Introduction to Machine Learning CS182

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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

Statistical Decision Theory

- Given:
  - random input vector $X \in \mathbb{R}^p$,
  - random output variable $Y \in \mathbb{R}$,
  - 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)*:

$$\mathrm{EPE}(f) = \mathrm{E}(Y - f(X))^2$$

$$= \int (y - f(x))^2 \Pr(dx, dy).$$

- Since $\Pr(X, Y) = \Pr(Y|X)\Pr(X)$, EPE can also be written as

$$\mathrm{EPE}(f) = \mathrm{E}_X \mathrm{E}_{Y|X}([Y - f(X)]^2|X).$$

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

$$f(x) = \mathrm{argmin}_c \, \mathrm{E}_{Y|X}([Y - c]^2|X = x)$$

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

Statistical Decision Theory

- 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.

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

Statistical Decision Theory

- Linear regression assumes that the regression function is approximately linear

$$f(x) \approx x^T\beta.$$

- This is a model-based approach.
- Plugging this $f(x)$ into EPE,

$$\mathrm{EPE}(f) = E(Y - f(X))^2$$

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

- Differentiating w.r.t. β, leads to

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

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

$$\mathrm{RSS}(\beta) = \sum_{i=1}^{N}(y_i - x_i^T\beta)^2$$

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Summary – approximation of $f(X)$

- Least squares: globally linear function
- Nearest neighbors: locally constant function.

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

Statistical Decision Theory

- What happens if we use absolute loss function?

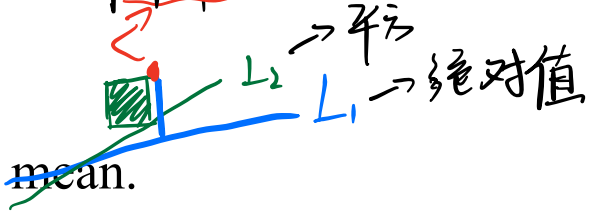
$$L_1(Y, f(X)) = |Y - f(X)|$$

- In this case,

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

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

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



Statistical Decision Theory

- Procedure for categorical output variable G with values from $\mathcal{G}$.
- Loss function is $K \times K$ matrix $\mathbf{L}$, 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 $\mathcal{G}_l$
  - $\mathbf{L}$ is zero on the diagonal
- Instead, we often use the zero-one loss function

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

where $\delta_{kl} = 1$ if $k = l$, otherwise $\delta_{kl} = 0$

分类正确是1
否则为0

- Expected prediction error (EPE)

$$\text{EPE} = \text{E}[L(G, \hat{G}(X))]$$

where expectation taken w.r.t. $\Pr(G, X)$

- Conditioning on X yields

$$\text{EPE} = \text{E}_X \sum_{k=1}^{K} L[\mathcal{G}_k, \hat{G}(X)] \Pr(\mathcal{G}_k | X)$$

- Again, it suffices to pointwise minimization

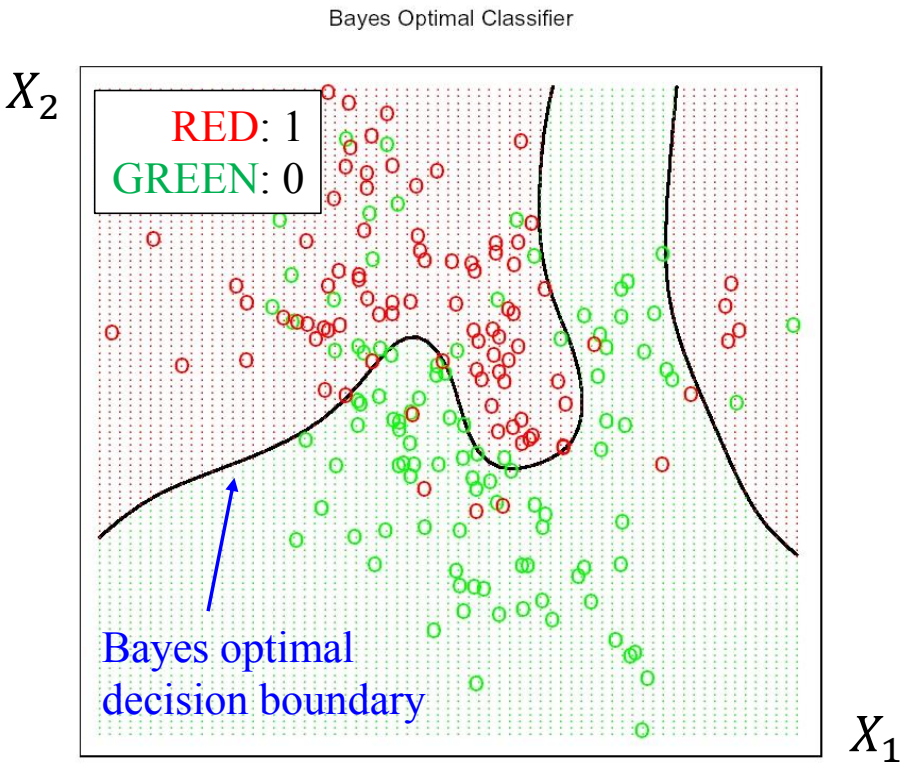
$$\hat{G}(x) = \text{argmin}_{g \in \text{G}} \sum_{k=1}^{K} L(\mathcal{G}_k, g) \Pr(\mathcal{G}_k | X = x)$$

- Or simply

$$\hat{G}(x) = \underset{g \in \text{G}}{\text{argmax}} \Pr(g | X = x)$$

Bayes classifier

Statistical Decision Theory



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

- Expected prediction error (EPE)

$$\text{EPE} = \text{E}[L(G, \hat{G}(X))]$$

where expectation taken w.r.t. $\Pr(G, X)$

- Conditioning on X yields

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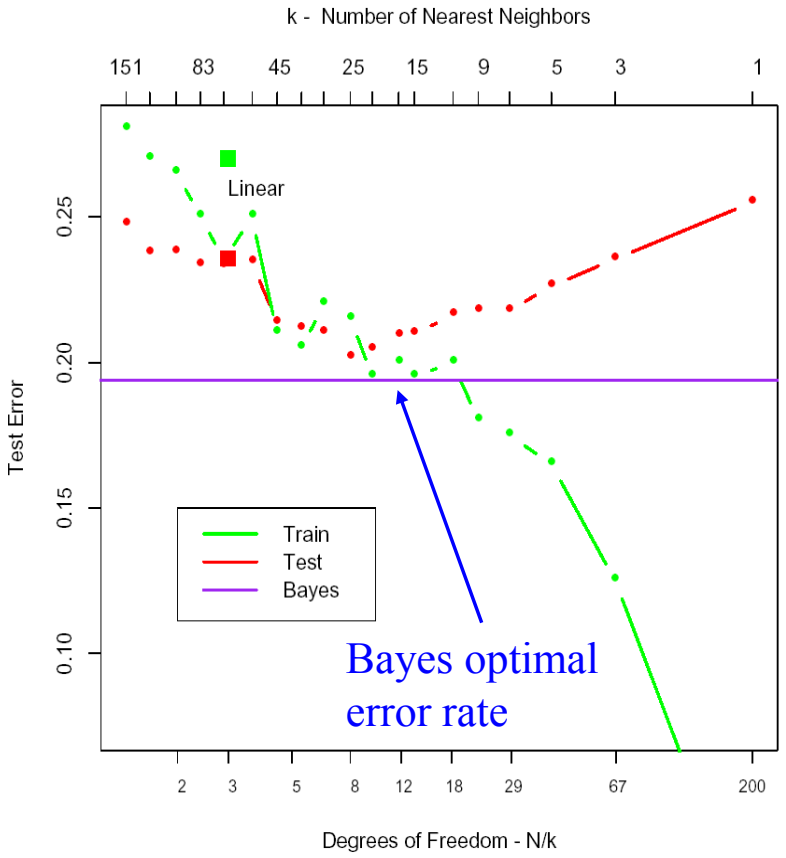
Statistical Decision Theory



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

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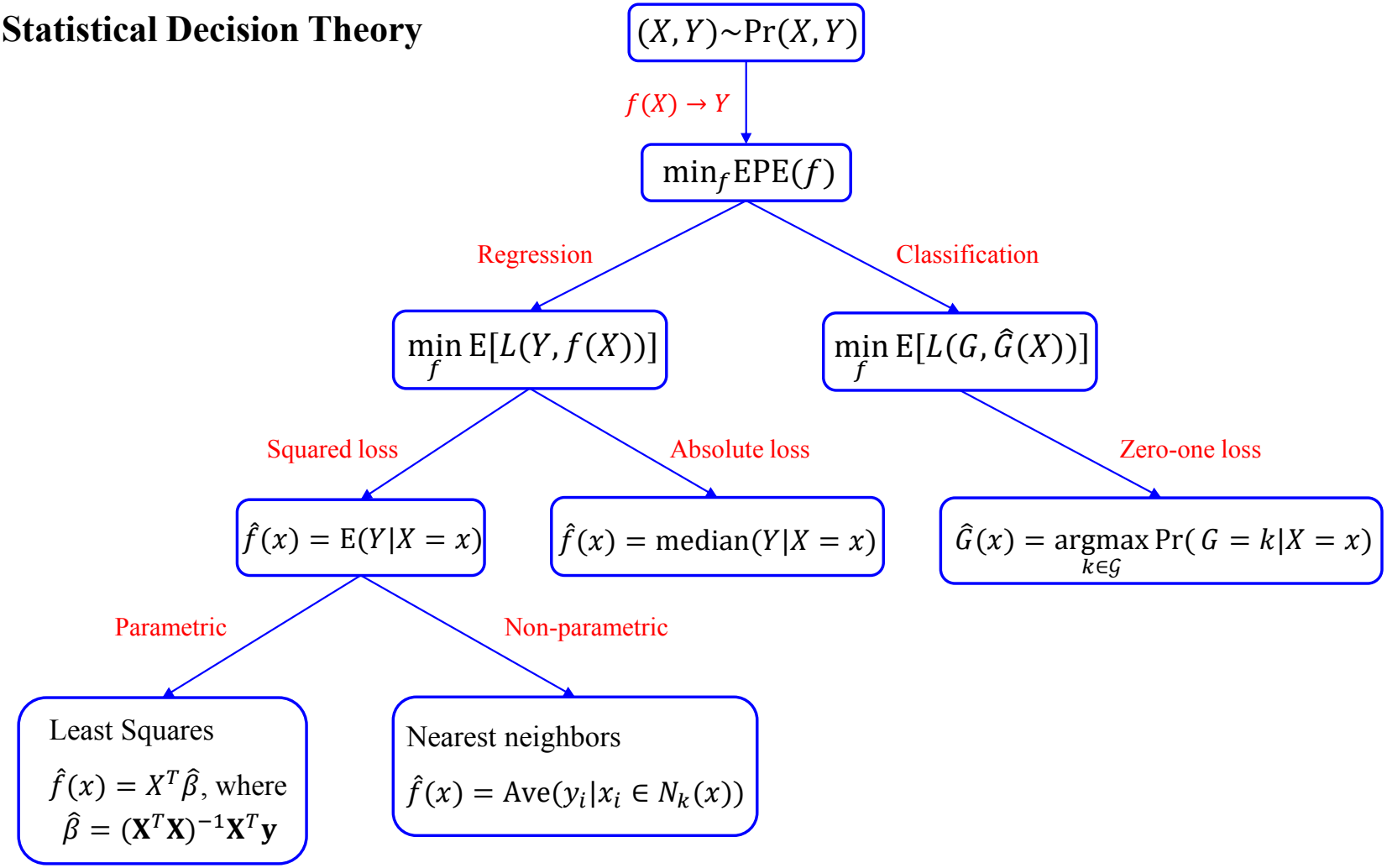
Bayes classifier

Statistical Decision Theory



Overview of Supervised Learning II

--- Local Methods in High Dimensions

$f(x)$：真实值 $Y = f(x) + \varepsilon$

y：观测值（引入噪声）

$\hat{y}$：预测值

EPE：y 与 $\hat{y}$ 之间的差异：$L(y, \hat{y})$

MSE：$(\hat{y} - f(x))^2$

RSS：残差平方和

loss function：一种损失函数

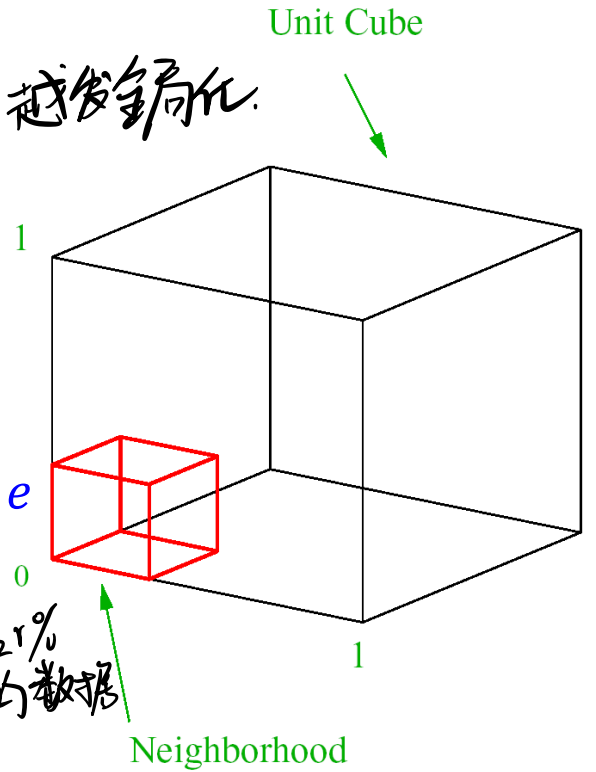
Local Models in High Dimensions

- Curse of Dimensionality: 随维数个邻域会越发全局化.
  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

  找一个小立方体覆盖r%的数据

  - edge length: $e_p(r) = r^{\frac{1}{p}}$ (小立方体邻域的边长)
  - $e_{10}(0.01) = 0.63$
  - $e_{10}(0.1) = 0.80$

  $e_1(0.01) = 0.01$

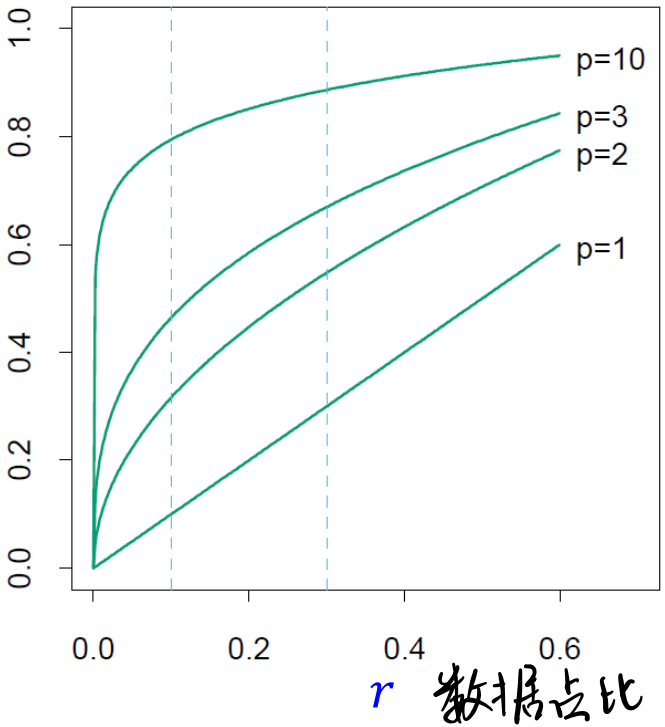


$$\frac{e^p}{1} = r$$

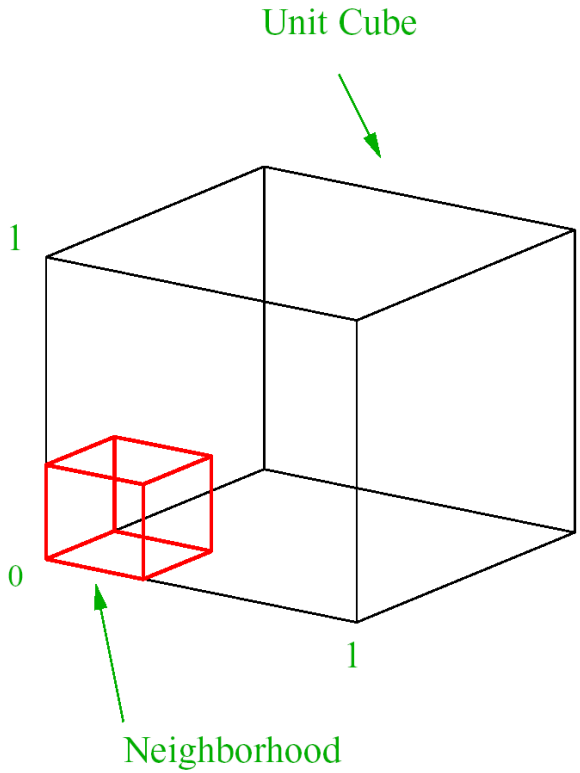
In ten dimensions we need to cover 63% (80%) of the range of each coordinate to capture 1% (10%) of the data.

$e_2(0.01) = 0.1$

Local Models in High Dimensions



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.

Local Models in High Dimensions

- In high dimensions, all sample points are close to the edge of the sample space
- 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) $(1 - r^p)^N = \frac{1}{2}$

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

Local Models in High Dimensions

- 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

采样密度指数增加.

- 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.

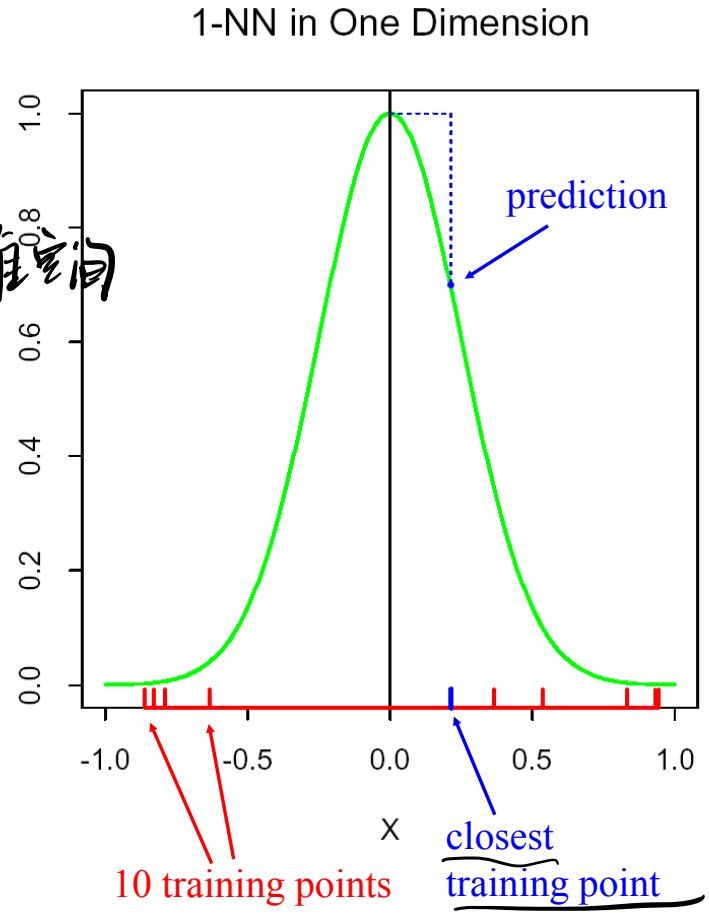
Local Models in High Dimensions

- Another example
- $\mathcal{T}$: set of training points x_i generated uniformly in $[-1,1]^p$ (red) 训练集合服从于[-1,1]的p维空间
- Functional relationship between X and Y (green) label 符合下面方程

$$Y = f(X) = e^{-8\|X\|^2}$$ (无观测误差)

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

使用KNN估计
↳ k=1: 1NN



Local Models in High Dimensions

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

期望

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

均方误差

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

(经过一定的分解)

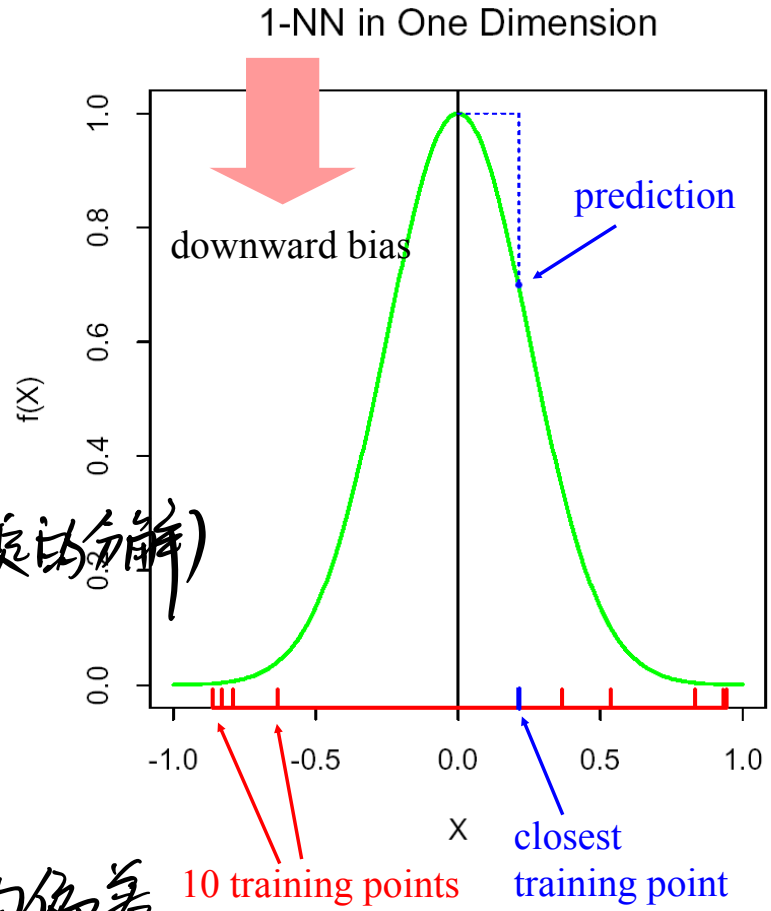
对点误差的估计

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

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

方差　　偏差的平方

描述波动情况　　期望与真实值的偏差



Local Models in High Dimensions

$$\begin{aligned}
\mathrm{MSE}(x_0) &= E_{\mathcal{T}}[f(x_0) - \hat{y}_0]^2 \\
&= E_{\mathcal{T}}[\hat{y}_0 - E_{\mathcal{T}}(\hat{y}_0) + E_{\mathcal{T}}(\hat{y}_0) - f(x_0)]^2 \\
&= E_{\mathcal{T}}\left[(\hat{y}_0 - E_{\mathcal{T}}(\hat{y}_0))^2 + 2(\hat{y}_0 - E_{\mathcal{T}}(\hat{y}_0))(E_{\mathcal{T}}(\hat{y}_0) - f(x_0)) + (E_{\mathcal{T}}(\hat{y}_0) - f(x_0))^2\right] \\
&= E_{\mathcal{T}}\left[(\hat{y}_0 - E_{\mathcal{T}}(\hat{y}_0))^2\right] + (E_{\mathcal{T}}(\hat{y}_0) - f(x_0))^2 \\
&= \mathrm{Var}_{\mathcal{T}}(\hat{y}_0) + \mathrm{Bias}^2(\hat{y}_0)
\end{aligned}$$

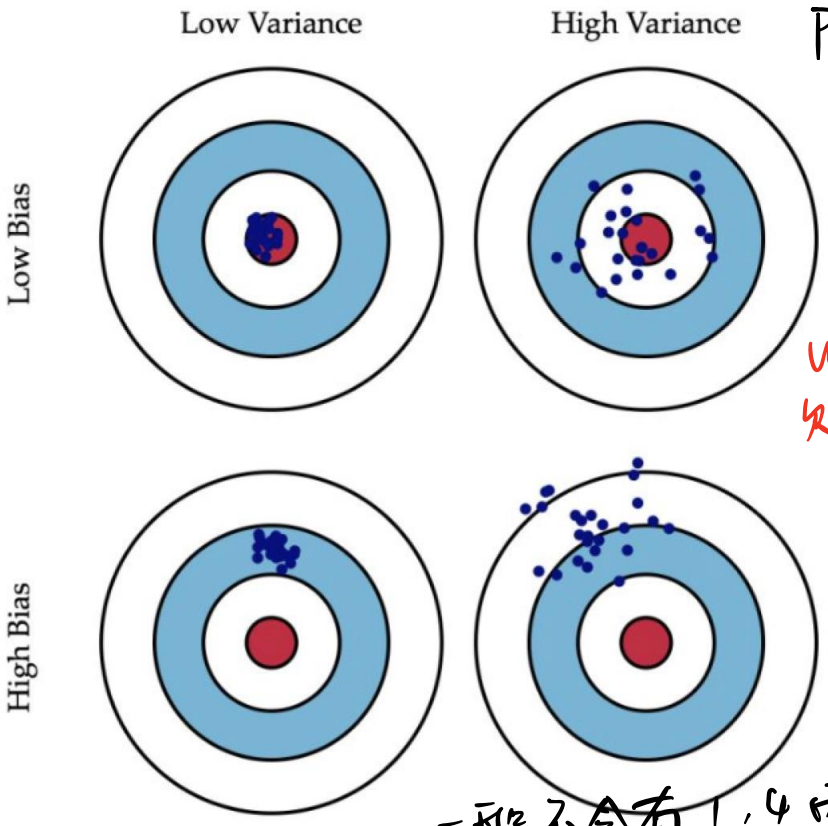
$E_{\mathcal{T}}(\hat{y}_0 - E_{\mathcal{T}}(\hat{y}_0))(E_{\mathcal{T}}(\hat{y}_0) - f(x_0)) = 0$

Constant

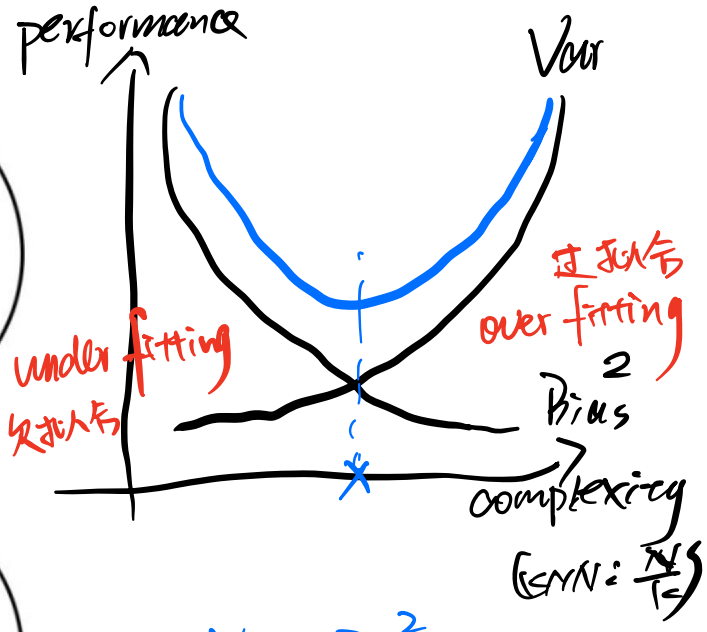
ground-truth.

This is known as the bias-variance decomposition.

Local Models in High Dimensions



KNN为例：



$MSE = Var + Bias^2$

为避免欠/过拟合，要有验证集.

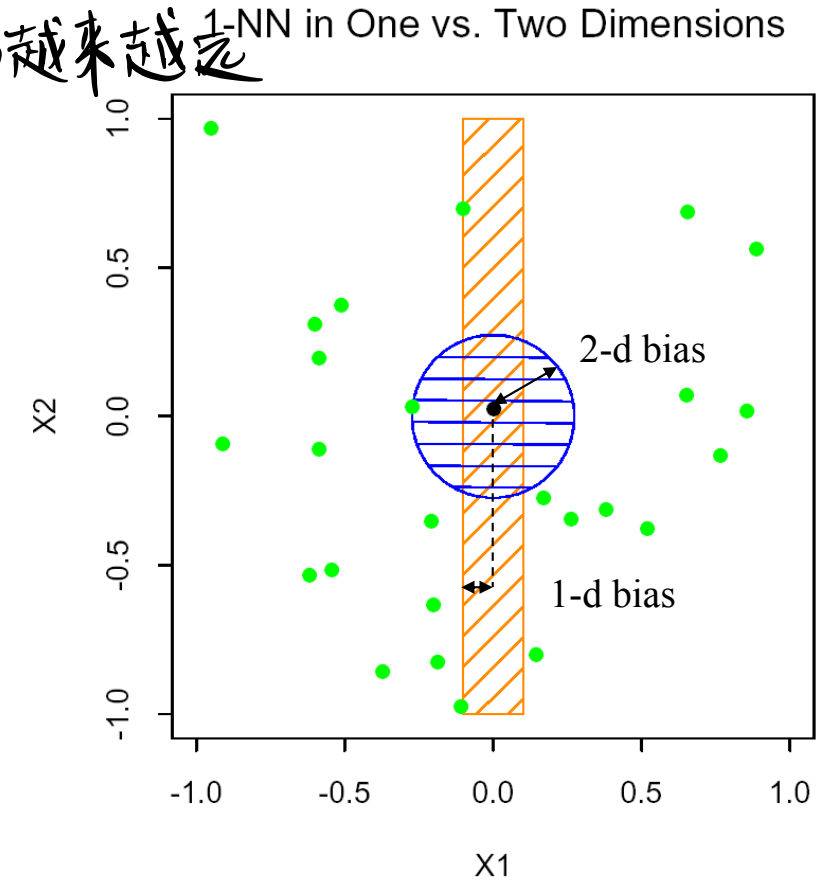
一般不会有1，4两种情况

The bias-variance decomposition: $\mathrm{MSE}(x_0) = \mathrm{Var}_{\mathcal{T}}(\hat{y}_0) + \mathrm{Bias}^2(\hat{y}_0)$

Local Models in High Dimensions

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

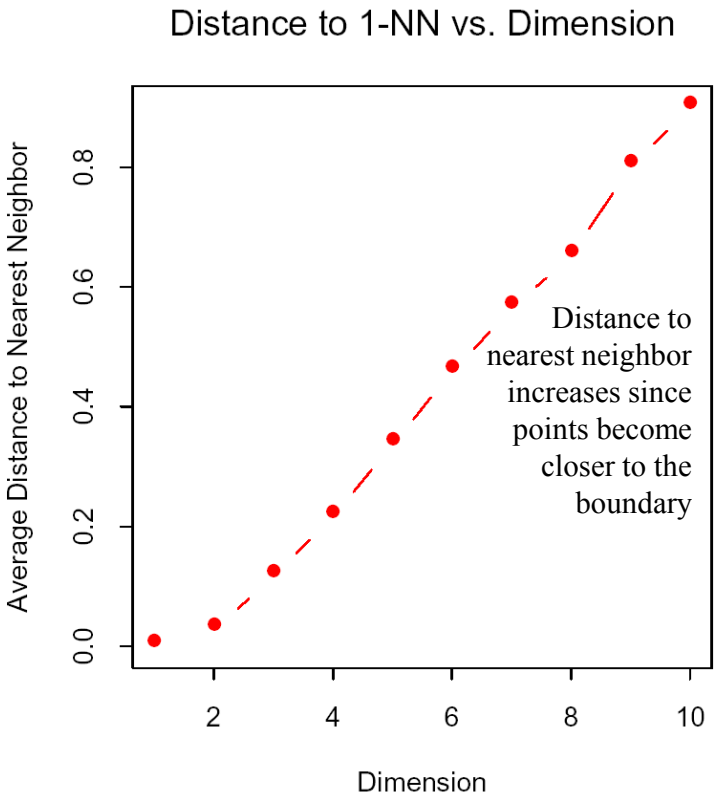
$$\begin{aligned}\mathrm{MSE}(x_0) &= \mathrm{E}_{\mathcal{T}}[f(x_0) - \hat{y}_0]^2 \\ &= \mathrm{E}_{\mathcal{T}}[\hat{y}_0 - \mathrm{E}_{\mathcal{T}}(\hat{y}_0)]^2 \\ &\quad + [\mathrm{E}_{\mathcal{T}}(\hat{y}_0) - f(x_0)]^2 \\ &= \mathrm{Var}_{\mathcal{T}}(\hat{y}_0) + \mathrm{Bias}^2(\hat{y}_0)\end{aligned}$$

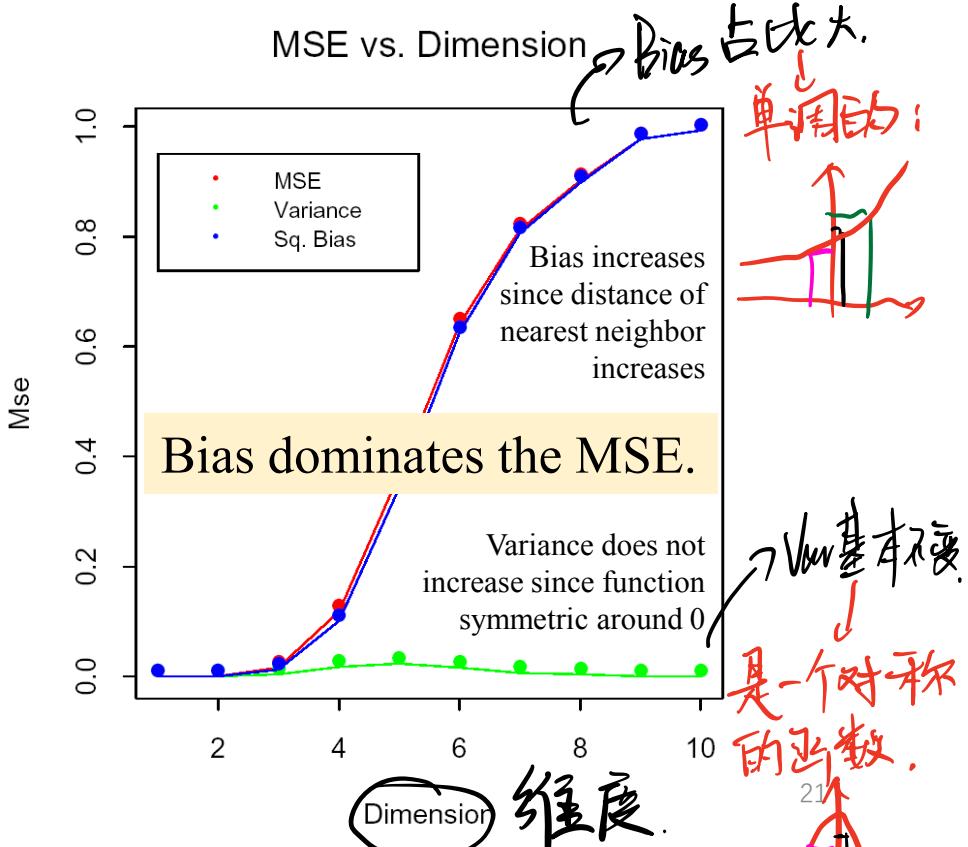


Local Models in High Dimensions

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

- The case on N=1000 training points

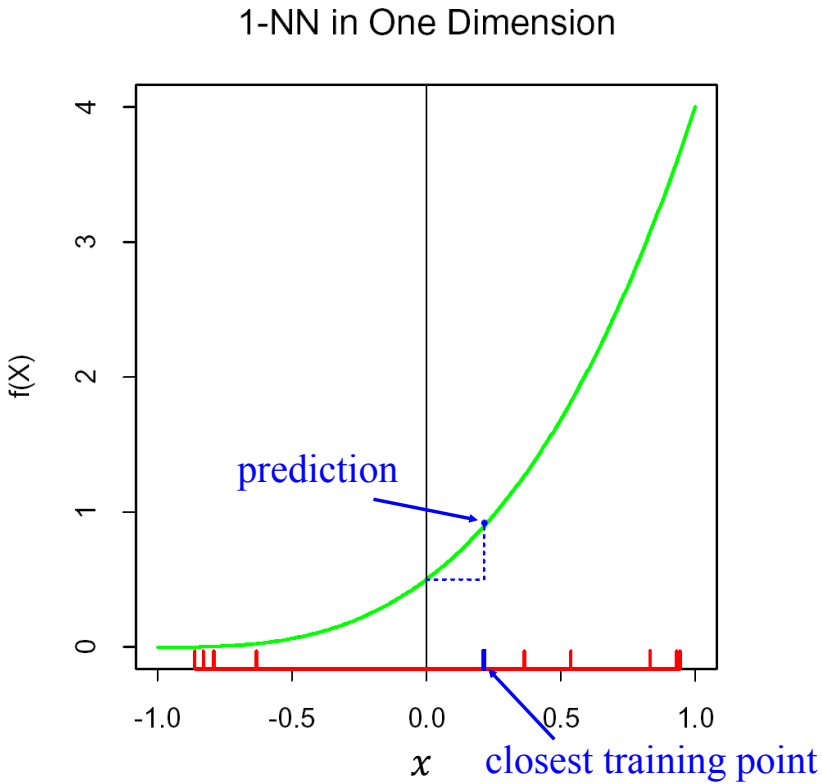


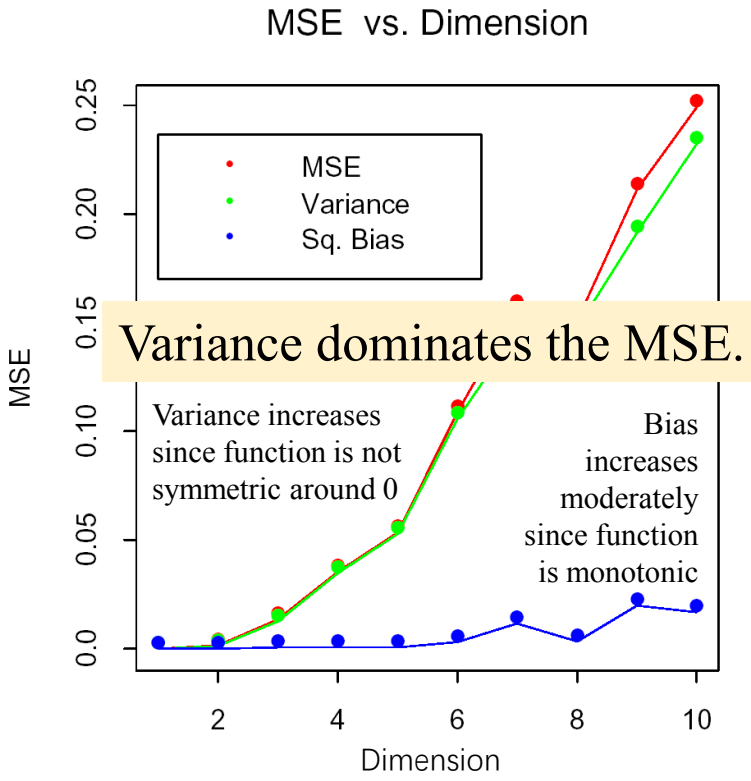


Local Models in High Dimensions

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

- Yet another example





无noise：deterministic 确定的

有noise：non-deterministic

Local Models in High Dimensions

使用参数模型（KNN是非参）

- Suppose a linear relationship with measurement error

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

高斯分布噪声

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

最小二乘法

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

不可控

  - Additional variance σ^2 originates from the nondeterministic part
  - Variance depends on x_0
  - No bias

↳ Var.

由于是线性模型，真实也为线性，故 Bias = 0

- If N is large, we get

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

当 $\frac{\sigma^2}{N}$ 很小（N在分母上）则无需在意维度（影响不大）

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

Local Models in High Dimensions

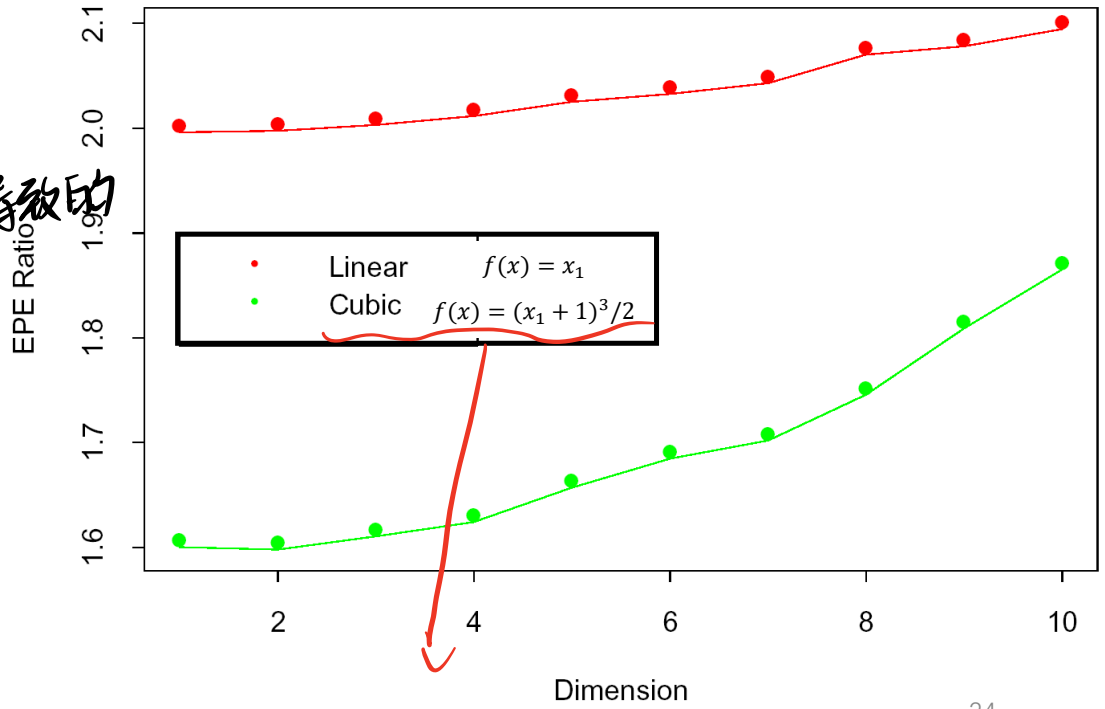
- More generally

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

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

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



故 EPE ratio会降低，
但在高维依然优于KNN

Local Models in High Dimensions

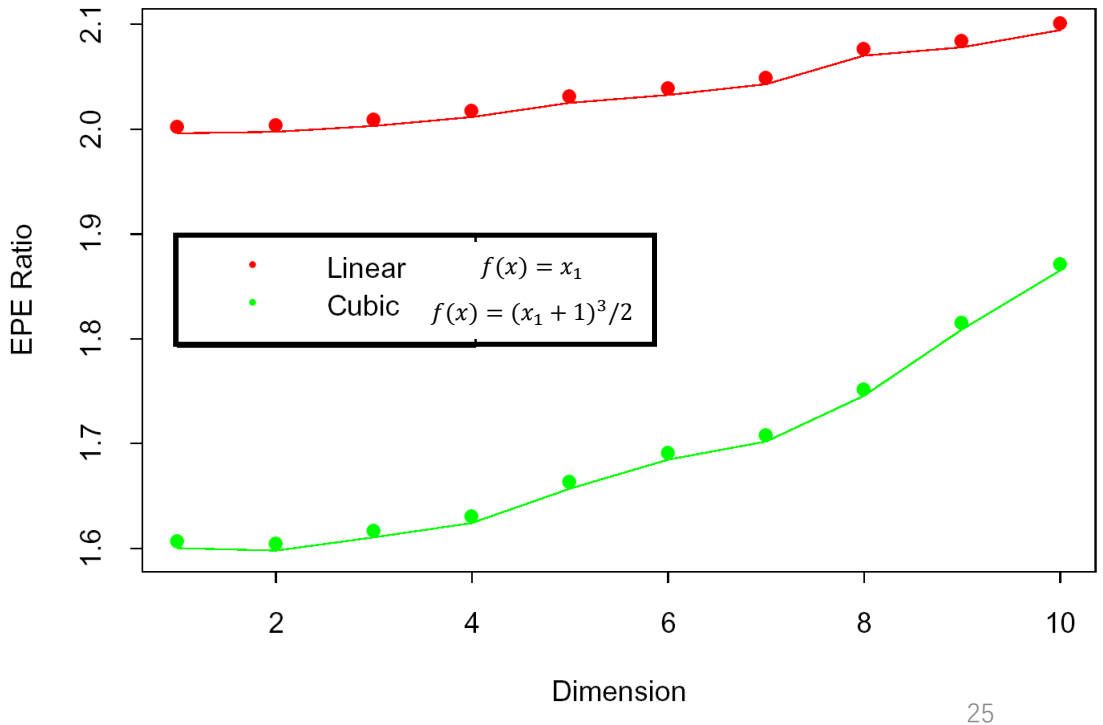
- More generally

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

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

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

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



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

$$\begin{aligned}\mathrm{EPE}(x_0) &= \mathrm{MSE}(x_0) \\ &= \mathrm{Var}_{\mathcal{T}}(\hat{y}_0) + \mathrm{Bias}^2(\hat{y}_0)\end{aligned}$$

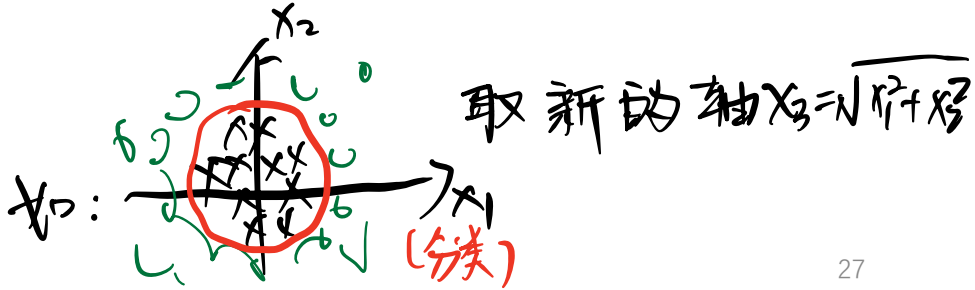
  2. Non-deterministic case

$$\begin{aligned}\mathrm{EPE}(x_0) &= \mathrm{MSE}(x_0) + \sigma^2 \\ &= \mathrm{Var}_{\mathcal{T}}(\hat{y}_0) + \mathrm{Bias}^2(\hat{y}_0) + \sigma^2\end{aligned}$$

- Least squares
  - Linear case: non-biased, negligible variance for large N
  - Non-linear case: biased
- Nearest neighbors
  - Symmetric on x_0: $\mathrm{Bias}^2(\hat{y}_0)$ dominates
  - Monotonic on x_0: $\mathrm{Var}_{\mathcal{T}}(\hat{y}_0)$ dominates

Overview of Supervised Learning II

--- Statistical Models



Statistical Models – Function Approximation

- Data: pairs (x_i, y_i) that are points in $(p+1)$-dimensional Euclidean space, we fit $f: \mathbb{R}^p \to \mathbb{R}$ by

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

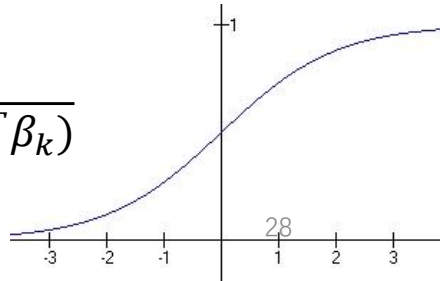
- Goal: a good approximation of $f(x)$ in some region of input space, given the training set $\mathcal{T}$
- Many models have certain parameters θ
  - E.g. for the linear model $f(x) = x^T\beta$ and $\theta = \beta$

- 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:

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



Statistical Models – Function Approximation

- Approximating f_θ by minimizing the residual sum of squares

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

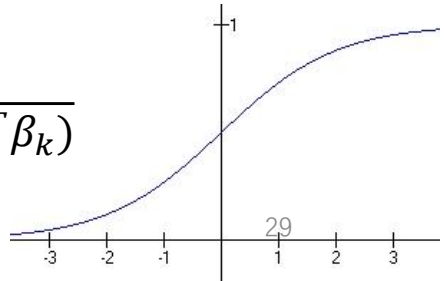
利用RSS取找拟合的θ

- 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:

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

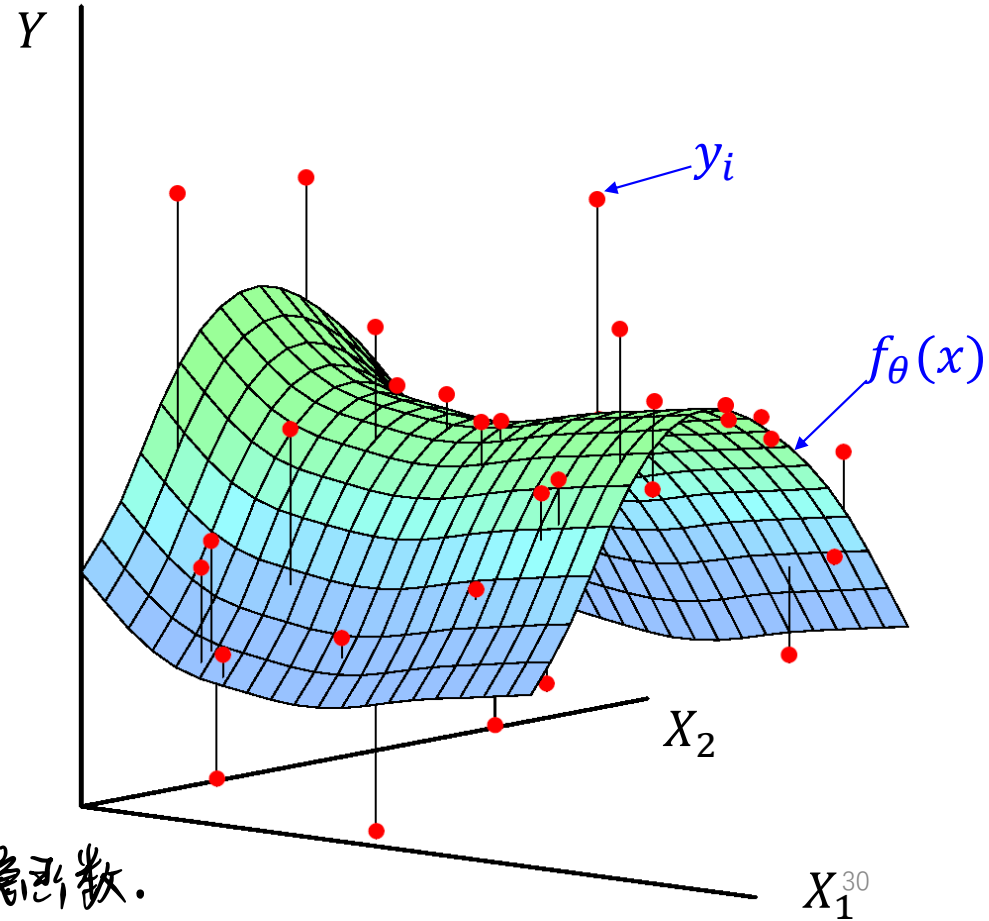


Statistical Models – Function Approximation

- Approximating f_θ by minimizing the residual sum of squares

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

- 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



但基函数大多都有隐函数.

Statistical Models – Function Approximation

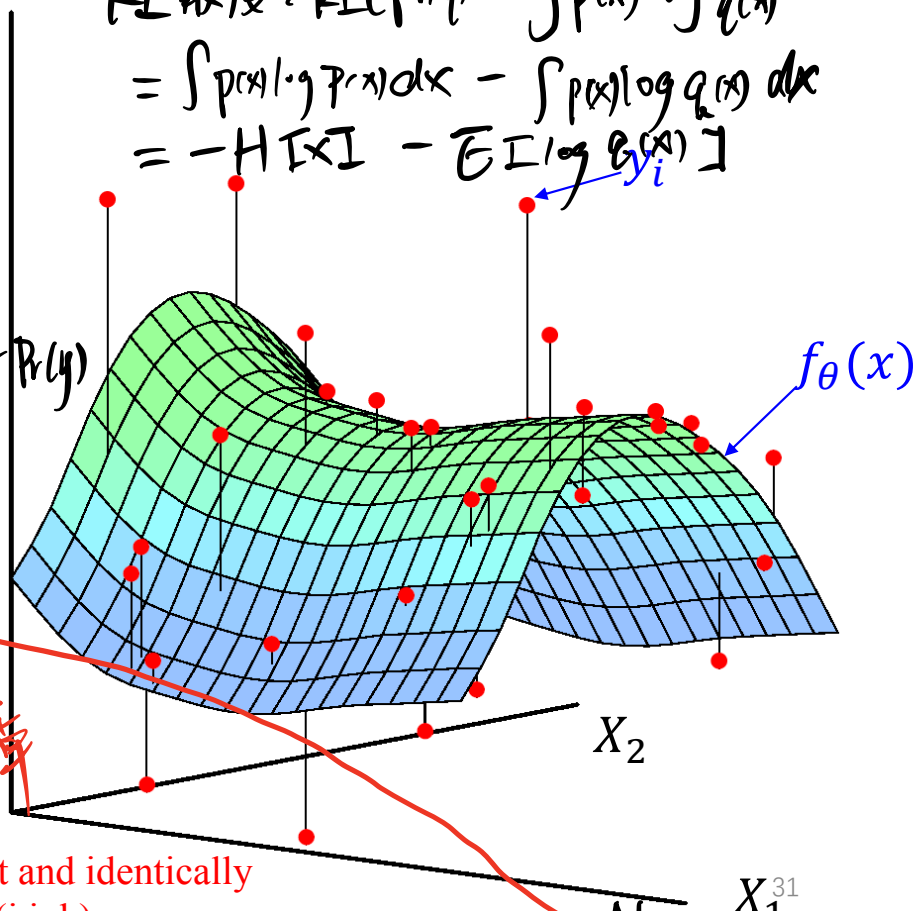
- Approximating f_θ by maximum likelihood estimation (MLE)
- Assume an independently drawn random sample $y_i, i = 1, \ldots, N$ from a probability density $\Pr_\theta(y)$.
- The log-probability of observing the sample is

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

$$\ell(\theta) = \log \Pr_\theta(y_1, y_2, \ldots, y_N)$$

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

independent and identically distributed (i.i.d.)



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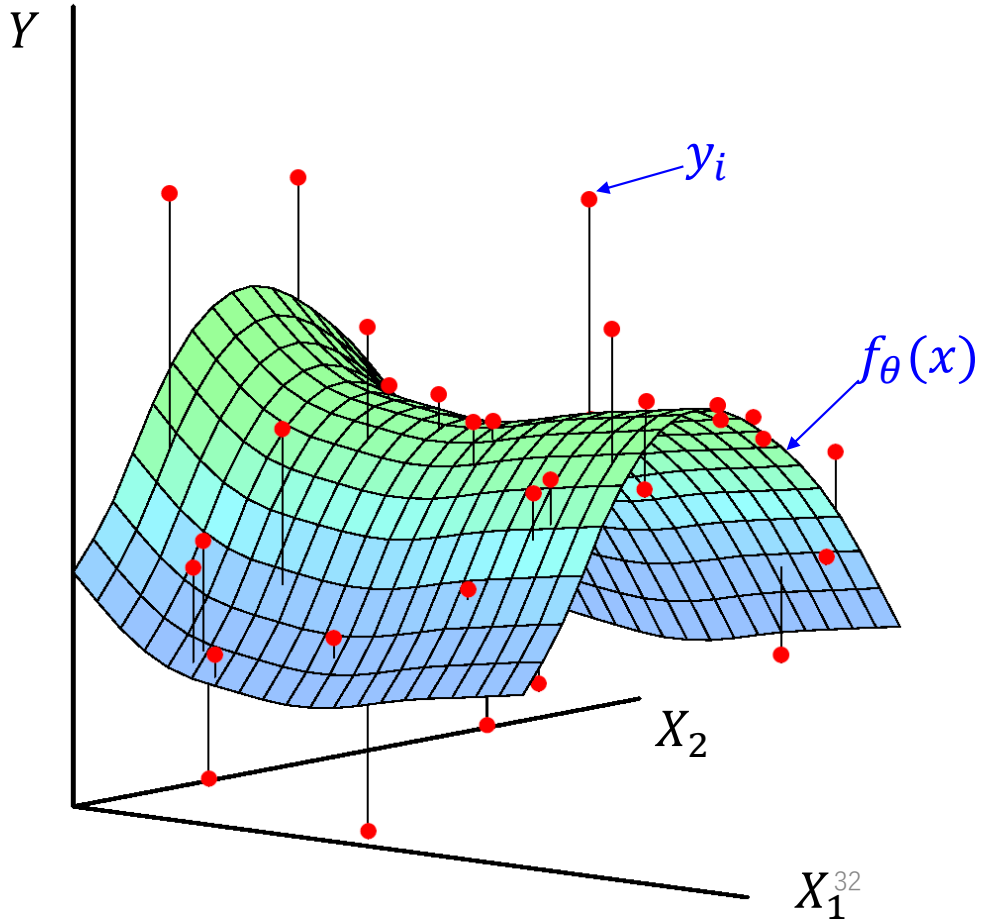
- Set θ to maximize $L(\theta)$

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



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- Set θ to maximize $L(\theta)$

- 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

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

给定X时Y的分布也是高斯分布

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

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

与θ无关，可去掉

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

与θ无关

因为是训练θ，所以可直接去掉P(xi)

训练数据集：T，则 $L(\theta|T) = \sum_{i=1}^{N} \log P(x_i, y_i) = \sum_{i=1}^{N} \log P_\theta(y_i|x_i)P(x_i) = \sum_{i=1}^{N} \log P_\theta(y_i|x_i)$

Statistical Models – Function Approximation

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Proportional to RSS

$$\operatorname{argmax}_\theta \ell(\theta) = \operatorname{argmin}_\theta \mathrm{RSS}(\theta) = \operatorname{argmin}_\theta \sum_{i=1}^{N}(y_i - f_\theta(x_i))^2$$

Overview of Supervised Learning II

--- Bayesian Methods and Roughness Penalty

Bayesian Methods and Roughness Penalty

- Bayesian methods
- Formula for joint probabilities

$$\Pr(A, B) = \Pr(B|A)\Pr(A)$$
$$= \Pr(A|B)\Pr(B)$$

- Bayes's theorem

Likelihood　　Prior probability for B

$$\Pr(B|A) = \frac{\Pr(A|B)\Pr(B)}{\Pr(A)}$$

Posterior probability for B　　Evidence

$$\text{Posterior} \propto \text{Likelihood} \times \text{Prior}$$

- RSS is penalized with a roughness penalty

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

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

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

  - Large second derivative is penalized

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)

对于过拟合的一次修正

$$\text{Posterior} \propto \text{Likelihood} \times \text{Prior}$$

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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

$$Y = f(X) + \varepsilon$$
$$\mathrm{E}(\varepsilon) = 0$$
$$\mathrm{Var}(\varepsilon) = \sigma^2$$

- Generalization error

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

irreducible error

mean-square error