中国科学院大学人工智能学院硕士课《模式识别》

第4章：非参数方法

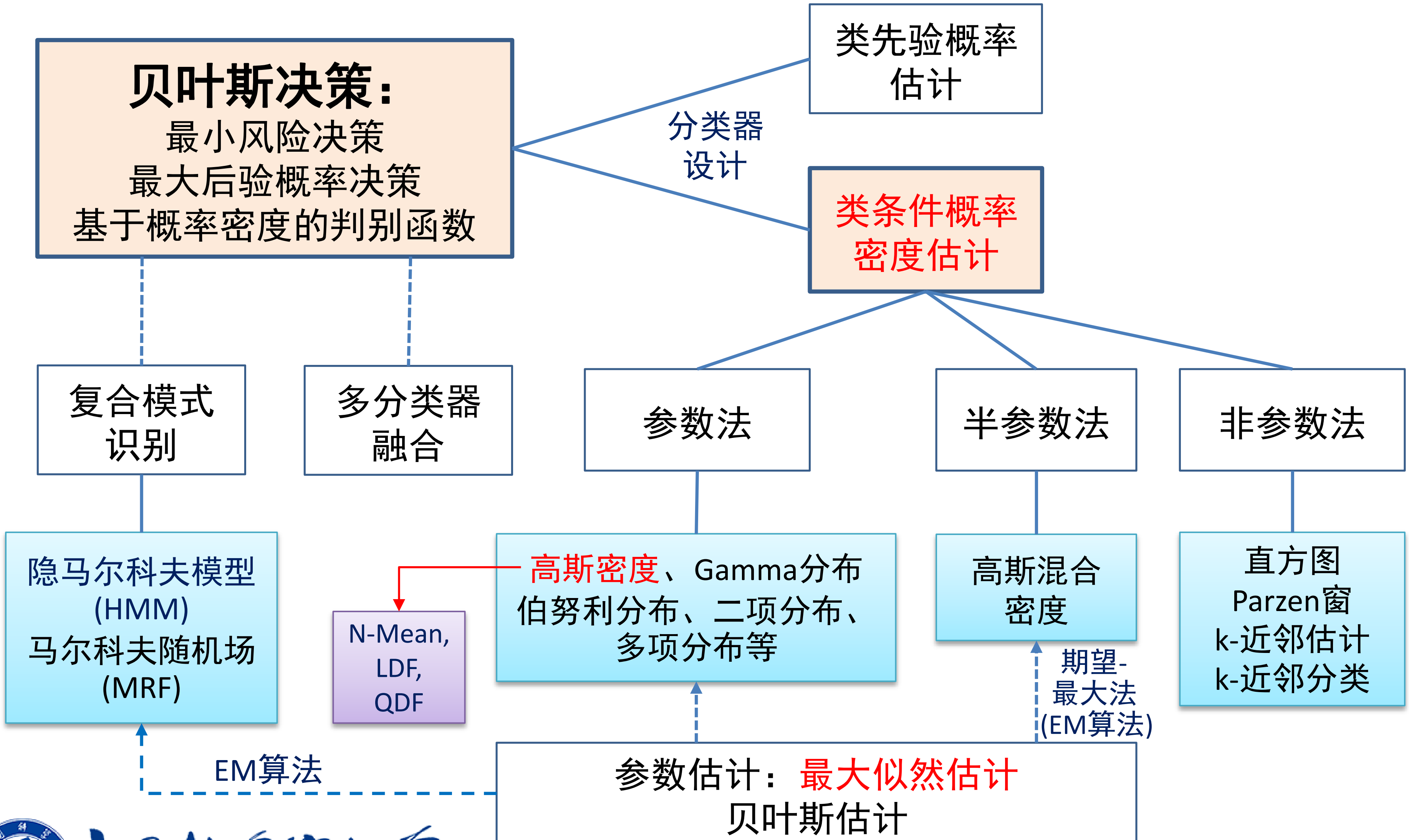
刘成林(liucl@nlpr.ia.ac.cn)

2019年10月9日

助教：王铁强(tieqiang.wang@nlpr.ia.ac.cn)
陈卓(zhuo.chen@nlpr.ia.ac.cn)
吴金文(jinwen.wu@nlpr.ia.ac.cn)

中国科学院大学
University of Chinese Academy of Sciences

基于贝叶斯决策的模式分类框架



上次课主要内容回顾

- 特征维数与过拟合
  - 增加特征带来更多判别信息
  - 克服过拟合的方法？
- 期望最大法(EM)
  - 对数似然度对缺失数据的期望
  - EM for Gaussian mixture
- 隐马尔可夫模型(HMM)
  - Three basic problems
  - Viterbi Algorithm (DP)
  - Extensions

提纲

- 第4章 非参数方法
  - 密度估计
  - Parzen窗方法
  - K近邻估计
  - 最近邻规则
  - 距离度量
  - Reduced Coulomb Energy Network
  - Approximation by Series Expansion

密度估计

- 概率和密度
  - 概率：特征空间中一定区域内样本的比率

$$P = \int_{\mathcal{R}} p(\mathbf{x}')\, d\mathbf{x}'$$

  - 假设局部区域（体积为V，样本数k）内等概率密度

$$\int_{\mathcal{R}} p(\mathbf{x}')\, d\mathbf{x}' \simeq p(\mathbf{x})V \qquad p(\mathbf{x}) \simeq \frac{k/n}{V}$$

  - 如何决定局部区域的大小：随样本数*n*变化
  - $p_n(\mathbf{x})$收敛到$p(\mathbf{x})$的条件

$$\lim_{n\to\infty} V_n = 0$$

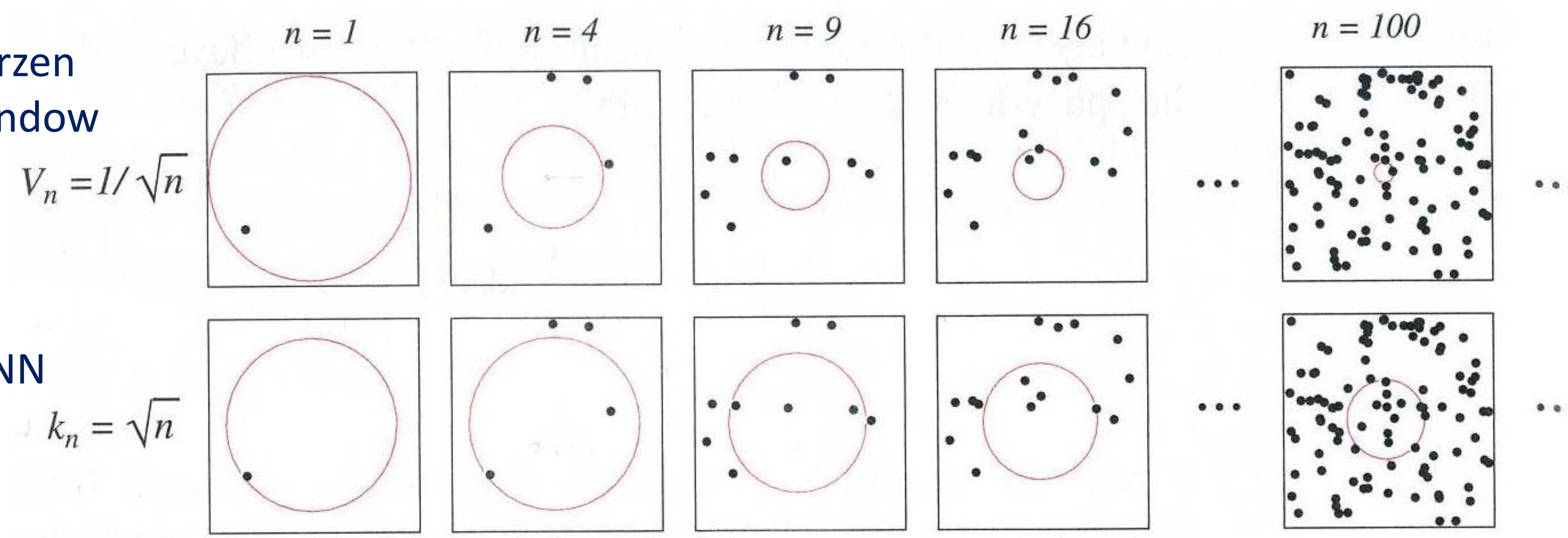
$$\lim_{n\to\infty} k_n = \infty$$

$$\lim_{n\to\infty} k_n/n = 0$$

- 非参数概率密度估计
  - Parzen window: 固定局部区域体积*V*，*k*变化
  - k-nearest neighbor: 固定局部样本数*k*，*V*变化

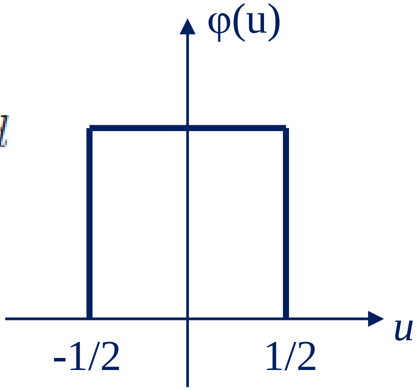
Parzen window

k-NN



Parzen Window

- 窗函数：hypercube



$$\varphi(\mathbf{u}) = \begin{cases} 1 & |u_j| \le 1/2 \qquad j = 1, ..., d \\ 0 & \text{otherwise.} \end{cases}$$

  – 满足条件

$$\varphi(\mathbf{x}) \ge 0 \qquad \int \varphi(\mathbf{u})\, d\mathbf{u} = 1$$

  – 以x为中心、体积为 $V_n = h_n^d$ 的局部区域内样本数

$$k_n = \sum_{i=1}^{n} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right)$$

  – 概率密度估计k_n/nV_n

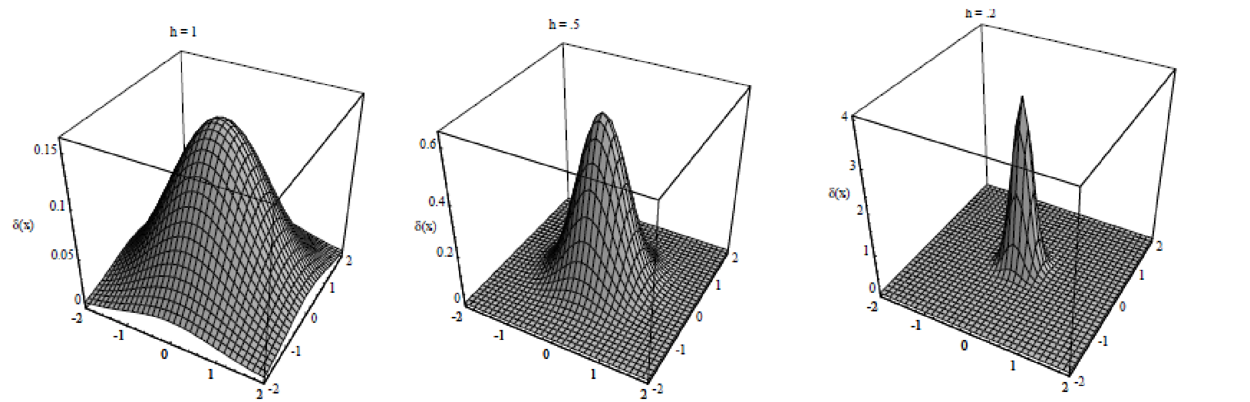
$$p_n(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{V_n} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right)$$

- 推广：满足密度函数要求的窗函数，如高斯函数

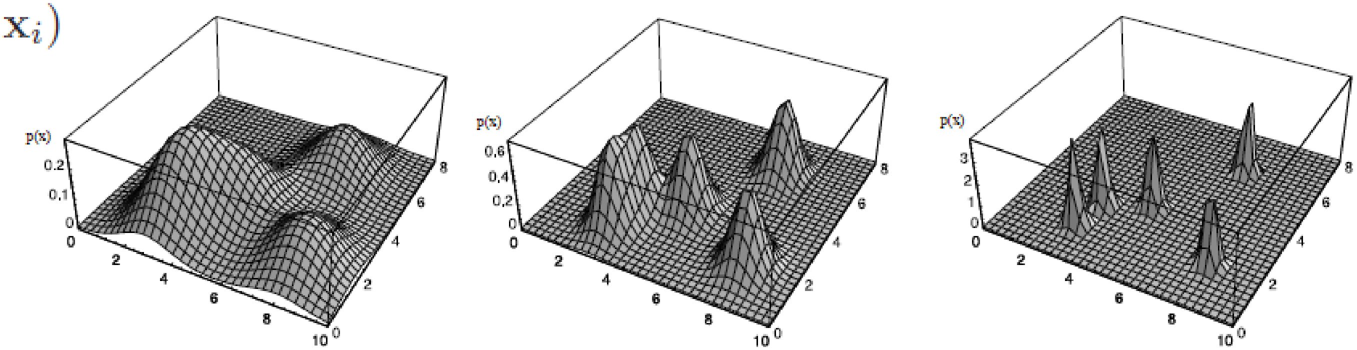
$$\varphi(\mathbf{x}) \ge 0 \qquad \int \varphi(\mathbf{u})\, d\mathbf{u} = 1$$

Gaussian window, variable width (*h*=1, 0.5, 0.2)

$$\delta_n(\mathbf{x}) = \frac{1}{V_n}\varphi\left(\frac{\mathbf{x}}{h_n}\right)$$



$$p_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\delta_n(\mathbf{x}-\mathbf{x}_i)$$



Large *h*: low variability, under fitting

Small *h*: high variability, overfitting

- Parzen窗密度估计的收敛性
  - $p_n(\mathbf{x})$的期望是$p(\mathbf{x})$的平滑（卷积）
    - Samples $\mathbf{x}_1,\ldots,\mathbf{x}_n$ are i.i.d from $p(\mathbf{x})$

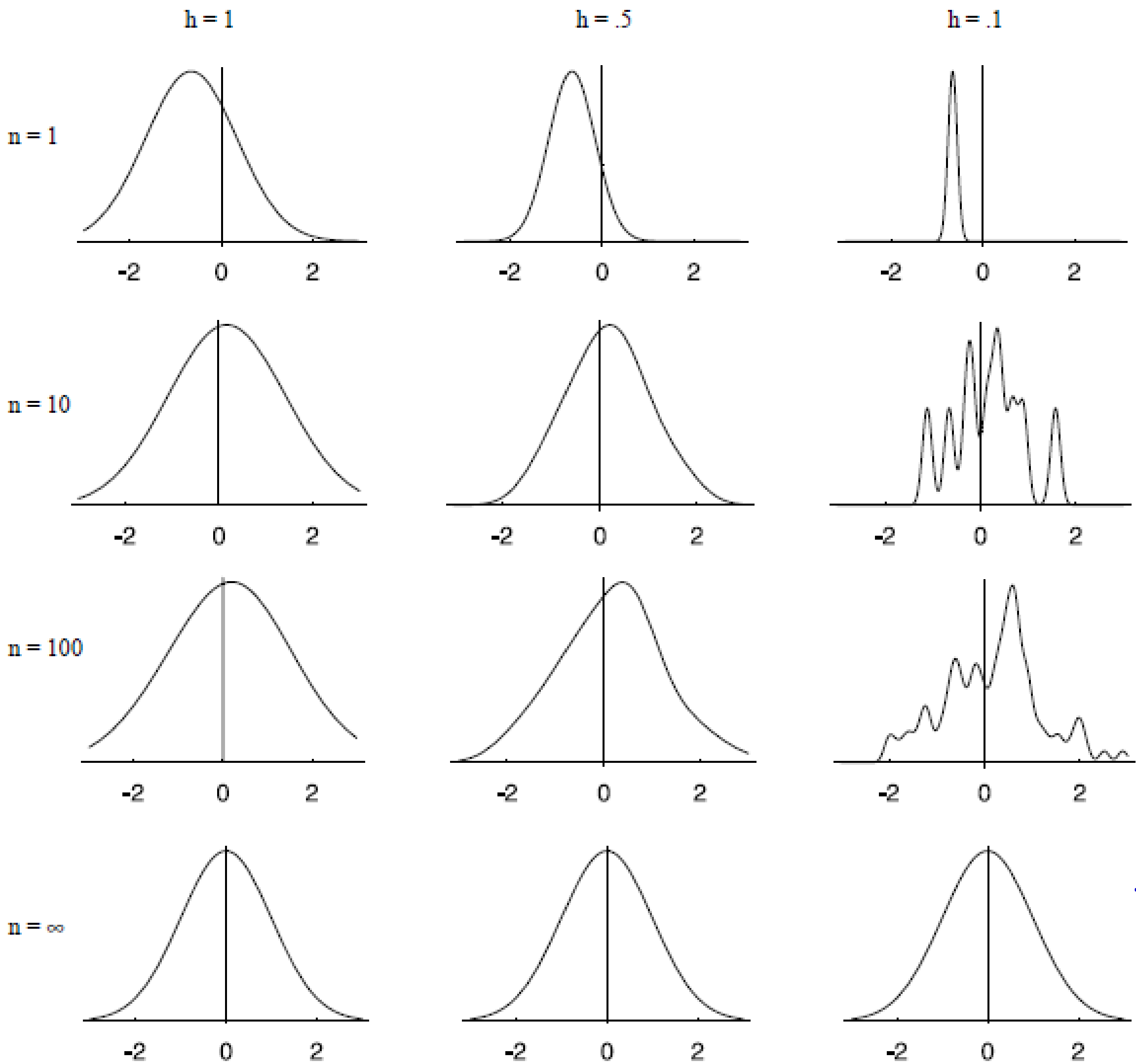
$$\begin{aligned}
\bar{p}_n(\mathbf{x}) &= \mathcal{E}[p_n(\mathbf{x})] \\
&= \frac{1}{n}\sum_{i=1}^{n}\mathcal{E}\Big[\frac{1}{V_n}\varphi\Big(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\Big)\Big] \\
&= \int \frac{1}{V_n}\varphi\Big(\frac{\mathbf{x}-\mathbf{v}}{h_n}\Big)\, p(\mathbf{v})\, d\mathbf{v} \\
&= \int \delta_n(\mathbf{x}-\mathbf{v})p(\mathbf{v})\, d\mathbf{v}.
\end{aligned}$$

When $n \to \infty$ $\quad \lim_{n\to\infty} V_n = 0 \quad \lim_{n\to\infty} nV_n = \infty$

$$\bar{p}_n(\mathbf{x}) \to p(\mathbf{x})$$

- 示例：高斯窗函数 $\varphi(u) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2}$

$$p_n(x) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h_n}\varphi\left(\frac{x - x_i}{h_n}\right) \qquad \underline{h_n = h_1/\sqrt{n}}$$



True p(x):
Gaussian

2D case

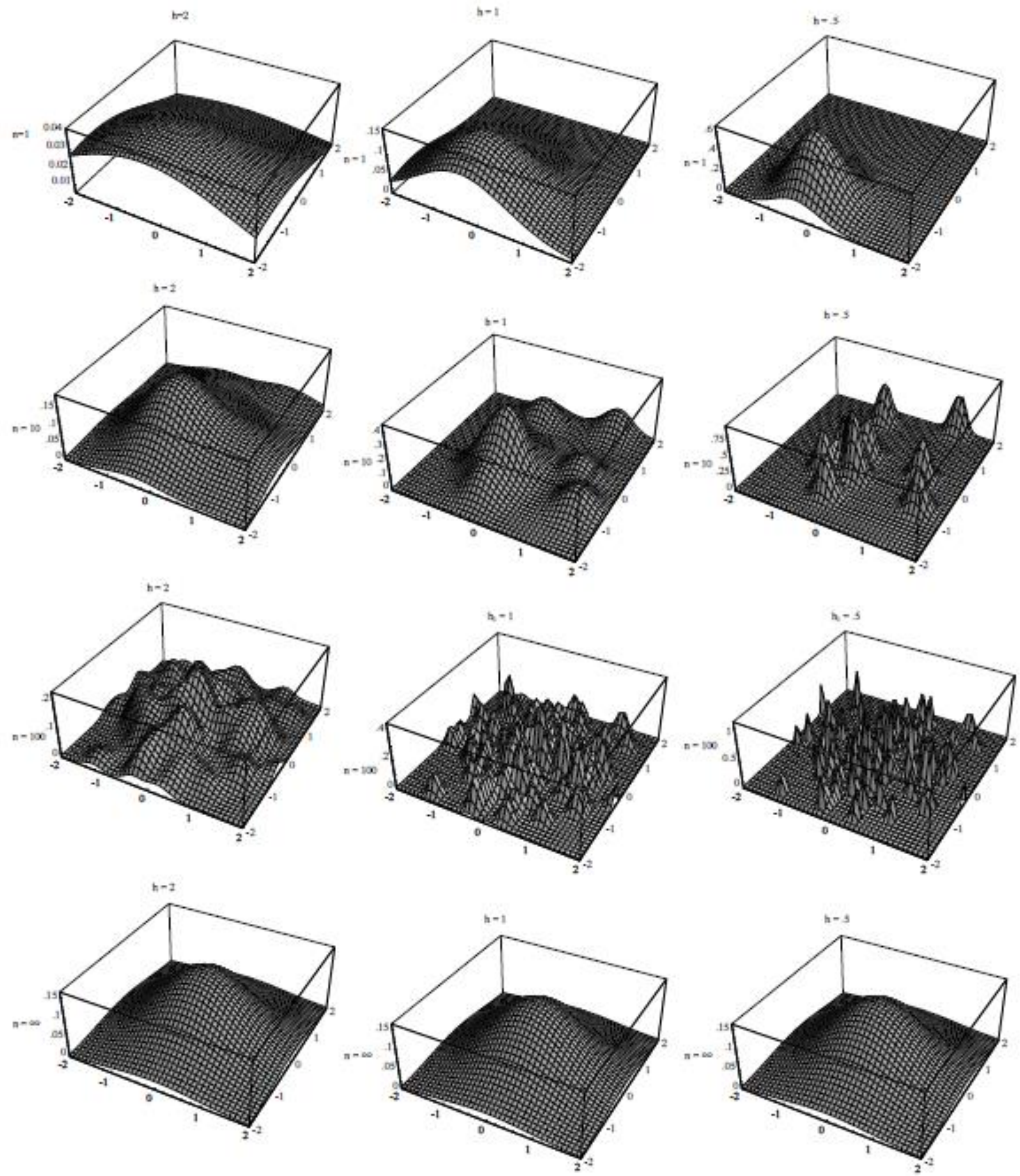
h=2 *h*=1.0 *h*=0.5

n=1

n=10

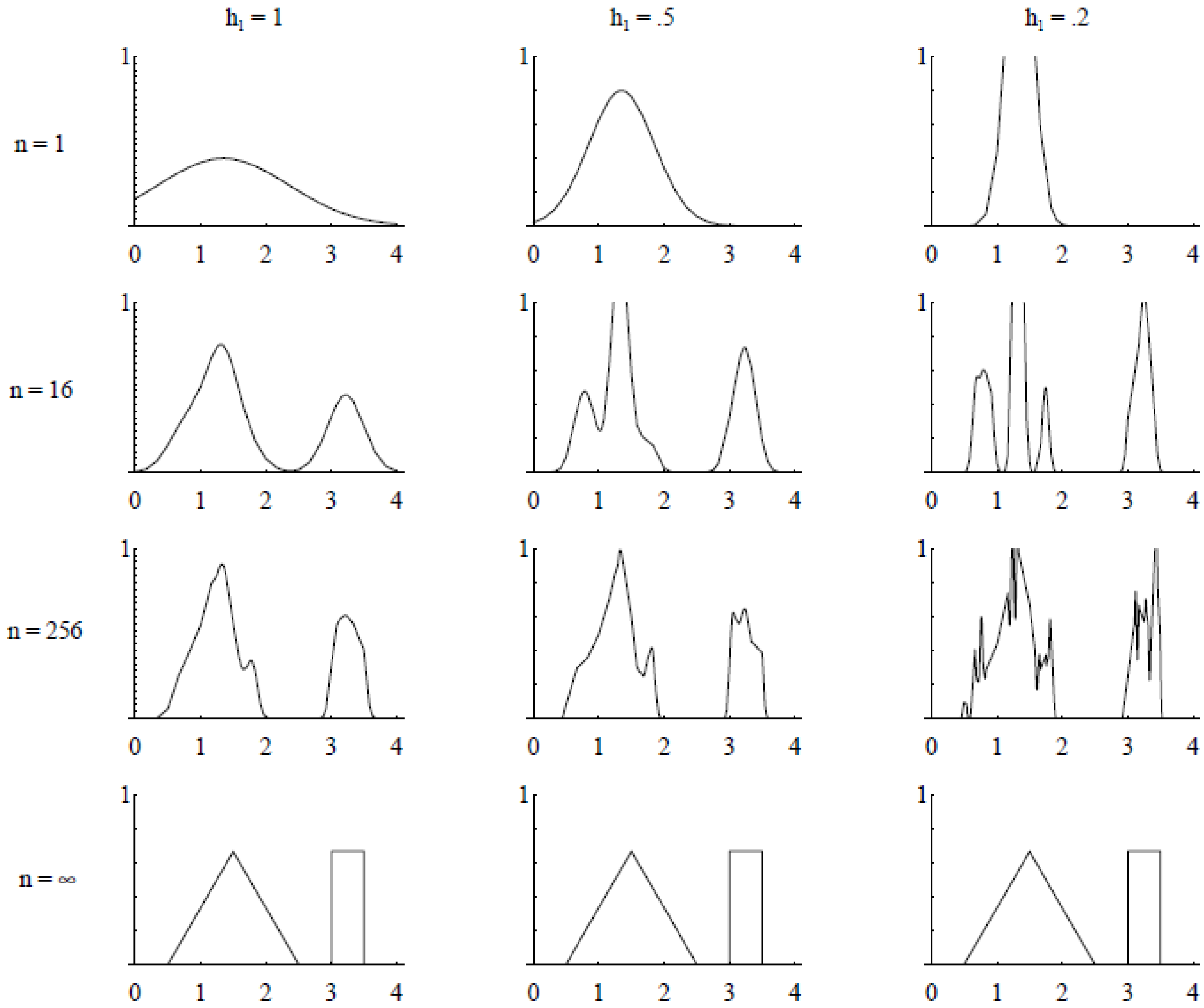
n=100

n=∞



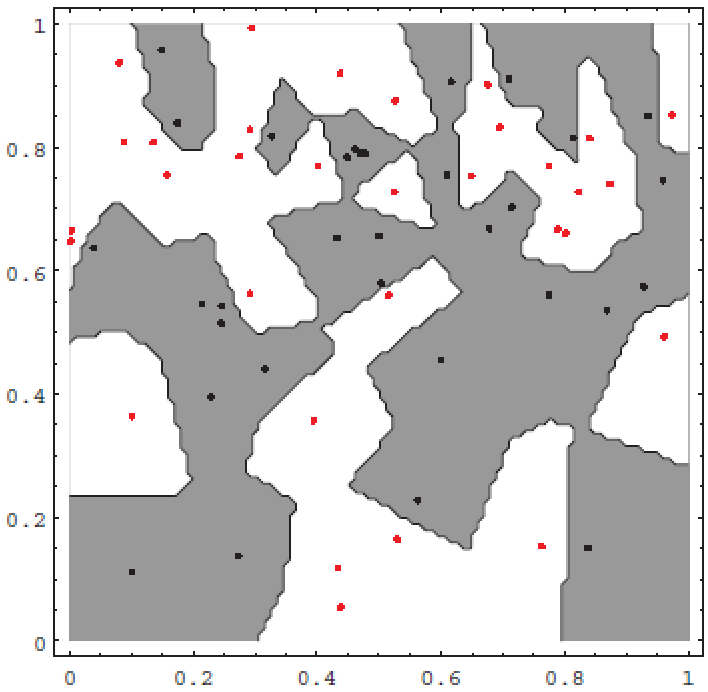
True $p(\mathbf{x})$: Gaussian

- Bimodal distribution



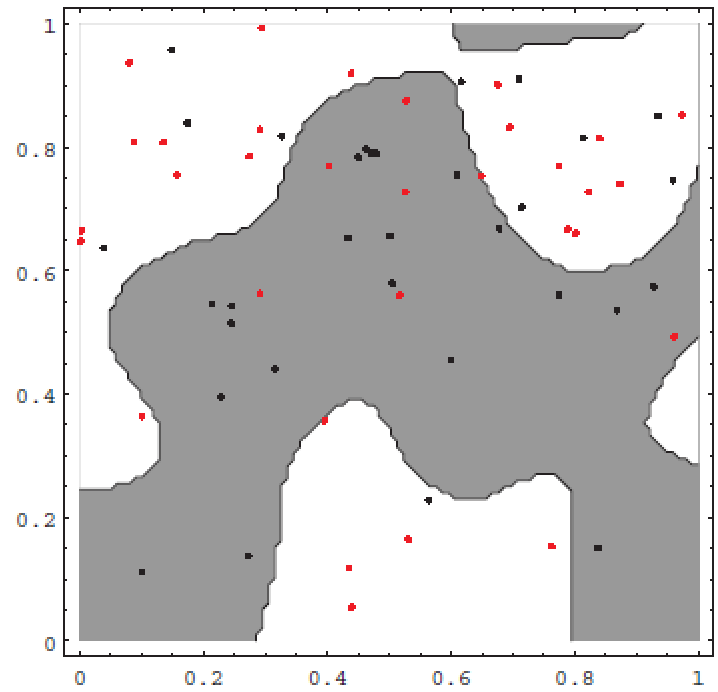
- 分类的例子 $\max_i p(\mathbf{x}|\omega_i)P(\omega_i)$

Small *h*



Decision regions

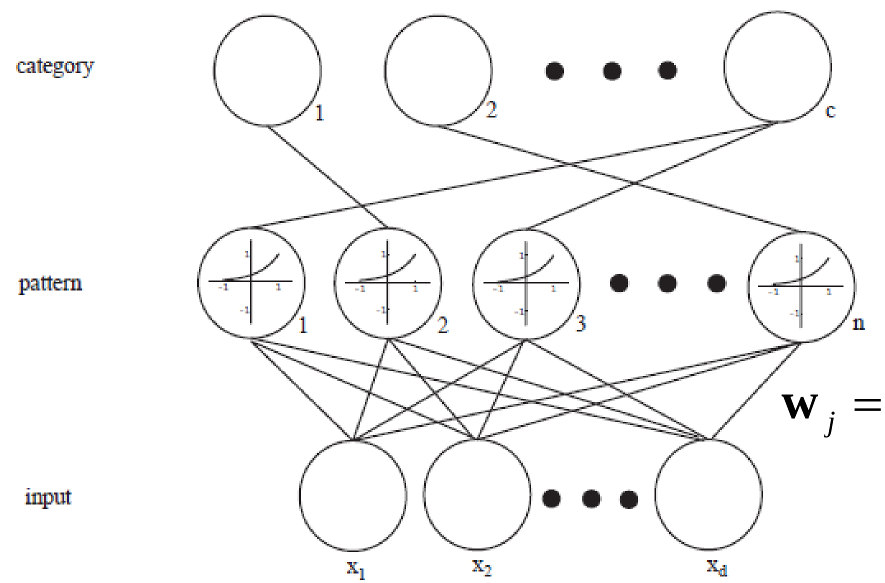
Large *h*



上部和下部密度区别大，适合不同的*h*值（考虑Generalization）

- 窗宽h_n选择经验
  - 一般原则：n越大或密度越大，h_n越小
  - 随n变化：$V_n = V_1/\sqrt{n}$
  - 随x变化：$h(\mathbf{x}), h(\mathbf{x}_i)$
    - $\mathbf{x}$测试样本，$\mathbf{x}_i$训练样本
    - 比如：根据k-NN的距离估计局部密度，h与局部密度成反比
  - 交叉验证(cross validation)
    - 比如选择V_1：设多个候选值，对每个值的效果进行交叉验证

- Probabilistic Neural Network (PNN)
  - 输出每个类别的概率密度
  - 隐节点：pattern unit, 对应Parzen窗函数
  - Normalized pattern: $\mathbf{x} \leftarrow \mathbf{x} / \|\mathbf{x}\|$



$$e^{(z_k-1)/\sigma^2}$$

$$z_k = \mathbf{w}_k^t \mathbf{x}$$

$$\mathbf{w}_j = \mathbf{x}_j$$

Why $e^{(z_k-1)/\sigma^2}$

$$\varphi\left(\frac{\mathbf{x}_k - \mathbf{w}_k}{h_n}\right) \propto \overbrace{e^{-(\mathbf{x}-\mathbf{w}_k)^t(\mathbf{x}-\mathbf{w}_k)/2\sigma^2}}^{\text{desired Gaussian}}$$

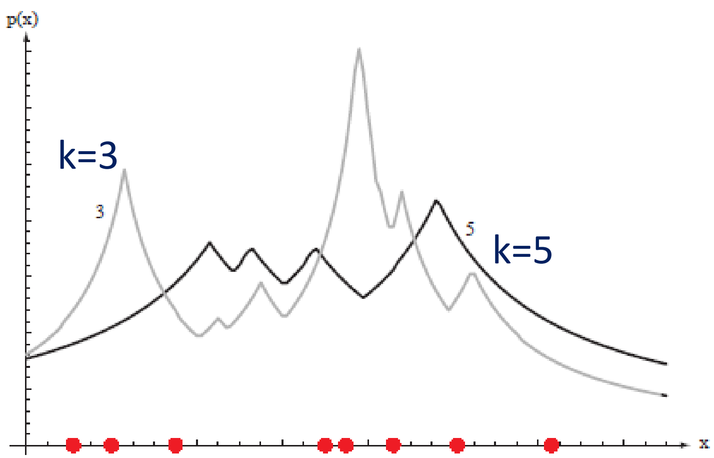
$$= e^{-(\mathbf{x}^t\mathbf{x}+\mathbf{w}_k^t\mathbf{w}_k-2\mathbf{x}^t\mathbf{w}_k)/2\sigma^2} = e^{(z_k-1)/\sigma^2}$$

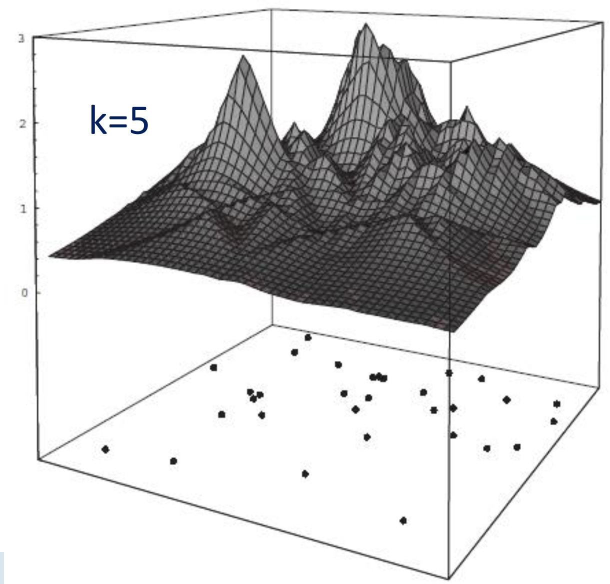
K近邻估计

- 概率密度估计
  - 固定局部区域样本数*k*, 体积*V*变化

$$p_n(\mathbf{x}) = \frac{k_n/n}{V_n}$$

  - 收敛到*p*(**x**)条件 $\lim_{n\to\infty} k_n = \infty$ and $\lim_{n\to\infty} k_n/n = 0$
  - 一种选择：$k_n = \sqrt{n} \quad V_n \simeq 1/(\sqrt{n}p(\mathbf{x}))$
  - 1D, 2D的例子

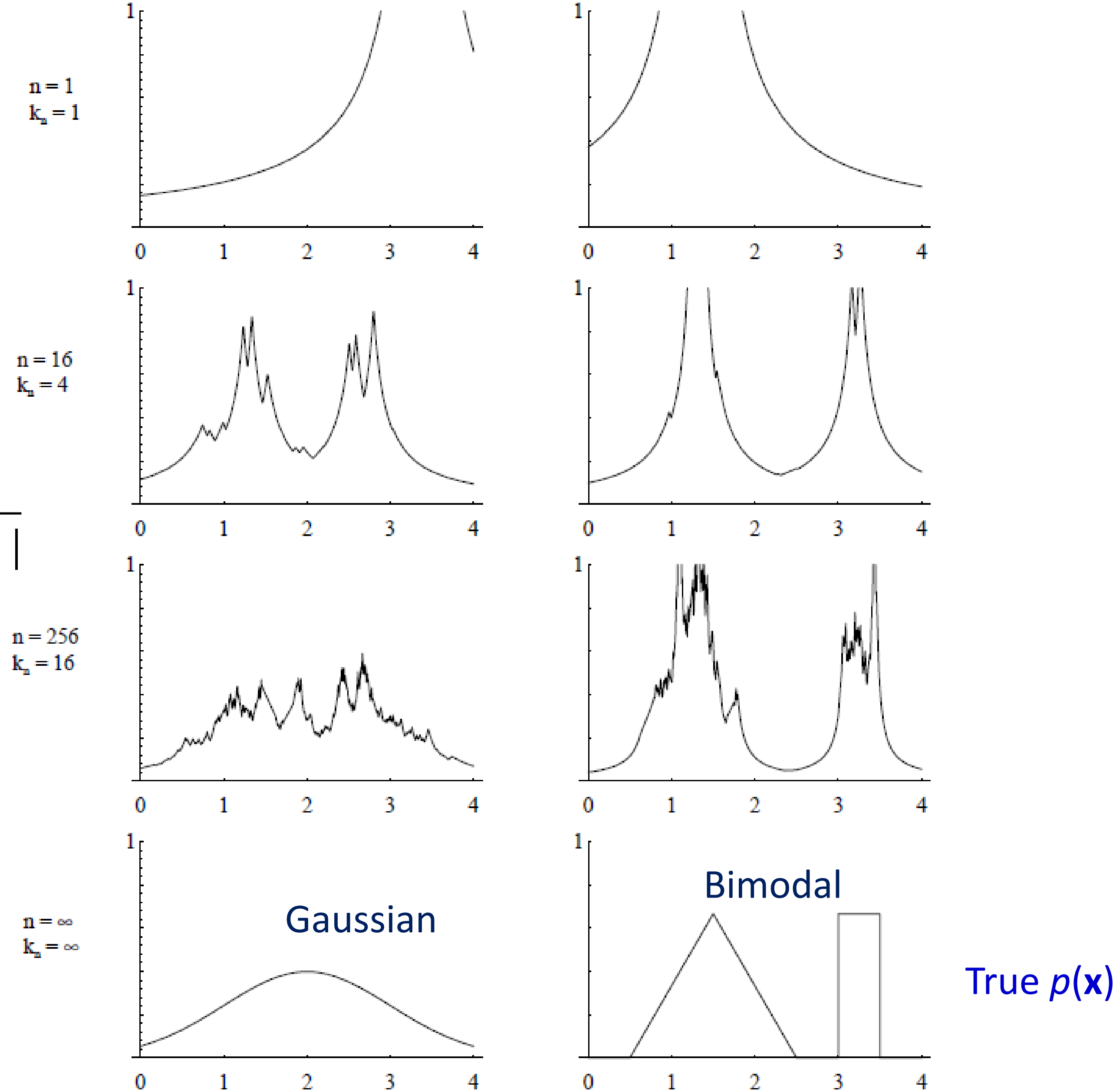




More 1D examples

$$k_n = \sqrt{n}$$

$$p_n(x) = \frac{\sqrt{n}/n}{2|x - x_{kNN}|}$$



- K-NN分类：后验概率
  - k_i NNs from class *i* $\quad k = \sum_{i=1}^{c} k_i$

$$p_n(\mathrm{x}, \omega_i) = \frac{k_i/n}{V}$$

$$\boxed{P_n(\omega_i|\mathrm{x}) = \frac{p_n(\mathrm{x}, \omega_i)}{\sum_{j=1}^{c} p_n(\mathrm{x}, \omega_j)} = \frac{k_i}{k}}$$

  - 分类错误率：当 $\lim_{n\to\infty} k_n = \infty$ and $\lim_{n\to\infty} k_n/n = 0$ 趋近贝叶斯错误率

K-NN分类规则里没有概率密度，但要注意，该规则是从非参数概率密度估计和贝叶斯决策过来的

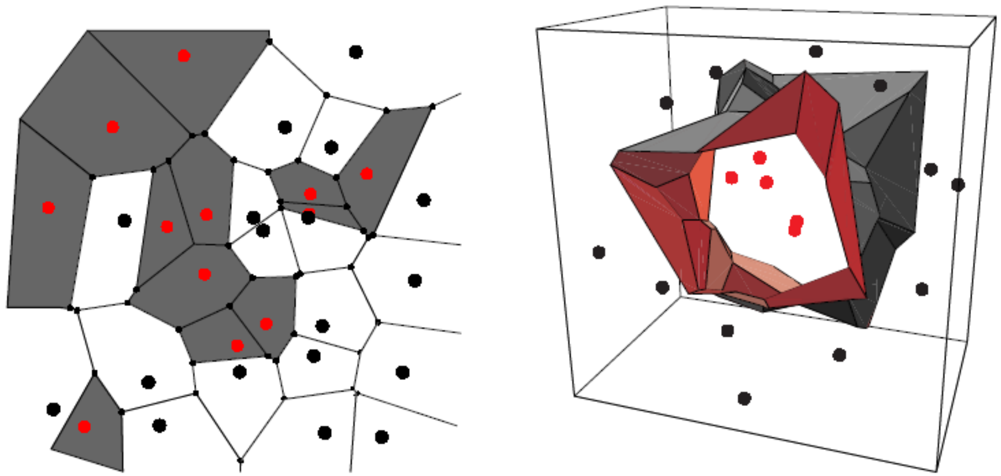
中国科学院大学
University of Chinese Academy of Sciences

最近邻规则

- Nearest Neighbor (1-NN) Rule
  - Among labeled data $\mathcal{D}^n = \{\mathrm{x}_1, \ldots, \mathrm{x}_n\}$ **x'** is the NN of **x**
  - Assume $P(\omega|\mathrm{x}') \simeq P(\omega_i|\mathrm{x})$
  - Classification: MAP

$$\omega_m = \arg\max_i P(\omega_i \mid \mathbf{x}) = \omega(\mathbf{x}')$$

  - Decision regions: Voronoi tesselation



- 最近邻规则的错误率

$$P(e) = \int P(e|\mathbf{x})p(\mathbf{x})\, d\mathbf{x}$$

$$P(e|\mathbf{x}) = \int \underline{P(e|\mathbf{x}, \mathbf{x}')}p(\mathbf{x}'|\mathbf{x})\, d\mathbf{x}'$$ **x**′: NN of **x**

  - 当n→∞, $p(\mathbf{x}'|\mathbf{x})$ 趋近以**x** 为中心的delta函数
  - 对$P(e|\mathbf{x},\mathbf{x}')$, 假设 **x** 和 $\mathbf{x}_j'$ (最近训练样本，与**x** 独立)的类别标号分别为 θ 和 θ_j'

$$P(\theta, \theta_j'|\mathbf{x}, \mathbf{x}_j') = P(\theta|\mathbf{x})P(\theta_j'|\mathbf{x}_j')$$

$$P_n(e|\mathbf{x}, \mathbf{x}_j') = 1 - \sum_{i=1}^{c} P(\theta = \omega_i, \theta' = \omega_i|\mathbf{x}, \mathbf{x}_j') = 1 - \sum_{i=1}^{c} P(\omega_i|\mathbf{x})P(\omega_i|\mathbf{x}_j')$$

$$\lim_{n\to\infty} P_n(e|\mathbf{x}) = \int \left[1 - \sum_{i=1}^{c} P(\omega_i|\mathbf{x})P(\omega_i|\mathbf{x}')\right] \underline{\delta(\mathbf{x}' - \mathbf{x})}\, d\mathbf{x}' = 1 - \sum_{i=1}^{c} P^2(\omega_i|\mathbf{x})$$

- 最近邻规则的错误率
  - Asymptotic error rate $\lim_{n\to\infty} P_n(e|\mathbf{x}) = 1 - \sum_{i=1}^{c} P^2(\omega_i|\mathbf{x})$

$$
\begin{aligned}
P &= \lim_{n\to\infty} P_n(e) \\
&= \lim_{n\to\infty} \int P_n(e|\mathbf{x})p(\mathbf{x})\, d\mathbf{x} \\
&= \int \Big[1 - \sum_{i=1}^{c} P^2(\omega_i|\mathbf{x})\Big] p(\mathbf{x})\, d\mathbf{x}
\end{aligned}
$$

- Error bound of 1-NN rule

$$\sum_{i=1}^{c} P^2(\omega_i|\mathbf{x}) = P^2(\omega_m|\mathbf{x}) + \boxed{\sum_{i\neq m} P^2(\omega_i|\mathbf{x})}$$

Minimized when P_i ($i \neq m$) are equal

$$P^*(e|\mathbf{x}) = 1 - P(\omega_m|\mathbf{x})$$

(Bayes error)

$$P(\omega_i|\mathbf{x}) = \begin{cases} \frac{P^*(e|\mathbf{x})}{c-1} & i \neq m \\ 1 - P^*(e|\mathbf{x}) & i = m \end{cases}$$

$$\sum_{i=1}^{c} P^2(\omega_i|\mathbf{x}) \geq (1 - P^*(e|\mathbf{x}))^2 + \frac{P^{*2}(e|\mathbf{x})}{c-1}$$

- Error bound of 1-NN rule

$$\sum_{i=1}^{c} P^2(\omega_i|\mathbf{x}) \geq (1 - P^*(e|\mathbf{x}))^2 + \frac{P^{*2}(e|\mathbf{x})}{c-1}$$

$$1 - \sum_{i=1}^{c} P^2(\omega_i|\mathbf{x}) \leq 2P^*(e|\mathbf{x}) - \frac{c}{c-1}P^{*2}(e|\mathbf{x})$$

  - Error rate

$$P = \int \left[1 - \sum_{i=1}^{c} P^2(\omega_i|\mathbf{x})\right] p(\mathbf{x})\, d\mathbf{x} \rightarrow P \leq 2P^*$$

$$\begin{aligned}\mathrm{Var}[P^*(e|\mathbf{x})] &= \int [P^*(e|\mathbf{x}) - P^*]^2 p(\mathbf{x})\, d\mathbf{x} \\ &= \int P^{*2}(e|\mathbf{x}) p(\mathbf{x})\, d\mathbf{x} - P^{*2} \geq 0 \rightarrow \int P^{*2}(e|\mathbf{x}) p(\mathbf{x})\, d\mathbf{x} \geq P^{*2}\end{aligned}$$

  - Error bound

$$\boxed{P^* \leq P \leq P^*\left(2 - \frac{c}{c-1}P^*\right)}$$

证明这个bound比较费劲，一般来说记住结论即可。
证明过程中有些思想很有启发，比如*P*(*e*|**x**,**x**')假设

Break

K近邻的快速计算

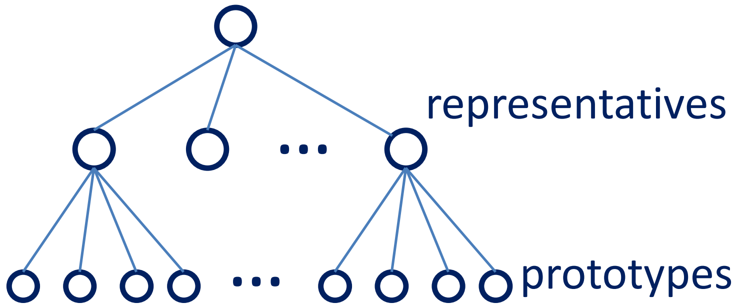
- 分类的计算复杂度$O(dn)$
- 近邻搜索的三种策略
  - Partial distance
  - Prestructuring
  - Editing (pruning, condensing)

Partial square distance (r<d)

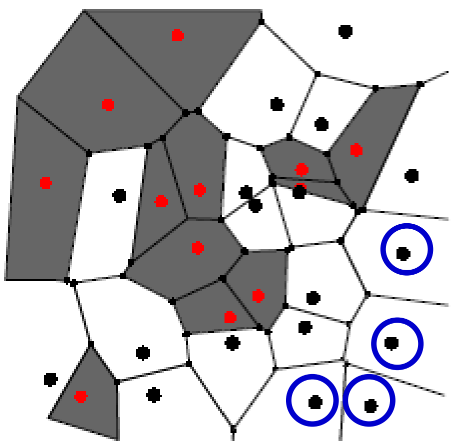
$$D_r^2(\mathbf{a},\mathbf{b}) = \sum_{i=1}^{r}(a_i - b_i)^2$$

Full distance to the current closest prototype $D^2(\mathbf{x},\mathbf{x}')$
Terminate computing if the partial square distance is greater than $D^2(\mathbf{x},\mathbf{x}')$

- Prestructuring
  - Search tree, prototypes are linked to the nodes, each labeled with a representative prototype
    - E.g. Constructed by clustering
  - 1-NN搜索：先找出到x的最近代表点，然后计算与最近代表点连接原型的距离，找出最近原型
  - 可结合partial distance
  - 为保证找到最近原型，应从多个代表点的原型中搜索



- Editing
  - Remove prototypes that are surrounded by samples (Voronoi neighbors) of same class



有更多近邻搜索的快速算法，如branch-and-bound, k-d tree等（在此省略）

距离度量

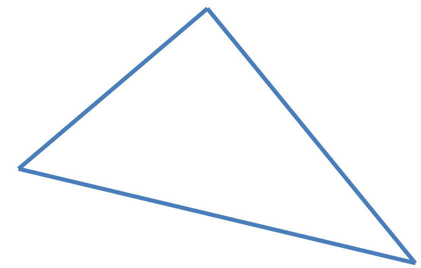
- 距离度量(metric)的性质

  non-negativity: $D(\mathbf{a}, \mathbf{b}) \geq 0$

  reflexivity: $D(\mathbf{a}, \mathbf{b}) = 0$ if and only if $\mathbf{a} = \mathbf{b}$

  symmetry: $D(\mathbf{a}, \mathbf{b}) = D(\mathbf{b}, \mathbf{a})$

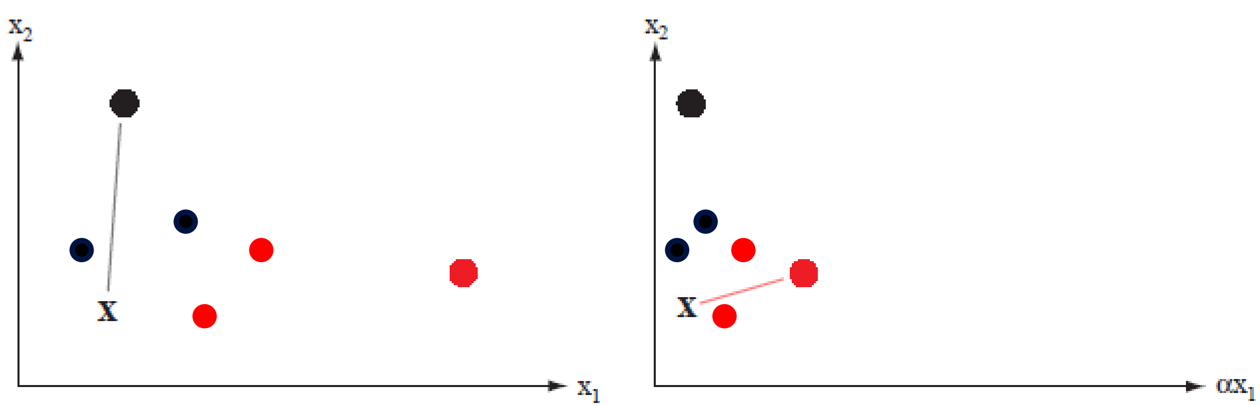
  triangle inequality: $D(\mathbf{a}, \mathbf{b}) + D(\mathbf{b}, \mathbf{c}) \geq D(\mathbf{a}, \mathbf{c})$



Euclidean metric

$$D(\mathbf{a}, \mathbf{b}) = \left(\sum_{k=1}^{d} (a_k - b_k)^2 \right)^{1/2}$$

- Metric影响分类性能
  - 比如，当特征变尺度



- 几种Metric
  - Minkowski (L_k norm)

$$L_k(\mathbf{a},\mathbf{b}) = \left(\sum_{i=1}^{d} |a_i - b_i|^k \right)^{1/k}$$

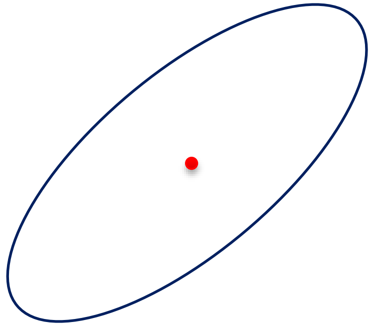
  - Manhattan (city block distance): k=1
  - Tanimoto metric (for binary features)

$$D_{Tanimoto}(\mathcal{S}_1,\mathcal{S}_2) = \frac{n_1 + n_2 - 2n_{12}}{n_1 + n_2 - n_{12}}$$

- Metric Learning
  - Parameters in metric optimized in learning (e.g., empirical risk minimization)

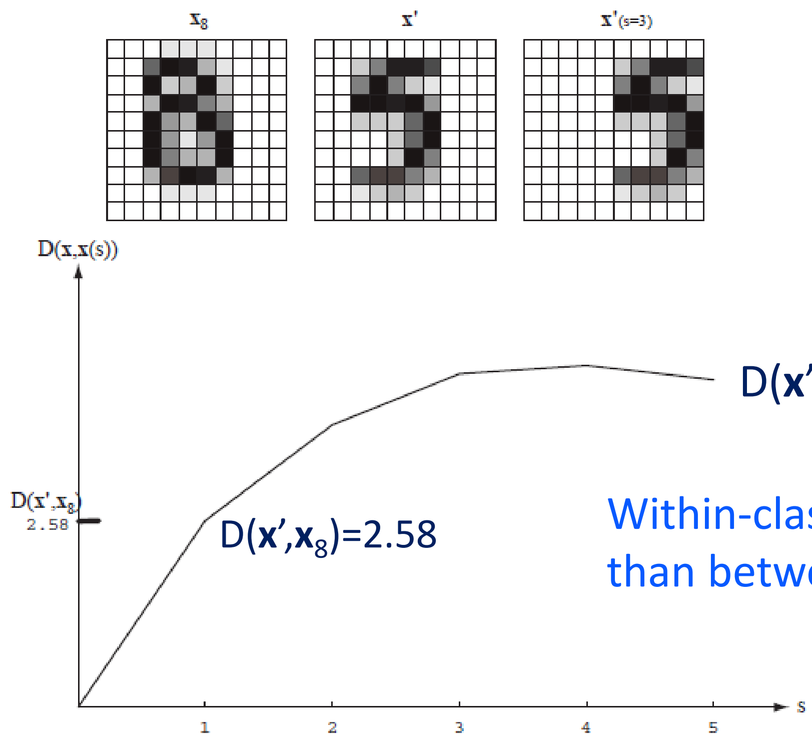
$$D_{\mathbf{w}}(\mathbf{a},\mathbf{b}) = \sum_{i=1}^{d} w_i (a_i - b_i)^2$$

$$D_{\Sigma}(\mathbf{a},\mathbf{b}) = (\mathbf{a}-\mathbf{b})^t \Sigma^{-1} (\mathbf{a}-\mathbf{b})$$



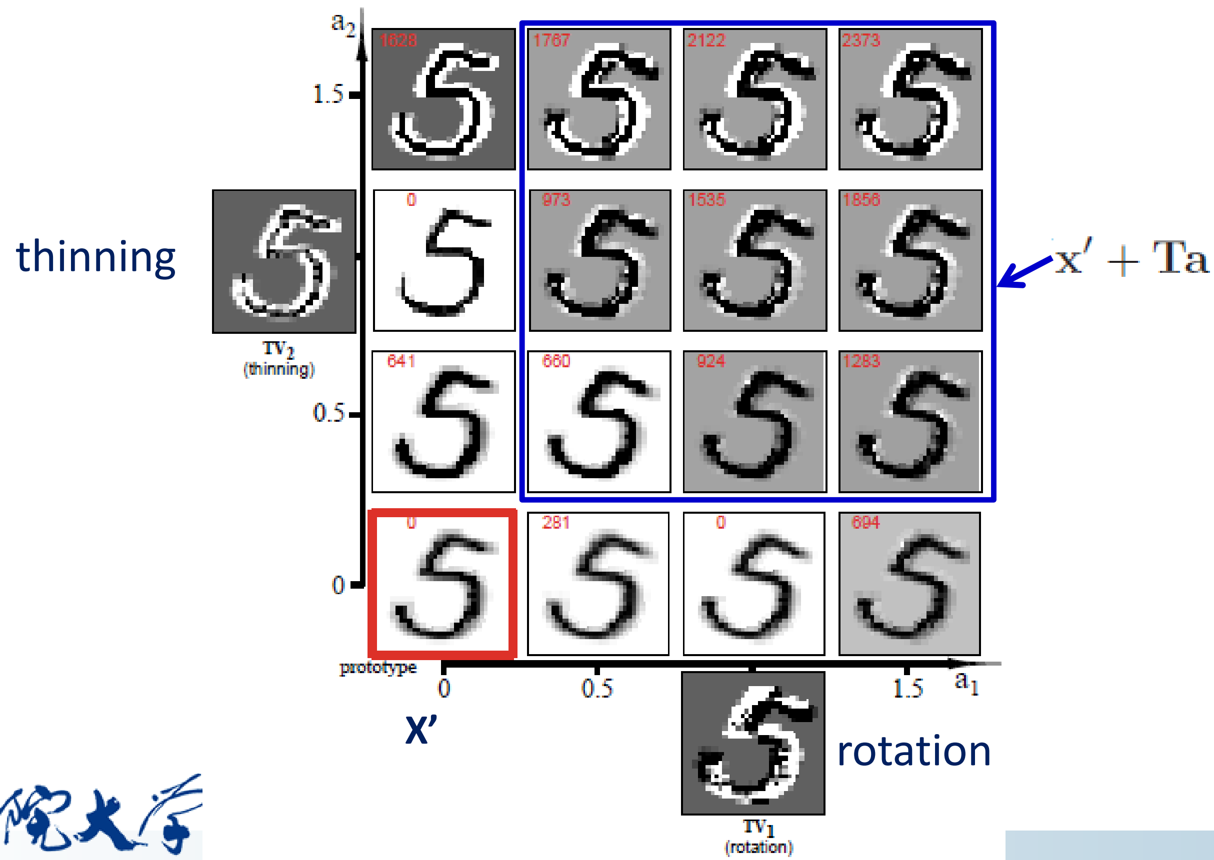
Tangent Distance

- Image Shape Transformation
  - Shift (translation), rotation, scaling, distortion
  - Distance sensitive to transformation



Within-class distance maybe larger than between-class distance

- Tangent distance
  - Search for optimal parameters for a combination of transformations for a prototype to minimize the distance to test sample
  - Parameterized transformation: $\mathcal{F}_i(\mathrm{x}';\ \alpha_i)$
  - Tangent vectors: $\mathbf{TV}_i = \mathcal{F}_i(\mathrm{x}';\ \alpha_i) - \mathrm{x}'$ 近似梯度方向
  - Linear combination in the space spanned by TVs: $\mathrm{x}' + \mathrm{Ta}$



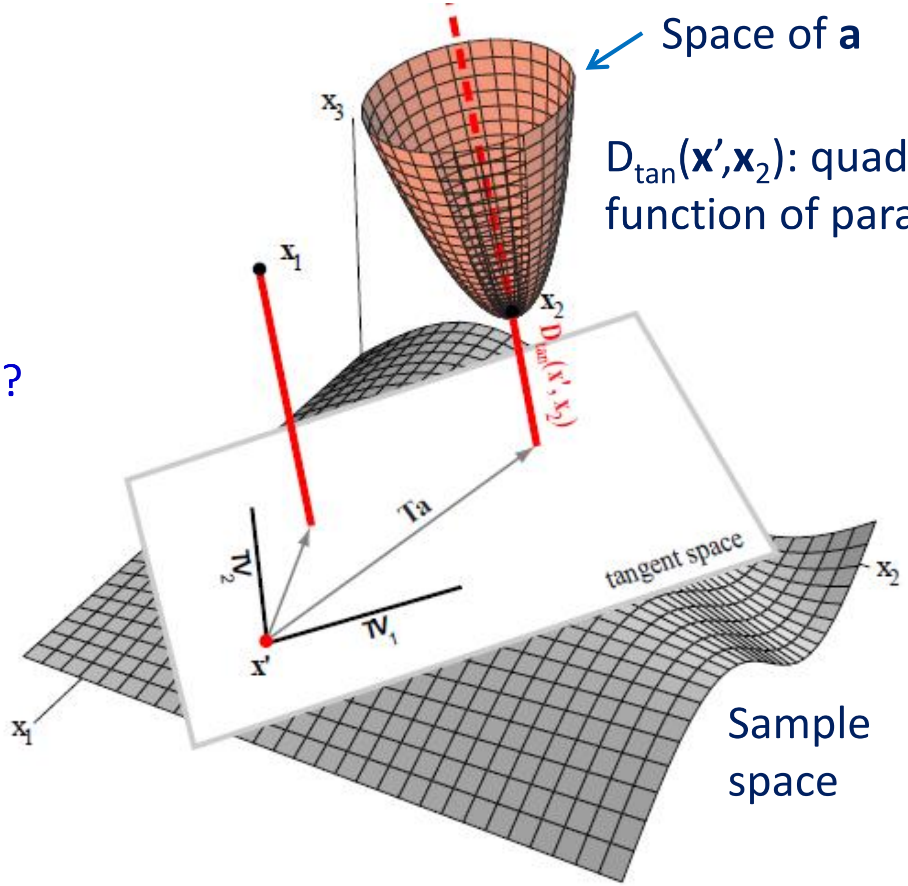
- Tangent distance
  - Euclidean distance to tangent space

$$D_{tan}(\mathrm{x}', \mathrm{x}) = \min_{\mathbf{a}} [\|(\mathrm{x}' + \mathrm{Ta}) - \mathrm{x}\|]$$

点到超平面的最近距离

  - Optimization: gradient search w.r.t **a**

为什么叫
tangent space?

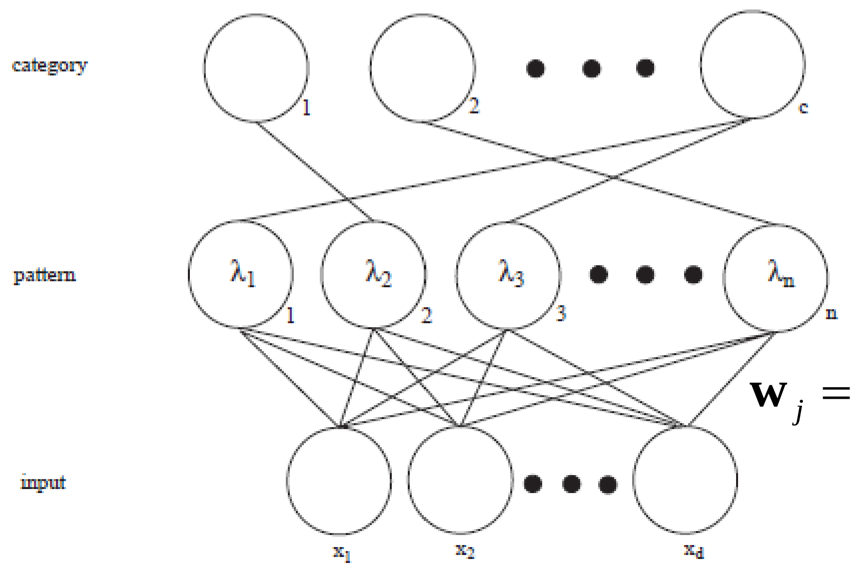


Reduced Coulomb Energy Network

- RCE Network
  - Hidden node (corresponding to a training sample): hypersphere with **radius** according to the distance to nearest point of different class

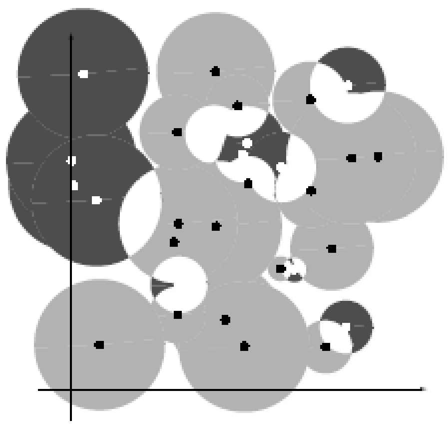
$$\epsilon = \text{small param}, \lambda_m = \text{max radius}$$

$$\lambda_j \leftarrow \min[\min_{\mathbf{x}\notin\omega_i} D(\mathbf{x},\mathbf{x}') - \varepsilon, \lambda_m]$$



$\mathbf{w}_j = \mathbf{x}_j$ (normalized)

- RCE分类规则
  - 找出包含x的隐节点（超球体），如果这些节点的类别标号一致，则分类到这个类别
    - 没有节点包含x，或者类别不一致（不同类别超球体重叠）的情况，则拒识



白色区域：
ambiguous

RCE Network: 与非参数方法(Parzen window, k-NN)的关系
与Probabilistic neural network的关系

Approximation by Series Expansion

- Parzen窗密度估计：计算量大
- 窗函数用序列展开

$$\varphi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right)=\sum_{j=1}^{m}a_j\psi_j(\mathbf{x})\chi_j(\mathbf{x}_i)$$

$$\sum_{i=1}^{n}\varphi\left(\frac{\mathbf{x}-\mathbf{x}_i}{h_n}\right)=\sum_{j=1}^{m}a_j\psi_j(\mathbf{x})\sum_{i=1}^{n}\chi_j(\mathbf{x}_i)$$

$$p_n(\mathbf{x})=\sum_{j=1}^{m}b_j\psi_j(\mathbf{x})\qquad b_j=\frac{a_j}{nV_n}\sum_{i=1}^{n}\chi_j(\mathbf{x}_i)$$

  – b_j可离线计算，p_n(x)只需m次计算($m<n$)

高斯窗函数的Taylor展开

$$\sqrt{\pi}\,\varphi(u) = e^{-u^2} \simeq \sum_{j=0}^{m-1} (-1)^j \frac{u^{2j}}{j!}$$

m=2

$$\sqrt{\pi}\varphi\left(\frac{x-x_i}{h}\right) \simeq 1-\left(\frac{x-x_i}{h}\right)^2 = 1+\frac{2}{h^2}x\,x_i-\frac{1}{h^2}\,x^2-\frac{1}{h^2}\,x_i^2$$

$$\boxed{\sqrt{\pi}p_n(x) = \frac{1}{nh}\sum_{i=1}^{n}\sqrt{\pi}\varphi\left(\frac{x-x_i}{h}\right) \simeq b_0+b_1x+b_2x^2}$$

$$b_0 = \frac{1}{h}-\frac{1}{h^3}\frac{1}{n}\sum_{i=1}^{n}x_i^2 \quad b_1 = \frac{2}{h^3}\frac{1}{n}\sum_{i=1}^{n}x_i \quad b_2 = -\frac{1}{h^3}$$

只有当max|x-x_i|<h时，展开的近似误差较小，然而这要求h比较大
当h较小，使用更多的展开项（m比较大）

这个方法实用价值不大，因为密度估计有误差，而从分类的角度，有很多分类器可以代替。但是思路值得借鉴。

总 结

- 非参数法的基本思想
  - 没有给定概率密度函数形式
  - 基于概率和密度的原始定义，以训练样本的局部分布近似x的局部密度
- Parzen window
- K-nearest neighbor (k-NN)
  - 1-nearest neighbor (1-NN), Error bound
  - 快速搜索
- 距离度量
  - Tangent distance
- Series expansion

统计模式识别的作用和地位

- 贝叶斯决策
  - MAP, 最小风险决策
  - 贝叶斯分类器：理想情况（样本无穷多、概率密度准确估计）下最优
  - 各种分类器性能分析的参照
- Parametric/Non-parametric统计分类器
  - 训练样本较少时比较competitive
- 概率密度估计
  - 概率密度模型：生成模型，可用于判别outlier ($p(\mathbf{x})<t$)
  - 信息论方法的基础，如熵、互信息等
  - K-NN: local density, local accuracy of classifier

统计模式识别的作用和地位

- 特征空间分析
  - 假设空间相邻的样本类别也相同(流形假设，Manifold assumption)
  - 基于特征空间划分的分类器设计，如tree classifier
  - 基于特征空间的分类器性能分析，如神经网络的决策面/决策区域
- 与其他分类方法的关系
  - 判别模型(SVM, 神经网络等)：近似后验概率，或输出可近似转换为后验概率
  - 基于距离/相似度的分类器：可从特征空间分析
  - 结构PR问题转换为统计PR: Dissimilarity embedding

统计模式识别方法

生成模型
(Density-based, Bayes decision)

Parametric
- ✓ Gaussian
- ✓ Dirichlet
- ✓ Bayesian network
- ✓ Hidden Markov model

Non-Parametric
- ✓ Histogram density
- ✓ Parzen window
- ✓ K-nearest neighbor

Semi-Parametric
- ✓ Gaussian mixture

判别模型
(discriminant/decision function)

- ✓ Linear methods
- ✓ Neural network
- ✓ Logistic regression
- ✓ Decision tree
- ✓ Kernel (SVM)
- ✓ Boosting

a.k.a. Non-parametric

下次课
（向世明老师）