Machine Learning

4771

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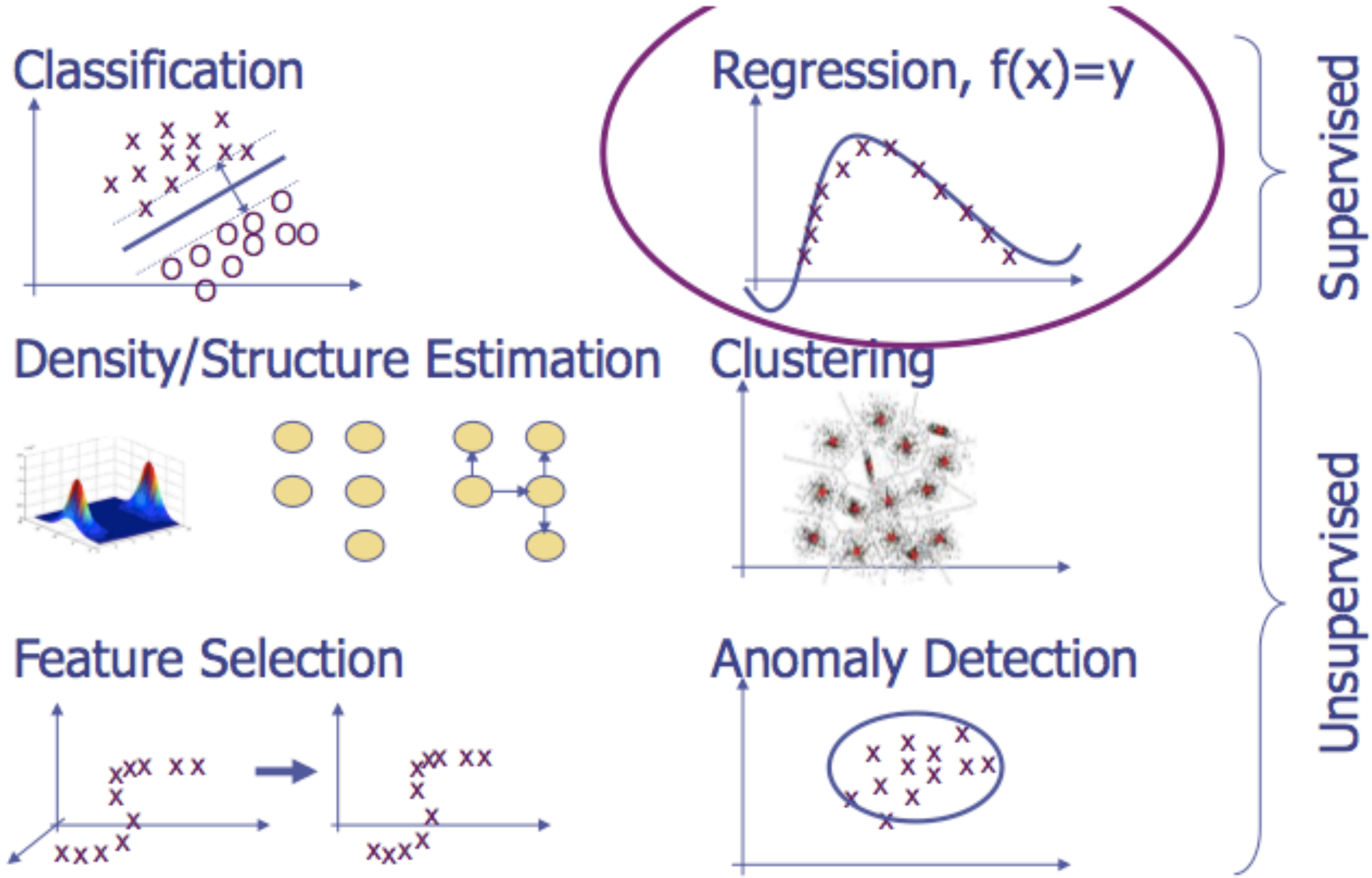
Lecture 3+4: Parametric Approaches to Statistical Inference

- Bayesian Decision Theory (Duda 2.1-2.4)
- Gaussian Distribution (Duda 2.5)
- Classification with Gaussians (Duda 2.6)
- Regression
- Polynomial Approximation (Bishop 1.1)
- Cornerstones of Parametric Statistics

Regression

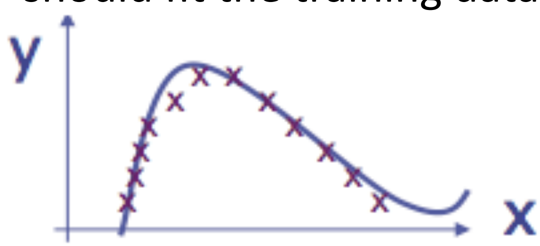

Classification
Regression, f(x)=y
Supervised
Density/Structure Estimation
Clustering
Unsupervised
Feature Selection
Anomaly Detection

Function Approximation

- Start with training dataset

$$\mathcal{X} = \left\{ \left(x_1, y_1\right), \left(x_2, y_2\right), \ldots, \left(x_N, y_N\right) \right\} \quad x \in \mathbb{R}^D = \begin{bmatrix} x(1) \\ x(2) \\ \ldots \\ x(D) \end{bmatrix} \quad y \in \mathbb{R}^1$$

- Have N (input, output) pairs
- Find a function f(x) to predict y from x
  - ➢ should fit the training data well



- Example: predict the price of house in dollars y using x = [#rooms; latitude; longitude; …]

- Need:
  a. Method (criterion) to evaluate how good a fit we have
  b. Class (set) of functions from which to select/search f(x)

Minimizing Training Error

- Idea: minimize 'loss' on the training data set
- Training = Empirical: use the training set to find the best fit
- Define a loss function for a single point (example):

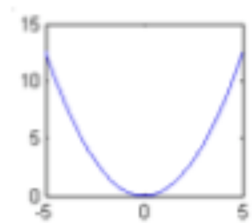
$$L\left(y_i, f\left(x_i\right)\right)$$

- Average loss over the dataset (empirical risk):

$$R = \frac{1}{N}\sum_{i=1}^{N} L\left(y_i, f\left(x_i\right)\right)$$

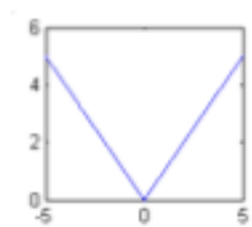
- Simplest loss: squared error from y value

$$L\left(y_i, f\left(x_i\right)\right) = \frac{1}{2}\left(y_i - f\left(x_i\right)\right)^2$$



- Other possible loss: absolute error

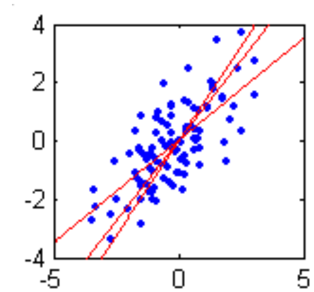
$$L\left(y_i, f\left(x_i\right)\right) = \left|y_i - f\left(x_i\right)\right|$$



Linear Function Class

- Linear is simplest class of functions to search over:

$$f(x;w) = w^T x + w_0 = \sum_{d=1}^{D} w_d x(d) + w_0$$

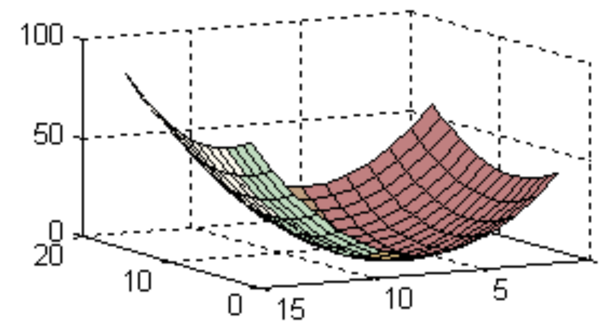


- Start with x being 1-dimensional (D=1):

$$f(x;w) = w_1 x + w_0$$

- Plug in the above & minimize empirical risk over ω

$$R(w) = \frac{1}{2N}\sum_{i=1}^{N}(y_i - w_1 x_i - w_0)^2$$



- Note: minimum occurs when R(w) gets flat (not always!)
- Note: when R(w) is flat, gradient $\nabla_w R = 0$

Minimize Risk ($\nabla_{\mathbf{w}} R = 0$)

- Gradient set to 0
  - all partial derivatives set to 0

$$\nabla_{\mathbf{w}} R = \begin{bmatrix} \frac{\partial R}{\partial w_0} \\ \frac{\partial R}{\partial w_1} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

- Take partials of empirical risk:

$$R(\mathbf{w}) = \frac{1}{2N} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0)^2$$

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$$\frac{\partial R}{\partial w_0} = 0 \Rightarrow \frac{1}{N} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0)(-1) = 0$$

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$$\frac{\partial R}{\partial w_1} = 0 \Rightarrow \frac{1}{N} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0)(-x_i) = 0$$

Minimize Risk ($\nabla_{\mathbf{w}} R = 0$)

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- Take partials of empirical risk:

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$$\frac{\partial R}{\partial w_0} = 0 \Rightarrow \frac{1}{N} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0)(-1) = 0 \qquad (1)$$

$$\frac{\partial R}{\partial w_1} = 0 \Rightarrow \frac{1}{N} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0)(-x_i) = 0 \qquad (2)$$

$$w_0 = \frac{1}{N} \sum y_i - w_1 \frac{1}{N} \sum x_i \qquad (3)$$

$$w_1 \sum x_i^2 = \sum y_i x_i - w_0 \sum x_i \qquad (4)$$

Minimize Risk ($\nabla_{\mathbf{w}} R = 0$)

- Gradient set to 0
  - ➢ all partial derivatives set to 0

$$\nabla_{\mathbf{w}} R = \begin{bmatrix} \frac{\partial R}{\partial w_0} \\ \frac{\partial R}{\partial w_1} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

- Take partials of empirical risk:

$$R(\mathbf{w}) = \frac{1}{2N} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0)^2$$

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$$w_1 \sum x_i^2 = \sum y_i x_i - w_0 \sum x_i \qquad (4)$$

$$w_1 \sum x_i^2 = \sum y_i x_i - \left(\frac{1}{N} \sum y_i - w_1 \frac{1}{N} \sum x_i\right) \sum x_i$$

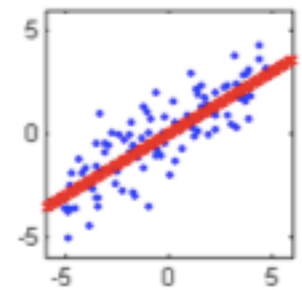
$$w_1\left(\sum x_i^2 - \frac{1}{N} \sum x_i \sum x_i\right) = \sum y_i x_i - \frac{1}{N} \sum y_i \sum x_i$$

$$w_1 = \frac{\sum y_i x_i - \frac{1}{N} \sum y_i \sum x_i}{\sum x_i^2 - \frac{1}{N} \sum x_i \sum x_i} \qquad (5)$$

Properties of the Solution

- Setting w* as before gives least squared error
- Define error on each data point as:

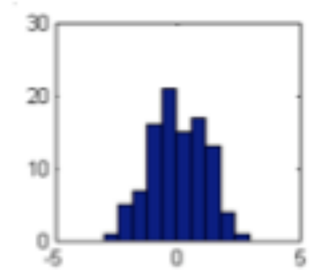
$$e_i = y_i - w_1^* x_i - w_0^*$$



- Note property #1:

$$\frac{\partial R}{\partial w_0} = \frac{1}{N} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0) = 0$$

...average error is zero $\quad \frac{1}{N} \sum e_i = 0$

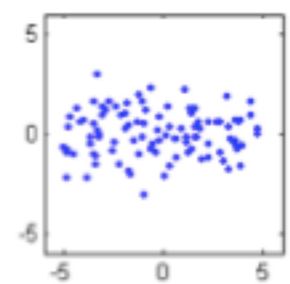


- Note property #2:

$$\frac{\partial R}{\partial w_1} = \frac{1}{N} \sum_{i=1}^{N} (y_i - w_1 x_i - w_0) x_i = 0$$

...error not correlated with data

$$\frac{1}{N} \sum e_i x_i = \frac{1}{N} e^T x = 0$$



Multi-Dimensional Regression

- More elegant/general to do $\nabla_{\mathbf{w}} R = 0$ with linear algebra
- Rewrite empirical risk in vector-matrix notation:
- Can add more dimensions by adding columns to X matrix and rows to w vector:

$$
\begin{aligned}
R(\mathbf{w}) &= \frac{1}{2N}\sum_{i=1}^{N}(y_i - w_1 x_i - w_0)^2 \\
&= \frac{1}{2N}\sum_{i=1}^{N}\left(y_i - [1, x_i]\begin{bmatrix} w_0 \\ w_1 \end{bmatrix}\right)^2 \\
&= \frac{1}{2N}\sum_{i=1}^{N}\left(y_i - [1, x_i(1)\ldots x_i(d)]\begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}\right)^2 \\
&= \frac{1}{2N}\left\|\begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} 1 & \mathbf{x}_1 \\ \vdots & \vdots \\ 1 & \mathbf{x}_N \end{bmatrix}\begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix}\right\|^2 \\
&= \frac{1}{2N}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2
\end{aligned}
$$

Multi-Dimensional Regression

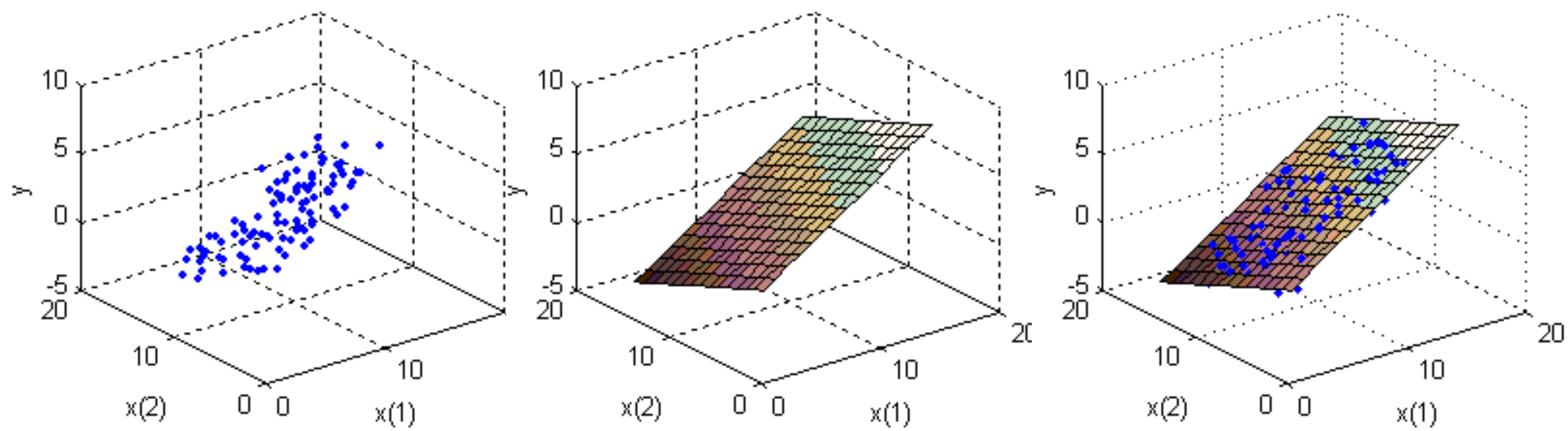
- More realistic dataset: many measurements
- Have N apartments each with D measurements
- Each row of X is [#rooms; latitude; longitude,…]

$$\mathbf{X} = \begin{bmatrix} 1 & x_1(1) & \ldots & x_1(D) \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_N(1) & \ldots & x_N(D) \end{bmatrix}$$

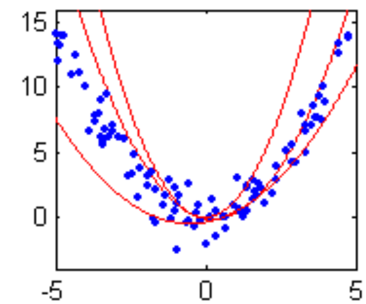
2D Linear Regression

- Once best w* is found, we can plug it into the function:

$$f(x; w^*) = w_2^* x(2) + w_1^* x(1) + w_0^*$$

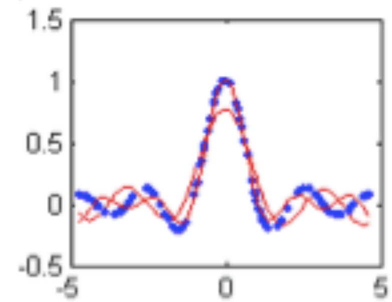


Polynomial Function Classes



- Back to 1-dim x (D=1) BUT Nonlinear Function Classes
- Polynomial: $f(x;w) = \sum_{p=1}^{P} w_p x^p + w_0$
- Writing Risk: $R(w) = \frac{1}{2N} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2, \quad X = \begin{bmatrix} 1 & x_1^1 & \cdots & x_1^p \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_N^1 & \cdots & x_N^p \end{bmatrix}$
- Order-P polynomial regression fitting for 1D variable is the same as P-dimensional linear regression!
- Construct a multidim x-vector from x scalar: $x_i = [x_i^0, x_i^1, x_i^2]^T$
- More generally any function: $x_i = [\phi_0(x_i), \phi_1(x_i), \phi_2(x_i)]^T$

Sinusoidal Basis Functions



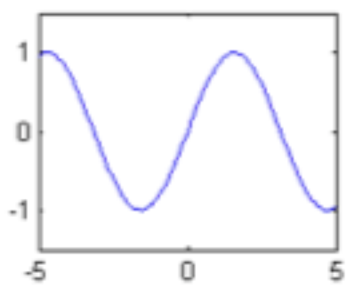
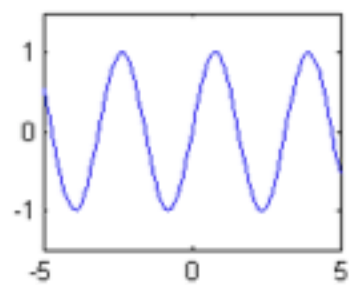
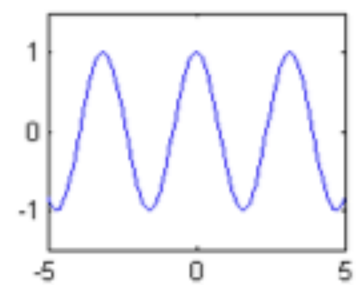
- More generally, we don't just have to deal with polynomials, use any set of basis fn's:

$$f(x;\theta) = \sum_{p=1}^{P} \theta_p \phi_p(x) + \theta_0$$

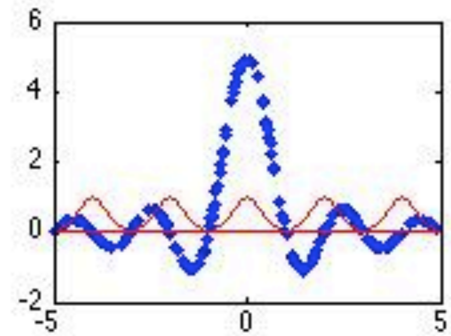
- These are generally called Additive Models
- Regression adds linear combinations of the basis fn's
- For example: Fourier (sinusoidal) basis

$$\phi_{2k}(x_i) = \sin(kx_i) \qquad \phi_{2k+1}(x_i) = \cos(kx_i)$$

- Note, don't have to be a basis per se, usually subset

$\theta_1 \times$  $+\theta_2 \times$  $+\theta_3 \times$ 

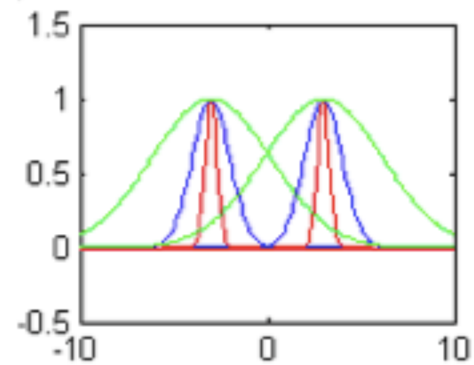
Radial Basis Functions



- Can act as prototypes of the data itself

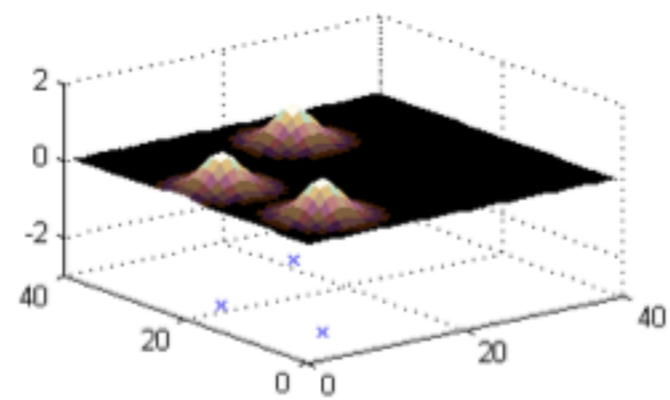
$$f(\mathbf{x};\theta) = \sum_{k=1}^{N} \theta_k \exp\left(-\frac{1}{2\sigma^2}\left\|\mathbf{x}-\mathbf{x}_k\right\|^2\right) + \theta_0$$

- Parameter σ = standard deviation
  σ^2 = covariance



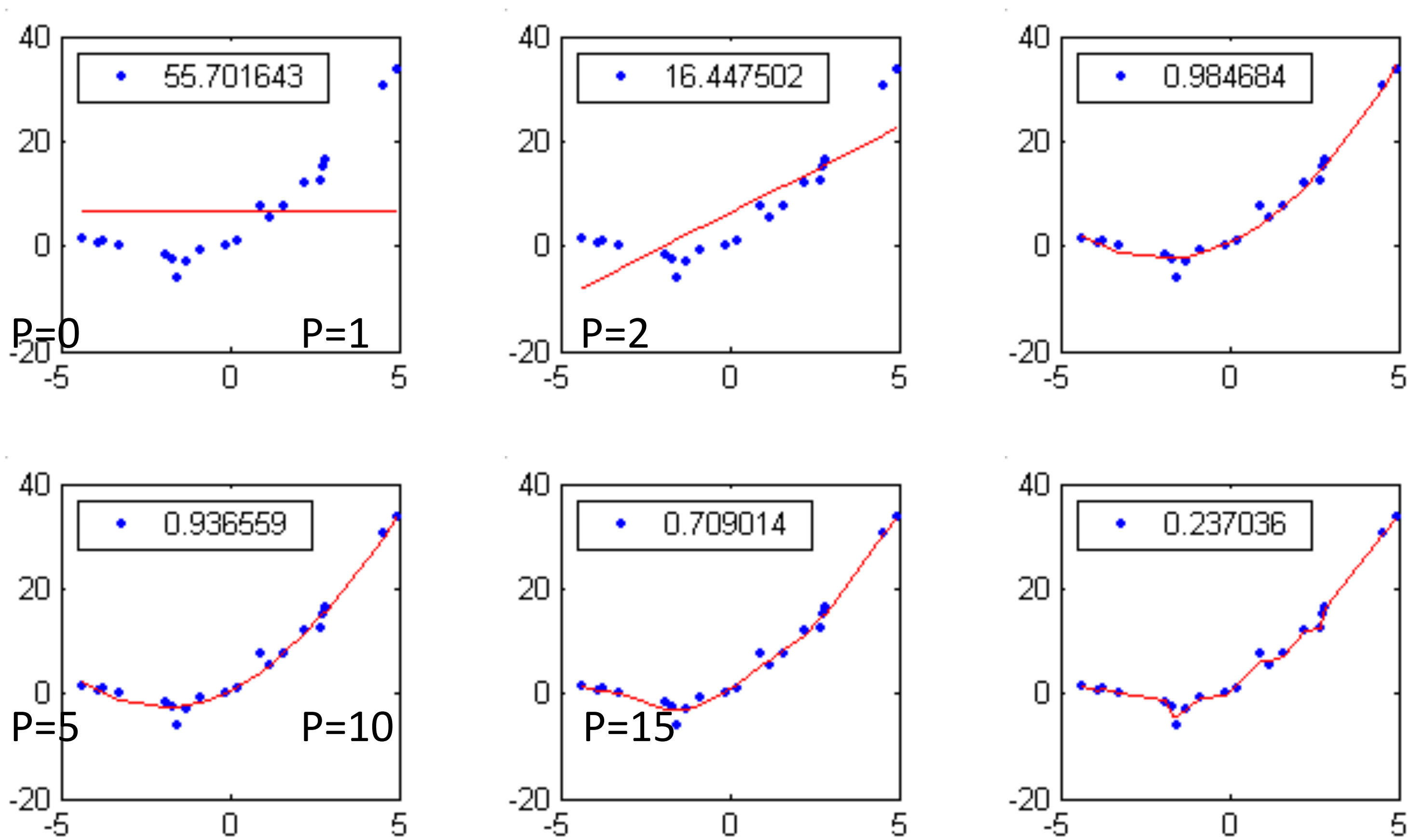
controls how wide bumps are
what happens if too big/small?

- Also works in multi-dimensions

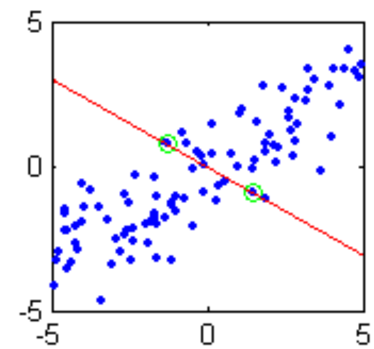


Underfitting/Overfitting

- Try varying P. Higher P fits a more complex function class
- Observe R(w*) drops with bigger P



Evaluating the Model



- Unfair to use training error to find best order P
- High P (vs. N) can overfit, even linear case!
- min R(w*) not on training but on future data
- Want model to *Generalize* to future data

Expected (true) loss: $R_{\text{expected}}(w) = \int L(y, f(x; w)) P(x, y)\, dx\, dy$

- One approach: split data into training / testing portion

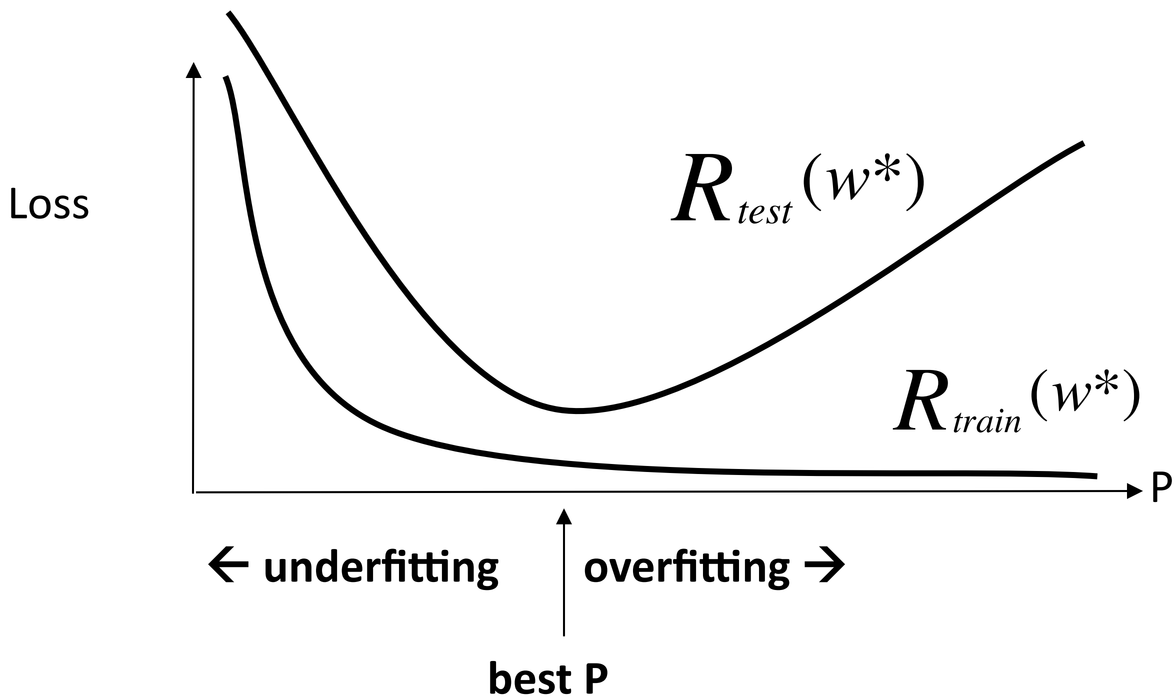
$\{(x_1, y_1), \ldots, (x_v, y_v)\}$ $\{(x_{v+1}, y_{v+1}), \ldots, (x_N, y_N)\}$

- Estimate ω* with training (empirical) loss: $R_{train}(w) = \frac{1}{2v} \sum_{i=1}^{v} (y_i - w^T x_i)^2$

- Evaluate P with testing loss: $R_{test}(w) = \frac{1}{2(N-v)} \sum_{i=v+1}^{N} (y_i - w^T x_i)^2$

Validation

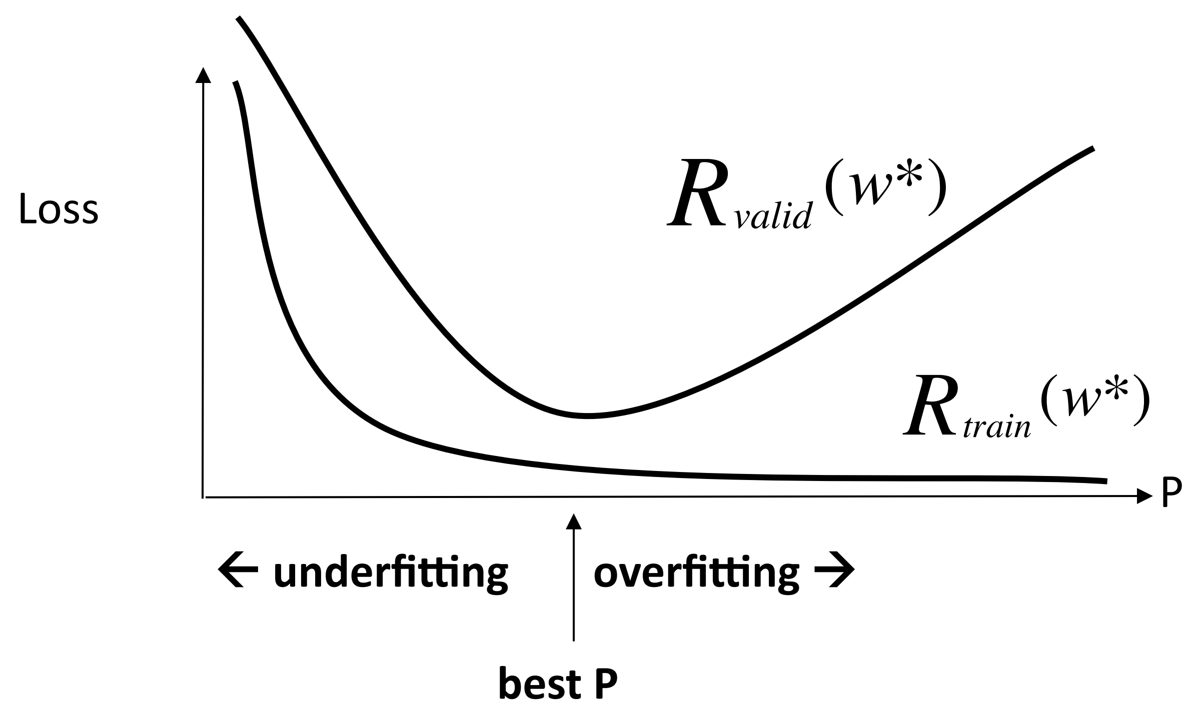
- Try fitting with different polynomial order P
- Select P which gives lowest $R_{test}(w^*)$



- Think of P as a measure of the complexity of the model
- Higher order polynomials are more flexible and complex

Cross-Validation

- Better idea: split data into three sets (training / validation / test)
- Even better idea: split data into two sets (training / test) but do *K-fold cross-validation* on the training set
  - ➢ K folds, K-1 for training, 1 for testing; repeat process K times; average error
- Best idea (sometimes): *leave-one-out cross-validation* on the training set
  - ➢ N examples, N-1 for training 1 for testing; repeat process N times; average error



The Weierstrass Approximation Theorem

- Theorem (1885):

  Suppose $f(x)$ is a continuous real-valued function defined on the real interval $[a,b]$. For every $\epsilon > 0$, there exists a polynomial function p over $\mathbb{R}$ such that $\forall x \in [a,b]$, we have $|f(x) - p(x)| < \epsilon$, or equivalently, $\|f(x) - p(x)\|_\infty < \epsilon$.

- Definition of supremum (infinity) norm:

  $$\|f(x) - p(x)\|_\infty = \sup\{|f(x) - p(x)|\}$$