# Optimization and Machine Learning SI151

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February 25, 2020

#### Today:

- Overview of supervised learning II
  - Statistical decision theory
  - Local methods in high dimensions
  - Statistical models
  - Model selection

#### Readings:

• The Elements of Statistical Learning (ESL), Chapter 2

# Overview of Supervised Learning II

--- Statistical Decision Theory

#### • Given:

- □ random input vector  $X \in \mathbb{R}^p$ ,
- □ random output variable  $Y \in \mathbb{R}$ ,
- $\Box$  joint distribution Pr(X, Y),
- Goal: we seek a function f(X) for predicting Y given values of X.
- To penalize prediction errors, we introduce the *loss function* L(Y, f(X)).
- Squared error loss:

$$L(Y, f(X)) = (Y - f(X))^2.$$

• Expected prediction error (EPE):

$$EPE(f) = E(Y - f(X))^{2}$$
$$= \int (y - f(x))^{2} Pr(dx, dy).$$

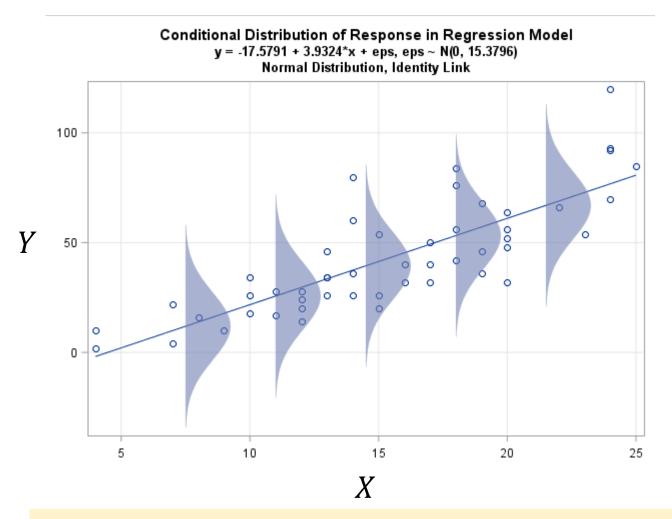
• Since Pr(X,Y) = Pr(Y|X) Pr(X), EPE can also be written as

$$EPE(f) = E_X E_{Y|X}([Y - f(X)]^2 | X).$$

• Thus, it suffices to minimize EPE *pointwise*:

$$f(x) = \operatorname{argmin}_{c} E_{Y|X} ([Y - c]^{2} | X = x)$$

Regression function: f(x) = E(Y|X = x).



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- Nearest neighbor methods try to directly implement this recipe  $\hat{f}(x) = \text{Ave}(y_i|x_i \in N_k(x)).$
- Two approximations:
  - expectation is approximated by averaging over sample data;
  - conditioning at a point is relaxed to conditioning on neighborhood.
- As  $N, k \to \infty$  and  $\frac{k}{N} \to 0$ , we have  $\hat{f}(x) \to E(Y|X=x)$ .

- But usually we do not have very large samples.
  - ➤ By making assumptions (linearity), we can reduce the required number of observations greatly.
- As increasing the number *p* of dimensions, the number *N* of observations required in the training data set increases exponentially.
  - Thus the *rate of convergence* to the true estimator (with increasing *p*) decreases.

- Linear regression assumes that the regression function is approximately linear  $f(x) \approx x^{T} e^{x}$ 
  - $f(x) \approx x^T \beta$
- This is a model-based approach.
- Plugging this f(x) into EPE,  $EPE(f) = E(Y - f(X))^{2}$

$$= E((Y - X^T \beta)^T (Y - X^T \beta))$$

• Differentiating w.r.t.  $\beta$ , leads to

$$\beta = [E(XX^T)]^{-1}E(XY)$$

 Again, linear regression replaces the theoretical expectation by averaging over the observed data

$$RSS(\beta) = \sum_{i=1}^{N} (y_i - x_i^T \beta)^2$$
$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

- Summary approximation of f(X)
  - Least squares:globally linear function
  - Nearest neighbors:locally constant function.

Regression function: f(x) = E(Y|X = x).

- Additional methods in our course are often model-based but more flexible than the linear model.
- For example, additive models

$$f(X) = \sum_{j=1}^{p} f_j(X_j)$$

- $\Box$  Coordinate function  $f_j$  is arbitrary.
- Approximate *univariate* conditional expectations simultaneously for each  $f_i$ .
- Model assumption: additivity.

• What happens if we use absolute loss function?

$$L_1(Y, f(X)) = E|Y - f(X)|$$

• In this case,

$$\hat{f}(x) = \text{median}(Y|X = x)$$

- More robust than the conditional mean.
- Summary:
  - $\Box$   $L_1$  criterion not differentiable.
  - Squared error is the most popular.

Q: How to obtain the  $\hat{f}(x)$  when absolute loss is used?

- Procedure for categorical output variable *G* with values from *G*.
- Loss function is  $K \times K$  matrix L, where  $K = \text{card}(\mathcal{G})$
- $\mathbf{L}(k, l)$  is the price paid for misclassifying an observation belonging to class  $\mathcal{G}_k$  as class  $\mathcal{G}_l$
- L is zero on the diagonal
- We often use the zero-one loss function

$$\mathbf{L}(k, l) = 1 - \delta_{kl}$$
 where  $\delta_{kl} = 1$  if  $k = l$ , otherwise  $\delta_{kl} = 0$ 

- Expected prediction error (EPE)  $EPE = E[L(G, \hat{G}(X))]$ where expectation taken w.r.t. Pr(G, X)
- Conditioning on *X* yields

$$EPE = E_X \sum_{k=1}^{K} L[\mathcal{G}_k, \widehat{G}(X)] \Pr(\mathcal{G}_k | X)$$

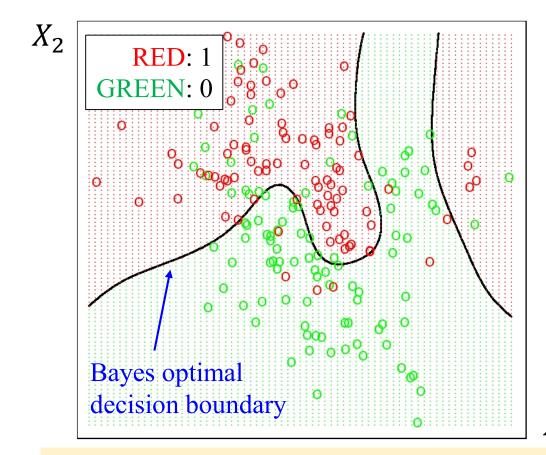
• Again, it suffices to pointwise minimization

$$\widehat{G}(x) = \operatorname{argmin}_{g \in G} \sum_{k=1}^{K} L(\mathcal{G}_k, g) \Pr(\mathcal{G}_k | X = x)$$
Or simply

Bayes classifier

Or simply  $\widehat{G}(x) = \operatorname{argmax} \Pr(g|X = x)$ 

Bayes Optimal Classifier



Since the generating density is known for each class, this boundary can be calculated exactly.

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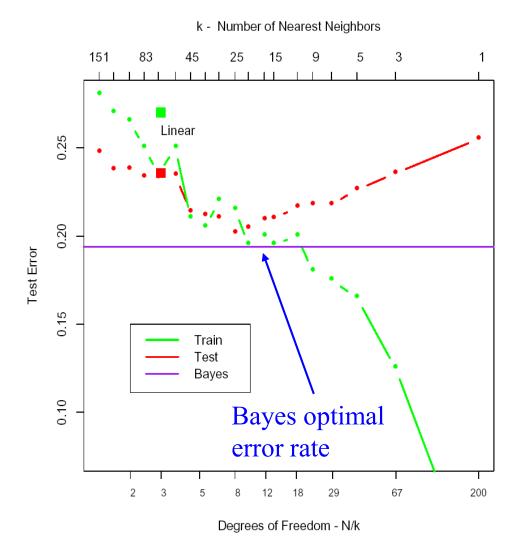
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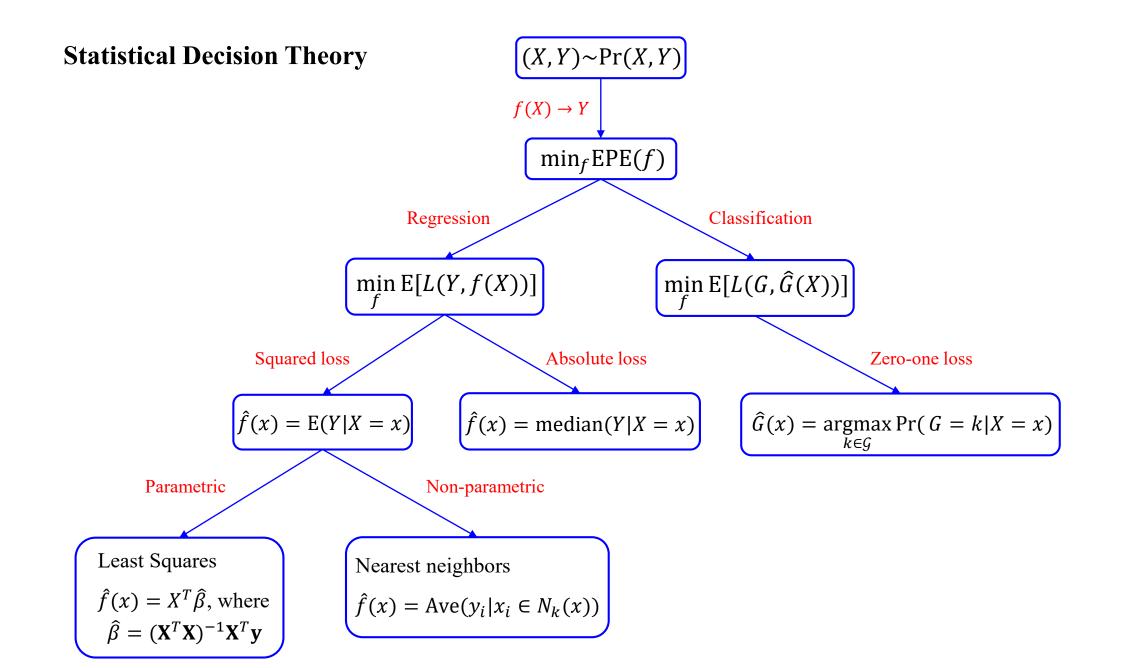
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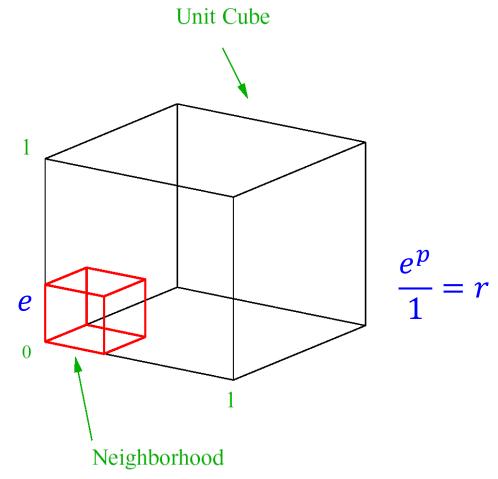
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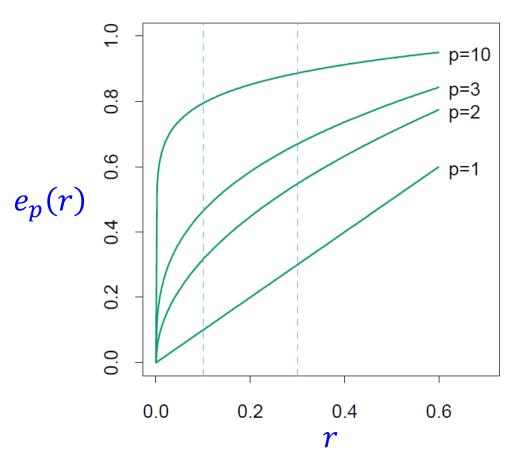
## Overview of Supervised Learning II

--- Local Methods in High Dimensions

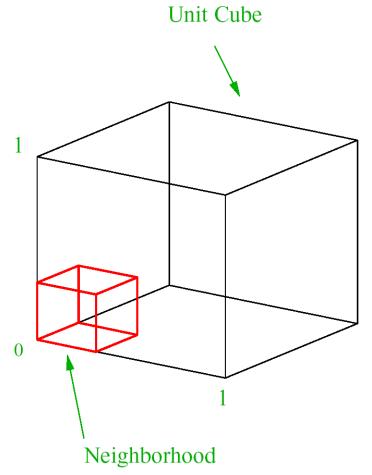
- Curse of Dimensionality:
   Local neighborhoods become increasingly global, as the number of dimension increases
- Example:
  Points uniformly distributed in a *p*-dimensional unit hypercube.
- Hypercubical neighborhood in *p* dimensions that captures a fraction *r* of the data
  - edge length:  $e_p(r) = r^{\frac{1}{p}}$   $e_{10}(0.01) = 0.63$   $e_{10}(0.1) = 0.80$



In ten dimensions we need to cover 63% (80%) of the range of each coordinate to capture 1% (10%) of the data.



Reducing *r* reduces the number of observations and thus the stability.



In ten dimensions we need to cover 63% (80%) of the range of each coordinate to capture 1% (10%) of the data.

- In high dimensions, all sample points are close to the edge of the sample
- *N* data points uniformly distributed in a *p*-dimensional unit ball centered at the origin
- Median distance from the closest point to the origin

$$d(p, N) = \left(1 - \frac{1}{2}^{1/N}\right)^{1/p}$$

•  $d(10,500) \approx 0.52$ : more than half the way to the boundary

(1) 
$$\prod_{i=1}^{N} \Pr(\|x_i\| > r) = \frac{1}{2}$$

(2) 
$$\Pr(\|x_i\| > r) = 1 - \Pr(\|x_i\| \le r)$$
  
=  $1 - r^p$ 

$$(3) \quad (1 - r^p)^N = \frac{1}{2}$$

Volume of a *p*-ball: 
$$V_p(r) = \frac{\pi^{\frac{p}{2}}}{\Gamma(\frac{p}{2}+1)} r^p$$

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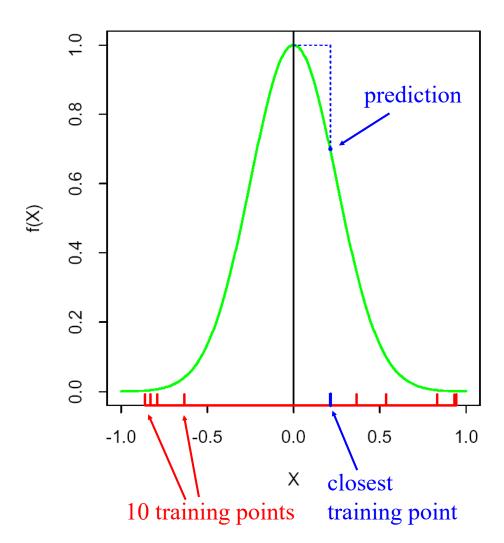
- Sampling density is proportional to  $N^{1/p}$
- If  $N_1 = 100$  is a dense sample for one input, then  $N_{10} = 100^{10}$  is an equally dense sample for 10 inputs.
- Thus in high dimensions all feasible training samples sparsely populate the input space.

- Another example
- $\mathcal{T}$ : set of training points  $x_i$  generated uniformly in  $[-1,1]^p$  (red)
- Functional relationship between X and Y (green)

$$Y = f(X) = e^{-8||X||^2}$$

- No measurement error
- Error of a 1-nearest neighbor classifier in estimating f(0) (blue)

#### 1-NN in One Dimension



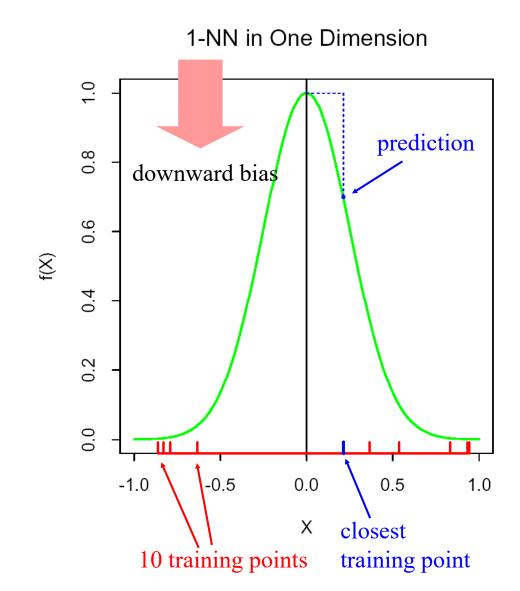
- Another example
- Problem deterministic: Prediction error is the meansquared error for estimating f(0)

$$MSE(x_0) = E_{\mathcal{T}}[f(x_0) - \hat{y}_0]^2$$

$$= E_{\mathcal{T}}[\hat{y}_0 - E_{\mathcal{T}}(\hat{y}_0)]^2$$

$$+ [E_{\mathcal{T}}(\hat{y}_0) - f(x_0)]^2$$

$$= Var_{\mathcal{T}}(\hat{y}_0) + Bias^2(\hat{y}_0)$$



$$MSE(x_{0}) = E_{T}[f(x_{0}) - \hat{y}_{0}]^{2}$$

$$= E_{T}[\hat{y}_{0} - E_{T}(\hat{y}_{0}) + E_{T}(\hat{y}_{0}) - f(x_{0})]^{2}$$

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$$= E_{T}[(\hat{y}_{0} - E_{T}(\hat{y}_{0}))^{2} + 2((\hat{y}_{0} - E_{T}(\hat{y}_{0}))(E_{T}(\hat{y}_{0}) - f(x_{0})) + (E_{T}(\hat{y}_{0}) - f(x_{0}))^{2}]$$

$$= E_{T}[(\hat{y}_{0} - E_{T}(\hat{y}_{0}))^{2}] + (E_{T}(\hat{y}_{0}) - f(x_{0}))^{2}$$

$$= Var_{T}(\hat{y}_{0}) + Bias^{2}(\hat{y}_{0})$$
Constant

This is known as the bias-variance decomposition.

- Another example
- 1-d (red) vs 2-d (blue)
- As p increases, the bias increases

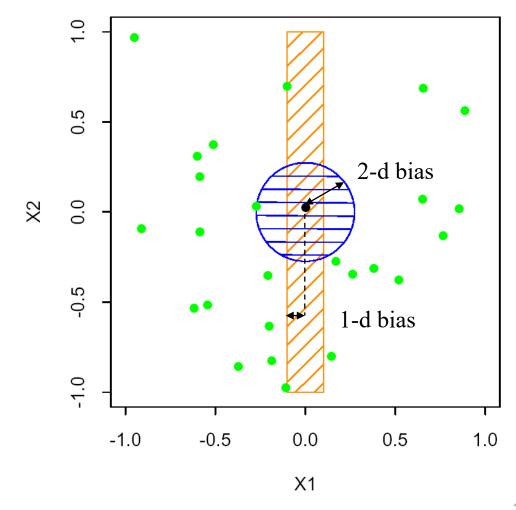
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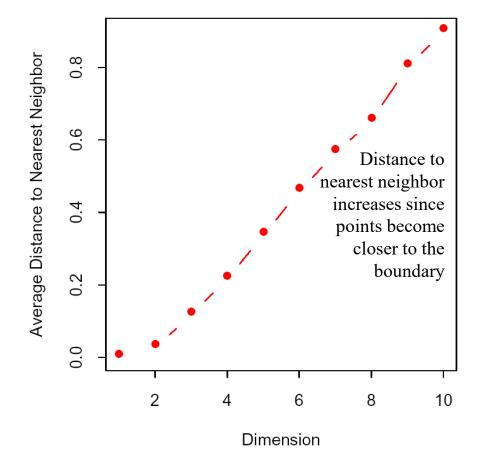
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#### 1-NN in One vs. Two Dimensions



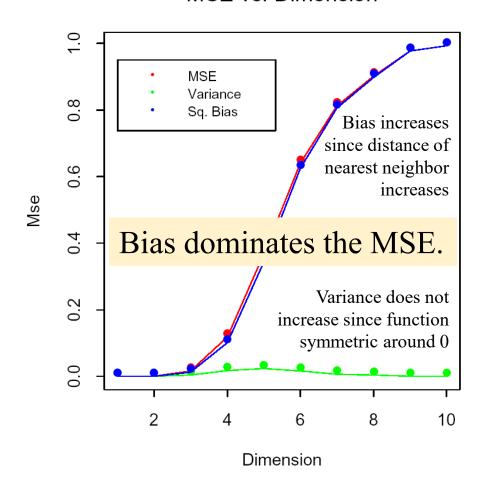
• The case on N=1000 training points

Distance to 1-NN vs. Dimension



$$Y = f(X) = e^{-8\|X\|^2}$$

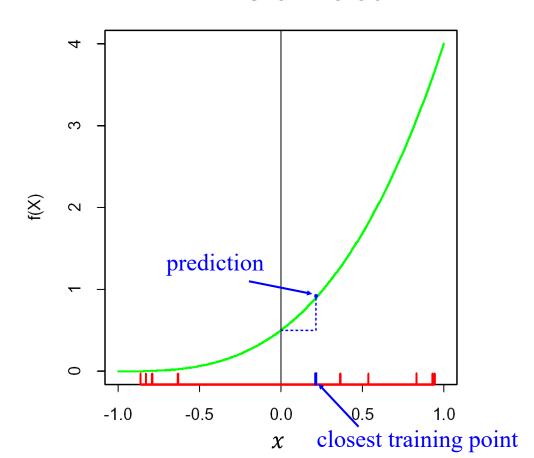
MSE vs. Dimension



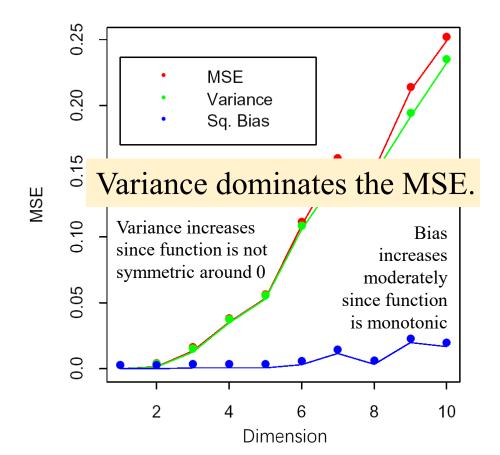
• Yet another example

$$Y = f(X) = \frac{1}{2}(X_1 + 1)^3$$

1-NN in One Dimension



MSE vs. Dimension



• Suppose a linear relationship with measurement error

$$Y = X^T \beta + \varepsilon$$
,  $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ 

• If the model is fitted by least squares, we find that

$$EPE(x_0) = \sigma^2 + E_T[x_0^T(\mathbf{X}^T\mathbf{X})^{-1}x_0]\sigma^2$$

- $\triangleright$  Additional variance  $\sigma^2$  originates from the nondeterministic part
- $\triangleright$  Variance depends on  $x_0$
- > No bias

• If *N* is large, we get

$$E_{x_0}EPE(x_0) \sim \frac{\sigma^2}{N}p + \sigma^2$$

- As p increases, variance grows negligible for large N or small  $\sigma^2$
- Curse of dimensionality controlled

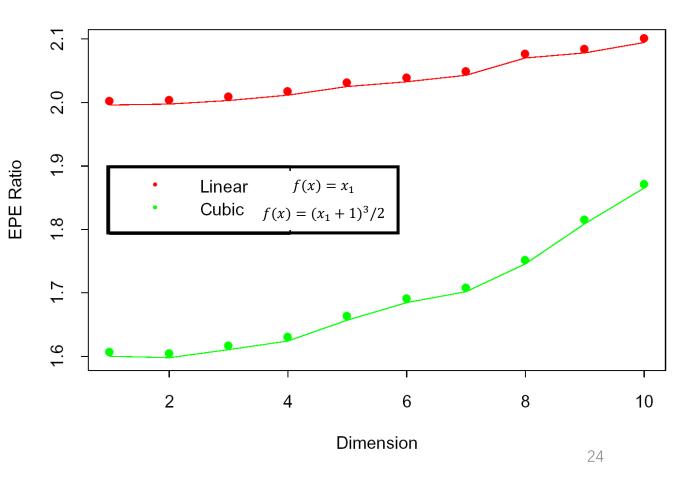
• More generally

$$Y = f(X) + \varepsilon$$
,

*X* uniform,  $\varepsilon \sim \mathcal{N}(0,1)$ 

- Sample size: N = 500
- Linear case
  - EPE (Least Squares)is slightly above 1, no bias
  - EPE (1-NN) always
     above 2, grows slowly
     as nearest training point strays
     from target

EPE ratio = 
$$\frac{\text{EPE (1-NN)}}{\text{EPE (least squares)}}$$
, at  $x_0 = 0$ 



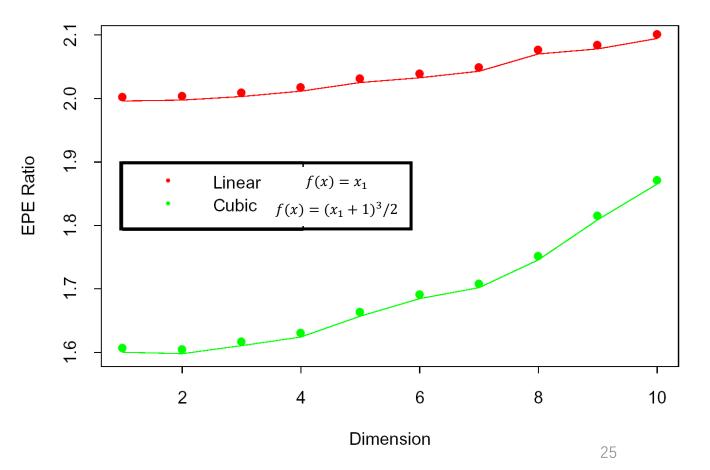
• More generally

$$Y = f(X) + \varepsilon,$$

*X* uniform,  $\varepsilon \sim \mathcal{N}(0,1)$ 

- Sample size: N = 500
- Cubic case
  - EPE (Least Squares)is biased, thus ratio is smaller

EPE ratio = 
$$\frac{\text{EPE (1-NN)}}{\text{EPE (least squares)}}$$
, at  $x_0 = 0$ 



### **Local Models in High Dimensions** – Summary

- Curse of Dimensionality
  - 1. Local neighborhoods become increasingly global, as the number of dimension increases
  - 2. In high dimensions, all samples are close to the edge of the sample
  - 3. Samples sparsely populate the input space

- The bias-variance decomposition
  - 1. Deterministic case

$$EPE(x_0) = MSE(x_0)$$
  
=  $Var_{\mathcal{T}}(\hat{y}_0) + Bias^2(\hat{y}_0)$ 

2. Non-deterministic case

$$EPE(x_0) = MSE(x_0) + \sigma^2$$
  
=  $Var_T(\hat{y}_0) + Bias^2(\hat{y}_0) + \sigma^2$ 

- Least squares
  - Linear case: non-biased, negligible variance for large *N*
  - Non-linear case: biased
- Nearest neighbors
  - > Symmetric on  $x_0$ : Bias<sup>2</sup>( $\hat{y}_0$ ) dominates
  - ightharpoonup Monotonic on  $x_0$ :  $Var_T(\hat{y}_0)$  dominates

# Overview of Supervised Learning II

--- Statistical Models

(p + 1)-dimensional Euclidean space, we fit  $f: \mathbb{R}^p \to \mathbb{R}$  by

$$y_i = f(x_i) + \varepsilon_i$$

- Goal: a good approximation of f(x) in some region of input space, given the training set  $\mathcal{T}$
- Many models have certain parameters  $\theta$ 
  - E.g. for the linear model  $f(x) = x^T \beta$ and  $\theta = \beta$

• Data: pairs  $(x_i, y_i)$  that are points in • Linear basis expansions have the more general form

$$f_{\theta}(x) = \sum_{k=1}^{K} h_k(x)\theta_k$$

- $h_k$ : a suitable set of functions or transformations of the input vector x.
- Examples:
  - Polynomial expansions:  $h_k(x) = x_1 x_2^2$
  - Trigonometric expansions:  $h_k(x) = \cos(x_1)$

Sigmoid expansion:

$$h_k(x) = \frac{1}{1 + \exp(-x^T \beta_k)}$$



• Approximating  $f_{\theta}$  by minimizing the residual sum of squares

$$RSS(\theta) = \sum_{i=1}^{N} (y_i - f_{\theta}(x_i))^2$$

• Linear basis expansions have the more general form

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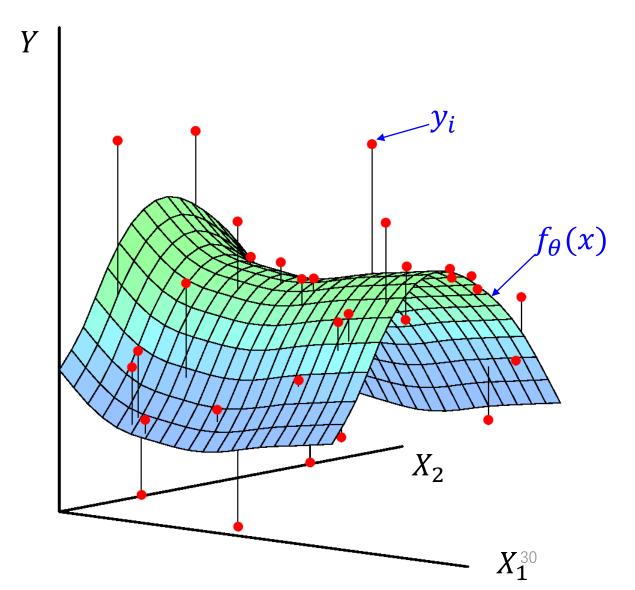
Sigmoid expansion:

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• Approximating  $f_{\theta}$  by minimizing the residual sum of squares

$$RSS(\theta) = \sum_{i=1}^{N} (y_i - f_{\theta}(x_i))^2$$

- Intuition
  - f surface in (p + 1) —space
  - Observe noisy realizations
  - Want fitted surface as close to the observed points as possible
  - Distance measured by RSS
- Methods
  - Closed form: if basis function have no hidden parameters
  - Iterative: otherwise

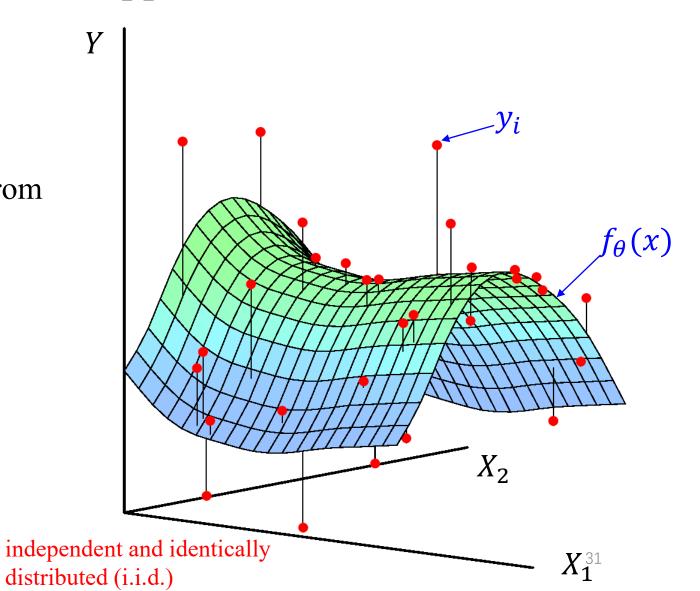


- Approximating  $f_{\theta}$  by maximum likelihood estimation (MLE)
- Assume an independently drawn random sample  $y_i$ , i = 1, ..., N from a probability density  $Pr_{\theta}(y)$ .
- The log-probability of observing the sample is

$$L(\theta) = \sum_{i=1}^{N} \log \Pr_{\theta}(y_i)$$

$$L(\theta) = \log \Pr_{\theta}(y_1, y_2, ..., y_N)$$

$$= \log \prod_{i=1}^{N} \Pr_{\theta}(y_i)$$



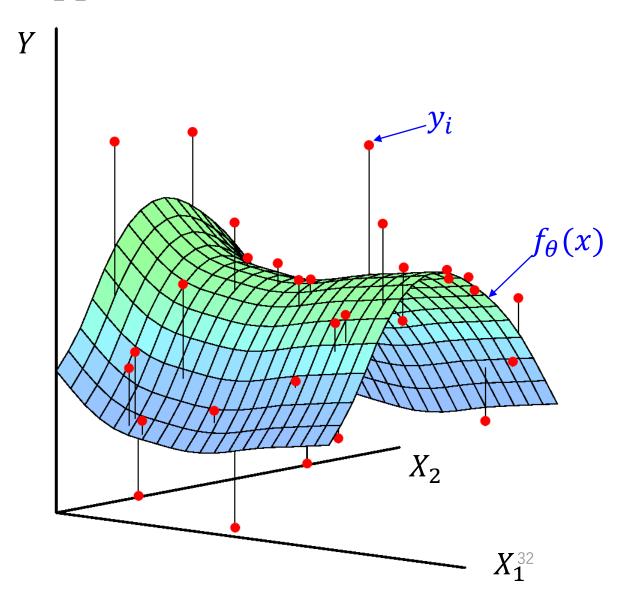
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• Set  $\theta$  to maximize  $L(\theta)$ 

#### Intuition:

Under the assumed statistical model, the observed data is most probable.



- Approximating  $f_{\theta}$  by maximum likelihood estimation (MLE)
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$$L(\theta) = \sum_{i=1}^{N} \log \Pr_{\theta}(y_i)$$

• Set  $\theta$  to maximize  $L(\theta)$ 

$$\Pr_{\theta}(y|X=x) = \frac{1}{\sigma\sqrt{2\pi}} \exp(-\frac{1}{2}(\frac{y - f_{\theta}(x)}{\sigma})^2)$$

Least squares with additive error model

$$Y = f_{\theta}(X) + \varepsilon$$
$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

is equivalent to maximum likelihood with the conditional likelihood

$$\Pr_{\theta}(Y|X) = \mathcal{N}(f_{\theta}(X), \sigma^2)$$

• This is, because in this case the *log-likelihood* of data is

$$L(\theta) = -\frac{N}{2}\log(2\pi) - N\log\sigma$$
$$-\frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - f_{\theta}(x_i))^2$$

- Approximating  $f_{\theta}$  by maximum likelihood estimation (MLE)
- Assume an independently drawn random sample  $y_i$ , i = 1, ..., N from a probability density  $Pr_{\theta}(y)$ .
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• Least squares with additive error model

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$$L(\theta) = -\frac{N}{2}\log(2\pi) - N\log\sigma$$

Proportional to RSS

$$-\frac{1}{2\sigma^2} \sum_{i=1}^{N} (y_i - f_{\theta}(x_i))^2$$

# Overview of Supervised Learning II

--- Bayesian Methods and Roughness Penalty

#### **Bayesian Methods and Roughness Penalty**

- Bayesian methods
- Formula for joint probabilities

$$Pr(X,Y) = Pr(Y|X) Pr(X)$$
$$= Pr(X|Y) Pr(Y)$$

Bayes's theorem

Likelihood Prior probability for Y  $Pr(Y|X) = \frac{Pr(X|Y) Pr(Y)}{Pr(X)}$ Posterior probability for Y
Evidence

• RSS is penalized with a roughness penalty

$$PRSS(f; \lambda) = RSS(f) + \lambda J(f)$$

- J(f) is large for ragged functions
  - E.g. cubic smoothing spline is the solution for the least-squares problem

$$PRSS(f; \lambda) = \sum_{i=1}^{N} (y_i - f(x_i))^2 + \lambda \int [f''(x)]^2 dx$$

Large second derivative is penalized

Posterior ∝ Likelihood × Prior

## **Bayesian Methods and Roughness Penalty**

- Introducing penalty functions is a type of regularization
  - It works against overfitting
  - It implements beliefs about unseen parts of the problem
- In a Bayesian framework
  - Penalty *J* is the log-prior (probability distribution)
  - PRSS is the log-posterior (probability distribution)

- RSS is penalized with a roughness penalty  $PRSS(f; \lambda) = RSS(f) + \lambda J(f)$
- J(f) is large for ragged functions
  - E.g. cubic smoothing spline is the solution for the least-squares problem

$$PRSS(f; \lambda) = \sum_{i=1}^{N} (y_i - f(x_i))^2 + \lambda \int [f''(x)]^2 dx$$

Large second derivative is penalized

# Overview of Supervised Learning II

--- Model Selection

#### **Model Selection**

- Smoothing and complexity parameters
  - Coefficient of the penalty term
  - Width of the kernel
  - Number of basis functions
- The setting of the parameters implements a trade-off between bias and variance
- Example: k-NN methods  $Y = f(X) + \varepsilon$   $E(\varepsilon) = 0$   $Var(\varepsilon) = \sigma^{2}$

• Generalization error

$$\begin{aligned} \text{EPE}_k(x_0) &= \text{E}[Y - \hat{f}_k(x_0) | X = x_0] \\ &= \sigma^2 + \left[ \text{Bias}^2(\hat{f}_k(x_0)) + \text{Var}_{\mathcal{T}}(\hat{f}_k(x_0)) \right] \\ &= \sigma^2 + \left[ f(x_0) - \frac{1}{k} \sum_{\ell=1}^k f(x_{(\ell)}) \right]^2 + \frac{\sigma^2}{k} \end{aligned}$$

#### irreducible error

#### mean-square error

