CS 189 Final Note Sheet

Bayesian Decision Theory

$$\begin{array}{l} \text{Bayes Rule: } P(\omega|x) = \frac{P(x|\omega)P(\omega)}{P(x)}, P(x) = \sum_{i} P(x|\omega_{i})P(\omega_{i}) \\ P(error) = \int_{-\infty}^{\infty} P(error|x)P(x)dx \\ P(error|x) = \left\{ \begin{array}{l} P(\omega_{1}|x) \text{ if we decide } \omega_{2} \\ P(\omega_{2}|x) \text{ if we decide } \omega_{1} \end{array} \right. \\ 0\text{-1 Loss: } \lambda(\alpha_{i}|\omega_{j}) = \left\{ \begin{array}{l} 0 \quad i=j \text{ (correct)} \\ 1 \quad i\neq j \text{ (mismatch)} \end{array} \right. \\ \text{Expected Loss (Risk): } R(\alpha_{i}|x) = \sum_{j=1}^{c} \lambda(\alpha_{i}|\omega_{j})P(\omega_{j}|x) \\ 0\text{-1 Risk: } R(\alpha_{i}|x) = \sum_{j\neq i}^{c} P(\omega_{j}|x) = 1 - P(\omega_{i}|x) \end{array}$$

Probabilistic Motivation for Least Squares

Note: The intercept term
$$x_0=1$$
 is accounted for in θ

$$\Rightarrow p(y^{(i)}|x^{(i)};\theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y^{(i)}-\theta^\mathsf{T}x^{(i)})^2}{2\sigma^2}\right)$$

$$\Rightarrow L(\theta) = \prod_{i=1}^m \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y^{(i)}-\theta^\mathsf{T}x^{(i)})^2}{2\sigma^2}\right)$$

$$\Rightarrow l(\theta) = m \log \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2} \sum_{i=1}^m (y^{(i)}-\theta^\mathsf{T}x^{(i)})^2$$

$$\Rightarrow \max_{\theta} l(\theta) \equiv \min_{\theta} \sum_{i=1}^m (y^{(i)}-h_{\theta}(x))^2$$
Gaussian noise in our data set $\{x^{(i)},y^{(i)}\}_{i=1}^m$ gives us least squares $\min_{\theta} ||X\theta-y||_2^2 \equiv \min_{\theta} \theta^\mathsf{T}X^\mathsf{T}X\theta - 2\theta^\mathsf{T}X^\mathsf{T}y + y^\mathsf{T}Y$

$$\nabla_{\theta} l(\theta) = X^\mathsf{T}X\theta - X^\mathsf{T}y = 0 \Rightarrow \begin{bmatrix} \theta^* = (X^\mathsf{T}X)^{-1}X^\mathsf{T}y \end{bmatrix}$$
Gradient Descent: $\theta_{t+1} = \theta_t + \alpha(y_t^{(i)} - h(x_t^{(i)}))x_t^{(i)}, \ h_{\theta}(x) = \theta^\mathsf{T}x^\mathsf{T}x$

Least Squares Solution

$$\min_{x} ||Ax - y||_2^2 \Longrightarrow x^* = A^{\dagger}y \text{ min norm sol'n}$$
 Sol'n set: $x_0 + N(A) = x^* + N(A)$
$$\left((A^{\intercal}A)^{-1}A^{\intercal} A \text{ full column r} \right)$$

$$A^{\dagger} = \left\{ \begin{array}{ll} (A^{\intercal}A)^{-1}A^{\intercal} & A \text{ full column rank} \\ A^{\intercal}(AA^{\intercal})^{-1} & A \text{ full row rank} \\ V\Sigma^{\dagger}U^{\intercal} & \text{any } A \end{array} \right.$$

L2 Reg: $\min_x ||Ax - y||_2^2 + \lambda ||x||_2^2 \implies x^* = (A^TA + \lambda I)^{-1}X^Ty$ The above variant is used when A contains a null space. L2 Reg falls out of the MLE when we add a Gaussian prior on x with $\Sigma = cI$. We get L1 Reg when x has a Laplace prior.

Logistic Regresion

Classify
$$y \in \{0, 1\} \Longrightarrow \text{Model } p(y = 1|x) = \frac{1}{1 + e^{-\theta^T x}} = h_{\theta}(x)$$

$$\frac{dh_{\theta}}{d\theta} = (\frac{1}{1 + e^{\theta^T x}})^2 e^{-\theta^T x} = \frac{1}{1 + e^{\theta^T x}} \left(1 - \frac{1}{1 + e^{-\theta^T x}}\right) = h_{\theta}(1 - h_{\theta})$$

$$p(y|x; \theta) = (h_{\theta}(x))^y (1 - h_{\theta}(x))^{1 - y} \Longrightarrow$$

$$L(\theta) = \prod_{i=1}^m (h_{\theta}(x^{(i)}))^{y^{(i)}} (1 - h_{\theta}(x^{(i)}))^{1 - y^{(i)}} \Longrightarrow$$

$$l(\theta) = \sum_{i=1}^m y^{(i)} \log(h_{\theta}(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)})) \Longrightarrow$$

$$\nabla_{\theta} l = \sum_{i} (y^{(i)} - h_{\theta}(x^{(i)})) x^{(i)} = X^{\mathsf{T}}(y - h_{\theta}(X)), \text{ (want max } l(\theta))$$
Stoch:
$$\theta_{t+1} = \theta_t + \alpha(y_t^{(i)} - h_{\theta}(x_t^{(j)})) x_t^{(j)}$$
Batch:
$$\theta_{t+1} = \theta_t + \alpha X^{\mathsf{T}}(y - h_{\theta}(X))$$

Multivariate Gaussian $X \sim \mathcal{N}(\mu, \Sigma)$

$$\begin{split} f(x;\mu,\Sigma) &= \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right) \\ \Sigma &= E[(X-\mu)(X-\mu)^T] = E[XX^T] - \mu\mu^T \\ \Sigma \text{ is PSD} &\Longrightarrow x^T \Sigma x \geq 0, \text{ if inverse exists } \Sigma \text{ must be PD} \\ \text{If } X \sim N(\mu,\Sigma), \text{ then } AX + b \sim N(A\mu + b, A\Sigma A^T) \end{split}$$

$$\implies \Sigma^{-\frac{1}{2}}(X-\mu) \sim N(0,I), \text{ where } \Sigma^{-\frac{1}{2}} = U\Lambda^{-\frac{1}{2}}$$

The distribution is the result of a linear transformation of a vector of univariate Gaussians $Z \sim \mathcal{N}(0, I)$ such that $X = AZ + \mu$ where we have $\Sigma = AA^{\mathsf{T}}$. From the pdf, we see that the level curves of the distribution decrease proportionally with $x^{\mathsf{T}}\Sigma^{-1}x$ (assume $\mu = 0$) \Longrightarrow

c-level set of
$$f \propto \{x : x^{\mathsf{T}} \Sigma^{-1} x = c\}$$

$$x^{\mathsf{T}} \Sigma^{-1} = c \equiv x^{\mathsf{T}} U \Lambda^{-1} U^{\mathsf{T}} x = c \Longrightarrow \lambda_1^{-1} (u_1^{\mathsf{T}} x)^2 + \dots + \lambda_n^{-1} (u_n^{\mathsf{T}} x)^2 = c$$
exist length: $\sqrt{\lambda_1}$
axis length: $\sqrt{\lambda_n}$

Thus we have that the level curves form an ellipsoid with axis lengths equal to the square root of the eigenvalues of the covariance matrix.

LDA and QDA

Classify
$$y \in \{0,1\}$$
, Model $p(y) = \phi^y \phi^{1-y}$ and $p(x|y=1;\mu_1) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} exp\left(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\right)$ $l(\theta,\mu_0,\mu_1,\Sigma) = \log \prod_{i=1}^m p(x^{(i)}|y^{(i)};\mu_0,\mu_1,\Sigma) p(y^{(i)};\Phi)$ gives us $\phi_{MLE} = \frac{1}{m}\sum_{i=1}^m 1\{y^{(i)} = 1\}, \mu_{k_{MLE}} = \text{avg of } x^{(i)}$ classified as k, $\Sigma_{MLE} = \frac{1}{m}\sum_{i=1}^m (x^{(i)} - \mu_{y_{(i)}})(x^{(i)} - \mu_{y_{(i)}})^T$. Notice the covariance matrix is the same for all classes in LDA. If $p(x|y)$ multivariate gaussian (w/ shared Σ), then $p(y|x)$ is logistic function. The converse is NOT true. LDA makes stronger assumptions about data than does logistric regression. $h(x) = arg \max_k -\frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k) + \log(\pi_k)$ where $\pi_k = p(y=k)$

For QDA, the model is the same as LDA except that each class has a unique covariance matrix.

$$h(x) = \arg\max_{k} -\frac{1}{2}\log|\Sigma_{k}| - \frac{1}{2}(x - \mu_{k})^{T}\Sigma_{k}^{-1}(x - \mu_{k}) + \log(\pi_{k})$$

Optimization

Newtons Method: $\theta_{t+1} = \theta_t - [\nabla^2_{\theta} f(\theta_t)]^{-1} \nabla_{\theta} f(\theta_t)$ Gradient Decent: $\theta_{t+1} = \theta_t - \alpha \nabla_{\theta} f(\theta_t)$, for minimizing Lagrange Multipliers:

Given, $\min_x f(x)$ s.t. $g_i(x) = 0$, $h_i(x) \leq 0$ the corresponding Lagrangian is: $L(x,\alpha) = f(x) + \sum_{i=1}^k \alpha_i g_i(x) + \sum_{i=1}^l \beta_i h_i(x)$ We min over x and max over the Lagrange multipliers α and β

Support Vector Machines

In the strictly separable case, the goal is to find a seperating hyperplane (like logistic regression) except now we don't just want any hyperplane, but one with the largest margin. $H = \{\omega^T x + b = 0\}$, since scaling ω and b in opposite directions doesn't change the hyperplane our optimization function should have scaling invariance built into it. Thus, we do it now and define the closest points to the hyperplane x_{sv} (support vectors) to satisfy: $|\omega^T x_{sv} + b| = 1$. The distance from any support vector to the hyper plane is now: $\frac{1}{|\omega||_2}$. Maximizing the distance to the hyperplane is the same as minimizing $|\omega||_2$. The final optimization problem is:

$$\frac{\min_{\omega,b} \frac{1}{2} ||\omega||_2 \ s.t. \ y^{(i)}(w^T x^{(i)} + b) \ge 1, i = 1, \dots, m}{\text{Primal: } L_p(\omega,b,\alpha) = \frac{1}{2} ||\omega||_2 - \sum_{i=1}^m \alpha_i (y^{(i)}(w^T x^{(i)} + b) - 1)}{\frac{\partial L_p}{\partial \omega} = \omega - \sum_i \alpha_i y^{(i)} x^{(i)} = 0 \implies \omega = \sum_i \alpha_i y^{(i)} x^{(i)}}$$

 $\begin{array}{l} \frac{\partial L_p}{\partial b} = -\sum \alpha_i y^{(i)} = 0, \quad \text{Note: } \alpha_i \neq 0 \text{ only for support vectors.} \\ \text{Substitute the derivatives into the primal to get the dual.} \\ \text{Dual: } L_d(\alpha) = \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m y^{(i)} y^{(j)} \alpha_i \alpha_j (x^{(i)})^T x^{(j)} \end{array}$

In the non-separable case we allow points to cross the marginal boundary by some amount ξ and penalize it.

$$\left| \min_{\omega, b} \frac{1}{2} ||\omega||_2 + C \sum_{i=1}^m \xi_i \quad s.t. \quad y^{(i)}(w^T x^{(i)} + b) \ge 1 - \xi_i \right|$$

The dual for non-separable doesn't change much except that each α_i now has an upper bound of $C \implies 0 \le \alpha_i \le C$

Loss Functions

In general the loss function consists of two parts, the loss term and the regularization term. $J(\omega) = \sum_{i} Loss_{i} + \lambda R(\omega)$

Nearest Neighbor

Key Idea: Store all training examples $\langle x_i, f(x_i) \rangle$

NN: Find closest training point using some distance metric and take its label.

k-NN: Find closest k training points and take on the most likely label based on some voting scheme (mean, median,...)

Behavior at the limit: 1NN $\lim_{N\to\infty}\epsilon^* \leq \epsilon_{NN} \leq 2\epsilon^*$ $\epsilon^* =$ error of optimal prediction, $\epsilon_{nn} =$ error of 1NN classifier KNN $\lim_{N\to\infty,K\to\infty},\frac{K}{N}\to 0,\epsilon_{knn}=\epsilon^*$

Curse of dimentionality: As the number of dimensions increases, everything becomes farther appart. Our low dimension intuition falls apart. Consider the Hypersphere/Hypercube ratio, it's close to zero at d=10. Solutions: 1) Get more data to fill all of that empty space. 2) Get better features, reducing the dimentionality and packing the data closer together. Ex: Bag-of-words,

Histograms,... 3) Use a better distance metric.

Minkowski:
$$Dis_p(x,y) = (\sum_{i=1}^d |x_i - y_u|^p)^{\frac{1}{p}} = ||x - y||_p$$

0-norm: $Dis_0(x,y) = \sum_{i=1}^d I|x_i = y_i|$

Mahalanobis: $Dis_M(x,y|\Sigma) = \sqrt{(x-y)^T \Sigma^{-1}(x-y)}$

In high-d we get "Hubs" s.t most points identify the hubs as their NN. These hubs are usually near the means (Ex: dull gray images, sky and clouds). To avoid having everything classified as these hubs, we can use cosine similarity.

Gradients

Gradients
$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} \triangleq \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_n} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}, \frac{\partial (Ax)}{\partial x} = A, \frac{\partial (x^T A)}{\partial x} = A^T,$$

$$\frac{\partial (x^T x)}{\partial x} = 2x, \frac{\partial (x^T A x)}{\partial x} = (A + A^T)x, \frac{\partial (trBA)}{\partial x} = B^T$$

Decision Trees

Given a set of points and classes $\{x_i,y_i\}_{i=1}^n$, test features x_j and branch on the feature which "best" separates the data. In new space (space without features x_j) repeat the process and continue splitting data until good classification accuracy is reached. Heurisitics:

1. Maximize Information Gain: \max_j infogain $(D|X_j)$

$$\max_{j} \ \ \mathrm{H}(D) \ - \sum_{x_j \in X_j} P(X_j = x_j) \cdot \mathrm{H}(D|X_j = x_j)$$

where $\mathrm{H}(D) = -\sum_{c \in C} P(y=c) \log(p(y=c))$ is the entropy of the data set, C is the set of classes each data point can take, and P(y=c) is the fraction of data points with class c.

- 2. Minimize Gini Impurity
- 3. Minimize Misclassification Impurity