i.i.d: independent and identically distributed

1 Math Basics

Eigenvectors: $Ax = \lambda x$

A matrix $A \in \mathbb{R}^n$ has eigenvectors if A is square and not singular $(\det(A) \neq 0).$

$$A = A^{\top} \implies \lambda_i \text{ is real} \qquad \operatorname{rank}(A) = n \implies \lambda_i \neq 0 \quad \forall i$$
$$x^{\top} A x > 0 \implies \lambda_i > 0 \qquad \qquad x^{\top} A x \geq 0 \implies \lambda_i \geq 0 \quad \forall i$$

Positive definite: $x^{\top}Ax > 0 \quad \forall x \neq 0$

Positive semidefinite: $x^{\top}Ax \geq 0$ $\forall x \neq 0$

Positive semidefinite:
$$\mathbf{x}^{\top} A \mathbf{x} \geq 0 \quad \forall \mathbf{x} \neq 0$$

Jacoobi-Matrix: $\mathbf{J}_f(\mathbf{x}) = \frac{df(\mathbf{x})}{d\mathbf{x}} = \begin{bmatrix} \frac{df_i(\mathbf{x})}{dx_j} \end{bmatrix}_{i=1...m;j=1...n}$

$$g(x) \circ f(x) \implies \mathbf{J}_{g \circ f}(\mathbf{x}) = \mathbf{J}_g(f(\mathbf{x})) \cdot \mathbf{J}_f(\mathbf{x})$$

$$\begin{aligned} \mathbf{Hessian\text{-}Matrix:} \ \mathbf{H}_f(\mathbf{x}) &= \frac{d^2 f(\mathbf{x})}{d\mathbf{x}^2} = \left[\frac{\partial^2 f_i(\mathbf{x})}{\partial x_j \partial x_k}\right]_{i=1...m;j,k=1...n} \end{aligned}$$

1.1 Statistics

Normal Distribution:
$$f_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Bernoulli Distribution: $f_X(x) = p^x (1-p)^{1-x} \ x \in \{0, \}$

Maximum likelihood estimation

$$L(x;\theta) = \prod_{i=1}^{N} f_{X_i}(x_i;\theta) \qquad l(x;\theta) = \sum_{i=1}^{N} \log f_{X_i}(x_i;\theta)$$

1.2 Convexity

1.3 Non-Linear Optimization

Kernel Trick

 $\kappa: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a **kernel function** if the following two conditions are fulfilled (with an arbitrary function $f \in L_2(\mathcal{X})$):

Positive definite: $\int_{\mathcal{X}\times\mathcal{X}} f(\mathbf{x}) \kappa(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) dx dy \geq 0$

Symmetry: $\kappa(\mathbf{x}, \mathbf{y}) = \kappa(\mathbf{y}, \mathbf{x})$

2.1 Common Kernels $(a, c, d \ge 0 \text{ and } \sigma > 0)$

Linear Kernel: $\kappa(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{y} + c$

Polynomial Kernel: $\kappa(\mathbf{x}, \mathbf{y}) = (a\mathbf{x}^T\mathbf{y} + c)^d$

Gaussian Kernel: $\kappa(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{||\mathbf{x} - \mathbf{y}||^2}{2\sigma^2}\right)$

Exponential Kernel: $\kappa(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{||\mathbf{x} - \mathbf{y}||^{\gamma}}{2\sigma^{2}}\right)$

2.2 Properties

Given the kernels κ_1 and κ_2 , c > 0 and an arbitrary function f the following combinations are valid kernels:

$$c\kappa_1(\mathbf{x})$$
 $c + \kappa_1(\mathbf{x})$ $f(\mathbf{x})f(\mathbf{y})$
 $\kappa_1(\mathbf{x})\kappa_2(\mathbf{x})$ $\kappa_1(\mathbf{x}) + \kappa_2(\mathbf{x})$

Mercer's Theorem: Let κ be a kernel, then there exists functions ϕ_i and a $\lambda_i \geq 0$ such that:

$$\kappa(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{\infty} \lambda_i \phi_i(\mathbf{x}) \phi_i(\mathbf{y})$$

3 Unsupervised Learning

3.1 K-Means

$$\mathcal{F} = \{f : \mathbb{R}^p \to \{\mathbf{c}_1, \dots, \mathbf{c}_k\} \subset \mathbb{R}^p\} \quad L(\mathbf{X}, f(\mathbf{X})) = ||\mathbf{X} - \mathbf{f}(\mathbf{X})||^2$$

Where \mathbb{R}^p is the feature space. \mathbf{c}_i is the center of cluster i.

Because f maps to a finite set, the volume of the set distribution is zero. Algorithms: Lloyd's algorithm, MaxQueen's algorithm

3.2 Principle Component Analysis

$$\mathcal{F} = \left\{ f : \mathbb{R}^p \to \mathbb{R}^k \subset \mathbb{R}^p \right\} \qquad L(\mathbf{X}, f(\mathbf{X})) = ||\mathbf{X} - \mathbf{U}_k \mathbf{U}_k^\top \mathbf{X}||_2^2$$

Where \mathbb{R}^p is the feature space. And $f(\mathbf{X}) = \mathbf{U}_k^{\top} \mathbf{X}$ is a (orthogonal) projection on to the subspace \mathbb{R}^k .

Principle components: $\mathbf{S} = \mathbf{U}_k^{\top} \mathbf{X} = \mathbf{\Sigma}_k \mathbf{V}_k^{\top}$

3.2.1 Kernel PCA

4 Supervised Learning

Expected Prediction Error: EPE(f) = E[L(Y, f(X))]

$$f(x) = \operatorname{argmin}_{f \in \mathcal{F}} \operatorname{EPE}(f) \approx \operatorname{argmin}_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} L(y_i, f(x_i)) = \hat{f}(x)$$

Quadratic Loss: $L_2(Y, f(X)) = (Y - f(X))^T$

Absolute Loss (l_1 -loss): $L_1(Y, f(X)) = |Y - f(X)|$

$$f_2(x) = \mathcal{E}_{Y|X=x}[Y]$$
 $f_1(x) = \text{median}_{Y|X=x}[Y]$

Generalization error: $G_N(f) = EPE(f) - \frac{1}{N} \sum_{i=1}^{N} L(y_i, f(x_i))$

4.1 Linear regression

$$\mathcal{F} = \left\{ f(\mathbf{x}) = \theta_0 + \sum_{k=1}^p \theta_k x_k \middle| \theta_k \in \mathbb{R}, p \in \mathbb{N} \right\}$$

4.2 K-nearest Neighbors

$$\hat{f}_k(x) = \frac{1}{k} \sum_{i \in N_k(x)} y_i \quad \forall i \text{ s.t. } x_i \in N_k(x)$$

Where $N_k(x)$ is the set of the k nearest neighbors of x

$$\lim_{N,k\to\infty,\frac{k}{N}\to 0} \hat{f}_k(x) = \mathrm{E}[Y|X=x]$$

4.3 Logistic regression

$$\mathcal{F} = \{ f(\mathbf{x}) = \mathbf{w}^{\top} \mathbf{x} + b \mid \mathbf{w} \in \mathbb{R}^p, b \in \mathbb{R} \}$$

$$\begin{split} L_{0,1}(Y,f(X)) &= \begin{cases} 1 & \text{if } Yf(X) \leq 0 \\ 0 & \text{otherwise} \end{cases} \ l(Y,f(X)) = \log\left(1 + e^{-Yf(X)}\right) \\ f \text{ could be an arbitrary function, but usually } f \text{ is chosen as defined above.} \end{split}$$

$$Pr(Y = y|\mathbf{x}) = \exp(-l(y, f(\mathbf{x}))) = \frac{1}{1 + e^{-yf(\mathbf{x})}} = \sigma(yf(\mathbf{x}))$$

Regularization: $\tilde{l}(y, f(\mathbf{x})) = l(y, f(\mathbf{x})) + \lambda (||\mathbf{w}||^2 + b^2)$

4.4 Feedforward Neural Network

$$f: \mathbb{R}^p \to \mathbb{R}^r \quad x \mapsto \sigma_l \circ \varphi_{\mathbf{w}_l} \circ \cdots \circ \sigma_1 \circ \varphi_{\mathbf{w}_1}(x)$$

$$\varphi_{\mathbf{w}}: \mathbb{R}^p \to \mathbb{R}^m \quad \mathbf{x} \mapsto \mathbf{W}\mathbf{x} \qquad \sigma: \mathbf{x} \mapsto [\sigma(x_1), \dots, \sigma(x_m)]^{\top}$$

Where m is the number of neurons in the layer and p is the number of input features/neurons from the previous layer.

Rectified Linear Unit (ReLU): $\sigma(x) = \max(0, x)$

Update rule:
$$\mathbf{W}_j \leftarrow \mathbf{W}_j - \alpha \pi_j^{-1} \left(\frac{d}{d\mathbf{W}_j} L(\mathbf{y}_i, f(\mathbf{x}_i)) \right)^{\top}$$

Softmax:
$$\mathbf{x} \mapsto \left(\sum_{\mathbf{x}} \exp(x_i)\right)^{-1} \left[\exp(x_1), \dots, \exp(x_C)\right]^{\top}$$

Cross entropy: $H(p, q) = -\sum_{i=1}^{n} p_i \log q_i$; $L(f(\mathbf{x}), \mathbf{y}_c) = -log(f(\mathbf{x})_c)$

Where c is the correct class in a multiclass classification problem with Cclasses

4.5 Support Vector machine