

1 Basics

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(x-\mu)^2}{\sigma^2}}, \quad \mathcal{N}(x|\mu, \sigma)$$

$$f(x) = \frac{1}{\sqrt{(2\pi)^d \det \Sigma}} e^{-\frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu)}, \quad \mathcal{N}(x|\mu, \Sigma)$$

$$\text{Condition number: } \kappa(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$$

$$f(x) \text{ on a: } f(a) + \frac{f'(a)}{1!} (x-a) + \frac{f''(a)}{2!} (x-a)^2 + \dots$$

$$\text{Binomial: } f(k, n, p) = \Pr(X = k) = \binom{n}{k} p^k (1-p)^{n-k}$$

$$\ln(p(x|\mu, \Sigma)) = -\frac{d}{2} \ln(2\pi) - \frac{\ln|\Sigma|}{2} - \frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu)$$
$$X \sim \mathcal{N}(\mu, \Sigma), Y = A + BX \Rightarrow Y \sim \mathcal{N}(A + B\mu, B\Sigma B^T)$$

$$// \text{ General p-norm: } \|x\|_p = (\sum_{i=1}^n |x_i|^p)^{1/p}$$

Moments

$$\bullet \text{ Var}[X] = \int_x (x - \mu)^2 p(x) dx$$

$$\bullet \text{ Var}[X] = E[(X - E[X])^2] = E[X^2] - E[X]^2$$

$$\bullet \text{ Var}[X+Y] = \text{Var}[X] + \text{Var}[Y] + 2\text{Cov}[X, Y]$$

$$\bullet \text{ Cov}[X, Y] = E[(X - E[X])(Y - E[Y])]$$

$$\bullet \text{ Cov}[aX, bY] = ab \text{Cov}[X, Y]$$

$$\bullet K_{XY} = \text{cov}(X, Y) = E[XY^T] - E[X]E[Y^T]$$

Calculus

$$\bullet \text{ Part.: } \int u(x)v'(x)dx = u(x)v(x) - \int v(x)u'(x)dx$$

$$\bullet \text{ Chain r.: } \frac{f(y)}{g(x)} = \frac{dz}{dx} \Big|_{x=x_0} = \frac{dz}{dy} \Big|_{z=g(x_0)} \cdot \frac{dy}{dx} \Big|_{x=x_0}$$

$$\bullet \frac{\partial}{\partial \mathbf{x}} (\mathbf{b}^T \mathbf{x}) = \frac{\partial}{\partial \mathbf{x}} (\mathbf{x}^T \mathbf{b}) = \mathbf{b} \bullet \frac{\partial}{\partial \mathbf{x}} (\mathbf{x}^T \mathbf{x}) = 2\mathbf{x}$$

$$\bullet \frac{\partial}{\partial \mathbf{x}} (\mathbf{x}^T \mathbf{A} \mathbf{x}) = (\mathbf{A}^T + \mathbf{A}) \mathbf{x} \stackrel{\text{A sym.}}{=} 2\mathbf{A} \mathbf{x}$$

$$\bullet \frac{\partial}{\partial \mathbf{x}} (\mathbf{b}^T \mathbf{A} \mathbf{x}) = \mathbf{A}^T \mathbf{b} \bullet \frac{\partial}{\partial \mathbf{x}} (\mathbf{c}^T \mathbf{X} \mathbf{b}) = \mathbf{c} \mathbf{b}^T$$

$$\bullet \frac{\partial}{\partial \mathbf{x}} (\mathbf{c}^T \mathbf{X}^T \mathbf{b}) = \mathbf{b} \mathbf{c}^T \bullet \frac{\partial}{\partial \mathbf{x}} (\|\mathbf{x} - \mathbf{b}\|_2) = \frac{\mathbf{x} - \mathbf{b}}{\|\mathbf{x} - \mathbf{b}\|_2}$$

$$\bullet \frac{\partial}{\partial \mathbf{x}} (\|\mathbf{x}\|_2^2) = \frac{\partial}{\partial \mathbf{x}} (\|\mathbf{x}^T \mathbf{x}\|_2) = 2\mathbf{x} \bullet \frac{\partial}{\partial \mathbf{x}} (\|\mathbf{x}\|_F^2) = 2\mathbf{X}$$

$$\bullet \mathbf{x}^T \mathbf{A} \mathbf{x} = \text{Tr}(\mathbf{x}^T \mathbf{A} \mathbf{x}) = \text{Tr}(\mathbf{x} \mathbf{x}^T \mathbf{A}) = \text{Tr}(\mathbf{A} \mathbf{x} \mathbf{x}^T)$$

$$\bullet \frac{\partial}{\partial \mathbf{A}} \text{Tr}(\mathbf{A} \mathbf{B}) = \mathbf{B}^T \bullet \frac{\partial}{\partial \mathbf{A}} \log|\mathbf{A}| = \mathbf{A}^{-T}$$

$$\bullet \text{ sigmoid}(x) = \sigma(x) = \frac{1}{1 + \exp(-x)}$$

$$\bullet \nabla \text{sigmoid}(x) = \text{sigmoid}(x)(1 - \text{sigmoid}(x))$$

$$\bullet \nabla \tanh(x) = 1 - \tanh^2(x) \bullet \tanh x = \frac{\sinh x}{\cosh x} = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

Probability / Statistics

$$\text{Bayes' Rule } P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)} = \frac{P(X|Y)P(Y)}{\sum_{i=1}^k P(X|Y_i)P(Y_i)}$$

$$\text{MGF } \mathbf{M}_X(t) = \mathbb{E}[e^{t^T \mathbf{X}}], \mathbf{X} = (X_1, \dots, X_n)$$

Jensen's inequality

X: random variable & φ : convex function $\rightarrow \varphi(\mathbb{E}[X]) \leq \mathbb{E}[\varphi(X)]$

2 Regression

Estimation

Consistency: $\hat{\theta}_n \xrightarrow{P} \theta$, i.e. $\forall \epsilon \in P\{|\hat{\theta}_n - \theta| \geq \epsilon\} \xrightarrow{n \rightarrow \infty} 0$

Asymptotic normality: $\sqrt{N}(\theta - \hat{\theta}_n) \rightarrow$

$$\mathcal{N}(0, J^{-1} I J^{-1})$$

Asymptotic efficiency: $\hat{\theta}_n$ has the smallest variance among all possible consistent estimators (for large enough N), i.e. $\lim_{n \rightarrow \infty} (V[\hat{\theta}_n] I(\theta))^{-1} = 1$ $\hat{\theta}_{MAP} := \arg \max_{\theta} \left\{ \sum_{i=1}^n \log(p(x_i|\theta)) + \log(p(\theta)) \right\}$

Rao-Cramer

$$\Lambda = \frac{\partial \log \mathbb{P}(x|\theta)}{\partial \theta} \text{ (score function), } E[\Lambda] = 0$$

$$\text{Fisher information: } I = \mathbb{V}[\Lambda]$$

$$J = E[\Lambda^2] = -E\left[\frac{\partial^2 \log \mathbb{P}(x|\theta)}{\partial \theta \partial \theta^T}\right] = -E\left[\frac{\partial \Lambda}{\partial \theta}\right]$$

variance of an estimator is bounded from below by the inverse of Fisher information

$$\text{MSE bound: } E[(\hat{\theta} - \theta)^2] \geq \frac{[1+b'(\theta)]^2}{nE[\Lambda^2]} + b_{\hat{\theta}}^2$$

$$\text{Biased estimators: } \text{var}(\hat{\theta}) \geq \frac{[1+b'(\theta)]^2}{I(\theta)}$$

$$\text{Efficiency: } e(\hat{\theta}) = \frac{I(\theta)^{-1}}{\text{var}(\hat{\theta})} \leq 1$$

$$\text{Cauchy-Schwarz: } |E(X, Y)|^2 \leq E(X^2)E(Y^2)$$

Regularized regression

$$\text{Error: } \hat{R}(w) = \sum_{i=1}^n (y_i - w^T x_i)^2 + \lambda \|w\|_2^2 \text{ (Ridge)}$$

$$\text{Closed form: } w^* = (X^T X + \lambda I)^{-1} X^T y \text{ (Ridge)}$$

$$\text{Shrinkage: } Xw^* = \sum_{j=1}^d u_j \frac{\sigma_j^2}{\sigma_j^2 + \lambda} u_j^T y, X = U \Sigma V^T$$

$$\text{LASSO: } w^* = \arg \min_w \sum_{i=1}^n (y_i - w^T x_i)^2 + \lambda \|w\|_1$$

Bayesian linear regression

Model: $y = X^T \beta + \epsilon$, with $\epsilon \sim \mathcal{N}(\epsilon|0, \sigma^2 I)$

or $P(y | X, \beta, \sigma) = \mathcal{N}(y|X^T \beta, \sigma^2 I)$ $P(\beta|\Lambda) = \mathcal{N}(\beta|0, \Lambda^{-1})$, Post: $P(\beta|X, y, \Lambda) = \mathcal{N}(\beta|\mu_{\beta}, \Sigma_{\beta})$

$$\mu_{\beta} = (X^T X + \sigma^2 \Lambda)^{-1} X^T y, \Sigma_{\beta} = \sigma^2 (X^T X + \sigma^2 \Lambda)^{-1}$$

$$\text{Prediction: } y_{\text{new}} = \hat{\beta}_{MAP}^T x_{\text{new}} = \mu_{\beta}^T x_{\text{new}}$$

$$P(y_{\text{new}}|x_{\text{new}}, X, y, \beta) = \mathcal{N}(\mu_{\beta}^T x_{\text{new}}, \sigma^2 + x_{\text{new}}^T \Sigma_{\beta} x_{\text{new}})$$

$$\text{Combination of Regression Models:}$$

$$\text{bias}[\hat{f}(x)] = \frac{1}{B} \sum_{i=1}^B \text{bias}[\hat{f}_i(x)]$$

$$\text{Var}[\hat{f}(x)] = \frac{1}{B^2} \sum_i \text{Var}[\hat{f}_i(x)] + \frac{1}{B^2} \sum_{i,j:i \neq j}$$

$$\text{Cov}[\hat{f}_i(x), \hat{f}_j(x)] \approx \frac{\sigma^2}{B}$$

RSS Estimator

$$\hat{\beta} \sim \mathcal{N}(\beta, (X^T X)^{-1} \sigma^2)$$

Bias vs. Variance

$$\mathbb{E}_D \mathbb{E}_{X,Y} (\hat{f}(X) - Y)^2 =$$

$$\mathbb{E}_D \mathbb{E}_X (\hat{f}(X) - \mathbb{E}(Y|X))^2 + \mathbb{E}_{X,Y} (Y - \mathbb{E}(Y|X))^2$$

$$= \mathbb{E}_X \mathbb{E}_D (\hat{f}(X) - \mathbb{E}_D(\hat{f}(X)))^2 \text{ (variance)}$$

$$+ \mathbb{E}_X (\mathbb{E}_D(\hat{f}(X)) - \mathbb{E}(Y|X))^2 \text{ (bias}^2)$$

$$+ \mathbb{E}_{X,Y} (Y - \mathbb{E}(Y|X))^2 \text{ (noise)}$$

Ridge Parametric to nonparametric

Ansatz: $w = \sum_i \alpha_i x$

$$w^* = \arg \min_w \sum_i (w^T x_i - y_i)^2 + \lambda \|w\|_2^2 =$$

$$\arg \min_{\alpha_{1:n}} \sum_{i=1}^n (\sum_{j=1}^n \alpha_j x_j^T x_i - y_i)^2 + \lambda \sum_i \sum_j \alpha_i \alpha_j (x_i^T x_j)$$

$$= \arg \min_{\alpha_{1:n}} \sum_{i=1}^n (\alpha^T K_i - y_i)^2 + \lambda \alpha^T K \alpha$$

$$= \arg \min_{\alpha} \|\alpha^T K - y\|_2^2 + \lambda \alpha^T K \alpha$$

$$\text{Closed form: } \alpha^* = (K + \lambda I)^{-1} y$$

$$\text{Prediction: } y^* = w^{*T} x = \sum_{i=1}^n \alpha_i^* k(x_i, x)$$

3 Gaussian Processes

Gaussian Process

$$[y_1, y_2, \dots]^T = X\beta + \epsilon \sim \mathcal{N}(y|0, X\Lambda^{-1}X^T + \sigma^2 I)$$

$$y \sim \mathcal{N}(y|m(X), K(X, X) + \sigma^2 I) = P(y|X, \Theta)$$

$$\begin{bmatrix} y \\ y_{n+1} \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} y \\ y_{n+1} \end{bmatrix} \middle| \begin{bmatrix} m(X) \\ m(x_{n+1}) \end{bmatrix}, \begin{bmatrix} C_n & k \\ k^T & c \end{bmatrix} \right)$$

$$p(y_{n+1}|x_{n+1}, X, y) = \mathcal{N}(y_{n+1}|\mu_{n+1}, \sigma_{n+1}^2)$$

$$\mu_{n+1} = m(x_{n+1}) + k^T C_n^{-1} (y - m(X))$$

$$\sigma_{n+1}^2 = c - k^T C_n^{-1} k, k = k(x_{n+1}, X)$$

$$c = k(x_{n+1}, x_{n+1}) + \sigma^2, C_n = K_n + \sigma^2 I$$

GP Hyperparameter Optimization

Log-likelihood:

$$l(Y|\theta) = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log|C_n| - \frac{1}{2} Y^T C_n^{-1} Y$$

Set of hyperparameters θ determine parameters C_n . Gradient descent: $\nabla_{\theta_i} l(Y|\theta) =$

$$-\frac{1}{2} \text{tr}(C_n^{-1} \frac{\partial C_n}{\partial \theta_i}) + \frac{1}{2} Y^T C_n^{-1} \frac{\partial C_n}{\partial \theta_i} C_n^{-1} Y$$

Kernels

$K(x, y) = \langle \phi(x), \phi(y) \rangle$ for some feature mapping $\phi(x)$

$$\text{Psd Gram Matrix: } c^T K c \geq 0, \sum_i \sum_j c_i c_j k(x_i, x_j) \geq 0$$

All principal minors of K need $\det \geq 0$;

$$k(x, y) = k(y, x); k(x, x) \geq 0; k(x, x)k(y, y) \geq k(x, y)^2 \text{ Closure Properties: psd prop. closed under}$$

pointwise limits (since each K_n is a kernel)

$$k(x, y) = k_1(x, y) + k_2(x, y), k(x, y) =$$

$$k_1(x, y)k_2(x, y)$$

$$k(x, y) = f(x)f(y), k(x, y) = k_3(\phi(x), \phi(y))$$

$$k(x, y) = \exp(\alpha k_1(x, y)), \alpha > 0, |X \cap Y| = \text{kernel}$$

$$k(x, y) = p(k_1(x, y)), p(\cdot) \text{ polynomial with pos. coeff.}$$

$$k(x, y) = k_1(x, y) / \sqrt{(k_1(x, x)k_1(y, y))}$$

$$\text{Gaussian (rbf): } k(x, y) = \exp(-\frac{\|x-y\|_2^2}{2\sigma^2}) \text{ inf.dim.}$$

$$\text{Sigmoid: } k(x, y) = \tanh(k \cdot x^T y - b) \text{ not valid for } \forall k, b$$

$$\text{Polynomial: } k(x, y) = (x^T y + c)^d, d \in \mathbb{N}, c \geq 0$$

$$\text{Periodic: } k(x, y) = \sigma^2 \exp(\frac{2 \sin^2(\pi|x-y|/p)}{c^2})$$

4 Numerical Estimating Methods

$$\text{Actual Risk: } \mathcal{R}(f) := \mathbb{E}_{x,y}[(y - f(x))^2]$$

$$\text{Empirical Risk: } \hat{\mathcal{R}}(f) = \frac{1}{n} \sum_i (y_i - f(x_i))^2$$

$$\text{Generalization Error: } G(f) = |\hat{\mathcal{R}}(f) - \mathcal{R}(f)|$$

K-fold cross validation

$$\hat{f}^{-v} \in \arg \min_f \frac{1}{|Z^{-v}|} \sum_{i \in Z^{-v}} (y_i - f(x_i))^2$$

$$\hat{\mathcal{R}}^{cv} = \frac{1}{n} \sum_i (y_i - \hat{f}^{-v(i)}(x_i))^2, k(i) \text{ is fold } i^{\text{th}} \text{ fold}$$

Problem: systematic tendency to underfit.

Leave-one-out

unbiased, high variance

$$\hat{f}^{-i} \in \arg \min_f \frac{1}{n-1} \sum_{j:j \neq i} L(y_j, f(x_j))$$

$$\hat{\mathcal{R}}^{LOOCV} = \frac{1}{n} \sum_i L(y_i, \hat{f}^{-i}(x_i))$$

Bootstrapping

Resampling with replacement from data D to produce B bootstrap datasets D^{*b} . $S(D)$ is expected generalization error of prediction model trained on D . Var: $\sigma^2(S) =$

$$\frac{1}{B-1} \sum_{b=1}^B (S(D^{*b}) - \bar{S})^2 \text{ with mean: } \hat{R}_{boot}(f) = \bar{S} = \frac{1}{B} \sum_{b=1}^B (\frac{1}{N} \sum_{i=1}^N L(y_i, \hat{f}_{D^{*b}}(x_i))) \text{ with } \hat{f}_{D^{*b}}(x_i)$$

being the prediction model. $\hat{R}_{boot}(f) =$

$$\frac{1}{N} \sum_{i=1}^N \frac{1}{|C^{-i}|} \sum_{b \in C^{-i}} L(y_i, \hat{f}_{D^{*b}}(x_i)) \text{ where } C^{-i}$$

denotes the set of bootstrap sets not containing data point i . Note: L can be $I_{\{c(x_i) \neq y_i\}}$.

\hat{R}_{boot} is optimistic. Hence use: $\hat{R}^{0.632} =$

$$0.368 \hat{R}_{boot} + 0.632 \hat{R}_{boot}^{(LOO)}$$

Prob. not to appear in set: $(1 - \frac{1}{n})^n = \frac{1}{e}$ for $n \rightarrow \infty$

Jackknife

Goal: Numerical estimate of bias of an estimator \hat{S}_n . Jackknife estimator: $\hat{S}_n^{JK} = \hat{S}_n -$

$$\text{bias}^{JK} \text{ with } \text{bias}^{JK} = (n-1)(\hat{S}_n - \hat{S}_n)$$

$$\hat{S}_n = \frac{1}{n} \sum_{i=1}^n \hat{S}_n^{(-i)} \text{ with } \hat{S}_n^{(-i)} \text{ being the leave-1-out estimator.}$$

Information Criteria

$$BIC = \ln(n)k - 2\ln(\hat{L}), AIC = 2k - 2\ln(\hat{L})$$

$$TIC = 2\text{trace}[I_1(\theta_k)J_1^{-1}(\theta_k)] - 2\ln(\hat{L}), \text{ where } k:$$

num. params, n: num. data points, likelihood:

$$\hat{L} = p(X|\theta_k, M)$$

5 Classification

Loss-Functions

$$\text{True class: } y \in \{-1, 1\}, \text{ pred. } z \in [-1, 1]$$

$$\text{Cross-entropy (log loss): } (y' = \frac{1+y}{2}) \text{ and } z' =$$

$$\frac{1+z}{2}) L(y', z') = -[y' \log(z') + (1-y') \log(1-z')]$$

$$\text{Hinge Loss: } L(y, z) = \max(0, 1 - yz)$$

$$\text{Perceptron Loss: } L(y, z) = \max(0, -yz)$$

Logistic loss: $L(y, z) = \log(1 + \exp(-yz))$
 Square loss: $L(y, z) = \frac{1}{2}(1 - yz)^2$
 Exponential loss: $L(y, z) = \exp(-yz)$
 Binomial deviance: $L(y, z) = 1 + \exp(-2yz)$
 0/1 Loss: $L(y, z) = \mathbb{I}\{\text{sign}(z) \neq y\}$

Perceptron

Gradient descent: $a(k+1) = a(k) - \eta(k) \nabla J(a(k))$
 $J(a) \approx J(a(k)) + \nabla J^T(a - a(k)) + \frac{1}{2}(a - a(k))^T H(a - a(k))$, $H = \frac{\partial^2 J}{\partial a_i \partial a_j}$

2^{nd} order algorithm: $\eta_{opt} = \frac{\|\nabla J\|^2}{\nabla J^T H \nabla J}$

Newton's rule: $a(k+1) = a(k) - H^{-1} \nabla J$

Perceptron criteria: $J_p(a) = \sum_{\tilde{x} \in \tilde{X}^{mc}} (-a^T \tilde{x})$

Perceptron rule: $a(k+1) = a(k) + \eta(k) \sum_{\tilde{x} \in \tilde{X}^{mc}} \tilde{x}$

Perceptron convergence: $\|a(k+1) - \alpha \hat{a}\|^2 = \|a(k) - \alpha \hat{a}\|^2 + 2(a(k) - \alpha \hat{a})^T \tilde{x}^k + \|\tilde{x}^k\|^2 \leq \|a(k) - \alpha \hat{a}\|^2 - 2\alpha\gamma + \beta^2$ where $\beta^2 = \max_i \|\tilde{x}_{i \in \tilde{X}^{mc}}\|^2$ and $\gamma = \min_{i \in \tilde{X}^{mc}} (\hat{a}^T \tilde{x}_i) > 0$ for $\alpha = \beta^2/\gamma$ then $k_0 = \alpha^2 \|\hat{a}\|^2 / \beta^2 = \beta^2 \|\hat{a}\|^2 / \gamma^2$

6 Design of Discriminant

Fisher's Linear Discriminant:

$\mathbb{R}^d \rightarrow \mathbb{R}^{(k-1)}$: $\vec{y}_i = \vec{w}_i^T \vec{x}_i, 1 \leq i \leq k-1, \vec{y} = W^T \vec{x}$
 Criterion: $J(W) = \frac{|W^T \Sigma_B W|}{|W^T \Sigma_W W|} = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2} \xrightarrow{\text{maximize}} d/dW = 0$

$\Sigma_B = \sum_i n_i (m_i - m)(m_i - m)^T$ (Between class variance)
 $\Sigma_W = \sum_i \sum_{x \in X_i} (x - m_i)(x - m_i)^T$ (Within class variance)
 $m_i = \frac{1}{n_i} \sum_{x \in X_i} x, m = \frac{1}{n} \sum_x x$

solution: $\hat{w} \stackrel{2 \text{ classes}}{=} \Sigma_W^{-1} (m_1 - m_2)$

7 SVM

Primal Problem: ($C \rightarrow \infty$: Hard Margin)

$\min_w \frac{1}{2} w^T w + C \sum_{i=1}^n \xi_i$ s.t. $z_i(w^T \phi(y_i) + w_0) \geq 1 - \xi_i, \xi_i \geq 0$

Dual Problem: $L(w, w_0, \xi, \alpha, \beta) = \frac{1}{2} w^T w + C \sum_{i=1}^n \xi_i - \sum_{i=1}^n \beta_i \xi_i - \sum_{i=1}^n \alpha_i (z_i(w^T \phi(y_i) + w_0) - 1 + \xi_i)$
 $\max_{\alpha} L(a) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n z_i z_j \alpha_i \alpha_j \phi(y_i, y_j)$
 s.t. $\sum_{j=1}^n z_j \alpha_j = 0 \wedge C \geq \alpha_i \geq 0$

optimal hyperplane: $w^* = \sum_{i=1}^n \alpha_i^* z_i \phi(y_i)$

$w_0^* = \frac{1}{n_s} \sum_{i \in S} (z_n - \sum_{j \in S} \alpha_j z_j \phi(y_i, y_j))$
 $\stackrel{\text{linear}}{=} -\frac{1}{2} (\min_{i: z_i=1} w^{*T} y_i + \max_{i: z_i=-1} w^{*T} y_i)$

Only for support vectors: $\alpha_i^* > 0$

Prediction: $z(y) = \text{sign}(\sum_{i=1}^n \alpha_i z_i \phi(y, y_i) + w_0)$

$\stackrel{\text{linear}}{=} \text{sign}(w^{*T} x + w_0)$

Homog. Coordinates: condition $\sum_{j=1}^n z_j \alpha_j = 0$

falls away.

8 Non-linear SVM

Multiclass SVM

$\min_{w, \eta} \frac{1}{2} w^T w + C \sum_i \xi_i$
 s.t. $\forall y_i \in Y: (w_{z_i}^T y_i) - \max_{z \neq z_i} (w_z^T y_i) \geq 1 - \xi_i$

Structured SVM

$\min_{w, \eta} \frac{1}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^n \eta_i, \eta \geq H_i(w) \forall i$, where $H_i(w) = \max_{y \in Y(x_i)} L(y_i, y) - w^T (\phi(x_i, y_i) - \phi(x_i, y))$

9 Ensemble method

Random Forest

for $b=1:B$ do:

draw a bootstrap sample D_b

repeat until node size $< n_{min}$:

1. select m features from p features
2. pick the best variable and split-point
3. Split the node accordingly

return the forest $\{\hat{c}_b(x)\}_{b=1}^B$

Boosting: Train weak learners sequentially on all data, but reweight misclassified samples higher, Bias \downarrow

Adaboost

Initialize weights $w_i = 1/n$, for $b=1:B$ do:

1. Fit classifier $c_b(x)$ with weights w_i
2. Compute error $\epsilon_b = \sum_i w_i \mathbb{I}_{[c_b(x_i) \neq y_i]} / \sum_i w_i$
3. Compute coeff. $\alpha_b = \log(\frac{1-\epsilon_b}{\epsilon_b})$
4. Update weights $w_i = w_i \exp(\alpha_b \mathbb{I}_{[y_i \neq c_b(x_i)]})$

Return $\hat{c}_B(x) = \text{sign}(\sum_{b=1}^B \alpha_b c_b(x))$

Loss: Exponential loss function

Model: Additive logistic regression

Bayesian approach (assumes posteriors)

Newtonlike updates (Gradient Descent)

Bagging

return ensemble class. $\hat{c}_B(x) = \text{sgn}(\sum_{i=1}^B c_i(x))$

Works: Covariance small (different subset for training), Variance small (similar behaviour of weak learners), biases weakly affected.

Bias \downarrow & Var. \downarrow : Use complex decision tree (bias \downarrow), ensemble mult. decision trees (var \downarrow)

Gaussian Mixtures

Estimate $\hat{\theta} = \{\mu_1, \dots, \mu_k, \Sigma_1, \dots, \Sigma_k\}$ that maximize the likelihood of sample feature vectors

$\mathcal{X} = \{x_1, \dots, x_n\}$:
 $p(\mathcal{X} | \pi_1, \dots, \pi_k, \theta_1, \dots, \theta_k) = \prod_{x \in \mathcal{X}} \sum_{c \leq k} \pi_c p(x | \theta_c)$
 Log-Likelihood: $L(\mathcal{X} | \pi, \theta) = \sum_{x \in \mathcal{X}} \log \sum_{c \leq k} \pi_c p(x | \theta_c)$

Expectation Maximization

$L(\mathcal{X}, M | \theta) = \sum_{x \in \mathcal{X}} \sum_{c=1}^k M_{xc} \log(\pi_c p(x | \theta_c))$

$Q(\theta; \theta^{(j)}) = \mathbb{E}_M[L(\mathcal{X}, M | \theta) | \mathcal{X}, \theta^{(j)}]$, M latent

variable

$M_{xc} = 1$ if cluster c has generated x , else $M_{xc} = 0$

$\mathbb{E}_M[M_{xc} | \mathcal{X}, \theta^{(j)}] = P(M_{xc} = 1) = P(c | x, \theta^{(j)}) = \frac{P(x | c, \theta^{(j)}) P(c | \theta^{(j)})}{P(x | \theta^{(j)})} = \frac{\pi_c P(x | c, \theta^{(j)})}{\sum_{c=1}^k \pi_c P(x | c, \theta^{(j)})} =: \gamma_{xc}$

- 1: **while** not converged **do**
- 2: E-Step: Compute γ_{xc} for all x, c Compute $m_c := \sum_x \gamma_{xc}$ for all c
- 3: M-Step: $\max_{\theta} Q(\theta; \theta^{(j)})$ s.t. $\sum_c \pi_c = 1$

$\mu_c^{(j+1)} = \frac{\sum_{x \in \mathcal{X}} \gamma_{xc} x}{\sum_c \gamma_{xc}} = \frac{\sum_{x \in \mathcal{X}} m_c \gamma_{xc} (x - \mu_c)(x - \mu_c)^T}{m_c} = \frac{1}{|\mathcal{X}|} m_c$

- 4: **end while**

Lagrangian with fixed γ_{xc}

$L = \sum_x \sum_c \gamma_{xc} \log(\pi_c P(x | c, \theta_c)) - \lambda (\sum_c \pi_c - 1)$

For GMM: $P(x | c, \theta^{(j)}) = \mathcal{N}(x | \mu_c, \Sigma_c)$

10 Neural Network

Backpropagation

For each unit j on the output layer:

- Compute error signal: $\delta_j = \ell'_j(f_j)$

- For each unit i on layer L : $\frac{\partial}{\partial w_{j,i}} = \delta_j v_i$

For each unit j on hidden layer $l = \{L-1, \dots, 1\}$:

- Error signal: $\delta_j = \phi'(z_j) \sum_{i \in \text{Layer}_{l+1}} w_{i,j} \delta_i$

- For each unit i on layer $l-1$: $\frac{\partial}{\partial w_{j,i}} = \delta_j v_i$

11 PAC Learning

Empirical error: $\hat{\mathcal{R}}_n(c) = \frac{1}{n} \sum_{i=1}^n \mathbb{I}_{\{c(x_i) \neq y_i\}}$

Expected error: $\mathcal{R}(c) = P\{c(x) \neq y\}$

ERM: $\hat{c}_n^* = \arg \min_{c \in \mathcal{C}} \hat{\mathcal{R}}_n(c)$

opt: $c^* \in \min_{c \in \mathcal{C}} \mathcal{R}(c)$, $|\mathcal{C}|$ finite

Generalization error: $\mathcal{R}(\hat{c}_n^*) = P\{\hat{c}_n^*(x) \neq y\}$

VC ineq.: $\mathcal{R}(\hat{c}_n^*) - \inf_{c \in \mathcal{C}} \mathcal{R}(c) \leq 2 \sup_{c \in \mathcal{C}} |\hat{\mathcal{R}}_n(c) - \mathcal{R}(c)|$

$P\{\mathcal{R}(\hat{c}_n^*) - \mathcal{R}(c^*) > \epsilon\} \leq P\{\sup_{c \in \mathcal{C}} |\hat{\mathcal{R}}_n(c) - \mathcal{R}(c)| > \frac{\epsilon}{2}\}$

$\leq 2|\mathcal{C}| \exp(-2n\epsilon^2/4) \leq 8s(\mathcal{A}, n) \exp(-n\epsilon^2/32)$
 and $s(\mathcal{A}, n) \leq n^{V_A}$

Markov ineq: $P\{X \geq \epsilon\} \leq \frac{\mathbb{E}[X]}{\epsilon}$ (for nonneg. X)

Boole's inequality: $P(\bigcup_i A_i) \leq \sum_i P(A_i)$

Hoeffding's lemma: $\mathbb{E}[e^{sX}] \leq \exp(\frac{1}{8} s^2 (b-a)^2)$

where $\mathbb{E}[X] = 0, P(X \in [a, b]) = 1$

Hoeffding's: $P\{|S_n - \mathbb{E}[S_n]| \geq t\} \leq \exp(-\frac{2t^2}{\sum_i (b_i - a_i)^2})$

Normalized: $P\{|\tilde{S}_n - \mathbb{E}[\tilde{S}_n]| \geq \epsilon\} \leq \exp(-\frac{2n^2 \epsilon^2}{\sum_i (b_i - a_i)^2})$

Error bound: $P\{\sup_{c \in \mathcal{C}} |\hat{\mathcal{R}}_n(c) - \mathcal{R}(c)| > \epsilon\} \leq 2|\mathcal{C}| \exp(-2n\epsilon^2)$

The VC dimension of a model f is the maximum number of points that can be arranged so that f shatters them.

12 Nonparametric Bayesian methods

$Dir(x | \alpha) = \frac{1}{B(\alpha)} \prod_{k=1}^n x_k^{\alpha_k - 1}, B(\alpha) = \frac{\prod_{k=1}^n \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^n \alpha_k)}$

$\mathbb{E}[1] = \sum_{i=1}^N \frac{\alpha_i}{\alpha + i} \sim (\alpha \log(N))$

de Finetti: $p(X_1, \dots, X_n) = \int (\prod_{i=1}^n p(x_i | G)) dP(G)$

$p(z_i = k | z_{-i}, x, \alpha, \mu) = \begin{cases} \frac{N_{k,-i}}{\alpha + N - 1} p(x_i | x_{-i,k}, \mu) & \exists k \\ \frac{\alpha}{\alpha + N - 1} p(x_i | \mu) & \text{otherwise} \end{cases}$

DP generative model:

- Centers of the clusters: $\mu_k \sim \mathcal{N}(\mu_0, \sigma_0)$
- Prob.s of clusters: $\rho = (\rho_1, \rho_2) \sim GEM(\alpha)$
- Assignments to clusters: $z_i \sim \text{Categorical}(\rho)$
- Coordinates of data points: $\mathcal{N}(\mu_{z_i}, \sigma)$

13 Generative Methods

Naive Bayes

All features independent.

$P(y|x) = \frac{1}{Z} P(y) P(x|y), Z = \sum_y P(y) P(x|y)$

$y = \arg \max_y P(y|x) = \arg \max_y \hat{P}(y) \prod_{i=1}^d \hat{P}(x_i | y)$

Discriminant Function

$f(x) = \log(\frac{P(y=1|x)}{P(y=-1|x)}), y = \text{sign}(f(x))$

14 Neural Networks

Learning features

Parameterize the feature maps and optimize over the parameters:

$w^* = \arg \min_{w, \Theta} \sum_{i=1}^n l(y_i, \sum_{j=1}^m w_j \Phi(x_i, \Theta_j))$

Reformulating the perceptron

Ansatz: $w = \sum_{j=1}^n \alpha_j y_j x_j$

$\min_{w \in \mathbb{R}^d} \sum_{i=1}^n \max[0, -y_i w^T x_i]$

$= \min_{\alpha_{1:n}} \sum_{i=1}^n \max[0, -y_i (\sum_{j=1}^n \alpha_j y_j x_j)^T x_i]$

$= \min_{\alpha_{1:n}} \sum_{i=1}^n \max[0, -\sum_{j=1}^n \alpha_j y_j y_i x_i^T x_j]$

$= \min_{\alpha_{1:n}} \sum_{i=1}^n \max[0, -\sum_{j=1}^n \alpha_j y_j y_i x_i^T x_j]$

Kernelized Perceptron

1. Initialize $\alpha_1 = \dots = \alpha_n = 0$

2. For t do

Pick data $(x_i, y_i) \in_{u.a.r} D$

Predict $\hat{y} = \text{sign}(\sum_{j=1}^n \alpha_j y_j k(x_j, x_i))$

If $\hat{y} \neq y_i$ set $\alpha_i = \alpha_i + \eta_t$