Probability

Bayes Theorem:

$$P(Y = \pm 1|X) = \frac{P(X|Y = \pm 1)P(Y = \pm 1)}{P(X|Y = +1)P(Y = +1) + P(X|Y = -1)P(Y = -1)}$$

Matrix calculus

$$f(\mathbf{x}) = \mathbf{x}'\mathbf{A}\mathbf{B} + \mathbf{A}\mathbf{B}\mathbf{x} + \mathbf{x}'\mathbf{A}\mathbf{B}\mathbf{x} \Leftrightarrow \frac{df(\mathbf{x})}{d\mathbf{x}} = \mathbf{A}\mathbf{B} + \mathbf{A}\mathbf{B} + 2\mathbf{A}\mathbf{B}\mathbf{x}$$

$$\mathbf{H}_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}; \, \nabla_x(a\mathbf{x}) = a\mathbf{I}$$

Perceptron

$$f(\mathbf{x}) = \boldsymbol{\theta} \cdot \mathbf{x} + \theta_0 = \sum_{i=1}^d \theta_i x_i + \theta_0, \ \hat{y} = \begin{cases} 1, & \text{if } f(x) \ge 0 \\ -1, & \text{if } f(x) < 0 \end{cases}$$

Decision boundary, a hyperplane in \mathbb{R}^d :

$$H = \{ \mathbf{x} \in \mathbb{R}^d : f(\mathbf{x}) = 0 \} = \{ \mathbf{x} \in \mathbb{R}^d : \boldsymbol{\theta} \cdot \mathbf{x} + \theta_0 = 0 \}$$

 θ is the **normal** of the hyperplane,

 θ_0 is the **offset** of the hyperplane from origin,

 $-\frac{\theta_0}{\|\theta\|}$ is the **signed distance** from the origin to hyperplane.

Perceptron algorithm,

Input: $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n) \in \mathbb{R}^d \times \{\pm 1\}$ while some $y_i \neq \operatorname{sign}(\boldsymbol{\theta} \cdot \mathbf{x}_i)$ pick some misclassified (\mathbf{x}_i, y_i) $\theta \leftarrow \theta + y_i \mathbf{x}_i$

Given a linearly separable data, perceptron algorithm will take no more than $\frac{R^2}{\gamma^2}$ updates to **converge**, where $R = \max_i \|\mathbf{x}_i\|$ is the radius of the data, $\gamma = \min_i \frac{y_i(\pmb{\theta} \cdot \mathbf{x}_i)}{\|\pmb{\theta}\|}$ is the margin.

Also, $\frac{\theta \cdot \mathbf{x}}{\|\mathbf{\theta}\|}$ is the signed distance from H to \mathbf{x} in the direction $\boldsymbol{\theta}$.

 $\boldsymbol{\theta} = \sum_i \alpha_i y_i \mathbf{x}_i$, thus any inner product space will work, this is a

Gradient descent view of perceptron, minimize margin cost function $J(\boldsymbol{\theta}) = \sum_{i} (-y_i(\boldsymbol{\theta} \cdot \mathbf{x}_i))_+$ with $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla J(\boldsymbol{\theta})$

Support Vector Machine

Hard margin SVM.

 $\min_{\boldsymbol{\theta}} \|\boldsymbol{\theta}\|^2$, such that $y_i \boldsymbol{\theta} \cdot \mathbf{x}_i \geq 1 (i = 1, \dots, n)$

Soft margin SVM,

$$\min_{\boldsymbol{\theta}} \|\boldsymbol{\theta}\|^2 + C \sum_{i=1}^n (1 - y_i \boldsymbol{\theta} \cdot \mathbf{x}_i)_+$$

Regularization and SVMs: Simulated data with many features $\phi(\mathbf{x})$; C controls trade-off between margin $1/\|\boldsymbol{\theta}\|$ and fit to data; Large C: focus on fit to data (small margin is ok). More overfitting. Small C: focus on large margin, less tendency to overfit. Overfitting increases with: less data, more features.

$$\theta = \sum_{i} \alpha_{i} y_{i} \mathbf{x}_{i}, \ \alpha_{i} \neq 0$$
 only for support vectors.

 $K(\mathbf{x}_i, \mathbf{x}_i) = \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_i)$, K is called a kernel. Solve α_j to determine $\sum_i \alpha_j y_j \phi(\mathbf{x}_j)$. Compute the classifier for a test point \mathbf{x} via $\boldsymbol{\theta} \cdot \phi(\mathbf{x}) = \sum_{j} \alpha_{j} y_{j} K(\mathbf{x}_{j}, \mathbf{x})$

degree-m polynomial kernel: $K_m(\mathbf{x}, \tilde{\mathbf{x}}) = (1 + \mathbf{x} \cdot \tilde{\mathbf{x}})^m$ radial basis function kernel: $K_{rhf}(\mathbf{x}, \tilde{\mathbf{x}}) = \exp(-\gamma ||\mathbf{x} - \tilde{\mathbf{x}}||^2)$

Decision Theory

Loss function: $l: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$, and $l(\hat{q}, y)$ is the cost of predicting \hat{y} when the outcome is y.

Assume (X, Y) are chosen i.i.d according to some probability distribution on $\mathcal{X} \times \mathcal{Y}$. **Risk** is misclassification probability: $R(f) = \mathbb{E}l(f(\mathbf{X}), \mathbf{Y}) = Pr(f(\mathbf{X}) \neq \mathbf{Y})$

Bayes Decision Rule is

$$f^*(x) = \begin{cases} 1, & \text{if } P(\mathbf{Y} = 1|x) > P(\mathbf{Y} = -1|x) \\ -1, & \text{otherwise.} \end{cases}$$

Excess risk is for any $f: \mathcal{X} \to \{-1, +1\}$,

 $R(f) - R^* = \mathbb{E}(1[f(x) \neq f^*(x)]|2P(\mathbf{Y} = +1|\mathbf{X}) - 1|)$ **Risk in Regression** is expected squared error:

Bias-variance decomposition:

 $R(f) = \mathbb{E}l(f(\mathbf{X}), \mathbf{Y}) = \mathbb{E}\mathbb{E}[f(\mathbf{X}) - \mathbf{Y}^2 | \mathbf{X}]$

$$R(f) = \mathbb{E}[\underbrace{(f(\mathbf{X}) - \mathbb{E}[\mathbf{Y}|\mathbf{X}])^{2}}_{\text{bias}^{2}}] + \mathbb{E}[\underbrace{(\mathbb{E}[\mathbf{Y}|\mathbf{X}] - \mathbf{Y})^{2}}_{\text{variance}}]$$

$$R(f) = \mathbb{E}[(f(\mathbf{X}) - f^{*}(\mathbf{X}))^{2}] + \mathbb{E}[(f^{*}(\mathbf{X}) - \mathbf{Y})^{2}]$$

$$R(f) = \mathbb{E}[(f(\mathbf{X}) - f^{*}(\mathbf{X}))^{2}] + R(f^{*})$$

$$R(f) - R(f^{*}) = \mathbb{E}[(f(\mathbf{X}) - f^{*}(\mathbf{X}))^{2}], f^{*}(\mathbf{X}) = \mathbb{E}[\mathbf{Y}|\mathbf{X}]$$

Generative and Discriminative

Discriminative models: P(X, Y) = P(X)P(Y|X).

Estimate $P(\mathbf{Y}|\mathbf{X})$, then pretend out estimate $\hat{P}(\mathbf{Y}|\mathbf{X})$ is the actual $P(\mathbf{Y}|\mathbf{X})$ and plug in bayes rule expression.

Generative model: P(X, Y) = P(Y)P(X|Y).

Estimate $P(\mathbf{Y})$ and $P(\mathbf{X}|\mathbf{Y})$, then use bayes theorem to calculate $P(\mathbf{Y}|\mathbf{X})$ and use discriminative model.

Gaussian class conditional densities $P(\mathbf{X}|Y=+1), P(\mathbf{X}|Y=-1)$ (with the same variance), the posterior probability is $\mathbf{logistic}$:

$$P(Y = +1|\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{x} \cdot \boldsymbol{\beta} - \beta_0)},$$

$$\boldsymbol{\beta} = \Sigma^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0), \, \beta_0 = \frac{\boldsymbol{\mu}_0' \Sigma^{-1} \boldsymbol{\mu}_0 - \boldsymbol{\mu}_1 \Sigma^{-1} \boldsymbol{\mu}_1}{2} + \log \frac{P(Y=1)}{P(Y=0)}$$

Estimation

Method of moments: Match moments of the distribution to momemnts measured in the data.

Maximum likelihood: Choose parameter so that the distribution it defines gives the obverved data the highest probability (likelihood).

Maximum log likelihood: Log of maximum likelihood, equilvalent to maximum likelihood since log is monotonically increase; it is useful since it can change \prod to \sum .

Penalized maximum likelihood: Add a penalty term in the maximum (log) likelihood equation; treat the penalty term as some imaginary data points crafted for desired probability.

Bayesian estimate: Treat parameter as a random variable, then update based on observed value (data).

Prior: $\pi(p) = 1$.

Posterior: $P(p|\mathbf{X}_1 = 1) = P(\mathbf{X}_1 = 1|p)\pi(p) / \int P(X_1 = 1|q)d\pi(q)$

Maximum a posterior probability: the mode of the posterior. If uniform prior, MAP is MLE; if not uniform prior, MAP is Penalized MLE.

Multivariate Normal Distribution

$$\mathbf{x} \in \mathbb{R}^d : p(x) = \frac{1}{(2\pi)^{d/2} |\mathbf{\Sigma}|^{1/2}} e^{\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})' \mathbf{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)}$$

Covariance matrix: $\Sigma = \mathbb{E}(X - \mu)(X - \mu)'$

Symmetric: $\Sigma_{i,j} = \Sigma_{j_i}$

Non-negative diagonal entries: $\Sigma i, i > 0$

Positive semidefinite: $\forall \mathbf{v} \in \mathbb{R}^d, \mathbf{v}' \Sigma \mathbf{v} > 0$

Super-level sets of pdf:

 $\boldsymbol{\xi}_r = \big\{ \mathbf{x} \in \mathbb{R}^d : (\mathbf{x} - \boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \leq r^2 \big\}.$ Volume of $\boldsymbol{\xi}_r \propto \prod_{i=1}^d \sigma_i = \sqrt{|\boldsymbol{\Sigma}|}$

Spectral Theorem for non-diagonal covariance:

 $U = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n], \mathbf{\Lambda} = \operatorname{diag}([\lambda_1, \lambda_2, \dots, \lambda_n]')$

We can eigen decompose $\Sigma^{-1} = U\Lambda^{-1}U'$, this is like to change to a different eigen spaces, where covariances (Λ) diagonal axis-alianed.

Assume independent,

$$\mathcal{N}(\boldsymbol{\mu}_x, \boldsymbol{\Sigma}) + \mathcal{N}(\boldsymbol{\mu}_y, \boldsymbol{\Sigma}_y) = \mathcal{N}(\boldsymbol{\mu}_x + \boldsymbol{\mu}_y, \boldsymbol{\Sigma}_x + \boldsymbol{\Sigma}_y)$$

Given a *d*-dimensional Gaussian
$$\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$
, write $\mathbf{X} = \begin{bmatrix} \mathbf{Y} \\ \mathbf{Z} \end{bmatrix}$, $\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_{\mathbf{Y}} \\ \boldsymbol{\mu}_{\mathbf{Z}} \end{bmatrix}$, $\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{\mathbf{YY}} & \boldsymbol{\Sigma}_{\mathbf{YZ}} \\ \boldsymbol{\Sigma}_{\mathbf{ZY}} & \boldsymbol{\Sigma}_{\mathbf{ZZ}} \end{bmatrix}$,

where $\mathbf{Y} \in \mathbb{R}^m$, and $\mathbf{Z} \in \mathbb{R}^{d-m}$. Then $\mathbf{Y} \sim \mathcal{N}(\mu_{\mathbf{Y}}, \Sigma_{\mathbf{YY}})$

Given a d-dimensional Gaussian $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, matrix $\mathbf{A} \in \mathbb{R}^{m \times d}$ and vector $\mathbf{b} \in \mathbb{R}^m$, define $\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{b}$. Then $\mathbf{Y} \sim \mathcal{N}(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}')$

Given a d-dimensional Gaussian $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, with Σ positive definite,

$$\mathbf{Y} = \mathbf{\Sigma}^{-\frac{1}{2}}(\mathbf{X} - \boldsymbol{\mu}) \sim \mathcal{N}(\mathbf{0}, \mathbf{I}, \mathbf{I})$$

Gaussian maximum likelihood estimation:

Sample mean: $\hat{\boldsymbol{\mu}} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i$;

Sample covariance: $\hat{\hat{\Sigma}} = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}) (\mathbf{x}_i - \hat{\boldsymbol{\mu}})'$

Linear Regression

Given $\mathbf{X} \in \mathbb{R}^p$, $Y \in \mathbb{R}$, consider linear(affine) prediction rules, $F_{\text{lin}} := \{ \mathbf{x} \mapsto \mathbf{x}' \boldsymbol{\beta} + \beta_0 : \boldsymbol{\beta} \in \mathbb{R}^p, \beta_0 \in \mathbb{R} \}$

Empirical risk minimization

Empirical risk is the sample average of squared error: $\hat{R}(f) = \hat{\mathbb{E}}_n \ell(f(\mathbf{X}), Y) = \frac{1}{n} \sum_{i=1}^{n} n(f(\mathbf{X}_i) - Y_i)^2$ Choose $\hat{f} := \arg \min_{f \in F_{\text{lin}}} \hat{\mathbb{E}}_n \ell(f(\mathbf{X}), Y)$

Find
$$\hat{f}: \mathbf{x} \mapsto \mathbf{x}' \hat{\boldsymbol{\beta}}$$
, such that $\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \sum_{i=1}^n (\mathbf{X}_i' \boldsymbol{\beta} - Y_i)^2 = \arg\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \underbrace{\|\mathbf{X} \boldsymbol{\beta} - \mathbf{y}\|^2}_{\text{RSS}}$

where design matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$ and response vector $\mathbf{y} \in \mathbb{R}^n$.

Normal equations:
$$X'X\beta = X'y \Rightarrow \hat{\beta} = (X'X)^{-1}X'y$$

Projection Theorem also leads to normal equations: $(\mathbf{y} - \hat{\mathbf{y}})^{-1}\mathbf{X} = 0 \Leftrightarrow \mathbf{X}'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = 0 \Leftrightarrow \mathbf{X}'\mathbf{y} = \mathbf{X}'\mathbf{X}\boldsymbol{\beta}$

Linear model with additive Gaussian noise

Model the conditional distribution of Y given $\mathbf{X} = \mathbf{x}$ as: $P(Y|\mathbf{X} = \mathbf{x}) = \mathcal{N}(\mathbf{x}'\boldsymbol{\beta}, \sigma^2)$ Equivalently: $Y = \mathbf{x}'\boldsymbol{\beta} + \epsilon$, where $\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma^2)$

Maximum likelihood is least square:

$$L(\boldsymbol{\beta}) = \prod_{i=1}^{n} p(Y_i | \mathbf{X}_i, \boldsymbol{\beta}) \Leftrightarrow \ell(\boldsymbol{\beta}) = g(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - \mathbf{X}' \boldsymbol{\beta})^2$$

Fix **X**. Provided
$$\mathbb{E}\mathbf{v} = \mathbf{X}\boldsymbol{\beta}$$
 and $Cov(\mathbf{v}) = \sigma^2 \mathbf{I}$

Bayesian analysis: Treat β as a r.v. with prior distribution $\mathcal{N}(\mathbf{0}, \tau^2 \mathbf{I})$, then compute posterior distribution $P(\boldsymbol{\beta}|\mathbf{X}, Y)$.

$$\begin{array}{l} P(\boldsymbol{\beta}|\mathbf{X}_1,Y_1,\ldots,\mathbf{X}_n,Y_n) \propto P(Y_1,\ldots,Y_n|\boldsymbol{\beta},\mathbf{X}_1,\ldots,\mathbf{X}_n)P(\boldsymbol{\beta}) \\ P(\boldsymbol{\beta}|\mathbf{X}_1,Y_1,\ldots,\mathbf{X}_n,Y_n) \propto exp(-\frac{1}{2}(\sum_{i=1}^n\frac{(Y_i-\mathbf{X}_i'\boldsymbol{\beta})^2}{\sigma^2}+\frac{1}{\tau^2}\|\boldsymbol{\beta}\|^2)) \end{array}$$

Linear Regression Regularization

Trading off bias and variance: some increase in bias can give a big decrease in variance.

Subset selection is like L0 regularization: RSS decreases as the complexity increases because the best fit with a smaller subset is always possible with a larger subset.

Find a path through subset space: using cross-validation and forward-stepwise selection or backward-stepwise selection (need n > p).

Ridge regression is like
$$L2$$
 regularization:

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \left(\sum_{i=1}^{n} (y_i - \mathbf{x}_i' \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^{n} p \beta_j^2 \right)$$

$$\hat{\boldsymbol{\beta}}^{\mathrm{ridge}} = (\mathbf{X}'\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{x}'\mathbf{y}$$

Lasso regression is like L1 regularization:

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \left(\sum_{i=1}^{n} (y_i - \mathbf{x}_i' \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^{n} p |\beta_j| \right)$$

While ridge regression leads to reduced, but non-zero values of the coefficients, Lasso regression forces some coefficients to be zero.

Bayesian analysis: Ridge regression is equivalent to a MAP estimate with a gaussian prior. Lasso regression is equivalent to a MAP estimate with a Laplace prior.

Logistic Regression

Model **log odds** ($\log p/(1-p)$) as an affine function of **x**.

$$P(Y=1|\mathbf{x}) = \frac{1}{1+\exp(\boldsymbol{\beta}'\mathbf{x})}$$
 Given data $(\mathbf{X}_1,Y_1),\ldots,(\mathbf{X}_n,Y_n) \in \mathbb{R}^p \times \{0,1\}$, estimate $\boldsymbol{\beta}$ with maximum likelihood.

Log likelihood:

$$\ell(\boldsymbol{\beta}) = \sum_{i=1}^{n} y_i \log \mu_i(\boldsymbol{\beta}) + (1 - y_i) \log(1 - \mu_i(\boldsymbol{\beta})),$$

where $\mu_i(\boldsymbol{\beta}) = P(Y = 1 | \mathbf{X} = \mathbf{x}_i, \boldsymbol{\beta}) = \frac{1}{1 + \exp(-\boldsymbol{\beta}' \mathbf{x}_i)}$

$$\nabla_{\boldsymbol{\beta}} \mu_{i}(\boldsymbol{\beta}) = \mu_{i}(\boldsymbol{\beta})(1 - \mu_{i}(\boldsymbol{\beta}))\mathbf{x}_{i}$$

$$\nabla_{\boldsymbol{\beta}} \ell(\boldsymbol{\beta}) = \sum_{i=1}^{n} (y_{i} - \mu_{i}(\boldsymbol{\beta}))\mathbf{x}_{i} = \mathbf{X}'(\mathbf{y} - \boldsymbol{\mu})$$

$$\nabla_{\boldsymbol{\beta}}^{2} \ell(\boldsymbol{\beta}) = \sum_{i=1}^{n} -\mu_{i}(\boldsymbol{\beta})(1 - \mu_{i}(\boldsymbol{\beta}))\mathbf{x}_{i}\mathbf{x}'_{i} = -\mathbf{X}'\operatorname{diag}(\boldsymbol{\mu}(1 - \boldsymbol{\mu}))\mathbf{X}$$

$$\hat{\boldsymbol{\beta}}^{\text{ml}} \text{ solves: } \sum_{i=1}^{n} y_{i}\mathbf{x}_{i} = \sum_{i=1}^{n} \mu_{i}\boldsymbol{\beta}\mathbf{x}_{i}$$

Gradient ascent:

$$\boldsymbol{\beta}^{(t+1)} = \boldsymbol{\beta}^{(t)} + \eta \nabla_{\boldsymbol{\beta}} \ell(\boldsymbol{\beta}^{(t)}) : O(np)/\text{step}$$

$$\boldsymbol{\beta}^{(t+1)} = \boldsymbol{\beta}^{(t)} + \eta(y_{i_t} - \mu_{i_t}(\boldsymbol{\beta}^{(t)}))\mathbf{x}_{i_t} : O(p)/\text{step}$$

$$\begin{array}{l} \textbf{Newton-Raphson method:} \\ \boldsymbol{\beta}^{(t+1)} = \boldsymbol{\beta}^{(t)} - [\nabla_{\boldsymbol{\beta}}^2 \ell(\boldsymbol{\beta}^{(t)})]^{-1} \nabla_{\boldsymbol{\beta}} \ell(\boldsymbol{\beta}^{(t)}) \end{array}$$

Prediction
$$\hat{p}(y|\mathbf{x}) = \begin{cases} P(Y=1|\mathbf{x}), & \text{if } y=1\\ P(Y=-1|\mathbf{x}), & \text{if } y=-1 \end{cases}$$

Log loss (Binomial Deviance): $\ell_{\log}(\hat{p}(\cdot|\mathbf{x}), y) = -\log(\hat{p}(y|\mathbf{x}))$ Minimize: $\frac{1}{n} \sum_{i=1}^{n} \log(1 + \exp(-y_i \boldsymbol{\beta}' \mathbf{x}_i))$

Linear Discriminant Analysis

Linear discriminant functions:

$$\delta_k(\mathbf{x}) = \boldsymbol{\mu}_k' \boldsymbol{\Sigma}^{-1} \mathbf{x} - \frac{1}{2} \boldsymbol{\mu}_k' \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k + \log \pi_k$$

Estimate with Maximum likelihood:

$$\pi_k = P(Y = k) \Leftrightarrow \hat{\pi}_k = \frac{n_k}{n}$$

$$\boldsymbol{\mu}_k = \mathbb{E}[\mathbf{X}|Y=k] \Leftrightarrow \hat{\boldsymbol{\mu}}_k = \frac{1}{n_k} \sum_{i:y_i=k} \mathbf{x}_i$$

$$\Sigma = \text{Var}[\mathbf{X}|Y=k] \Leftrightarrow \hat{\Sigma} = \frac{1}{n} \sum_{k} \sum_{i} i : y_i = k(\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)'$$

SVM with Convex Optimization

Lagrangian: rewrite constraint as penalties for a convex optimization problem such that $L(x, \lambda) = f_0(x) + \sum_{i=1}^m \lambda_i f_i(x)$.

Weak duality:
$$\underbrace{p^* = \min \max_{x} L(x, \lambda)}_{\text{primal}} \geq \underbrace{\max_{\lambda \geq 0} \min_{x} L(x, \lambda) = d^*}_{\text{dual}}$$

Strong duality:

if there is a saddle point (x^*, λ^*) such that for all x and $\lambda > 0$, $L(x^*,\lambda) \leq L(x^*,\lambda^*) \leq L(x,\lambda^*)$, then primal and dual have the same value ($p^* = d^*$). Karush-Kuhn-Tucker optimality

Primal feasibility: $f_i(x) < 0$; Dual feasibility: $\lambda_i > 0$ Complementary slackness: $\lambda_i f_i(x) = 0$ Stationarity: $\nabla f_0(x) + \sum_i \lambda_i \nabla f_i(x) = 0$

Hard margin SVM:

$$L(\boldsymbol{\theta}, \alpha) = \frac{1}{2} ||\boldsymbol{\theta}||^2 + \sum_{i=1}^n \alpha_i (1 - y_i \boldsymbol{\theta}' \mathbf{x}_i)$$

$$g(\alpha) = \min_{\boldsymbol{\theta}} L(\boldsymbol{\theta}, \alpha)$$
setting $\boldsymbol{\theta}^* = \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i,$

$$g(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i' \mathbf{x}_j$$

Hard margein SVM dual problem:

$$\max_{\alpha} \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{x}'_{i} \mathbf{x}_{j}, \text{ s.t. } \alpha_{i} \geq 0 \text{ } (i = 1, \dots, n).$$

$$\min_{\alpha} \frac{1}{2} \boldsymbol{\alpha}' \operatorname{diag}(\mathbf{y}) \mathbf{K} \operatorname{diag}(\mathbf{y}) \boldsymbol{\alpha} - \boldsymbol{\alpha}' \mathbf{1}, \text{ s.t. } \boldsymbol{\alpha} \geq \mathbf{0}.$$

Soft margin SVM:

$$L(\boldsymbol{\theta}, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\lambda}) = \frac{1}{2} \|\boldsymbol{\theta}\|^2 + \frac{C}{n} \sum_{i=1}^n \xi_i + \sum_{i=1}^n \alpha_i (1 - y_i \boldsymbol{\theta}' \mathbf{x}_i - \xi_i) - \sum_{i=1}^n \lambda_i \xi_i$$

Soft margein SVM dual problem:

$$\min_{\alpha} \frac{1}{2} \alpha' \operatorname{diag}(\mathbf{y}) \mathbf{K} \operatorname{diag}(\mathbf{y}) \alpha - \alpha' \mathbf{1}$$
, s.t. $\mathbf{0} \le \alpha \le \frac{C}{n}$.