Probability

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

Perceptron

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

Decision boundary, a **hyperplane** in $\mathbb{R}^d$:
$H = \{\mathbf{x}\in\mathbb{R}^d : f(\mathbf{x})=0\} = \{\mathbf{x}\in\mathbb{R}^d : \boldsymbol{\theta}\cdot\mathbf{x}+\theta_0=0\}$

$\boldsymbol{\theta}$ is the **normal** of the hyperplane,
θ_0 is the **offset** of the hyperplane from origin,
$-\frac{\theta_0}{\|\boldsymbol{\theta}\|}$ is the **signed distance** from the origin to hyperplane.

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

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, $\gamma = \min_i \frac{y_i(\boldsymbol{\theta}\cdot\mathbf{x}_i)}{\|\boldsymbol{\theta}\|}$ is the margin.
Also, $\frac{\boldsymbol{\theta}\cdot\mathbf{x}}{\|\boldsymbol{\theta}\|}$ 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 **kernel**.

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 $y_i\boldsymbol{\theta}\cdot\mathbf{x}_i \geq 1 (i=1,\ldots,n)$
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.

$\boldsymbol{\theta} = \sum_j \alpha_j y_j \mathbf{x}_j$, $\alpha_j \neq 0$ only for support vectors.

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

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

Decision Theory

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

Assume $(\mathbf{X}, \mathbf{Y})$ 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
$f^*(x) = \begin{cases} 1, & \text{if } P(\mathbf{Y}=1|x) > P(\mathbf{Y}=-1|x) \\ -1, & \text{otherwise.} \end{cases}$,
and the optimal risk (Bayes risk) $R^* = \inf_f R(f) = R(f^*)$

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

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

Generative and Discriminative

Discriminative models: $P(\mathbf{X}, \mathbf{Y}) = P(\mathbf{X})P(\mathbf{Y}|\mathbf{X})$.
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: $P(\mathbf{X}, \mathbf{Y}) = P(\mathbf{Y})P(\mathbf{X}|\mathbf{Y})$.
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.

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

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

Covariance matrix: $\boldsymbol{\Sigma} = \mathbb{E}(\mathbf{X}-\boldsymbol{\mu})(\mathbf{X}-\boldsymbol{\mu})'$
Symmetric: $\boldsymbol{\Sigma}_{i,j} = \boldsymbol{\Sigma}_{j_i}$
Non-negative diagonal entries: $\boldsymbol{\Sigma}i, i \geq 0$
Positive semidefinite: $\forall\mathbf{v}\in\mathbb{R}^d, \mathbf{v}'\boldsymbol{\Sigma}\mathbf{v} \geq 0$

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

Spectral Theorem for **non-diagonal covariance**:
$U = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n]$, $\boldsymbol{\Lambda} = \text{diag}([\lambda_1, \lambda_2, \ldots, \lambda_n]')$
We can eigen decompose $\boldsymbol{\Sigma}^{-1} = U\boldsymbol{\Lambda}^{-1}U'$, this is like to change to a different eigen spaces, where covariances ($\boldsymbol{\Lambda}$) 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-dimensaional Gaussian $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$,
write $\mathbf{X} = \left[\begin{smallmatrix}\mathbf{Y}\\ \mathbf{Z}\end{smallmatrix}\right]$, $\boldsymbol{\mu} = \left[\begin{smallmatrix}\boldsymbol{\mu}_\mathbf{Y}\\ \boldsymbol{\mu}_\mathbf{Z}\end{smallmatrix}\right]$, $\boldsymbol{\Sigma} = \left[\begin{smallmatrix}\boldsymbol{\Sigma}_{\mathbf{YY}} & \boldsymbol{\Sigma}_{\mathbf{YZ}}\\ \boldsymbol{\Sigma}_{\mathbf{ZY}} & \boldsymbol{\Sigma}_{\mathbf{ZZ}}\end{smallmatrix}\right]$,
where $\mathbf{Y}\in\mathbb{R}^m$, and $\mathbf{Z}\in\mathbb{R}^{d-m}$. Then $\mathbf{Y} \sim \mathcal{N}(\mu_\mathbf{Y}, \boldsymbol{\Sigma}_{\mathbf{YY}})$

Given a d-dimensaional 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-dimensaional Gaussian $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$,
with $\boldsymbol{\Sigma}$ positive definite,
$\mathbf{Y} = \boldsymbol{\Sigma}^{-\frac{1}{2}}(\mathbf{X}-\boldsymbol{\mu}) \sim \mathcal{N}(\mathbf{0}, \mathbf{I},)$

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

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:
$\hat{R}(f) = \hat{\mathbb{E}}_n\ell(f(\mathbf{X}), Y) = \frac{1}{n}\sum_{i=1} n(f(\mathbf{X}_i) - Y_i)^2$

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

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

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

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

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:
$\hat{\boldsymbol{\beta}} = \arg\ \min_{\boldsymbol{\beta}}(\sum_{i=1}^{n}(y_i - \mathbf{x}_i'\boldsymbol{\beta})^2 + \lambda\sum_{j=1}^{p}\beta_j^2)$
$\hat{\boldsymbol{\beta}}^{\text{ridge}} = (\mathbf{X}'\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{x}'\mathbf{y}$

Lasso regression is like $L1$ regularization:
$\hat{\boldsymbol{\beta}} = \arg\ \min_{\boldsymbol{\beta}}(\sum_{i=1}^{n}(y_i - \mathbf{x}_i'\boldsymbol{\beta})^2 + \lambda\sum_{j=1}^{p}|\beta_j|)$

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.