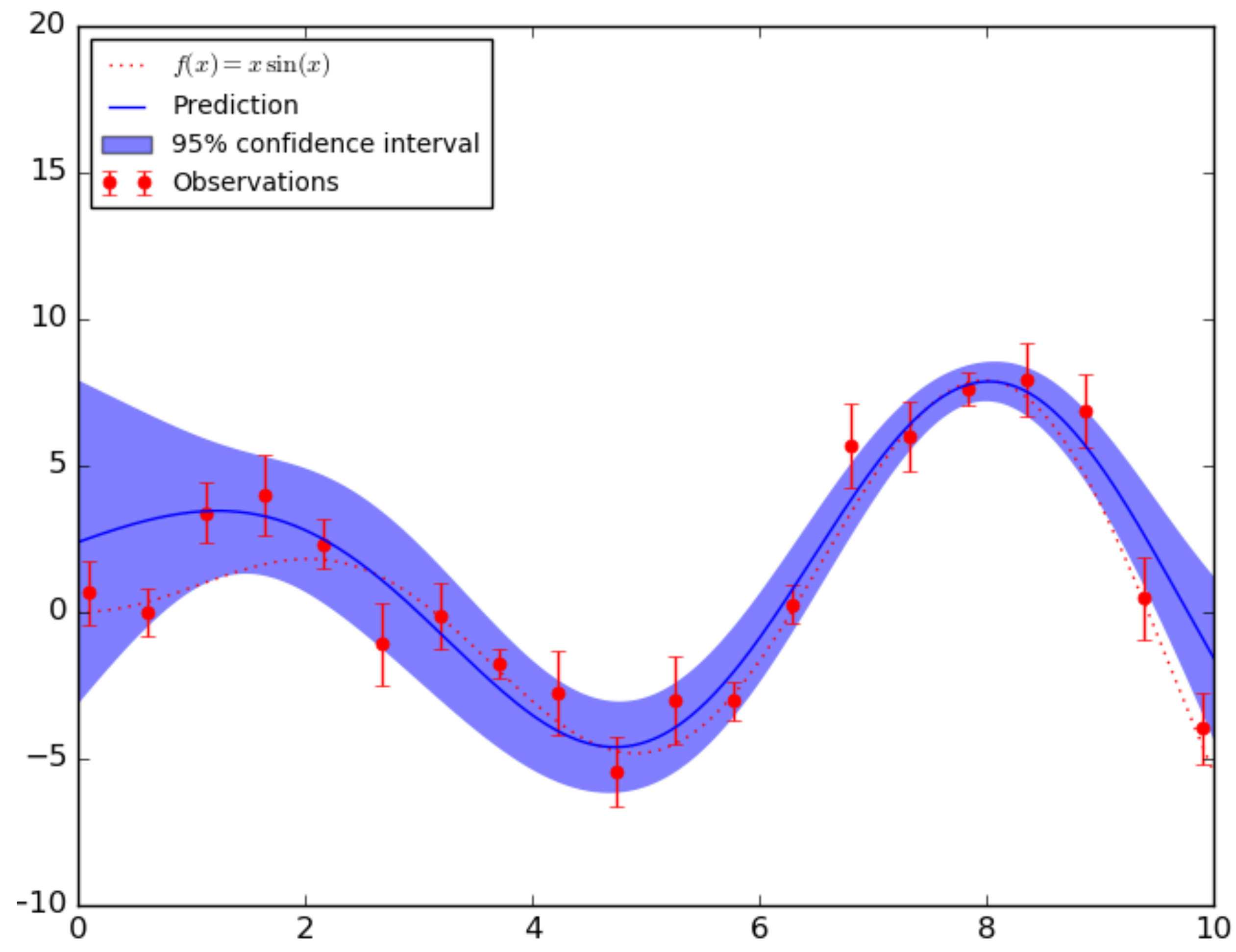
Nonparametric Regression



As *k* increases, *f* gets smoother.

Gaussian Processes





Applications

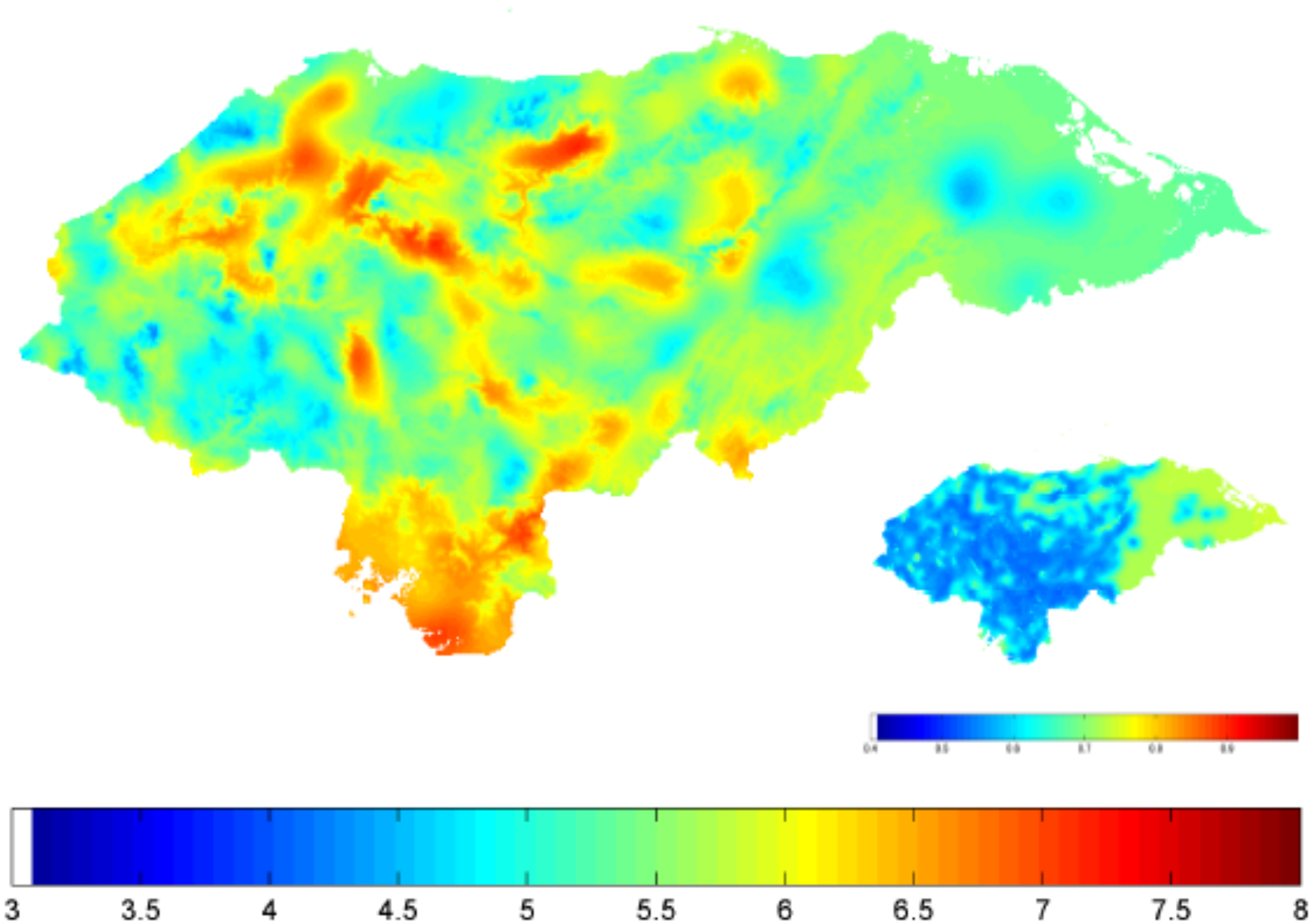


Fig. 3. Predicted map of pH in topsoil and 67% confidence interval

model and predict variations in pH, clay, and sand content in the topsoil

(Gonzalez et al., 2007)