### Intro to ML

Objective Function for Vanilla Linear Regression:

$$J(\omega) = \frac{1}{2} ||t - X\omega||_2^2 \tag{1}$$

We solve for the optimal  $\omega$  by taking the derivative of the objective function with respect to  $\omega$  and setting it to zero:

$$\frac{\partial J(\omega)}{\partial \omega} = 0, (X^T X)^{-1} X^T t = \omega \tag{2}$$

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} t = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_n \end{bmatrix}$$
 (3)

$$(X^T X + \lambda I)^{-1} X^T t = \omega \tag{4}$$

# Experimental Design and Analysis

#### **Basis Functions**

$$\phi(x) = \begin{bmatrix} \phi_0(x) \\ \phi_1(x) \\ \vdots \\ \phi_M(x) \end{bmatrix}$$

$$\phi_j(x) = \exp{-\frac{\|x - \mu\|^2}{2\sigma^2}}$$
 (6)

$$\phi_j(x) = x^j \tag{7}$$

#### **Model Selection**

$$\min_{\omega} \frac{1}{2} \|t - X\omega\|_2^2 + \lambda \|\omega\|_1 \tag{8}$$

$$\min_{\omega} \frac{1}{2} \|t - X\omega\|_2^2 + \lambda_1 \|\omega\|_1 + \lambda_2 \|\omega\|_2^2, \quad \lambda_1 + \lambda_2 = 1 \quad (9)$$

#### Metrics of Regression

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (t_i - \hat{t}_i)^2$$
 (10)

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |t_i - \hat{t}_i|$$
 (11)

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (t_{i} - \hat{t}_{i})^{2}}{\sum_{i=1}^{n} (t_{i} - \bar{t})^{2}}, \quad \bar{t} = \frac{1}{n} \sum_{i=1}^{n} t_{i}$$
 (12)

$$R^{2} = 1 - \frac{\|t - X\omega\|_{2}^{2}}{\|t - \bar{t}\|_{2}^{2}}$$
 (13)

### **Bayesian Learning**

$$\omega_{MLE} = \arg_{\omega} \max \prod_{i=1}^{n} p(t_i|x_i, \omega)$$
 (14)

$$\omega_{MLE} = \arg_{\omega} \max \sum_{i=1}^{N} \ln p(t_i|x_i, \omega)$$
 (15)

$$\omega_{MLE} = \arg_{\omega} \min \mathbb{E}_{\phi(x)} [\ln p(t|x,\omega)]$$

$$\omega_{\text{MAP}} \propto \arg_{\omega} \max \prod_{i=1}^{N} \mathcal{N}(t_i; y_i, 1) \mathcal{N}(\omega_j; 0, \frac{1}{\lambda})$$
 (16)

- 1. Gaussian-Gaussian
- 2. Gaussian-Exponential
- 3. Gaussian-Gamma
- 4. Gaussian-Beta
- 5. Gaussian-Dirichlet
- 6. Gaussian-Wishart
- 7. Gaussian-Inverse Wishart
- 8. Gaussian-Student's t
- 9. Gaussian-Laplace
- 10. Gaussian-Cauchy

### (5) Generative Models

$$p(t|x,\omega) = \mathcal{N}(t;\omega^T \phi(x), \beta^{-1})$$
(17)

$$p(x|\omega) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x; \mu_k, \Sigma_k)$$

$$\Theta = \{\pi_1, \pi_2, \dots, \pi_K, \mu_1, \mu_2, \dots, \mu_K, \Sigma_1, \Sigma_2, \dots, \Sigma_K\}, \quad \sum_{k=1}^K \pi_k = 1$$

$$\mathcal{L}_0 = \prod_{i=1}^{N} \sum_{k=1}^{K} \pi_k \mathcal{N}(x_i; \mu_k, \Sigma_k)$$

$$\ln \mathcal{L}_0 = \sum_{i=1}^N \ln \sum_{k=1}^K \pi_k \mathcal{N}(x_i; \mu_k, \Sigma_k)$$

 $z_i$  = label of the Gaussian component for the  $i^{th}$  data point  $x_i$ 

$$\mathcal{L}^c = \prod_{i=1}^N \pi_{z_i} \mathcal{N}(x_i; \mu_{z_i}, \Sigma_{z_i})$$

$$Q(\Theta, \Theta^{(t)}) = \mathbb{E}_z[\ln p(x, z|\Theta)|X, \Theta^{(t)}]$$

(12) 
$$P(z_i|x_i, \Theta^{(t)}) = \frac{P(x_i|z_i, \Theta^t)P(z_i|\Theta^t)}{P(x_i|\Theta^t)} = \frac{\pi_{z_i}\mathcal{N}(x_i; \mu_{z_i}, \Sigma_{z_i})}{\sum_{k=1}^K \pi_k \mathcal{N}(x_i; \mu_k, \Sigma_k)}$$

$$C_{ik} = P(z_i|x_i, \Theta^{(t)}) = \frac{\pi_k \mathcal{N}(x_i; \mu_k, \Sigma_k)}{\sum_{j=1}^K \pi_j \mathcal{N}(x_i; \mu_j, \Sigma_j)}$$

$$\arg_{\Theta} \max Q(\Theta, \Theta^{(t)}) = \sum_{z_i}^K \ln(\mathcal{L}^c) P(z_i | x_i, \Theta^{(t)})$$

$$= \sum_{z_i=1}^K \ln(\prod_{i=1}^N \pi_{z_i} G(x_i; \mu_{z_i}, \Sigma_{z_i})) P(z_i | x_i, \Theta^{(t)})$$

$$= \sum_{k=1}^{K} \sum_{i=1}^{N} (\ln(\pi_k) + \ln(G(x_i; \mu_k, \Sigma_k))) C_{ik}$$

$$= \sum_{k=1}^{K} \sum_{i=1}^{N} (\ln(\pi_k) - \frac{d}{2} \ln(2\pi) - \frac{d}{2} \ln(\sigma_k^2) - \frac{1}{2\sigma_k^2} \|x_i - \mu_k\|_2^2) C_{ik}$$

$$\mu_K = \frac{\sum_{i=1}^{N} \mathbf{x}_i C_{ik}}{\sum_{i=1}^{N} C_{ik}}$$

$$\sigma_k^2 = \frac{\sum_{i=1}^{N} C_{ik} ||x_i - \mu_k||_2^2}{d \sum_{i=1}^{N} C_{ik}}$$

$$\pi_k = \frac{\sum_{i=1}^{N} C_{ik}}{N}$$

## Non-Parametric Models

$$J(\Theta, U) = \sum_{i=1}^{N} \sum_{k=1}^{K} u_{ik} d^{2}(x_{i}, \theta_{k}) = \sum_{i=1}^{N} \sum_{k=1}^{K} u_{ik} ||x_{i} - \theta_{k}||_{2}^{2}$$

$$\theta_k = \frac{\sum_{x_i \in C_k} x_i}{N_k}$$

- 1.  $b_i$  = average distance from  $x_i$  to all other points in the same cluster
- 2.  $a_i$  = average distance from  $x_i$  to all other points in the nearest cluster

Silhouette = 
$$\frac{1}{N} \sum_{i=1}^{N} \frac{b_i - a_i}{\max(a_i, b_i)}$$

- 1. a = number of pairs of elements in S that are in the same cluster and in the same set in S'
- 2. b = number of pairs of elements in S that are in different clusters and in different sets in S'
- 3. c = number of pairs of elements in S that are in the same cluster and in different sets in S'
- 4. d = number of pairs of elements in S that are in different clusters and in the same set in S'

Rand Index = 
$$\frac{a+b}{a+b+c+d}$$

$$Jaccard = \frac{TP}{TP + FP + FN}$$