# EE5907 Pattern Recognition

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# 1 Statistical Learning

#### 1.1 Basics

A random variable x is a quantity that is uncertain. Some values occur more than others; this information captured by probability distribution p(x).

Bernoulli:  $Pr(x) = \lambda^x (1 - \lambda)^{1-x}$ ; Categorical:  $Pr(x = k) = \lambda_k$ ; Gaussian:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}.$$
 Marginalization: 
$$p(x) = \sum_y p(x,y).$$
 Conditional probability:

$$\begin{array}{l} p\left( {x|y = y^* } \right) = \frac{{p\left( {x,y = y^* } \right)}}{{p\left( {y = y^* } \right)}} = \frac{{p\left( {x,y = y^* } \right)}}{{\int {p\left( {x,y = y^* } \right)dx}}} \text{ or } \\ p(x|y) = \frac{{p(x,y)}}{{p(y)}}. \text{ Bayes' rule:} \end{array}$$

$$p(x|y) = \frac{p(y)}{p(y)}$$
. Bayes rule:  

$$p(y|x) = \frac{p(y)p(x|y)}{p(x)} = \frac{p(y)p(x|y)}{\sum_y p(y)p(x|y)}$$

Independence: 
$$p(x,y) = p(x)p(y|x) = p(x)p(y)$$
.  
Expectation:  $E[f(x)] = \sum_{x} f(x)p(x)$ , if

$$f(x) = x$$
, mean; if  $f(x) = (x - \mu_x)^2$ , variance.  
 $Cov(x, y) = E(xy) - E(x)E(y)$ . Conditional  
 $E[f(x, y)|y] \triangleq E_{p(x|y)}[f(x, y)]$ 

expectation:

$$\triangleq \int_{x} f(x,y)p(x|y)dx.$$

Conditional independent:

 $p(x_1, x_2|x_3) = p(x_1|x_3) p(x_2|x_3).$ 

Suppose Y = g(X), where g is monotonic;

Change of variable: If  $X \sim f(x)$ , then

$$Y \sim \left| \frac{d}{dy} \left( g^{-1}(y) \right) \right| f \left( g^{-1}(y) \right).$$

$$Ga(x|a,b) = \frac{b^a}{\Gamma(a)}x^{a-1}e^{-xb}, \ \Gamma(t+1) = t\Gamma(t).$$

KL divergence:

$$D_{\mathrm{KL}}(P||Q) = \sum_{x \in \mathcal{X}} P(x) \log \left(\frac{P(x)}{Q(x)}\right).$$

Leibniz rule: 
$$\frac{d}{dx} \left( \int_{a(x)}^{b(x)} f(x,t) dt \right) = f(x,b(x)) \cdot \frac{d}{dx} b(x) - f(x,a(x)) \cdot \frac{d}{dx} a(x) + \int_{a(x)}^{b(x)} \frac{\partial}{\partial x} f(x,t) dt$$

# 1.2 Estimation and Conjugate Priors

MAP estimation:  $y_{MAP} \triangleq \underset{y}{\operatorname{argmax}} p(y|x) =$ 

 $\underset{y}{\operatorname{argmax}} \frac{p(y)p(x|y)}{p(x)} = \underset{y}{\operatorname{argmax}} p(y)p(x|y). \text{ If the }$ 

 $\begin{aligned} & \text{prior } p(y) \text{ is constant (uniform)}, \\ & y_{MAP} = \text{argmax} p(x|y) \triangleq y_{ML}. \end{aligned}$ 

Much of ML is about how to choose a model for p(y|x) and how to optimize model parameters. To model posterior  $p(y|x, \theta)$ , we have

**generative** (model  $p(x|y, \theta)$  and  $p(y|\theta)$  so that can generate new data

 $p(x, y|\boldsymbol{\theta}) = p(y|\boldsymbol{\theta})p(x|y, \boldsymbol{\theta}))$  and **discriminative** models  $(P(y|x, \boldsymbol{\theta}) \text{ only})$ . We treat the parameter  $\boldsymbol{\theta}$  as random variable and perform probabilistic estimation.

• Beta-Binomial Generative Model  $p(D|\theta) = \text{Bin}(N_1|N,\theta) = \binom{N}{N_1} \theta^{N_1} (1-\theta)^{N_0},$ 

$$\begin{split} p(\theta|a,b) &= \operatorname{Beta}(\theta|a,b) = \frac{1}{B(a,b)} \theta^{a-1} (1-\theta)^{b-1}, \\ p(\theta|D) &= \operatorname{Beta}(\theta|N_1+a,N_0+b). \\ \text{For } \operatorname{Beta}(x|c,d), \quad \operatorname{mode} = \frac{c-1}{c+d-2}, \operatorname{mean} = \frac{c}{c+d}, \\ \text{so } \hat{\theta}_{MAP} &= \underset{\theta}{\operatorname{argmax}} p(\theta|D) = \frac{N_1+a-1}{N+a+b-2} \text{ and} \\ \hat{\theta}_{ML} &= \frac{N_1}{N} \text{ by setting } a = b = 1 \text{ (uniform prior)} \ . \\ \hat{\theta}_{MAP} &= (1-\lambda)\hat{\theta}_{ML} + \lambda m_0, \\ m_0 &= \frac{a-1}{a+b-2} \text{ (prior mode)} \ . \quad \textbf{To predict future} \\ \text{coin toss, plug-in: } p(\tilde{x}=1) = \theta_{ML} \text{ or} \\ p(\tilde{x}=1) &= \theta_{MAP}; \text{ posterior predictive:} \\ p(\tilde{x}=1|D) &= E(\theta|D) = \frac{N_1+a}{N+a+b}. \\ &\bullet \text{ Dirichlet-Multinomial Generative Model} \\ p(D|\theta) &= \frac{N!}{N_1! \cdots N_K!} \prod_{k=1}^K \theta_k^{N_k}, \end{split}$$

$$\begin{split} p(\theta|D) &= \text{Dir}\,(\theta|N_1 + \alpha_1, \cdots, N_K + \alpha_K). \\ \hat{\theta}_k^{MAP} &= \frac{N_k + \alpha_k - 1}{N + \sum_k \alpha_k - K}, \\ \hat{\theta}_k^{ML} &= \frac{N_k}{N} \text{ by setting } \alpha_k = 1 \text{ (uniform prior) }. \\ \text{Again, posterior predictive:} \\ p(\tilde{x} = i|D) &= \frac{N_i + \alpha_i}{N + \sum_k \alpha_k}. \text{ (more important since the data is more sparse).} \\ \text{Posterior predictive:} \\ p\left(x_{n+1}|D\right) &= \int p\left(x_{n+1}|\lambda\right)p(\lambda|D)d\lambda, \text{ or} \\ p\left(x_{N+1}|D\right) &= \frac{p\left(x_{N+1}|\lambda\right)D\left(\lambda|D\right)}{N} \end{split}$$

 $p(\theta|\alpha) = Dir(\theta|\alpha), \alpha = {\alpha_k}_{k=1:K}, \alpha_k > 0,$ 

$$p(x_{n+1}|D) = \int p(x_{n+1}|\lambda) p(\lambda|D) d\lambda,$$

$$p(x_{N+1}|D) = \frac{p(x_{N+1}|\lambda, D) p(\lambda|D)}{p(\lambda|x_{N+1}, D)}$$

$$= \frac{p(x_{N+1}|\lambda) p(\lambda|D)}{p(\lambda|x_{N+1}, D)}.$$

# 1.3 Univariate Gaussian and Naive Bayes

 $p(x) = \mathcal{N}\left(x|\mu,\sigma^2\right), \text{ ML estimation:} \\ \hat{\mu} = \frac{1}{N}\sum_{n=1}^{N}x_n, \hat{\sigma}^2 = \frac{1}{N}\sum_{n=1}^{N}(x_n - \hat{\mu})^2; \\ p\left(\mu,\sigma^2\right) = \text{NormInvGam}\left(\mu,\sigma^2|\alpha,\beta,\gamma,\delta\right), \text{ MAP} \\ \text{estimation:} \quad \hat{\mu} = \frac{\sum_{n=1}^{N}x_n+\gamma\delta}{N+\gamma}, \hat{\sigma}^2 = \frac{\sum_{n=1}^{N}(x_n - \hat{\mu})^2 + 2\beta + \gamma(\delta - \hat{\mu})^2}{N+3+2\alpha}. \text{ To predict future} \\ \text{Gaussian sample, ML:} p\left(x^*\right) = \mathcal{N}\left(\mu_{ML},\sigma_{ML}^2\right); \\ \text{MAP:} \quad p\left(x^*\right) = \mathcal{N}\left(\mu_{MAP},\sigma_{MAP}^2\right); \text{ or posterior} \\ \text{predictive:} \quad p\left(x^*|D\right). \quad (\text{omitted here}). \end{aligned}$ 

• Naive Bayes Classifier
We need to model
1) class prior:  $P(Y = c_k)$ ,  $k = 1, 2, \dots, K$  and
2) feature likelihood:  $P(X = x | Y = c_k) = \prod_{j=1}^{n} P(X^{(j)} = x^{(j)} | Y = c_k)$  (Naive). To classify:  $y = \sum_{j=1}^{n} P(X^{(j)} = x^{(j)} | Y = c_k)$ 

# 1.4 Logistic Regression

$$p(y=1|x) = \frac{1}{1+e^{-wT_x}}, p(y=0|x) = \frac{1}{1+e^{wT_x}}.$$
 Log odds is  $\log \frac{p(y=1|x)}{p(y=0|x)} = w^T x$ .  $NLL(w) = -\sum_{i=1}^{N} [y_i \log \mu_i + (1-y_i) \log (1-\mu_i)],$  where  $\mu_i = \frac{1}{1+\exp(-w^T x_i)}$ . We want to minimize  $NNL(w)$  as optimization problem.  $g = \frac{d}{dv} NLL(w) = X^T (\mu - y),$ 

$$\begin{split} H &= \frac{d}{dw} g(\mathbf{w})^T = X^T S X, \text{ where } \\ S &= diag_{N \times N} (\mu_i \left(1 - \mu_i\right)). \text{ Impose } \\ \text{regularization to avoid overfitting: } \\ NLL_{reg}(\mathbf{w}) &= NLL(\mathbf{w}) + \frac{1}{2} \lambda \mathbf{w}^T \mathbf{w}, \\ g_{reg}(\mathbf{w}) &= g(\mathbf{w}) + \lambda \begin{pmatrix} 0_{1 \times 1} \\ w_{D \times 1} \end{pmatrix}, \\ H_{reg}(\mathbf{w}) &= H(\mathbf{w}) + \lambda \begin{pmatrix} 0_{1 \times 1} & \cdots \\ \vdots & I_{D \times D} \end{pmatrix}. \end{split}$$

#### 1.5 Non-parametric Techniques

In density estimation, we don't know the type of the distribution; in classification, we don't know the kind of mapping function  $\rightarrow$ 

**non-parametric** approach (does not mean no parameter!; number and nature of parameters change with data!).

Given  $x_1, \dots, x_N$  i.i.d from unknown p(x), For particular x, count number of samples k falling in window of volume V centered at x.  $p(x) \approx \frac{k/N}{V}$ .

• Parzen window: fix V, estimate k Hypercude:

$$\phi(u) = \begin{cases} 1 & |u_j| \le 0.5, j = 1, \dots, d \\ 0 & \text{otherwise} \end{cases},$$

$$k(x) = \sum_i \phi\left(\frac{x - x_i}{h}\right) =$$

# samples in hypercube centered at x,

# samples in hypercube centered at 
$$x$$
,
$$p(x) = \frac{k(x)/N}{V} = \frac{\sum_{i} \phi\left(\frac{x-x_{i}}{h}\right)/N}{h^{d}} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{h^{d}} \phi\left(\frac{x-x_{i}}{h}\right)$$
. Can take different  $h$  and test it on  $\sum_{i} \log p_{h}(x_{i})$ , pick highest  $\log$ 

probability. • k-NN: grow V until capture a certain k  $p_N(x) = \frac{k_N(x)/N}{V_N}$ . Mostly used for non-parametric classification:

Joint probability  $p(x, y = c) = \frac{k_c/N}{V}$ Posterior  $p(y = c|x) = \frac{p(x, y = c)}{\sum_{c'=1}^C p(x, y = c')} = \frac{\frac{(k_c/N)/V}{\sum_{c'=1}^C (k_{c'}/N)/V}}{\sum_{c'=1}^C (k_{c'}/N)/V} = \frac{k_c}{\sum_{c'=1}^C k_{c'}} = \frac{k_c}{K}$ Distance metric:  $\operatorname{dist}(a, b) = \left(\sum_{j=1}^D |a_j - b_j|^p\right)^{1/p}.$ 

#### 1.6 Bayesian Statistics

2) feature likelihood:  $P(X = x|Y = c_k) = \prod_{j=1}^{n} P\left(X^{(j)} = x^{(j)}|Y = c_k\right)$  (Naive). To Bayesian way is to use posterior, one of which is classify:  $y = \max_{c_k} P(Y = c_k) \prod_{j=1}^{n} P\left(X^{(j)} = x^{(j)}|Y = c_k\right)$  and sensitive to parametrization. But ML or posterior predictive don't have such problem.

Bayesian model selection.  $\hat{m} = \underset{m}{\operatorname{argmax}} p(m|D) = \underset{m}{\operatorname{argmax}} p(D|m)p(m) = \underset{m}{\operatorname{argmax}} p(D|m), \ p(D|m)$  is called **marginal likelihood**. Previously, if we want to estimate model parameter  $\theta$ :  $\theta_{MAP} = \underset{\theta}{\operatorname{argmax}} p(\theta|D) = \underset{\theta}{\operatorname{argmax}} \frac{p(\theta)p(D|\theta)}{p(D)} \text{ and we can drop } p(D); \text{ but consider the implicit}$ 

model choice, becomes:  $\frac{p(\theta|m)p(D|\theta,m)}{p(D|m)},$  and the one we drop is actually marginal likelihood p(D|m) (because it's constant when we only consider one model).

$$\begin{split} BIC(M,\mathcal{D}) &\triangleq \log p\left(\mathcal{D}|\hat{\pmb{\theta}}_{MLE}\right) - \frac{\operatorname{dof}(M)}{2}\log N,\\ \text{larger BIC, better model. Bayesian factor:} \\ BF_{1,0} &= \frac{p(D|M_1)}{p(D|M_0)}. \end{split}$$

Bayesian decision theory. Bayes' estimator:  $\delta(x) = \operatorname{argmin} \rho(a|x)$ , where

 $\begin{array}{l} \rho(a|x) = \mathbb{E}_{p(y|x)}[L(y,a)] = \sum_y L(y,a)p(y|x). \\ \text{[nature picks } y \in \mathcal{Y} \text{ and generates observation } \\ x \in \mathcal{X}, \text{ we choose action } a \in \mathcal{A} \text{ with minimum loss.]} \end{array}$ 

MAP minimizes 0-1 loss: 
$$\rho(a|x) = \sum_y L(y,a) p(y|x) = p(y \neq a|x)$$
 
$$= 1 - p(y = a|x)$$

MMSE corresponds to posterior mean, which minimizes  $l_2$  loss:

$$\rho(a|x) = \sum_{y} L(y, a)p(y|x)$$

$$= E\left[(y-a)^{2}|x\right] ,$$

$$= E\left(y^{2}|x\right) - 2aE(y|x) + a^{2}$$

$$\frac{\partial}{\partial a}\rho(a|x) = -2E(y|x) + 2a = 0$$

$$\Rightarrow a = E(y|x) ,$$
posterior

median minimizes  $l_1$  loss.

We can threshold the decision by false negative loss and false positive loss:  $\frac{p(y=1|x)}{p(y=0|x)} > \frac{L_{FP}}{L_{FN}} = \tau$ . We can vary  $\tau$  to draw ROC.

Mixture of conjugate priors.

 $p(\theta) = \sum_{k} p(z=k)p(\theta|z=k)$ , so posterior  $p(\theta|D) = \sum_{k} p(z=k|D)p(\theta|D,z=k)$ .

# 2 Representation Learning

# 2.1 Unsupervised: PCA, NMF (& ICA)

In PCA, we want to capture the big variability and ignore the small variability, and after ordering, we choose the first k "direction" to project the raw data on. Each PC is **orthogonal** to each other. Given data:  $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$  Using  $1^{st}$  PC we project data onto  $z_1 = a_1^T x, a_1$  is chosen such that  $\text{var}[z_1] = a_1^T Sa_1$  is maximized (under the constraint  $a_1^T a_1 = 1$ ), where S is the covariance matrix. The solution:  $a_1$  is the eigenvector of S corresponding to the largest eigenvalue. And in general,  $\text{var}[z_k] = a_k^T Sa_k = \lambda_k$ , the  $k^{th}$  PC  $z_k$  retains the  $k^{th}$  greatest variation. STEPS:

1. covariance matrix:  $S = \frac{1}{n} \sum_{i=1}^{n} (x_i - \overline{x}) (x_i - \overline{x})^T$  2. eigenvectors:  $\{a_i\}_{i=1}^d$ 

3. first p eigenvectors:  $\{a_i\}_{i=1}^p$ 

4. transformation:  $G \leftarrow [a_1, a_2, \dots, a_p]_{d \times p}$ 

5.  $y = G^T x$ 

Using SVD:

• centering:  $X_{d,n} = [(x_1 - \overline{x}), \dots, (x_n - \overline{x})]$ 

• SVD:  $X = U_{d,d}D_{d,n}(V_{n,n})^T$  $(S = XX^T = UD^2U^T)$ 

• reconstruct:  $\tilde{x}_i = \overline{x} + U_{d,p}U_{d,p}^T(x_i - \overline{x})$ 

A criterion for p:  $\frac{\sum_{i=1}^{p} \lambda_i}{\sum_{i=1}^{d} \lambda_i} \ge Threshold(e.g.0.95)$ In NMF, we express an image vector as the

linear combination of a set of basis images. Unlike PCA, the coefficients are positive only (PCA involves subtraction due to some negative values after de-mean). Factorization:

 $V_{n,m} \approx W_{n,r}H_{r,m}$ . V contains m images, one of which has n non-negative pixel values; W has rcolumns of basis images; each column in H is called encoding.

STEPS:

1. objective:

$$\min_{W,H} \|V - WH\|^2 \text{ s.t. } W \ge 0, H \ge 0$$
  
2. a pixel:  $V_{i\mu} = (WH)_{i\mu} = \sum_{a=1}^r W_{ia} H_{a\mu}$ 

3. gradient descent:  $H_{a\mu} \leftarrow$ 

$$H_{a\mu} + \eta_{a\mu} \left[ \left( W^T V \right)_{a\mu} - \left( W^T W H \right)_{a\mu} \right]$$
4. multiplicative update rule:

$$H_{a\mu} \leftarrow H_{a\mu} \frac{(\hat{W}^T V)_{a\mu}}{(W^T W H)_{a\mu}}$$
$$(\eta_{a\mu} = \frac{H_{a\mu}}{(W^T W H)_{a\mu}})$$

In summary: PCA has holistic representation, while NMF has part-based; PCA uses eigenfaces as basis image, while NMF uses locallized features: each face in PCA is a linear combination of all eigenfaces, while in NMF only additive combinations.

# 2.2 Supervised: LDA, GE

**LDA** finds the most discriminative projection by maximizing between-class distance and minimizing within-class distance. We define: Class-specific mean:  $\mu_i = \frac{1}{n_i} \sum_{\mathbf{x} \in C_i} \mathbf{x}$ 

Class-specific covariance:

 $\mathbf{S}_i = \frac{\hat{\mathbf{I}}}{n_i} \sum_{\mathbf{x} \in C_i} (\mathbf{x} - \mu_i) (\mathbf{x} - \mu_i)^T$ 

Total mean:  $\mu = \frac{1}{N} \sum_{\mathbf{x}} \mathbf{x}$ 

Within-class scatter:  $\mathbf{S}_{W} = \sum_{i=1}^{C} \frac{n_{i}}{N} \mathbf{S}_{i} = \sum_{i=1}^{C} P_{i} \mathbf{S}_{i}$ Between-class scatter:  $\mathbf{S}_{B} = \sum_{i=1}^{C} P_{i} (\mu_{i} - \mu) (\mu_{i} - \mu)^{T}$ 

 $\mathbf{S}_T = \frac{1}{N} \sum_{\mathbf{x}} (\mathbf{x} - \mu)(\mathbf{x} - \mu)^T$ Total covariance:

$$= \mathbf{S}_W + \mathbf{S}_B$$

In two-class case, given data:  $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{R}^d$ , we seek a projection w(onto a scalar):  $y = w^T x$ . Thus within-class scatter:  $\tilde{S}_i^2 = \sum_{x \in c_i} (w^T x - w^T \mu_i)^2$ ; between-class scatter:  $J(w) = |\tilde{\mu}_1 - \tilde{\mu}_2| = |w^T (\mu_1 - \mu_2)|$ . And Fisher

linear discriminant is to maximize  $J(w) = \frac{|\tilde{\mu}_1 - \tilde{\mu}_2|^2}{\tilde{S}_1^2 + \tilde{S}_2^2} = \frac{w^T S_B w}{w^T S_W w}$ . (NOTE that  $S_B$  is the outer product of two vectors, its rank is at most 1). Taking derivative and setting to zero yield:  $(w^T S_W w) S_B w - (w^T S_B w) S_W w =$  $S_B w - J(w)S_W w = 0 \Rightarrow S_W^{-1} S_B w = J(w)w$ (Eigenvalue decomposition - since  $\hat{S}_B$  is at most rank 1, only take the first eigenvalue) In multi-class case, we can project on  $[y_1, y_2, \dots y_{C-1}]$ , hence projection is a matrix  $W = [w_1 | w_2 | \dots | w_{C-1}]$ . We want to maximize  $J(W) = \frac{\left|\tilde{S}_B\right|}{\left|\tilde{S}_W\right|} = \frac{\left|W^TS_BW\right|}{\left|W^TS_WW\right|},$  and the optimal projection  $W^*$  is the one whose columns are the eigenvectors corresponding to the largest eigenvalues of the following generalized eigenvalue problem  $W^* = \arg \max \frac{|W^T S_B W|}{|W^T S_W W|}$  $(S_B - \lambda_i S_W) w_i^* = 0$ , where  $\lambda_i = J(w_i) = \text{scalar. Limitations of LDA are 1}$ at most C-1 feature projections; 2) parametric

(assumes unimodal Gaussian likelihoods). Graph embedding is a general framework for feature extraction. We define intrinsic graph  $G = [x_i, S_{ij}]$  and penalty graph  $G^P = [x_i, S_{ij}^P],$ 

S and  $S^{P}$  are similarity matrices, L and B are Laplacian matrices from S and  $S^P$  $(L = D - S, \quad D_{ii} = \sum_{j \neq i} S_{ij} \quad \forall i)$ . Data in high-dimensional space and low-dimensional space (1-D assumed):

 $X = [x_1, x_2, \dots, x_N]$   $y = [y_1, y_2, \dots, y_N]^T$ To preserve graph similarity:

$$y^* = \underset{y^T y=1 \text{ or } y^T B y=1}{\arg \min} \sum_{i \neq j} ||y_i - y_j||^2 S_{ij}$$
$$= \underset{y^T y=1 \text{ or } y^T B y=1}{\arg \min} y^T L y$$

After linearization  $y = X^{\mathrm{T}}w$ , arg min  $w^T w = 1$  or  $w^T X B X^T w = 1$ Solution can be obtained by solving  $\tilde{\boldsymbol{L}}\boldsymbol{v} = \lambda \tilde{\boldsymbol{B}}\boldsymbol{v}$  where  $\tilde{L} = XLX^T$  and  $\tilde{B} = XBX^T$ Letting L = D - W and  $B = D^P - W^P$ , we have Marginal Fisher Criterion:

 $\overline{w^* = \arg\min_{w} \frac{w^T X (D - W) X^T w}{w^T X (D^P - W^P) X^T w}}, \text{ where}$  $W_{ij} = W_{ji} = 1$  if  $x_i$  is among the  $k_1$ -nearest neighbours of  $x_j$  in the same class (intraclass compactness);  $W_{ij}^p = 1$  for the pair (i, j) if  $x_i$  is among the  $k_2$ -nearest neighbours of  $x_i$  in different classes. Compared to LDA no distribution assumption, more projection directions, interclass margin can better characterize the separability of different classes.

#### 2.3Clustering

There is an important distinction between hierarchical (organized as a hierarchical tree) and partitional (into non-overlapping subsets)

sets of clusters. Clusters can also be fuzzy such that a point belongs to every cluster with some probability. Some types of clusters: well-separated, center-based, contiguous, density-based. **K-means** is a partitional clustering method,

which simply initialize K random centroids, and

repeats 1) assigning all points to the closest centroid; 2) recompute the centroid of each cluster. Solutions to initial centroid problem: a) multiple runs; b) use hierarchical clustering to determine initial centroids; c) select more than k initial centroids then choose from them. Most common measure for evaluation is Sum of Squared Error:  $SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$ . We can use the "elbow finding" method to decide K. Hierarchical clustering can be visualized as a dendrogram, which is a tree-like diagram that records the sequence of merges or splits. Clusters are produced when cutting at proper level. It can be agglomerative or divisive. Algorithm for agglomerative clustering: 1) compute proximity matrix; 2) let each point be a cluster; 3) repeat: a. merge two closest clusters, b. update the proximity matrix until only one cluster remains. We can use MIN (noise-sensitive), MAX (biased towards globular clusters), Group Average (same as MAX) or Distance Between Centroid to define the inter-cluster similarity.

### Models

# 3.1 Gaussian Mixture Model, Boosting

GMM is generative while boosting is discriminative.

**GMM**:  $P(y|\theta) = \sum_{k=1}^{K} \alpha_k \phi(y|\theta_k)$ , where  $\alpha_k \geqslant 0, \quad \sum_{k=1}^K \alpha_k = 1 \text{ and } \phi(y|\theta_k) =$  $\phi\left(y|\left(\mu_k, \sigma_k^2\right)\right) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{\left(y - \mu_k\right)^2}{2\sigma_k^2}\right)$ 

EM algorithm: After initializing  $\theta^{(0)}$ , compute  $Q(\theta, \theta^{(i)}) = E_Z \left[ \log P(Y, Z|\theta) | Y, \theta^{(i)} \right]$  $= \sum \log P(Y, Z|\theta) P\left(Z|Y, \theta^{(i)}\right), \text{ and }$ 

then update  $\theta^{(i+1)} = \arg \max_{\theta} Q(\theta, \theta^{(i)})$  until convergence.

Back in GMM, the latent variable is r.v.  $\gamma_{jk} = \left\{ \begin{array}{l} 1, \text{observation j from component k} \\ 0, \text{otherwise} \end{array} \right.$  . Its

expectation  $\hat{\gamma}_{jk} = \frac{\alpha_k \phi(y_j | \theta_k)}{\sum_{k=1}^K \alpha_k \phi(y_j | \theta_k)}$ . To maximize the Q function (partial and set to zero):  $\hat{\mu}_k = \frac{\sum_{j=1}^{N} \hat{\gamma}_{jk} y_j}{\sum_{j=1}^{N} \hat{\gamma}_{jk}}, \hat{\sigma}_k^2 = \frac{\sum_{j=1}^{N} \hat{\gamma}_{jk} (y_j - \mu_k)^2}{\sum_{j=1}^{N} \hat{\gamma}_{jk}}$  $\hat{\alpha}_k = \frac{n_k}{N} = \frac{\sum_{j=1}^{N} \hat{\gamma}_{jk}}{\sum_{k=1}^{N} \hat{\gamma}_{jk}}.$ 

Boosting defines a strong classifier using an additive model of many weak classifier. (Omitted

### 3.2 Support Vector Machines

Separating hyper-plane:  $w^* \cdot x + b^* = 0$  or decision function  $f(x) = \text{sign}(w^* \cdot x + b^*)$  for binary classification. Functional margin:  $\hat{\gamma}_i = y_i (w \cdot x_i + b)$ ; geometric margin:  $\gamma_i = y_i \left( \frac{w}{\|w\|} \cdot x_i + \frac{b}{\|w\|} \right)$ . If we want to maximize the geometric margin, we need  $\min_{w,b} \frac{1}{2} ||w||^2$ s.t.  $y_i(w \cdot x_i + b) - 1 \ge 0, \quad i = 1, 2, \dots, N$ 

to find  $w^*$  and  $b^*$ . Lagrange function:  $L(w, b, \alpha) =$ 

 $\frac{1}{2} \|w\|^2 - \sum_{i=1}^{N} \alpha_i y_i \left( w \cdot x_i + b \right) + \sum_{i=1}^{N} \alpha_i,$ partial  $\nabla_w L(w, b, \alpha) = w - \sum_{i=1}^{N} \alpha_i y_i x_i = 0$  $\nabla_b L(w, b, \alpha) = \sum_{i=1}^{N} \alpha_i y_i = 0$ 

$$L(w, b, \alpha) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (x_i \cdot x_j) -$$

$$\sum_{i=1}^{N} \alpha_i y_i \left( \left( \sum_{j=1}^{N} \alpha_j y_j x_j \right) \cdot x_i + b \right) + \sum_{i=1}^{N} \alpha_i$$

$$= -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j (x_i \cdot x_j) + \sum_{j=1}^{N} \alpha_i$$

min  $\alpha$  =  $\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_{i}\alpha_{j}y_{i}y_{j}$   $(x_{i}\cdot x_{j}) - \sum_{i=1}^{N}\alpha_{i}$  s.t.  $\sum_{i=1}^{N}\alpha_{i}y_{i} = 0, \alpha_{i} \geq 0, i = 1, 2, \cdots, N$  The resulted separating hyper-plane:  $\sum_{i=1}^{N} \alpha_{i}^{*} y_{i} (x \cdot x_{i}) + b^{*} = 0 \text{ and decision function}$ 

 $f(x) = \operatorname{sign}\left(\sum_{i=1}^{N} \alpha_i^* y_i (x \cdot x_i) + b^*\right)$ . For non-linearly separable data, introduce slack

variable:  $\begin{array}{ll} \min_{w,b,\xi} & \frac{1}{2} ||w||^2 + C \sum_{i=1}^N \xi_i \\ \text{s.t.} & y_i \left( w \cdot x_i + b \right) \geqslant 1 - \xi_i, \xi_i \geqslant 0, i = \cdots \end{array},$ and its dual is  $\min_{\alpha} \quad \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \left( x_i \cdot x_j \right) - \sum_{i=1}^{N} \alpha_i \\ \text{s.t.} \quad \sum_{i=1}^{N} \alpha_i y_i = 0, 0 \leqslant \alpha_i \leqslant C, i = 1, 2, \cdots, N$ 

Using kernel trick, the kernel function  $K(x,z) = \phi(x) \cdot \phi(z)$  and the mapping  $\phi(x): \mathcal{X} \to \mathcal{H}$ . The objective function becomes  $W(\alpha) =$ 

 $\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_{i}\alpha_{j}y_{i}y_{j}K\left(x_{i},x_{j}\right)-\sum_{i=1}^{N}\alpha_{i}$ , and the separating hyper-plane becomes

 $f(x) = \operatorname{sign}\left(\sum_{i=1}^{N_s} a_i^* y_i \phi(x_i) \cdot \phi(x) + b^*\right) =$  $\operatorname{sign}\left(\sum_{i=1}^{N_s} a_i^* y_i K\left(x_i, x\right) + b^*\right).$ 

#### 3.3 Neural Networks

Simple neuron:

 $h_{w,b}(x) = f(W^T x) = f(w^T x + b)$ . f can be sign activation, sigmoid  $(f(x) = \frac{1}{1 + \exp(-x)}),$ ReLU ... Weight updating:  $w_i = w_i + \Delta w_i$ ;  $\Delta w_i = \eta \sum_d (y_d - o_d) \, x_{id}; \, o_d = f \left( \sum_{i=0}^n w_i x_{id} \right).$  Softmax (probability of class k given input):  $P \left( c_k = 1 | x \right) = \frac{e^{o_k}}{\sum_{j=1}^c e^{o_j}}; \, \text{crossentropy loss:}$  $L(x, y; \theta) = -\sum_{j=1}^{c} y_j \log p(c_j|x)$ . So learning is to find  $\theta^* = \operatorname{argmin}_{\theta} \sum_{n=1}^{N} L(x^n, y^n; \theta)$