Machine Learning

LI Tao

July 14, 2013

Chapter 1

Bayesian Decision Theory

Bernoulli : $P(X) = p_0^X(1-p_0)^{1-X}$, p_0 is the param.

Estimation of p_0 form $\mathcal{X} = \{x^{(l)}\}_{l=1}^N$:

$\hat{p_0} = \frac{\#\text{heads}}{\#\text{tosses}} = \frac{\sum_{l=1}^N x^{(l)}}{N}$

Predict outcome = head if $P_0 > 1/2$, tail otherwise.

Baye's Rule :

Posterior$P(C|\mathbf{x}) = \frac{\text{likelihood}\times\text{prior}}{\text{evidence}} = \frac{p(\mathbf{x}|C)P(C)}{p(\mathbf{x})}$

Baye for $K > 2$ classes:

$P(C_i|\mathbf{x}) = \frac{p(\mathbf{x}|C_i)P(C_i)}{\sum_{k=1}^K p(\mathbf{x}|C_k)P(C_k)}$

Optimal decision: Choose C_i if $P(C_i|\mathbf{x}) = \max_k(C_k|\mathbf{x})$

Losses and Risks :

$R(\alpha_i|\mathbf{x}) = \sum_{k=1}^K \lambda_{ik}P(C_k|\mathbf{x})$,

α_i the action assigned to class C_i, λ_{ik} loss for α_i if C_k

Optimal:α_i if $R(\alpha_i|\mathbf{x}) = \min_k R(\alpha_k|\mathbf{x})$

0-1 loss : $R(\alpha_i|\mathbf{x}) = \sum_{k=1}^K \lambda_{ik}P(C_k|\mathbf{x}) = 1 - P(C_i|\mathbf{x})$,

$\lambda_{ik} = 1$ if $i \neq k$, 0 otherwise

Reject Option : Loss:

$$\lambda_{ik} = \begin{cases} 1 & \text{if } i = k \\ \lambda & \text{if } i = K+1 \\ 0 & \text{otherwise} \end{cases}$$

λ is the loss for choosing reject.

Expected risk:

$$R(\alpha_i|\mathbf{x}) = \begin{cases} \sum_{k=1}^K \lambda P(C_k|\mathbf{x}) = \lambda & \text{if } i = K+1 \\ \sum_{k\neq 1} P(C_k|\mathbf{x}) = 1 - P(C_i|\mathbf{x}) & \text{if } i \in 1,\dots,K \end{cases}$$

Optimal Decision: choose C_i if

$R(\alpha_i|x) = \min_{1\leq k\leq K} R(\alpha_i|\mathbf{x}) < R(\alpha_{K+1}|\mathbf{x})$,

Reject otherwise.

Discriminant Functions : choose C_i if $g_i(\mathbf{x}) = \max_k g_k(x)$

$g_i(\mathbf{x}) = -R(\alpha_i|x) = P(C_i|\mathbf{x}) = p(\mathbf{x}|C_i)P(C_i)$

Two class may define single discriminant functions: $g(\mathbf{x}) = g_1(\mathbf{x}) - g_2(\mathbf{x})$, choose C_i if it greater than zero.

Decision Regions $\mathcal{R}_i = \{\mathbf{x}|g_i(\mathbf{x}) = \max_k g_k(\mathbf{x})\}$

Bayesian Network joint:

$P(X_1,\dots,X_d) = \prod_{i=1}^d P(X_i|parents(X_i))$

Chapter 2

Parameter Estimation

Setting Assume data follow a distribution model.$\mathcal{X} = \{\mathbf{x}^{(l)}\}$, $\mathbf{x}^l \sim p(\mathbf{x})$, Assume some parametric form for $p(\mathbf{x}|\theta)$, θ is estimated using $\mathcal{X}$

Param Approach to classification In Baye's rule for classification, $p(\mathbf{x}|C_i)$(likelihood) and $P(C_i)$ (prior) need to be estimated from the sample $\mathcal{X}$

MLE seeks to find θ that makes sampling from $p(\mathbf{x}|\theta)$ as likely as possible

likelihood:
$L(\theta|\mathcal{X}) \equiv p(\mathcal{X}|\theta) = \prod_{l=1}^{N} p(\mathbf{x}^{(l)}|\theta)$

log likelihood: $\mathcal{L} \equiv \log L(\theta|X) = \sum_{l=1}^{N} \log p(\mathbf{x}^{(l)}|\theta)$

Max Likelihood estimate: $\hat{\theta} = arg\max_\theta \mathcal{L}(\theta|\mathcal{X})$

Bernoulli $x \in \{0, 1\}, P(x = 1)$ for $p(C_1)$,
$P(x|p_0) = p_0^x(1 - p_0)^{1-x}$

Log Likelihood:
$\mathcal{L}(p_0|\mathcal{X}) = \sum_{l=1}^{N}[x^{(l)} \log p_0 + (1 - x^{(l)}) \log(1 - p_0)]$

ML estimation: $\hat{p_0} = \frac{1}{N}\sum_{l=1}^{N} x^{(l)}$

Multinomial Ran Var. $\mathbf{x}$ with $K \geq 2$ possible value

Indicator var: $x_i = 1$ if outcome is state i, 0 if not

$P(\mathbf{x}|\theta) = P(X_1, \ldots, x_K|p_1, \ldots, p_K) = \prod_{i=1}^{K} p_i^{x_i}$, $\sum_{i=1}^{K} p_i = 1$

Log likelihood: $\mathcal{L}(p_0|\mathcal{X}) = \sum_{l}^{N}\sum_{i=1}^{K} x_i^{(l)} \log p_i$

ML estimate: $\hat{p_i} = \frac{1}{N}\sum_{l=1}^{N} x_i^{(l)}$

Normal pdf: $p(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-\frac{(x-\mu)^2}{2\sigma^2}]$

$\mathcal{L}(\mu, \sigma|\mathcal{X}) = -\frac{N}{2}\log(2\pi) - N \log\sigma - \frac{1}{2\sigma^2}\sum_{l=1}^{N}(x^{(l)} - \mu)^2$

ML Estimates: $\hat{\mu} = \frac{1}{N}\sum_{l=1}^{N} x^{(l)}$
$\hat{\sigma^2} = \frac{1}{N}\sum_{l=1}^{N}(x^{(l)} - \hat{\mu})^2$

Multivariable Normal $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, $\boldsymbol{\mu}$ mean vec, $\boldsymbol{\Sigma}$ covariance matrix

$p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp[-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})]$

$\mathcal{L}(\boldsymbol{\mu}, \boldsymbol{\Sigma}|\mathcal{X}) = \frac{Nd}{2}\log(2\pi) - \frac{N}{2}\log|\boldsymbol{\Sigma}| - \frac{1}{2}\sum_{l=1}^{N}(\mathbf{x}^{(l)} - \boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}^{(l)} - \boldsymbol{\mu})$

ML estimates: $\hat{\boldsymbol{\mu}} = \frac{1}{N}\sum_{l=1}^{N}\mathbf{x}^{(l)}$,
$\hat{\boldsymbol{\Sigma}} = \frac{1}{N}\sum_{l=1}^{N}(\mathbf{x}^{(l)} - \hat{\boldsymbol{\mu}})(\mathbf{x}^{(l)} - \hat{\boldsymbol{\mu}})^T$

Bias and Variance Bias: $b_\theta(d) = E[d] - \theta$
Variance: $E[d - E[d]^2]$(d is estimator of param θ)

Mean Squared error:
$r(d,\theta) = E[(d-\theta)^2] = \text{bias}^2 + \text{variance}^2$

Bayesian Estimation Treat θ as a Ran Var. Prior $p(\theta)$

Posterior:
$p(\theta|\mathcal{X}) = \frac{p(\mathcal{X}|\theta)p(\theta)}{p(\mathcal{X})} = \frac{p(\mathcal{X}|\theta)p(\theta)}{\int p(\mathcal{X}|\theta')p(\theta')d\theta'}$

Estimation of density at x:
$p(x|\mathcal{X}) = \int p(x|\theta)p(\theta|\mathcal{X})d\theta$

Regression $y = g(x|\theta)$: $y = \int g(x|\theta)p(\theta|\mathcal{X})d\theta$

Computational Considerations

Max a posteriori (MAP): $\theta_{MAP} = arg\max_\theta p(\theta|\mathcal{X})$,
$p(x|\mathcal{X}) \approx p(x|\theta_{MAP})$, $y \approx y_{MAP} = g(x|\theta_{MAP})$

ML estimation: $\theta_{ML} = arg\max_\theta p(\theta|\mathcal{X})$

Bayes' estimation – expectation w.r.t. posterior density:

$$\theta_{Bayes} = E[\theta|\mathcal{X}] = \int \theta p(\theta|\mathcal{X})d\theta$$

Example: Bayesian estimation with known μ, σ and σ_0
$x^{(l)} \sim \mathcal{N}(\theta, \sigma_0^2)$, $\theta \sim \mathcal{N}(\mu, \sigma^2)$
MLE: $\theta_{ML} = \frac{1}{N}\sum_{l=1}^N \mathbf{x}^{(l)} = m$
$\theta_{Map} = \theta_{Bayes} = E(\theta|\mathcal{X}) = \frac{N/\sigma_0^2}{N/\sigma_0^2+1/\sigma^2}m + \frac{1/\sigma^2}{N/\sigma_0^2+1/\sigma^2}\mu$

Classification with Discriminant Functions Gaussian density for each class: $p(x|C_i) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left[-\frac{(x-\mu_i)^2}{2\sigma_i^2}\right]$

Discriminant functions: $g_i(x) = \log\left[p(x|C_i)p(C_i)\right] = -\frac{1}{2}\log 2\pi - \log\sigma_i - \frac{(x-\mu_i)^2}{2\sigma_i^2} + \log P(C_i)$

Sample $\mathcal{X} = \left\{(x^{(l)}, \mathbf{y}^{(l)})\right\}_{l=1}^N (y_i^{(l)} = 1 \text{ if } x^{(l)} \in C_i)$

ML Estimates: $\hat{P}(C_i) = \frac{1}{N}\sum_{l=1}^N y_i^{(l)}$
$m_i = \frac{\sum_{l=1}^N x^{(l)} y_i^{(l)}}{\sum_{l=1}^N y_i^{(l)}} \qquad s_i^2 = \frac{\sum_{l=1}^N (x^{(l)}-m_i)^2 y_i^{(l)}}{\sum_{l=1}^N y_i^{(l)}}$
Discriminant Functions:

$$g_i(x) = -\log s_i - \frac{(x-m_i)^2}{2s_i^2} + \log\hat{P}(C_i)$$

Additive Parametric Model Functional relationship in additive form: $r = f(x) + \epsilon$

Parametric modeling: $f(x) \approx g(x|\theta)$, $\epsilon \sim \mathcal{N}(0, \sigma^2)$

Conditional probability of output given input:

$$p(r|x) \sim \mathcal{N}(g(x|\theta), \sigma^2)$$

Log likelihood given: $\mathcal{X} = \left\{(x^{(l)}, r^{(l)})\right\}$:

$$\mathcal{L}(\theta|\mathcal{X}) = \log\prod_{l=1}^N p(x^{(l)}, r^{(l)}) = \frac{1}{2\sigma^2}\sum_{l=1}^N \left[r^{(l)} - g(x^{(l)}|\theta)\right]^2 + \text{const}$$

Equivalent to minimizing error function:

$$E(\theta|\mathcal{X}) = \frac{1}{2}\sum_{l=1}^N \left[r^{(l)} - g(x^{(l)}|\theta)\right]^2$$

Called least squares estimates

Polynomial Regression

$$g(x^{(l)}|w_0, w_1, \ldots, w_k) = w_k(x^{(l)})^k + \cdots + w_2(x^{(l)})^2 + w_1 x^{(l)} + w_0$$

Least square estimate: $\hat{\mathbf{w}} = (\mathbf{D}^T\mathbf{D})^{-1}\mathbf{D}^T\mathbf{r}$, where:

$$D = \begin{bmatrix} 1 & x^{(1)} & (x^{(1)})^2 & \ldots & (x^{(l)})^k \\ 1 & x^{(2)} & (x^{(2)})^2 & \ldots & (x^{(l)})^k \\ \ldots \\ 1 & x^{(N)} & (x^{(N)})^N & \ldots & (x^{(l)})^k \end{bmatrix}$$

$$\mathbf{r} = \left(r^{(1)}, r^{(2)}, \ldots, r^{(N)}\right)^T$$

Bias and Variance Expected squared error of sample $\mathcal{X}$ $E\left[(r - g(x))^2|x\right] = \left(E\left[r|x\right] - g(x)\right)^2 + E\left[(r - E\left[r|x\right])^2|x\right] =$ squared err + noise

Average over $\mathcal{X}$: $E_{\mathcal{X}} = \left[(E[r|x] - g(x))^2|x\right] = \left(E[r|x] - E_{\mathcal{X}}[g(x)]\right)^2 + E_{\mathcal{X}}\left[(g(x) - E_{\mathcal{X}}[g(x)])^2\right] =$ bias + variance

Chapter 3

Multivariate Method

Multivariate Data N i.i.d. instances:

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \dots x_d^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \dots x_d^{(2)} \\ \dots & & \\ x_1^{(N)} & x_2^{(N)} & \dots x_d^{(N)} \end{bmatrix}$$

Parameters Mean Vector: $E[x] = \mu = (\mu_1, \dots, \mu_d)^T$

Covariance of x_i and x_j:

$$\sigma_{ij} = E\left[(x_i - \mu_i)(x_j - \mu_j)\right] = E[x_i x_j] - \mu_i \mu_j$$

Variance of x_i: $\sigma_i^2 = E\left[(x_i - \mu_i)^2\right]$

Covariance matrix:

$$\begin{aligned} \boldsymbol{\Sigma} &= Cov(\mathbf{x}) = E\left[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T\right] \\ &= \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \dots & \sigma_{1d} \\ \sigma_{21} & \sigma_2^2 & \dots & \sigma_{2d} \\ \dots & & & \\ \sigma_{d1} & \sigma_{d2} & \dots & \sigma_d^2 \end{bmatrix} \end{aligned}$$

Correlation: $\rho_{ij} = \frac{\sigma_{ij}}{\sigma_i \sigma_j}$

x_i and x_j are independent $\Rightarrow \sigma_{ij} = \rho_{ij} = 0$

Parameter Estimation Sample Mean $\mathbf{m} = \frac{1}{N} \sum_{l=1}^{N} \mathbf{x}^{(l)}$

Sam. Cov.: $\mathbf{S} = [s_{ij}]_{i,j=1}^d = \frac{1}{N} \sum_{l=1}^{N} (\mathbf{x}^{(l)} - \mathbf{m})(\mathbf{x}^{(l)} - \mathbf{m})^T$

Multivariate Normal Distribution $\mathbf{x} \sim \mathcal{N}_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$p(x) = \frac{1}{(2\pi)^{d/2} |\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right]$

Mahalanobis distance: $(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$(d-dimensional hyperellipsoid.)

Bivariate Normal Distribution Covariance matrix:

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$$

$p(x_1, x_2) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \exp\left[-\frac{1}{2(1-\rho^2)}(z_1^2 - 2\rho z_1 z_2 + z_2^2)\right]$, where $z_i = \frac{x_i - \mu_i}{\sigma_i}$

Parametric Classification Class-conditional densities:$p(\mathbf{x}|C_i) \sim \mathcal{N}_d(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$:

$$p(\mathbf{x}|C_i) = \frac{1}{(2\pi)^{d/2} |\boldsymbol{\Sigma}_i|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^T \boldsymbol{\Sigma}_i^{-1} (\mathbf{x} - \boldsymbol{\mu}_i)\right]$$

Discriminant functions: $g_i(\mathbf{x}) = \log p(\mathbf{x}|C_i) + \log P(C_i)$
$= -\frac{1}{2}\log 2\pi - \frac{1}{2}\log|\boldsymbol{\Sigma}_i| - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_i)^T \boldsymbol{\Sigma}_i^{-1} (\mathbf{x} - \boldsymbol{\mu}_i) + \log P(C_i)$

Estimation of Parameters $\hat{P}(C_i) = \frac{1}{N}\sum_l r_i^{(l)}$

$\mathbf{m}_i = \frac{\sum_l r_i^{(l)}\mathbf{x}^{(l)}}{\sum_l r_i^{(l)}}$

$\mathbf{S}_i = \frac{\sum_l r_i^{(l)} r_i^{(l)}(\mathbf{x}^{(l)}-\mathbf{m}_i)(\mathbf{x}^{(l)}-\mathbf{m}_i)^T}{\sum_l r_i^{(l)}}$

Quadratic Discriminant Functions

$$g_i(\mathbf{x}) = \mathbf{x}^T\mathbf{W}_i\mathbf{x} + \mathbf{w}_i^T\mathbf{x} + w_0$$

where $\mathbf{W}_i = -\frac{1}{2}\mathbf{S}_i^{-1}$

$\mathbf{w}_i = \mathbf{S}_i^{-1}\mathbf{m}_i$

$w_{i0} = -\frac{1}{2}\mathbf{m}_i^T\mathbf{S}_i^{-1}\mathbf{m}_i - \frac{1}{2}\log|\mathbf{S}_i| + \log\hat{P}(C_i)$

Chapter 4

Dimensionality reduction

Forward Search Start with no features, add them one by one, at each step adding the one that decreases most.

Backward Search Start with all features and so a similar process

Principle Component Analysis Projection of $\mathbf{x}$ on the direction of $\mathbf{w}$: $z = \mathbf{w}^T\mathbf{x}$

Finding the first principle component $\mathbf{w_1}$ such that $Var(z_1)$ is maximized:

$$\begin{aligned} Var(z_1) &= Var(\mathbf{w}^T\mathbf{x}) = E[(\mathbf{w}^T\mathbf{x} - \mathbf{w}^T\boldsymbol{\mu})^2] \\ &= \mathbf{w}^T E[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^T]\mathbf{w} = \mathbf{w}^T\boldsymbol{\Sigma}\mathbf{w} \end{aligned}$$

$Cov(\mathbf{x}) = E[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^T] = \boldsymbol{\Sigma}$

Lagrangian: $\mathbf{w}_1^T\boldsymbol{\Sigma}\mathbf{w}_1 - \alpha(\mathbf{w}_1^T\mathbf{w}_1 - 1)$

Taking derivative:$\boldsymbol{\Sigma}\mathbf{w}_1 = \alpha\mathbf{w}_1$ (eigenvalue equation) $\mathbf{w}_1^T\boldsymbol{\Sigma}\mathbf{w}_1 = \alpha\mathbf{w}_1^T\mathbf{w}_1 = \alpha(\mathbf{w}_1$ is unit)

We choose the eigenvector with the largest eigenvalue for the variance to be maximum.

Second PC: $\mathbf{w}_2^T\boldsymbol{\Sigma}\mathbf{w}_2 - \alpha(\mathbf{w}_2^T\mathbf{w}_2 - 1) - \beta(\mathbf{w}_2^T\mathbf{w}_1 - 0)$

Derivative: $2\boldsymbol{\Sigma}\mathbf{w}_2 - 2\alpha\mathbf{w}_2 - \beta\mathbf{w}_1 = 0$ (times $\mathbf{w}_1^T$ on both side, $\mathbf{w}_1^T\mathbf{w}_2 = 0$

Then $\Sigma\mathbf{w}_2 = \alpha\mathbf{w}_2$, $\mathbf{w}_2$ is the second largest eigenvalue.

Proportion of variance (PoV) Explained:$\frac{\lambda_1,\ldots,\lambda_k}{\lambda_1,\ldots,\lambda_d}$

Factor Analysis Assume latent factors z_j Sample $\mathcal{X} = \{\mathbf{x}^{(l)}\}$, $E(\mathbf{x}) = \boldsymbol{\mu}$, $Cov(\mathbf{x}) = \boldsymbol{\Sigma}$
Factors z_j, $E[z_j] = 0$, $Var(z_j) = 1$
Noise: ϵ_i: $E[\epsilon_i] = 0$, $Var(\epsilon_i) = \Psi_i$, $Cov(\epsilon_i, \epsilon_j) = 0$
$x_i - \mu_i = \sum_{j=1}^k v_{ij}z_j + \epsilon_i$, assume $\boldsymbol{\mu} = 0$, v_{ij} are called factor loading
$Var(x_i) = \sum_{j=1}^k v_{ij}^2 Var(z_j) + Var(\epsilon_i) = \sum_{j=1}^k v_{ij}^2 + \Psi_i$
Covariance Matrix: $\boldsymbol{\Sigma} = Cov(\mathbf{Vz} + \boldsymbol{\epsilon}) = \mathbf{VV}^T + \boldsymbol{\Psi}$
Factor loading: $Cov(\mathbf{x}, \mathbf{z}) = \mathbf{V}$
Dim reduc: Given $\mathbf{S}$ as the estimator of $\boldsymbol{\Sigma}$, we want to find $\mathbf{V}$ and $\boldsymbol{\Psi}$ s.t. $\mathbf{S} = \mathbf{VV}^T + \boldsymbol{\Psi}$, $\boldsymbol{\Psi} = diag(\Psi_i)$

Multidimensional Scaling lower dimension preserve pairwise distances.
Sample $\mathcal{X} = \{\mathbf{x}^{(l)} \in \mathbb{R}^d\}_{l=1}^N$
Squared Euclidean distance between point r and s:

$$d_{rs}^2 = \sum_{j=1}^d (x_j^{(r)} - x_j^{(s)})^2 = b_{rr} + b_{ss} - 2b_{rs}$$

$b_{rs} = \sum_{j=1}^d x_j^{(r)} x_j^{(s)}$, or matrix form $\mathbf{B} = \mathbf{XX}^T$
Constraint: $\sum_l^N x_j^{(l)} = 0, \forall j$, define: $T = \sum_{l=1}^N b_{ll}$
Then $\sum_r d_{rs}^2 = T + Nb_{ss}$, $\sum_r \sum_s = d_{rs}^2 = 2NT$
defining:

$d^2_{*s} = \frac{1}{N}\sum_r d^2_{rs}$, $d_{r*} = \frac{1}{N}\sum_s d^2_{rs}$, $d^2_{**} = \frac{1}{N^2}\sum_r\sum_s d^2_{rs}$
So $b_{rs} = \frac{1}{2}(d^2_{r*} + d^2_{*s} - d^2_{**} - d^2_{rs})$ $\mathbf{B} = \mathbf{X}\mathbf{X}^T$ is p.s.d. :

$$\mathbf{B} = \mathbf{C}\mathbf{D}\mathbf{C}^T = (\mathbf{C}\mathbf{D}^{1/2})(\mathbf{C}\mathbf{D}^{1/2})^T$$

Ignore small eigenvalues, let $\mathbf{c}_j$ be the k eigenvectors chosen with eigenvalues λ_j, the new dimensions:$z_j^{(l)} = \sqrt{\lambda_j}c_j^{(l)}$

LDA Sample mean after projection:

$$m_1 = \mathbf{w}^T\mathbf{m}_1, m_2 = \mathbf{w}^T\mathbf{m}_2$$

Between class scatter: $(m_1 - m_2) = \mathbf{w}^T\mathbf{S}_B\mathbf{w}$, $\mathbf{S}_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T$
Within Class Scatter: $s_1^2 = \mathbf{w}^T\mathbf{S}_1\mathbf{w}$, $\mathbf{S}_1 = \sum_l(\mathbf{x}^{(l)} - \mathbf{m}_1)(\mathbf{x}^{(l)} - \mathbf{m}_1)^T y^{(l)}$, similarly $\mathbf{S}_2 = \sum_l(\mathbf{x}^{(l)} - \mathbf{m}_2)(\mathbf{x}^{(l)} - \mathbf{m}_2)^T(1 - y^{(l)})$, so

$$s_1^2 + s_2^2 = \mathbf{w}^T\mathbf{S}_w\mathbf{w}$$

, $\mathbf{S}_w = \mathbf{S}_1 + \mathbf{S}_2$

Fisher's LD $J(\mathbf{w}) = \frac{(m_1-m_2)^2}{s_1^2+s_2^2} = \frac{\mathbf{w}^T\mathbf{S}_B\mathbf{w}}{\mathbf{w}^T\mathbf{S}_W\mathbf{w}}$, take derivative of J w.r.t. $\mathbf{w}$ setting it to 0: $\mathbf{S}_B\mathbf{w} = \lambda\mathbf{S}_W\mathbf{w}$,
or $\mathbf{S}_W^{-1}\mathbf{S}_B\mathbf{w} = \lambda\mathbf{w}$ (Eigen equation)

$K > 2$ Within-class scatter $\mathbf{S}_i = \sum_l y_i^{(l)}(\mathbf{x}^{(l)} - \mathbf{m}_i)(\mathbf{x}^{(l)} - \mathbf{m}_i)^T$, $y_i^{(l)} = 1$ if $\mathbf{x}^{(l)} \in C_i$
Total class scatter: $\mathbf{S}_W = \sum_{i=1}^K \mathbf{S}_i$
Between Class Scatter: $\mathbf{S}_B = \sum_{i=1}^K N_i(\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^T$
Optimal is $\mathbf{W}$ that max: $J(\mathbf{W}) = \frac{Tr(\mathbf{W}^T\mathbf{S}_B\mathbf{W})}{Tr(\mathbf{W}^T\mathbf{S}_W\mathbf{W})}$ Corresponds to eigenvectors of $\mathbf{S}_W^{-1}\mathbf{S}_B$

Chapter 5

Non Parametric Method

Nonparametric Density Estimation Sample: $\mathcal{X} = \{x^{(l)}\}_{l=1}^{N}$, Probability density: $p(X)$, cumulative distribution: $F(X)$

Estimator of $F(X)$: $\hat{F}(x) = \frac{\#\{x^{(l)} leqx)\}}{N}$

Estimator of $p(X)$: $\hat{p}(x) = \frac{1}{h}[\frac{\#\{x^{(l)}+h\leq x\} - \#\{x^{(l)}\leq x\}}{N}]$, where h is the interval and instances $x^{(l)}$ that fall in this interval are assumed to be close enough

Histogram Estimator bin: $[x_0 + mh, x_0 + (m+1)h]$, x_0 origin, h bin width

$\hat{p}(x) = \frac{\#\{x^{(l)}\text{in the same bin as x}\}}{Nh}$

Naive Estimator: $\hat{p}(x) = \frac{\#\{x - h/2 < x^{(l)} \leq x + h/2\}}{Nh}$

Alternative form: $\hat{p}(x) = \frac{1}{Nh}\sum_{t=1}^{N} w(\frac{x - x^{(l)}}{h})$ with weight function

$$w = \begin{cases} 1 & if |u| < 1/2 \\ 0 & otherwise \end{cases}$$

Kernel Estimator Kernel $K(u) = \frac{1}{2\pi}\exp(-\frac{u^2}{2})$,
Estimator:$\hat{p} = \frac{1}{Nh}\sum_{l=1}^{N} K(\frac{x - x^{(l)}}{h})$

KNN $\hat{p}(x) = \frac{k}{2Nd_k(x)}$, $d_k(x)$ is the distance from x to the kth nearest instannce.

KNN with kernel:$\hat{p}(\mathbf{x}) = \frac{1}{Nh^d}\sum_{l=1}^{N} K(\frac{\mathbf{x} - \mathbf{x}^{(l)}}{h})$, with $\int_{\mathbb{R}^d} K(\mathbf{x})d\mathbf{x} = 1$,

Multivariate ellipsoidal Gaussin kernel:
$K(\mathbf{u}) = \frac{1}{(2\pi)^{d/2}|\mathbf{S}|^{1/2}}\exp\left(-\frac{1}{2}\mathbf{u}^T\mathbf{S}^T\mathbf{u}\right)$

Nonparammetric Classification Kernel estimator of class-conditional densities: $\hat{p}(\mathbf{x}|C_i) = \frac{1}{N_i h^d}\sum_{l=1}^{N} K(\frac{\mathbf{x} - \mathbf{x}^{(l)}}{h})y_i^{(l)}$, $y_i^{(l)} = 1$ if $\mathbf{x}^{(l)}$ is in C_i, and $N = \sum_l y_i^{(l)}$, $\hat{P}(C_i) = \frac{N_i}{N}$

Discriminant:
$g_i(\mathbf{x}) = \hat{p}(\mathbf{x}|C_i)\hat{P}(C_i) = \frac{1}{Nh^d}\sum_{l=1}^{N} K(\frac{\mathbf{x} - \mathbf{x}^{(l)}}{h})y_i^{(l)}$

KNN classifier $\hat{p}(\mathbf{x}|C_i) = \frac{k_i}{N_i V^k(\mathbf{x})}$, $\hat{P}(C_i|\mathbf{x}) = \frac{k_i}{k}$, Choose C_i if $i = arg\max_j \hat{P}(C_j|\mathbf{x}) = arg\max_j k_j$

Non param regression $y^{(l)} = g(\mathbf{x}^{(l)}) + \epsilon$,
$\hat{g}(x) = \frac{\sum_{l=1}^{N} K(\frac{x - x^{(l)}}{h})y^{(l)}}{\sum_{l=1}^{N} K(\frac{x - x^{(l)})}{h}}$

Regularized cost function balance bias and variance:
$\sum_l \left[y^{(l)} - \hat{g}(x^{(l)})\right]^2 + \lambda\int_a^b [\hat{g}''(x)]^2 dx$

Chapter 6

Decision Trees

6.1 Constructing Decision Trees

6.1.1 Basic alogrithm

Can be expressed recursively.

1. select an attribute to place at the root node
   - Make one branch for each possible value.
   - This splits up the example set into subsets, one for each possible value.
2. Repeat the process recursively for each branch
3. If at any tie all instances at a node have the same classification, stop.

Only thing: how to determine which attribute to split on.

6.1.2 Measure of purity

If we had a measure of the purity of each node, we could choose the attribute that produces the purest daughter nodes.

We use *information* measured with unit of *bits*.

- It represents the expected amount of information that would be needed to specify whether a new instance should be classified yes or noo
- Given the example reached that node.
- The value is often less than 1

We calculate the information gained on different splits and choose the one that gain most.

Calculating Information

Properties we expect to have:

- When the number of either *yes*'s or *no*'s is zer, the information is zero
- When the number of *yes*'s and *no*'s equal, the information reaches a maximum
- The information should obey the multistage property that we have illustrated.

Highly Branching Attributes

The information gain measure tends to prefer attributes with large numbers of possible values.

To compensate for this, a modification of the measure called the gain ratio is widely used. The gain raeio is derived by taking into account the number and size of of daughter nodes into which an attribute splits the dataset, disregarding any information about the class.

6.2 Pruning

Fully expanded decision trees often contain unnecessary structure, and it is generally advisable to simplify them before they are deployed.

- Prepruning would involve trying to decide during the tree building process when to stop developing subtrees. – avoid all the work of developing subtrees only to throw them away afterward.
- Postpruning:situations occur in which attributes individually seem to have nothing to contribute but are powerful predictors when combined.

Two operations that have been considered for postpruning: *subtree replacement* and *subtree raising.*

At each node, a learning scheme might decide whether it should perform subtree replacement, subtree raising, or leave the subtree as it is, unpruned.

Subtree replacement The idea is to select some subtrees and replace them with single leaves. This will certainly cause the accuracy on the training set to decrease, however, it may **increase the accuracy on an independently chosen test set.**

When subtree replacement is implemented, it proceeds **from the leaves and works back up toward the root.**

Subtree raising Replace an internal node by one of the nodes below it.

6.2.1 Estimating Error Rates

How to decide whether to replace an internal node by a leaf.

Estimate the error rate that would be expected at a particular node given an independently chosen test set, at internal nodes and at leaf nodes.

If we had such an estimate, it would be clear whether to replace, or raise. A particular subtree simply by comparing the estimated error of the subtree with that of its proposed replacement.

Standard verification technique: Hold back some of the data originally given and use it as an independent test set to estimate the error at each node. Drawback: the actual tree is based on less data.

Alternative: try to make some stimate of error based on the training data itself. It is a heuristic based on some statistical reasoning.

The idea is to consider the set of instances that reach each node and imagine that the majority class is chosen to represent the node. That gives us a certain number of errors, E, out of the total number of instances, N.

Now imagine the true probability of error at the node is q and that N instances are generated by a Bernoulli process with parameter q, of which E turn out to be errors.

Given a particular confidence c, we find confidence limits z such that:

$$Pr\left[\frac{f-q}{\sqrt{q(1-q)/N}} > z\right] = c$$

Where N is the number of samples, $f = E/N$ is the observed error rate, and q is the true error rate.

Now we use that upper confidence limit as a estimate for the error e at the node:

$$e = \frac{f + \frac{z^2}{2N} + z\sqrt{\frac{f}{N} - \frac{f^2}{N} + \frac{z^2}{4N^2}}}{1 + \frac{z^2}{N}}$$

Classification Trees for node m, N_m training instances, N_m^i instances belong to class C_i, estimate for the probability of class C_i $\hat{P}(C_i|\mathbf{x}, m) = \frac{N_m^i}{N_m} = p_m^j$, pure if $p_m^j = 1$

Entropy $\mathcal{T}_m = -\sum_{i=1}^{K} p_m^j \log_2 p_m^j$, assume $0 \log 0 = 0$, largest is $\log_2 K$ when all $p_m^i = 1/K$

Other Impurity Measures Properties: $\phi(1/2, 1/2) \geq \phi(p, 1-p)$, $\phi(0,1) = \phi(1,0) = 0$, $\phi(p, 1-p)$ increase in p on $[0, 1/2]$ and decrease o$[1/2, 1]$

Best Split Node m, N_{mj} take branch j, if $f_m(\mathbf{x}) = j$, the estimate for the probability of class C_i is: $\hat{P}(C_i|\mathbf{x}, m, j) = p_{mj}^i = \frac{N_{mj}^i}{N_{mj}}$,total impurity after split:
$\mathcal{T}'_m = -\sum_{i=1}^{n} \frac{N_{mj}}{N_m} \sum_{i=1}^{K} p_{mj}^i \log p_{mj}^i$

Regression Trees $b_m(\mathbf{x}) = 1$ if in $\mathcal{X}_m$,
estimated value at node m:

$$g_m = \frac{\sum_l b_m(\mathbf{x}^{(l)}) y^{(l)}}{\sum_l b_m(\mathbf{x}^{(l)})}$$

,
mean square error after split:

$$E_m = \frac{1}{N_m} \sum_l (y^{(l)} - g_m)^2 b_m(\mathbf{x}^{(l)})$$

tree expansion:

$$b_{mj}(\mathbf{x}) = 1 \text{if } \mathbf{x} \in \mathcal{X}_{mj}$$

,
estimate val in branch j: $g_{mj} = \frac{\sum_l b_{mj}(\mathbf{x}^{(l)}) y^{(l)}}{\sum_l b_{mj}(\mathbf{x}^{(l)})}$,
error after split $E'_m = \frac{1}{N_m} \sum_j \sum_l (y^{(l)} - g_{mj}^2 b_{mj}(\mathbf{x}^{(l)})$
Best split: split that resuts in smallest error, or worst possible error.

Pruning Prepruning stop split when the number of instances reaching a node is belong a certain percentage. Post pruning: Replace subtree by a leaf node, if the leaf node does not perform worse, the subtree is pruned and replaced by leaf.

Chapter 7

Linear Model

7.1 Linear Discriminant functions

A discriminant is a function that take an input vector $\mathbf{x}$ and assignes it to one of K classes:

$$g_i(\mathbf{x}|\mathbf{w}_i, w_{i0}) = \mathbf{w}_i^T\mathbf{x} + w_{i0}$$

generalized use base function $g_i(\mathbf{x}) = \sum_{j=1}^{k} w_j\phi_{ij}(\mathbf{x})$

7.1.1 Two classes

$$g(\mathbf{x}) = g_1(\mathbf{x}) - g_2(\mathbf{x})$$

, C_1 if $g(\mathbf{x}) > 0$

7.1.2 Geometry Interpretation

The decision boundary is defined by

$$g(\mathbf{x}) = 0$$

Corresponds to a $(D-1)$ dimensional hyperplane within the D-dimensional space.

Express any point as

$$\mathbf{x} = \mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|}$$

where x_p is the projection of $\mathbf{x}$ onto hyperplane. r distance from $\mathbf{x}$ to hyper plane.plane, we have $r = \frac{g(\mathbf{x})}{\|\mathbf{w}\|}$

7.1.3 Multi classes

K discriminant:

$$g_i(\mathbf{x}|\mathbf{w}_i, w_{i0}) = \mathbf{w}_i^T + w_{i0}$$

Linear separable:

$$g_i(\mathbf{x}|\mathbf{w}_i, \mathbf{w}_{i0}) > 0$$

if $\mathbf{x} \in C_i$

Choose C_i if

$$g_i(\mathbf{x}) = \max_{j=1}^{K} g_i(\mathbf{x})$$

7.1.4 Pairwise Separation

Discriminant function for class i and j:

$$g_{ij}(\mathbf{x}|\mathbf{w}_{ij}, w_{ij0}) = \mathbf{w}_{ij}^T\mathbf{x} + w_{ij0} = \begin{cases} > 0 & \text{if } \mathbf{x} \in C_i \\ \leq 0 & \text{if } \mathbf{x} \in C_j \\ \text{don't care} & \text{if } \mathbf{x} \in C_k, k \neq i, k \neq j \end{cases}$$

7.2 Logistic Discrimination

7.2.1 Two classes

Assume that the log likelihood ratio is linear:

$$\log \frac{p(\mathbf{x}|C_1)}{p(\mathbf{x}|C_2)} = \mathbf{w}^T\mathbf{x} + w_0^o$$

Using Baye's rule we have;

$$\begin{aligned} logit(P(C_1|x)) &= \log \frac{p(C_1|\mathbf{x})}{1 - p(C_1|\mathbf{x})} \\ &= \log \frac{p(\mathbf{x}|C_1)}{p(\mathbf{x}|C_2)} + \log \frac{p(C_1)}{p(C_2)} \\ &= mathbfw^T\mathbf{x} + w_0 \end{aligned}$$

where $w_0 = w_0^o + \log \frac{P(C_1)}{P(C_2)}$

Rearranging terms:

$$\begin{aligned} y &= sigmoid(mathbfw^T\mathbf{x} + w_0) \\ &= \hat{P}(C_1|\mathbf{x}) = \frac{1}{1 + \exp\left[-(mathbfw^T\mathbf{x} + w_0)\right]} \end{aligned}$$

As our estimator of $P(C_1|\mathbf{x})$

Gradient Decent

In the discriminant-based approach, the parameters are those of the discriminants, and they are *optimized to minimize the classification error*

Error $\mathbf{w}$ denotes the set of parameters and $E(\mathbf{w}|\mathcal{X})$ is the error parameters $\mathbf{w}$ on the given training set $\mathcal{X}$, we look for:

$$\mathbf{w}* = arg \min_{\mathbf{w}} E(\mathbf{w}|\mathcal{X})$$

No analytical solution

Gradient Vector When $E(\mathbf{w})$ is a differentiable function of a vector of variables, we have the gradient vector composed of the partial derivatives:

$$\nabla_{\mathbf{w}} E = \left[\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \ldots, \frac{\partial E}{\partial w_d}\right]^T$$

Gradient Descent starts from a *random* $\mathbf{w}$, at each step, update w in a *opposite direction* of the gradient:

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}, \forall i$$

$$w_i = w_i + \Delta w_i$$

η is *step size*, or *learning factor*

When we get to minimum, the derivative is 0 and the procedure terminates.

This indicates that the procedure finds the nearest minimum that can be *local minimum*. There is no guarantee of finds the nearest minimum that can be a local minimum

Learning parameters Given a sample of two classes, $\mathcal{X} = \mathbf{x}^{(l)}, \mathbf{r}^{(l)}$, where $\mathbf{r}^{(l)} = 1$ if $\mathbf{x} \in C_1$

We assume $\mathbf{r}^{(l)}$, given $\mathbf{x}^{(l)}$ is Bernoulli with probability $y^{(l)} = p(C_1|\mathbf{x}^{(l)})$:

$$\mathbf{r}^{(l)}|\mathbf{x}^{(l)} \sim Bernoulli(y^{(l)})$$

Note that in this discriminant-based approach, we model directly $\mathbf{r}|\mathbf{x}$ The sample likelihood is:

$$L(mathbfw, w_0|\mathcal{X}) = \prod_t (y^{(l)})^{(r^{(l)})}(1 - y^{(l)})^{1-r^{(l)}}$$

We can always turn it in an error function to minimize: $E = -\log L$ So we have *cross-entropy*:

$$E(mathbfw, w_0|\mathcal{X}) = -\sum_t \mathbf{r}^{(l)} \log y^{(l)} + (1 - r^{(l)}) \log(1 - y^{(l)})$$

We use gradient descent to minimize cross-entropy If $y = sigmoid(a) = \frac{1}{1+exp(-a)}$, its derivative is given as:

$$\frac{dy}{da} = y(1 - y)$$

and we get the following update equations:

$$\begin{aligned}\Delta w_j &= -\eta \frac{\partial E}{\partial w_j} = \eta \sum_t (\frac{r^{(l)}}{y^{(l)}} - \frac{1 - r^{(l)}}{1 - y^{(l)}} x_j^{(l)} \\ &= \eta \sum (r^{(l)} - y^{(l)}) x_j^{(l)}, \ = 1, \ldots, d \\ \Delta w_0 &= -\eta \frac{\partial E}{\partial w_0} = \eta \sum (r^{(l)} - y^{(l)})\end{aligned}$$

7.2.2 Multiple Classes

Generalization of sigmoid

Take one of the classes C_k, as reference class and assume that:
$\log \frac{p(\mathbf{x}|C_i)}{p(\mathbf{x}|C_K)} = mathbfw_i^T \mathbf{x} + w_{i0}^o$, $i = 1, \ldots, K - 1$
Then we have:

$$\frac{P(C_i|\mathbf{x})}{P(C_K|\mathbf{x})} = \exp[mathbfw_i^T \mathbf{x} + w_{i0}]$$

With $w_{i0} = w_{i0}^o + \log \frac{P(C_i)}{P(C_K)}$

Summing over i we can deduce:

$$P(C_K|\mathbf{x}) = \frac{1}{1 + \sum_{i=1}^{K-1} \exp(\mathbf{w}_i^T \mathbf{x} + w_{i0})}$$

$$P(C_i|\mathbf{x}) = \frac{\exp(\mathbf{w}_i^T + w_{i0})}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{w}_j^T \mathbf{x} + w_{j0})}$$

, where $k = 1, \ldots, K - 1$

Softmax

Treat all classes uniformly
$y_i = \hat{P}(C_i|\mathbf{x}) = \frac{\exp(\mathbf{w}_i^T + w_{i0})}{\sum_{j=1}^K \exp(\mathbf{w}_j^T + w_{j0})}$, $i = 1, \ldots, K$

Learning

$$\frac{\partial y_i}{\partial a_j} = y_i(\delta_{ij} - y_i)$$

$\Delta \mathbf{w}_j = \eta \sum_l (r_j^{(l)} - y_j^{(l)}) \mathbf{x}^{(l)}$, $\Delta w_{j0} = \eta \sum_l (r_j^{(l)} - y_j^{(l))}$

Regression for two-class Classification $r^{(l)} = y^{(l)} + \epsilon$, $r^{(l)} \in \{0,1\}$, $\epsilon \sim \mathcal{N}(0, \sigma^2)$, $y^{(l)} = sigmoid(\mathbf{w}^T\mathbf{x}^{(l)} + w_0)$,

Likelihood:$L(\mathbf{w}, w_0|\mathcal{X}) = \prod_l \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(r^{(l)}-y^{(l)})^2}{2\sigma^2}\right]$,

Error: $E(\{\mathbf{w}_i, w_{i0}\}_i|\mathcal{X}) = \frac{1}{2}\sum_l (r^{(l)} - y^{(l)})^2$,

Learning $\Delta\mathbf{w} = \eta\sum_l (r^{(l)} - y^{(l)})y^{(l)}(1 - y^{(l)})\mathbf{x}^{(l)}$,
$\Delta w_0 = \eta\sum_l (r^{(l)} - y^{(l)})y^{(l)}(1 - y^{(l)})$

$K > 2$ **classes** $\mathbf{r}^{(l)} = \mathbf{y}^{(l)} + \boldsymbol{\epsilon}$,
$\epsilon \sim \mathcal{N}_K(0, \sigma^2\mathbf{I}_K)$, $y_i^{(l)} = \frac{1}{1+\exp\left[-(\mathbf{w}_i^T\mathbf{x}^{(l)}+w_{i0})\right]}$,
Likelihood:
$L(\{\mathbf{w}_i, w_{i0}\}_i|\mathcal{X}) = \prod_l \frac{1}{(2\pi)^{K/2}|\mathbf{\Sigma}|^{1/2}} \exp\left[-\frac{\|\mathbf{r}^{(l)}-\mathbf{y}^{(l)}\|^2}{2\sigma^2}\right]$
Error Func: $E(\{\mathbf{w}_i, w_{i0}\}|\mathcal{X}) = \frac{1}{2}\sum_l \|\mathbf{r}^{(l)} - \mathbf{y}^{(l)}\|^2$
Learning $\Delta\mathbf{w}_i = \eta\sum_l (r_i^{(l)} - y_i^{(l)})y_i^{(l)}(1 - y_i^{(l)})\mathbf{x}^{(l)}$,
$\Delta w_0 = \eta\sum_l (r_i^{(l)} - y_i^{(l)})y_i^{(l)}(1 - y_i^{(l)})$

Chapter 8

Multilayer Perceptrons

8.1 Perceptron

The output y is a **weighted sum** of the input $\mathbf{x} = (x_0, x_1, \ldots, x_d)^T$:

$$y = \sum_{j=1}^{d} w_j x_j + w_0 = \mathbf{w}^T \mathbf{x}$$

where x_0 is a special *bias unit* with $x_0 = 1$ and $\mathbf{w} = (x_0, w_1, \ldots, w_d)^T$ are called **connection weight or synaptic weights**

To implement a linear discriminant function, we need threshold function:

$$s(a) = \begin{cases} 1 & \text{if } a > 0 \\ 0 & \text{otherwise} \end{cases}$$

to define the following decision rule:

$$\text{Choose} \begin{cases} C_1 & \text{if } s(\mathbf{w}^T\mathbf{x}) = 1 \\ C-2 & \text{otherwise} \end{cases}$$

Use **sigmoid** instead of threshold to gain differentiability:

$$y = sigmoid(\mathbf{w}^T\mathbf{x}), \text{ where } sigmoid(a) = \frac{1}{1 + \exp(-a)}$$

The output may be interpreted as the *posterior probability* that the input $\mathbf{x}$ belongs to C_1

8.1.1 $K > 2$ Outputs

K perceptrons, each with a weight vector $\mathbf{w}_i$,

$$y_i = \sum_{j=1}^{d} w_{ij} x_j + w_{i0} = \mathbf{w}_i^T \mathbf{x}, \text{ or } \mathbf{y} = \mathbf{W}\mathbf{x}$$

where w_{ij} is the weight from input x_j to output y_i and each row of the $K \times (d+1)$ matrix $\mathbf{W}$ is the weight vector of one perceptron.

Choose C_i if $y_i = \max_k y_k$

Posterior probability Use softmax to define y_i as:

$$y_i = \frac{\exp(\mathbf{w}_i^T)}{\sum_{k=1}^{K} \exp(\mathbf{w}_k^T \mathbf{x})}$$

8.1.2 Stochastic Gradient Descent

Gradient descent for online learning, for regression, the error on a single instance

$$E^{(l)}(\mathbf{w}|\mathbf{x}^{(l)}, r^{(l)}) = \frac{1}{2}(r^{(l)} - y^{(l)})^2 = \frac{1}{2}\left[r^{(l)} - (\mathbf{w}^T\mathbf{x}^{(l)})\right]^2$$

gives the online update rule:

$$\Delta w_j^{(l)} = \eta(r^{(l)} - y^{(l)})x_j^{(l)}$$

where η is step size.

For Binary classification:

Likelihood:

$$L = (y^{(l)})^{r^{(l)}}(1 - y^l)^{1-r^{(l)}}$$

Cross Entropy:

$$E^{(l)}(\mathbf{w}|\mathbf{x}^{(l)}, r^{(l)}) = -\log L = -r^{(l)}\log y^{(l)} - (1 - r^{(l)})\log(1 - y^{(l)})$$

Online update rule:

$$\Delta w_j^{(l)} = \eta(r^{(l)} - y^{(l)})x_j^{(l)}$$

$K > 2$

$$y_i^{(l)} = \frac{\exp(\mathbf{w}_i^T\mathbf{x}^{(l)})}{\sum_k \exp(\mathbf{w}_k^T\mathbf{x}^{(l)})}$$

Likelihood:

$$L = \prod_i (y_i^{(l)})^{r_i^{(l)}}$$

Cross Entropy:

$$E^{(l)}(\{\mathbf{w}_i\}|\mathbf{x}^{(l)}, \mathbf{r}^{(l)}) = -\sum_i r_i^{(l)}\log y_i^{(l)}$$

Online update rule:

$$\Delta w_{ij}^{(l)} = \eta(r_i^{(l)} - y^{(l)})x_j^{(l)}$$

8.2 Multilayer Perception

MLP has a hidden layer between the input and output.

Input to hidden:

$$z_h = sigmoid(\mathbf{w}_h^T\mathbf{x}) = \frac{1}{1 + \exp\left[-(\sum_{j=1}^d w_{hj}x_j + w_{h0}\right]}$$

Hidden to output:

$$y_i = \mathbf{v}_i^T\mathbf{z} = \sum_{h=1}^H v_{ih}z_h + v_{i0}$$

Backward, hidden-to-output weight: treating hidden unit as input

Input-to-hidden, chain rule:

$$\frac{\partial E}{\partial w_{hj}} = \frac{\partial E}{\partial y_i}\frac{\partial y_i}{\partial z_h}\frac{\partial z_h}{\partial w_{hj}}$$

8.2.1 MLP for Nonlinear Regression(Multi output)

outputs:

$$
\begin{aligned}
y_i^{(l)} &= \sum_{h=1}^{H} v_{ih} z_h^{(l)} + v_{i0} \\
z_h^{(l)} &= sigmoid(\mathbf{w}_h^T \mathbf{x}^{(l)})
\end{aligned}
$$

Error function:

$$E(\mathbf{W}, \mathbf{v}|\mathcal{X}) = \frac{1}{2} \sum_l \sum_i (r_i^{(l)} - y_i^{(l)})^2$$

Update rule for second layer:

$$\Delta v_{ih} = \eta \sum_l (r_i^{(l)} - y_i^{(l)}) z_h^{(l)}$$

Update rule for first layer:

$$\Delta w_{hj} = -\eta \frac{\partial E}{\partial w_{hj}} = \eta \sum_l \left[\sum_i (r_i^{(l)} - y_i^{(l)}) v_{ih} \right] z_h^{(l)} (1 - z_h^{(l)} (1 - z_h^{(l)}) x_j^{(l)}$$

8.2.2 MLP for NonLinear Multi-class Discrimination

Outputs:

$$y_i^{(l)} = \frac{\exp(o_i^{(l)})}{\sum_k \exp(o_k^{(l)})}$$

,

$$o_i^{(l)} = \sum_h^H v_{ih} z_h^{(l)} + v_{i0}$$

Error Function:

$$E(\mathbf{W}, \mathbf{V}|\mathcal{X}) = -\sum_l \sum_i r_i^{(l)} \log y_i^{(l)}$$

, update rules are the same us regression.

Chapter 9

Support Vector Machine

Optimal Separating Hyperplane results from *statistical learning* theory showing that the separating hyperplane with the *largest margin* generalizes best.

Hard-margin case points are **linearly separable** with proper scaling of $\mathbf{w}$ and w_0, the points cloest to the hyper plane satisfy $|\mathbf{w}^T\mathbf{x} + w_0| = 1 \Rightarrow$ **canoical separating hyperplane.**

The one max the margin: **canonical optimal separating hyperplane**

$\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ be two closest point on each side:

$$\mathbf{w}^T\mathbf{x}^{(1)} + w_0 = +1$$

$$\mathbf{w}^T\mathbf{x}^{(2)} + w_0 = -1$$

So $\mathbf{w}^T(x^{(1)} - \mathbf{w}^{(2)}) = 2$, the margin is given by:

$$\gamma = \frac{1}{2}\frac{\mathbf{w}^T(\mathbf{x}^{(1)} - \mathbf{x}^{(2)})}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}$$

Maximizing the margin is equivalent to minimizing $\|\mathbf{w}\|$

Inequality constraint

$$\mathbf{w}^T\mathbf{x}^{(l)} + w_0 \begin{cases} \geq +1 & \text{if } y^{(l)} = +1 \\ \leq -1 & \text{if } y^{(l)} = -1 \end{cases}$$

Equivalent to:

$$y^{(l)}(\mathbf{w}^T\mathbf{x}^{(l)} + w_0) \geq 1$$

Primal Optimization

$$\begin{aligned} \text{Minimize} \quad & \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{Subject to} \quad & y^{(l)}(\mathbf{w}^T\mathbf{x}^{(l)} + w_0) \geq 1, \forall l \end{aligned}$$

Lagrangian

$$\begin{aligned} L_p(\mathbf{w}, w_), \alpha_l) &= \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{l=1}^{N} \alpha_l \left[y^{(l)}(\mathbf{w}^T\mathbf{x}^{(l)} + w_0) - 1 \right] \\ &= \frac{1}{2}\mathbf{w}^T\mathbf{w} - \mathbf{w}^T \sum_l \alpha_l y^{(l)}\mathbf{x}^{(l)} - w_0 \sum_l \alpha_l y^{(l)} + \sum_l \alpha_l \end{aligned}$$

Eliminating Primal Var

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} = \sum_l \alpha_l y^{(l)}\mathbf{x}^{(l)}$$

$$\frac{\partial L_p)}{\partial w_0} = 0 \Rightarrow \sum_l \alpha_l y^{(l)} = 0$$

Dual Optimization Problem Setting gradient of L_p w.r.t. $\mathbf{w}$ and w_0 to 0, then plugging, we get duel optimization problem:

$$\begin{aligned} \text{Maximize} \quad & \sum_l \alpha_l - \frac{1}{2}\sum_l \sum_{l'} \alpha_l \alpha_{l'} y^{(l)} y(l')(\mathbf{x}^{(l)})^T \mathbf{x}^{(l')} \\ \text{subject to} \quad & \sum_l \alpha_l y^{(l)} = 0 \text{and } \alpha_l \geq 0, \forall l \end{aligned}$$

Support Vector Most of the Dual Variables vanish with $\alpha_l = 0$. They are points lying beyond the margin, Support vectors: $\mathbf{x}^{(l)}$ with $\alpha_l > 0$.
Computation of primal variables: $\mathbf{w} = \sum_{l=1}^N \alpha_l y^{(l)} \mathbf{x}^{(l)} = \sum_{\mathbf{x}^{(l)} \in SV} \alpha_l y^{(l)} \mathbf{x}^{(l)}$
Support vector on margin:$y^{(l)}(\mathbf{w}^T\mathbf{x}^{(l)} + w_0) = 1$ or $w_0 = y^{(l)} - \mathbf{w}^T\mathbf{x}^{(l)}$, Then:

$$w_0 = \frac{1}{|SV|} \sum_{x^{(l)} \in SV} (y^{(l)} - \mathbf{w}^T \mathbf{x}^{(l)})$$

Discriminant Function $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$ (plug in $\mathbf{w}$ and w_0 above), choose C_1 if $g(\mathbf{x}) > 0$

$K > 2$ An SVM $g_i(\mathbf{x})$ is learned for each two-class problem. Choose C_j if $j = arg\max_k g_k(\mathbf{x})$

Slack Variables Relaxed constraint:
$y^{(l)}(\mathbf{w}^T\mathbf{x}^{(l)} + w_0) \geq 1 - \zeta_l$,
minimize: $C\sum_l \zeta_l + \frac{1}{2}\|\mathbf{w}\|^2$
Lagrangian(Primal):
$L_p = \frac{1}{2}\|\mathbf{w}\|^2 +$
$C\sum_l \zeta_l - \sum_{l=1}^N \alpha_l \left[y^{(l)}(\mathbf{w}^T\mathbf{x}^{(l)} + w_0) - 1 + \zeta_l\right] - \sum \mu_l \zeta_l$,
C is the regularization parameter, μ_l is the new Lagrange multipiler to guarantee that $\zeta \geq 0$
Dual: Max $\sum_l \alpha_l - \frac{1}{2}\sum_l \sum_{l'} \alpha_l \alpha_{l'} y^{(l)} y^{(l')} (\mathbf{x}^{(l)})^T \mathbf{x}^{(l')}$
subject to: $\sum_l \alpha_l y^{(l)} = 0$ and $0 \leq \alpha_l \leq C, \forall l$

Kernel Functions Dual Problem:
Max: $\sum_l \alpha_l - \frac{1}{2}\sum_l \sum_{l'} \alpha_l \alpha_{l'} y^{(l)} y^{(l')} \phi(\mathbf{x}^{(l)})^T \phi(\mathbf{x}^{(l')})$
subject to: $\sum_l y^{(l)} = 0$ and $0 \leq \alpha_l \leq C, \forall l$
Kernel: $K(\mathbf{x}^{(l)}, \mathbf{x}^{(l')} = \phi(\mathbf{x}^{(l)})^T \phi(\mathbf{x}^{(l')})$

$\epsilon - InsensitiveLoss$

$$\varepsilon_\epsilon(y^{(l)}, f(\mathbf{x}^{(l)}) = \begin{cases} 0 & \text{if } |y^{(l)} - f(\mathbf{x}^{(l)})| \leq \epsilon \\ |y^{(l)} - f(\mathbf{x}^{(l)})| - \epsilon & otherwise \end{cases}$$

Primal: Max $\frac{1}{2}\|\mathbf{w}\|^2 + C\sum_l (\zeta_l^+ + \zeta_l^-)$
Subject to: $y^{(l)} - (\mathbf{w}^T\mathbf{x}^{(l)} + w_0) \leq \epsilon + \zeta_l^+, \forall l$
$(\mathbf{w}^T\mathbf{x}^{(l)} + w_0) - y^{(l)} \leq \epsilon + \zeta_l^-, \forall l$, $\zeta_l^+, \zeta_l^- \geq 0, \forall l$
Two slack variables: ζ_l^+ such that $y^{(l)} - (\mathbf{w}^T\mathbf{x}^{(l)} + w_0) > \epsilon$, ζ_l^- such that $(\mathbf{w}^T\mathbf{x}^{(l)} + w_0) - y^{(l)} > \epsilon$

Chapter 10

Performance Evaluation and Comparison

K-Fold Cross Validation The data set $\mathcal{X}$ is randomly partitioned into K equal-sized subsets $\mathcal{X}_i$, **Stratification** the class distribution different subsets are kept roughly the same.
Use $\mathcal{X}_1, \dots, \mathcal{X}_K$ as validation sets, and the remaining as training respectively.
If N is small, K should be large to allow large enough training sets.
Leave one out: one instance if left out as validation and $N-1$ for training.

5×2 **Cross Validation** For each fold i, Split into two equal-sized parts, $\mathcal{X}_i^{(1)}$, $\mathcal{X}_i^{(2)}$, 10 training/validation set pairs: $\mathcal{T}_1 = \mathcal{X}_1^{(1)}, \mathcal{V}_1 = \mathcal{X}_1^{(2)}, \mathcal{T}_2 = \mathcal{X}_1^{(2)}, \mathcal{V}_2 = \mathcal{X}_1^{(1)}, \mathcal{T}_3 = \mathcal{X}_2^{(1)}, \mathcal{V}_3 = \mathcal{X}_2^{(2)}, \mathcal{T}_4 = \mathcal{X}_2^{(2)}, \mathcal{V}_4 = \mathcal{X}_2^{(1)}, \dots$

Bootstrapping Generates new samples, each of size N, by drawing randomly with replacement. Multiple bootstrap sammples are used to max the change that the system is trained on all instances.

Error Measure TP: True positive, FP: False postivie, FN:False Negative, TN: True Negative, Error rate: $\frac{|FN|+|FP|}{N}$

Receiver Operating characteristics curve Hit rate: $\frac{|TP|}{|TP|+|FN|}$ False alarm rate: $\frac{|FP|}{|FP|+|TN|}$, area under the curve is often used.

Point vs Interval estimator Point specifies a value for θ, intervale specifies an interval within which θ lines with a certain degree of confidence.

Confidence Interval Define z_α,
Two sided: $P(\mathcal{Z} > z_\alpha) = \alpha$, then for level of confidence $1-\alpha$,

$$P(-z_{\alpha/2} < \sqrt{N}\frac{m-\mu}{\sigma} < z_{\alpha/2}) = 1-\alpha$$

One-sided $P(m - z_{alpha}\frac{\sigma}{\sqrt{N}} < \mu) = 1-\alpha$

t Distribution σ^2 replaced by sample var $S^2 = \frac{\sum_l (x^{(l)}-m)^2}{N-1}$, $\sqrt{N}(m-\mu)/S$ follows a t distribution with $N-1$ degree of freedom: $\sqrt{N}\frac{m-\mu}{S} \sim t_{N-1}$ For $\alpha \in (0, 1/2)$,

$$P(m - t_{\alpha/2,N-1}\frac{S}{\sqrt{N}} < \mu < m + t_{\alpha/2,N-1}\frac{S}{\sqrt{N}}) = 1-\alpha$$

Hypothesis Testing Test some hypothesis concerning the parameters.

1. Define a statistics obey a certain distribution
2. Random sample is consistent with the hypothesis under consideration, accept(not reject)
3. Otherwise reject

Given normal $\mathcal{N}(\mu, \sigma^2)$, σ known, μ unknown. **Null Hypothesis**:$H_0 : \mu = \mu_0$, $H_1 : \mu \neq \mu_0$ Accept H_0 if the sample mean is not too far from μ_0. Accept H_0 with level of significance α if μ_0 lies in the $100(1-\alpha)$,

$$\sqrt{N}\frac{m-\mu_0}{\sigma} \in (-z_{\alpha/2}, z_{\alpha/2})$$

Error Type I, rejected when it is correct, α defines how much type I can tolerate. Type II accepted when incorrect.

One Sided $H_0 : \mu \leq \mu_0$, $H_1 : \mu > \mu_0$, accept $\frac{\sqrt{N}(m-\mu_0)}{\sigma} \in (-\infty, z_\alpha)$

t-test If σ^2 is not known, $H_0 : \mu = \mu_0$, $H_1 : \mu \neq \mu_0$, accept at α if

$$\sqrt{N}\frac{m-\mu_0)}{S} \in (-t_{\alpha,N-1}, t_{\alpha,N-1})$$

Binomial Test Single test/validation:Classifier is trained on a training set $\mathcal{T}$ and tested on validation set $\mathcal{V}$. p be the probability that the classifier makes a misclassification error..Define $x^{(l)}$ as a B ernoulli variable to denote the correctness, $x^{(l)} = 1$ with probability p and $x^{(l)} = 0$ with probability $1-p$, point estimation: $\hat{p} = \frac{\sum_l x^{(l)}}{|\mathcal{V}|} = \frac{\sum_l x^{(l)}}{N}$

Hypothesis test: $H_0 : p \leq p_0$ vs. $H_1 : p > p_0$, $X = \sum_{l=1}^{N} x^{(l)}$ denote the number of errors on $\mathcal{V}$.,

$$P(X = j) = \binom{N}{j} p^j (1-p)^{N-j}$$

Under the null hypothesis $p \leq p_0$, so the probability that there are e errors or less is:

$$P(X \leq e) = \sum_{j=1}^{e} \binom{N}{j} p_0^j (1-p_0)^{N-j}$$

Binomial test: accept H_0 if $P(X \leq e) < 1-\alpha$

Paired t Test Multiple training/validation set pairs: run the algorithm K times on K T/V set pairs, we get K error probabilities, $p_i, i = 1, \ldots, K$ on K validation sets.

Paired t test to determine whether to accept the null hypothesis H_0 that the classifier has error probability p_0 or less at significane level α.

$$x_i^{(l)} = \begin{cases} 1 & \text{if classifier trained on } \mathcal{V}_i \text{ makes an error on instance} l \text{ of } \mathcal{V}_i \\ 0 & \text{otherwise} \end{cases}$$

Test statistic: $\sqrt{K}\frac{(m-p_0)}{S} \sim t_{K-1}$, where $p_i = \frac{\sum_{l=1}^{N} x_i^{(l)}}{N}$, $m = \frac{\sum_{i=1}^{K} p_i}{K}$, $S^2 = \frac{\sum_{i=1}^{K}(p_i-m)^2}{K-1}$

K-Fold Cross-Validated Paired t Test Given two classification algorithms and a data set, we want to compare and test whether the two algorithms constuct classifiers that have the same expected error rate on a new instance.

K-fold cross validation is used to obtain K training/validation set pairs $\{(\mathcal{T}_i, \mathcal{V}_i)\}_{i=1}^{K}$, run two algorithms, error probabilities p_i^1 and p_i^2, define $p_i = p_i^1 - p_i^2$, p_i with mean μ

$H_0 = \mu = 1$, $H_1 = \mu \neq 0$. Test statistic: $\sqrt{K}\frac{(m-0)}{S} \sim t_{K-1}$, where $m = \frac{\sum_{i=1}^{K} p_i}{K}$, $S^2 = \frac{\sum_{i=1}^{K}(p_i-m)^2}{K-1}$, accept H_0 at significance level α if $\sqrt{K}m/S \in -t_(\alpha/2, K-1, t_{\alpha/2,K-1})$

Chapter 11

Ensemble Learning

Combining Base Learners Multiexpert combination method: base learners work in parallel, give decision and combined to give a final.

Multistage combinations: Base learners work serially, sorted increasing complexity, complex is used when simple is not confident.

Voting Takes a convex combination of the base learners:

$$y = f(d_1, \ldots, d_L|\mathbf{\Phi}) = \sum_{j=1}^{L} w_j d_j(\mathbf{x})$$

, with $w_j \geq 0$ and $\sum_{j=1}^{L} w_j = 1$, $\mathbf{\Phi} = (w_1, \ldots, w_L)^T$ are the parameters and y is the final prediction.

Voting for Classification for class C_i $y_i = \sum_{j=1}^{L} w_j d_{ij}(\mathbf{x})$, where d_{ij} is the vote of learner j for C_i

Simple voting $w_j = \frac{1}{L}$

Bayesian model combination: $P(C_i|x) = \sum_{models \mathcal{M}_j} P(C_i|x, \mathcal{M}_j)P(\mathcal{M}_|)$, weight w_j can be seen as approximation of the prior $P(\mathcal{M}_j)$, Analysis, as L increase, bias does not change but the variance decreases.

Bagging bootstrap aggregation, a voting method whereby the base learners are made different by training on slightly different training sets.

AdaBoost Modifies the probabilities of drawing instances for classifier training as a function of the error of the pre-

Training:

  For all $\{x^t, r^t\}_{t=1}^{N} \in \mathcal{X}$, initialize $p_1^t = 1/N$

  For all base-learners $j = 1, \ldots, L$

    Randomly draw $\mathcal{X}_j$ from $\mathcal{X}$ with probabilities p_j^t

    Train d_j using $\mathcal{X}_j$

    For each (x^t, r^t), calculate $y_j^t \leftarrow d_j(x^t)$

    Calculate error rate: $\epsilon_j \leftarrow \sum_t p_j^t \cdot 1(y_j^t \neq r^t)$

    If $\epsilon_j > 1/2$, then $L \leftarrow j - 1$; stop

    $\beta_j \leftarrow \epsilon_j / (1 - \epsilon_j)$

    For each (x^t, r^t), decrease probabilities if correct:

      If $y_j^t = r^t$ $p_{j+1}^t \leftarrow \beta_j p_j^t$ Else $p_{j+1}^t \leftarrow p_j^t$

    Normalize probabilities:

      $Z_j \leftarrow \sum_t p_{j+1}^t$; $p_{j+1}^t \leftarrow p_{j+1}^t / Z_j$

Testing:

  Given x, calculate $d_j(x), j = 1, \ldots, L$

  Calculate class outputs, $i = 1, \ldots, K$:

    $y_i = \sum_{j=1}^{L} \left(\log \frac{1}{\beta_j} \right) d_{ji}(x)$

vious base learner.

11.1 Matrices Properties

Basic Matrix $(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$, $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$, $(\mathbf{A}^T)^{-1} = (\mathbf{A}^{-1})^T$, $\mathbf{P}^{-1}+\mathbf{B}^T\mathbf{R}^{-1}\mathbf{B})^{-1}\mathbf{B}^T\mathbf{R}^{-1} = \mathbf{PB}^T(\mathbf{BPB}^T + \mathbf{R})^{-1}$,

Traces and Determinants $Tr(\mathbf{AB}) = Tr(\mathbf{BA})$, $Tr(\mathbf{ABC}) = Tr(\mathbf{CBA}) = Tr(\mathbf{BCA})$, $|\mathbf{A}^{-1}| = \frac{1}{|\mathbf{A}|}$, $\mathbf{a}^T\mathbf{A}\mathbf{a} = Tr(\mathbf{A}\mathbf{a}\mathbf{a}^T)$

Matrix Derivatives $\frac{\partial}{\partial \mathbf{x}}(\mathbf{x}^T\mathbf{a}) = \frac{\partial}{\partial \mathbf{x}}(\mathbf{a}^T\mathbf{x}) = \mathbf{a}$, $\frac{\partial}{\partial \mathbf{x}}(\mathbf{AB}) = \frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{B} + \mathbf{A}\frac{\partial \mathbf{B}}{\partial \mathbf{x}}$, $\frac{\partial}{\partial x}(\mathbf{A}^{-1}) = -\mathbf{A}^{-1}\frac{\partial \mathbf{A}}{\partial x}\mathbf{A}^{-1}$, $\frac{\partial}{\partial x}\ln|\mathbf{A}| = Tr(\mathbf{A}^{-1}\frac{\partial \mathbf{A}}{\partial x})$, $\frac{\partial}{\partial A_{ij}}Tr(\mathbf{AB}) = B_{ji}$, $\frac{\partial}{\partial \mathbf{A}}Tr(\mathbf{AB}) = \mathbf{B}^T$, $\frac{\partial}{\partial \mathbf{A}}Tr(\mathbf{A}) = \mathbf{I}$, $\frac{\partial}{\partial \mathbf{A}}Tr(\mathbf{ABA}^T) = \mathbf{A}(\mathbf{B} + \mathbf{B}^T)$, $\frac{\partial}{\partial \mathbf{A}}\ln|\mathbf{A}| = (\mathbf{A}^{-1})^T$

Chapter 12

Convolutional Neural Networks

12.1 Motivation

There exist a complex arrangement of cells within the visual cortex. These cells are sensitive to small sub-regions of the input space, called a **receptive field**, and are tiled in such a way as to cover the entire visual field. These filters are local in input space and are thus better suited to exploit the strong spatially local correlation present in natural images.

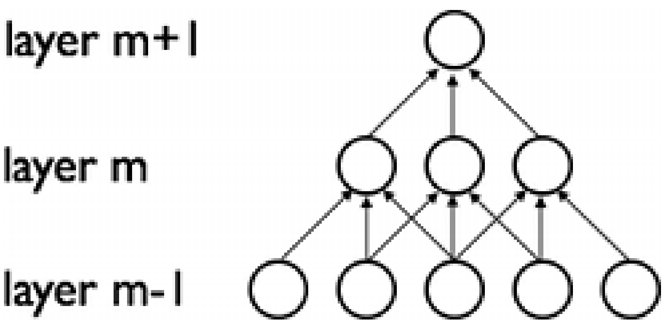
Two basic cell types: Simple cells (S) and complex cells (C).

- Simple Cells(S) respond maximally to specific edge-like stimulus patterns within their receptive field.
- Complex cells(C) have larger receptive fields and are locally invariant to the exact position of stimulus.

12.2 Sparse Connectivity

CNNs exploit spatially local correlation by **enforcing a local connectivity pattern between neurons of adjacent layers**.

Input hidden units in the m-th layer are connected to a local subset of units in the $(m-1)$-th layer, which have spatially contiguous receptive fields.



- Layer $m-1$ is the input retina.
- Units in layer m have receptive fields of width 3. Thus only connected to 3 adjacent neurons in the $(m-1)$-th layer.
- Layer m have a similar connectivity with the layer below. $(m+1)$

We say that their receptive field with respect tot he layer below is 3, but their receptive field with respect to the input is larger (it is 5). The architecture thus confines the learnt “filters” to the spatially local pattern.

12.3 Shared Weights

In CNNs, each sparse filter h_i is additionally replicated across the entire visual field. These "replicated" units form a **feature map**, which share the same parameterization. (the receptive fields in the same feature map share the same weight and bias for the sensitive region)

Gradient descent can still be used to learn such shared parameters, and requires only a small change to the original algorithm. The gradient of a shared weight is simply the sum of the gradients of the parameters being shared.

Replicating units in this way allows for feature to be detected regardless of their position in the visual field. Additionally, weight sharing offers a very efficient way to do this, since it greatly reduces the number of free parameter

12.4 Details and notation

The k-th feature map at a given layer as h^k, whose filter with weights W^k and bias b_k, then the feature map h^k is obtained as follows (for $tanh$ non-linearities)

$$h_{ij}^k = tanh\left(\left(W^k * x\right)_{ij}\right) + b_k\right)$$

To form a richer representation of the data, hidden layers are composed of a set of multiple feature maps $\left\{h^{(k)}, k = 0 \dots K\right\}$

The weights of this layer can be parameterized as a 4D tensor (Tensors are geometric objects that describe linear relations between vectors, scalars, and other tensors. Elementary examples of such relations include the dot product, the cross product and linear maps, vectors and scalars themselves are also tensors.)

- Destination feature map index
- Source feature map index
- Source vertical position index
- Source horizontal position index

12.5 MaxPooling

MaxPooling is a form of non-linear down-sampling. MaxPooling partitions the input image into a set of non-overlapping rectangles and, for each such sub-region, outputs the maximum value.

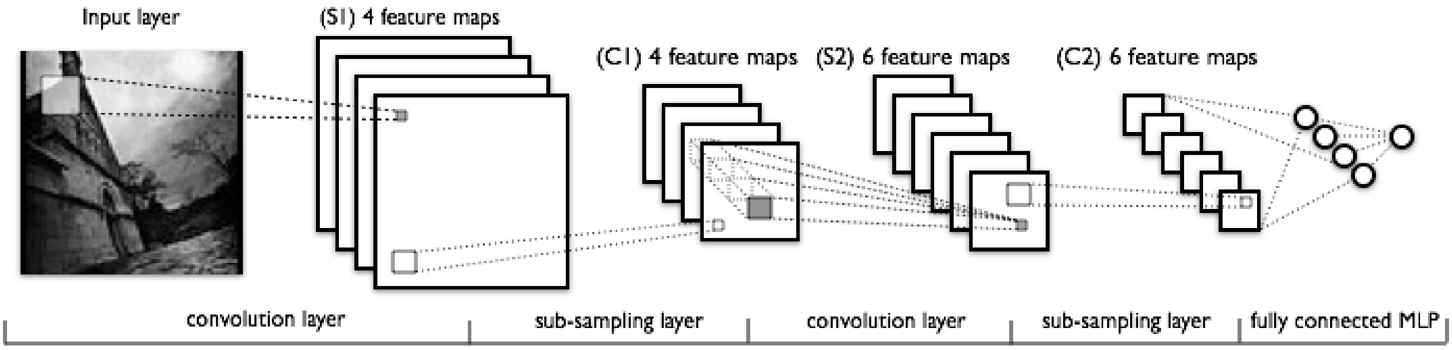
Useful for two reasons:

- Reduces the computational complexity for upper layers
- Provides a form of translation invariance

Why it works: Imagine cascading a max-pooling layer with a convolutional layer. There are 8 directions in which one can translate the input image into a single pixel. If max-pooling is done over a 2×2 region, 3 out of these 8 possible configurations will produce exactly the same output at the convolutional layer. For max-pooling over a 3×3

12.6 The Full Model: LeNet

Graphical depiction:



The lower layers are composed to alternating convolution and max-mpooling layers.

The upper layers however are fully-connected and correspond to a traditional MLP

Chapter 13

Denoising Autoencoders

An extension of a classical autoencoder and it was introduced as a building block for deep networks.

13.1 Autoencoders

An auto-encoder is trained to encode the input $\mathbf{x}$ into some representation $\mathbf{c}(\mathbf{x})$ so that the input can be reconstructed from that representation. Hence the target output of the auto-encoder is the auto-encoder input itself.

An autoencoder takes an input $\mathbf{x} \in [0,1]^d$

First maps it with an encoder to a hidden representation $\mathbf{y} \in [\mathbf{0},\mathbf{1}]^{\mathbf{d}'}$ through a deterministic mapping:

$$\mathbf{y} = s(\mathbf{W}\mathbf{x} + \mathbf{b})$$

Where s is a non-linearity such as the sigmoid.

The latent representation $\mathbf{y}$, or **code** is then mapped back (with a decorder) into a **reconstruction** $\mathbf{z}$ of same shape as $\mathbf{x}$ though a similar transformation:

$$\mathbf{z} = s(\mathbf{W}'\mathbf{y} + \mathbf{b}')$$

. Where $'$ does NOT indicate transpose, and $\mathbf{z}$ should be seen as prediction of $\mathbf{x}$, given the code $\mathbf{y}$

The parameter of the model W are optimized such that **the average reconstruction error is minimized**.

Measure the reconstruction error using the traditional squared error $L(\mathbf{x}, \mathbf{z}) = \|\mathbf{x} - \mathbf{z}\|$

If the input is interpreted as either bit vectors or vectors of bit probability by the reconstruction cross-entropy defined as (if $\mathbf{x}|\mathbf{y}$ is in Gaussian):

$$L_H(\mathbf{x}, \mathbf{z}) = -\log P(\mathbf{x}|\mathbf{y}) = -\sum_{k=1}^{d} [\mathbf{x}_k \log \mathbf{z}_k + (1 - \mathbf{x}_k) \log(1 - \mathbf{z}_k)]$$

The hope: $\mathbf{y}$ is a distributed representation that captures the coordinates along the main factors of variation in the data.

13.2 Denoising Autoencoder

The idea behind denoising autoencoders is that in order to force the hidden layer to discover more robust features and prevent it from simply learning the identity (copy the input to output), we train the autoencoder to reconstruct the input from a corrupted version of it.

The denoising auto-encoder is a stochastic version of the auto encoder. It does two things:

- Try to encode the input (preserve the information)
- Try to undo the effect of a corruption process stochastically applied to the input of the auto-encoder.

The stochastic corruption process consists in randomly setting some of the inputs (as many as half of them) to zero. Hence the denoising auto-encoder is trying to **predict corrupted values from the uncorrupted values**, for randomly selected subsets of missing patterns. Note how being able to predict any subset of variables from the rest is a sufficient condition for completely capturing the joint distribution between a set of variables.

To convert the autodecoder class into a denoising autoencoder class, all we need to do is to add a stochastic corruption step operating on the input.

Chapter 14

Stacked Denoising Autoencoders(SDA)

The denoising autoencoders can be stacked into form a deep network by **feeding the latent representation(output code)** of the denoising autoencoder found on the layer below as input to the current layer.

The unsupervised pre-training of such an architecture is done one layer at a time.

Each layer is trained as a denoising auto-encoder by minimizing the reconstruction of its input (output code of the previous layer).

Once the first k-layers are trained, we can train the $(k+1)$-th layer because we can now compute the code (latent representation) from the layer below.

Once all layers are pre-trained, the network goes through a second stage of training called **fine-tuning**.

Supervised fine-tuning Minimize the prediction error on a supervised task.

1. Add a logistic regression layer on top of the network (the out put code of the output layer)
2. Train the entire network as we would train a multilayer perceptron.
3. At this point, we only consider the encoding parts of each auto-encoder.

Chapter 15

Restricted Boltzmann Machines

15.1 Energy-Based Models (EBM)

- Associate a scalar energy to each configuration of the variables
- Learning: modify that energy so that its shape has desired properties.

Define a probability distribution through an energy function as follows:

$$p(x) = \frac{e^{-E(x)}}{Z}$$

The normal factor Z – partition function

$$Z = \sum_x e^{-E(x)}$$

An EBM can be learnt by performing stochastic gradient descent on the empirical negative log-likelihood

As for logistic regression, log-likelihood:

$$\mathcal{L}(\theta, \mathcal{D}) = \frac{1}{N} \sum_{x^{(i)} \in \mathcal{D}} \log p(x^{(i)}$$

Loss function as being the negative log-likelihood:

$$l(\theta, \mathcal{D}) = -\mathcal{L}(\theta, \mathcal{D})$$

Using the stochastic gradient:

$$-\frac{\partial \log p(x^{(i)}}{\partial \theta}$$

15.1.1 EBMs with Hidden Units

Consider an observed part x and a hidden part h:

$$P(x) = \sum_h P(x, h) = \sum_h \frac{e^{-E(x,h)}}{Z}$$

Free Energy

$$\mathcal{F}(x) = -\log \sum_h e^{-E(x,h)}$$

Then

$$P(x) = \frac{e^{-\mathcal{F}(x)}}{Z}$$

with $Z = \sum_x e^{-\mathcal{F}(x)}$

Negative log-likelihood gradient:

$$-\frac{\partial \log p(x)}{\partial \theta} = \frac{\partial \mathcal{F}(x)}{\partial \theta} - \sum_{\hat{x}} p(\hat{x}) \frac{\partial \mathcal{F}(\hat{x})}{\partial \theta}$$

The positive and negative phase reflect their effect on the probability of training data.

It is usually difficult to determine this gradient analytically, as it involves the computation of $E_p \left[\frac{\partial \mathcal{F}(x)}{\partial \theta} \right]$, an expectation over all possible configuration of the input x.

Making this computation tractable is to **estimate the expectation** using a fixed number of model samples.

- Samples used to estimate the negative phase gradient are referred to as negative particles, denoted as $\mathcal{N}$
- The gradient can be written as:

$$-\frac{\partial \log p(x)}{\partial \theta} \approx \frac{\partial \mathcal{F}(x)}{\partial \theta} - \frac{1}{|\mathcal{N}|} \sum_{\hat{x} \in \mathcal{N}} \frac{\partial \mathcal{F}(\hat{x})}{\partial \theta}$$

15.2 Restricted Boltzmann Machines (RBM)

A particular form of log-linear Markov Random Field, for which the **energy function is linear** in its free parameters.

Two-layer network, in which stochastic, binary *feature detectors* using weighted connections.

- The pixels correspond to visible units
- The feature detectors correspond to hidden units

Assume that the hidden and visible variables are binary.

1. **Energy** Joint Configuration $(\mathbf{v}, \mathbf{h})$ (visible and hidden)

$$E(\mathbf{v}, \mathbf{h}) = -\sum_{i \in visible} a_i v_i - \sum_{j \in hidden} b_j h_j - \sum_{i,j} v_i h_j w_{ij}$$

   a_i and b_j are bias and w_{ij} is the weight

2. Probability to every pair of a visible and a hidden vector:

$$p(\mathbf{v}) = \sum_{\mathbf{h}} p(\mathbf{v}, \mathbf{h}) = \frac{1}{Z} \sum_{\mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}$$

   Z is given by:

$$Z = \sum_{\mathbf{v}, \mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}$$

3. Network assigns to a visible vector $\mathbf{v}$:

$$p(\mathbf{v}) = \frac{1}{Z} \sum_{\mathbf{h}} e^{-E(\mathbf{v}, \mathbf{h})}$$

4. Raise the probability of the network assigns a training image: lower the energy of that image and raise the energy of other images => By adjusting the weights and biases.

5. Derivative of the log probability:

$$\frac{\partial \log p(\mathbf{v})}{\partial w_{ij}} = \langle v_i h_j \rangle_{data} - \langle v_i h_j \rangle_{model}$$

   Angle brackets denote expectations under the distribution specified by the subscript that follows

6. The learning rule:

$$\Delta w_{ij} = \epsilon(\langle v_i h_j \rangle_{data} - \langle v_i h_j \rangle_{model})$$

   Where ϵ is the learning rate.

7. Ease to get a unbiased sample of $\langle v_i h_j \rangle$

$$p(h_j = 1|\mathbf{v}) = \sigma(b_j + \sum_i v_i w_{ij} p(v_i = 1|\mathbf{h}) = \sigma(a_i + \sum_j h_j w_{ij}$$

Energy function:

$$E(v,h) = -b'v - c'h - h'Wv$$

W – The weights connecting hidden and visible units and
b, c – the offsets of the visible and hidden layers respectively.

Free energy formula:

$$\mathcal{F}(v) = -b'v - \sum_i \log \sum_{h_i} e^{h_i(c_i + W_i v)}$$

Visible and hidden units are conditionally independent given one-another:

$$p(h|v) = \prod_i p(h_i|v) p(v|h) = \prod_j p(v_j|h)$$

15.2.1 Binary Units

In the case of binary units $v_j, h_i \in \{0, 1\}$:

$$P(h_i = 1|v) = sigm(c_i + W_i v) P(v_j = 1|h) = sigm(b_j + W_j' h)$$

Free energy can be simplifies to:

$$\mathcal{F}(v) = -b'v - \sum_i \log(1 + e^{c_i + W_j v})$$

15.3 Contrastive divergence multi-layer RBMs

15.3.1 Boltzmann machines

X observed and H hidden. Their joint given by Boltzmann distribution associate with energy:

$$P(X = x, H = h) = \frac{\exp\left[-E(x,h)\right]}{Z}$$

Z is the appropriate normalization constant:

$$Z = \sum_{x,h} \exp\left(-E(x,h)\right)$$

Energy function is a quadratic polynomial, $z = (x, h)$

$$E(z) = -\sum_i b_i z_i - \sum_{ij} w_{ij} z_i z_j$$

$z_i \in 0, 1$

If $X = x$ observed, H remains hidden, the likelihood involves a sum over all configurations of H:

$$P(X = x) = \sum_h P(X = x, H = h) = \sum_h \frac{\exp\left(-E(x,y)\right)}{Z}$$

Summing over h and x (in denominator Z) are both intractable.

Restricted Boltzmann Machine: interactions between hidden units are removed, so the sum over h becomes tractable.

Derivatives(non-tractable):

$$
\begin{aligned}
\frac{\partial - \log P(x)}{\partial \theta} &= \frac{\partial - \log \sum_h \frac{\exp(-E)}{Z}}{\partial \theta} \\
&= \frac{\partial \left\{ - \log [\sum_h \exp(-E)] + \log Z \right\}}{\partial \theta} \\
&= \sum_h \frac{exp(-E)}{\sum_h \exp(-E)} \cdot \frac{\partial E}{\partial \theta} - \frac{1}{Z} \sum_{x,h} \exp\left[-E(x,h)\right] \frac{\partial E}{\partial \theta} \\
&= \sum_h \left[\frac{\exp(-E)}{\sum_h \exp(-E)} \frac{\partial E}{\partial H} \right] \frac{\partial E}{\partial \theta} - \sum_{x,h} \frac{\exp[-E(x,h)]}{Z} \frac{\partial E}{\partial \theta} \\
&= \sum_h P(H=h|X=x) \frac{\partial E(h,x)}{\partial \theta} \text{ [this is the POSITIVE phase contribution]} \\
&\quad - \sum_{h,x} P(H=h, X=x) \frac{\partial E(h,x)}{\partial \theta} \text{ [this is the NEGATIVE phase contribution]}
\end{aligned}
$$

The standard way to estimate the gradient, is to avoid perform an MCMC scheme to obtain one or more samples from $P(h|x)$ scheme

15.3.2 Restricted Boltzmann Machines

If we set the weight between h_i and h_j and the weight between x_i and x_j we obtain a RBM.

All the H_i's become independent when conditioning on X, and all the X_i become independent when conditioning on H.

15.3.3 Energy functions for RBM

Note that $w_{ij} = w_{ji}$

Energy term for binomial unit i with value v_i and inputs u_j.

$$E(v_i, u_j) = -b_i v_i - \sum_j w_{ij} v_i u_j$$

$$==> P(v_i = 1|u) = \frac{exp(b_i + \sum_j w_{ij} u_j)}{1 + exp(b_i + \sum_j w_{ij} u_j)} = sigmoid \left(b_i + \sum_j w_{ij} u_j \right)$$

Energy term for fixed-variance Gaussian unit i with value v_i and inputs u_i:

$$a_i^2 v_i^2 - b_i v_i - \sum_j w_{ij} v_i u_j$$

$$P(y|x) = \frac{\exp(-E(x,y))}{\sum_y \exp(-E(x,y))}$$

15.3.4 Update Rule

Use $Z = \sum_{x,y} \exp[-E(x,y)]$:

$$P(x,y) = \frac{\exp[-E(x,y)]}{Z}$$

For any energy-based Boltzmann distribution:

$$\begin{aligned}
\frac{\partial}{\partial\theta}(-\log P(x)) &= \frac{\partial}{\partial\theta}\left(-log\sum_y P(x,y)\right) \\
&= \frac{\partial}{\partial\theta}\left(-\log\sum_y \frac{\exp(-E(x,y))}{Z}\right) \\
&= -\frac{Z}{\sum_y \exp[-E(x,y)]}\left(\sum_y \frac{1}{Z}\frac{\partial\exp[-E(x,y)]}{\partial\theta} - \sum_y \frac{\exp[-E(x,y)]}{Z^2}\frac{\partial Z}{\partial\theta}\right) \\
&= \sum_y\left(\frac{\exp[-E(x,y)]}{\sum_{\hat{y}}\exp[-E(x,\hat{y})]}\frac{\partial E(x,y)}{\partial\theta}\right) + \frac{1}{Z}\frac{\partial Z}{\partial\theta} \\
&= \sum_y P(y|x)\frac{\partial E(x,y)}{\partial\theta} - \frac{1}{Z}\sum_{x,y}\exp[-E(x,y)]\frac{\partial E(x,y)}{\partial\theta} \\
&= \sum_y P(y|x)\frac{\partial E(x,y)}{\partial\theta} - \sum_{x,y} P(x,y)\frac{\partial E(x,y)}{\partial\theta} \\
&= \mathbb{E}\left[\frac{\partial E(x,y)}{\partial\theta}\,\middle|\, x\right] - \mathbb{E}\left[\frac{\partial E(x,y)}{\partial\theta}\right]
\end{aligned}$$