CS 189 Final Note Sheet

Bayesian Decision Theory

Bayes Rule: $P(\omega|x) = \frac{P(x|\omega)P(\omega)}{P(x)}, P(x) = \sum_i P(x|\omega_i)P(\omega_i)$
$P(x,w) = P(x|w)P(w) = P(w|x)P(x)$
$P(error) = \int_{-\infty}^{\infty} P(error|x)P(x)dx$

$$P(error|x) = \begin{cases} P(\omega_1|x) \text{ if we decide } \omega_2 \\ P(\omega_2|x) \text{ if we decide } \omega_1 \end{cases}$$

0-1 Loss: $\lambda(\alpha_i|\omega_j) = \begin{cases} 0 & i = j \text{ (correct)} \\ 1 & i \neq j \text{ (mismatch)} \end{cases}$

Expected Loss (Risk): $R(\alpha_i|x) = \sum_{j=1}^{c} \lambda(\alpha_i|\omega_j)P(\omega_j|x)$
0-1 Risk: $R(\alpha_i|x) = \sum_{j\neq i}^{c} P(\omega_j|x) = 1 - P(\omega_i|x)$

Probabilistic Motivation for Least Squares

$y^{(i)} = \theta^\intercal x^{(i)} + \epsilon^{(i)}$ with noise $\epsilon(i) \sim \mathcal{N}(0, \sigma^2)$
Note: The intercept term $x_0 = 1$ is accounted for in θ

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

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

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

$\implies \max_\theta l(\theta) \equiv \min_\theta \sum_{i=1}^{m} (y^{(i)} - h_\theta(x))^2$

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

$\nabla_\theta l(\theta) = X^\intercal X\theta - X^\intercal y = 0 \implies \boxed{\theta^* = (X^\intercal X)^{-1} X^\intercal y}$

Gradient Descent: $\theta_{t+1} = \theta_t + \alpha(y_t^{(i)} - h(x_t^{(i)}))x_t^{(i)}, \quad h_\theta(x) = \theta^\intercal x$

Least Squares Solution

$\min_x ||Ax - y||_2^2 \implies x^* = A^\dagger y$ min norm sol'n
Sol'n set: $x_0 + N(A) = x^* + N(A)$

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

L2 Reg: $\min_x ||Ax - y||_2^2 + \lambda||x||_2^2 \implies x^* = (A^T A + \lambda I)^{-1} X^T y$
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 $y \in \{0,1\} \implies$ Model $p(y = 1|x) = \frac{1}{1+e^{-\theta^T x}} = h_\theta(x)$

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

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

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

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

$\nabla_\theta l = \sum_i (y^{(i)} - h_\theta(x^{(i)}))x^{(i)} = X^\intercal(y - h_\theta(X))$, (want max $l(\theta)$)

Stoch: $\boxed{\theta_{t+1} = \theta_t + \alpha(y_t^{(j)} - h_\theta(x_t^{(j)}))x_t^{(j)}}$

Batch: $\boxed{\theta_{t+1} = \theta_t + \alpha X^\intercal(y - h_\theta(X))}$

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

$f(x;\mu,\Sigma) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$
$\Sigma = E[(X-\mu)(X-\mu)^T] = E[XX^T] - \mu\mu^T$

Σ is PSD $\implies x^T\Sigma x \geq 0$, if inverse exists Σ must be PD
If $X \sim N(\mu, \Sigma)$, then $AX + b \sim N(A\mu + b, A\Sigma A^T)$
$\implies \Sigma^{-\frac{1}{2}}(X - \mu) \sim N(0, I)$, 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 $\Sigma = AA^\intercal$. From the pdf, we see that the level curves of the distribution decrease proportionally with $x^\intercal\Sigma^{-1}x$ (assume $\mu = 0$) $\implies$

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

$$x^\intercal\Sigma^{-1} = c \equiv x^\intercal U\Lambda^{-1}U^\intercal x = c \implies$$

$$\underbrace{\lambda_1^{-1}(u_1^\intercal x)^2}_{\text{axis length: } \sqrt{\lambda_1}} + \cdots + \underbrace{\lambda_n^{-1}(u_n^\intercal x)^2}_{\text{axis length: } \sqrt{\lambda_n}} = c$$

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
$p(x|y = 1;\mu_1) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} exp\left(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\right)$
$l(\theta, \mu_0, \mu_1, \Sigma) = log\ \Pi_{i=1}^{m} p(x^{(i)}|y^{(i)};\mu_0,\mu_1,\Sigma)p(y^{(i)};\Phi)$ gives us
$\phi_{MLE} = \frac{1}{m}\sum_{i=1}^{m} 1\{y^{(i)} = 1\}, \mu_{k_{MLE}} =$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 logisitic 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: $\theta_{t+1} = \theta_t - [\nabla_\theta^2 f(\theta_t)]^{-1}\nabla_\theta f(\theta_t)$
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:

$$\boxed{\min_{\omega,b} \frac{1}{2}||\omega||_2 \ s.t.\ y^{(i)}(w^T x^{(i)} + b) \geq 1, i = 1, \ldots, m}$$

Primal: $L_p(\omega, b, \alpha) = \frac{1}{2}||\omega||_2 - \sum_{i=1}^{m}\alpha_i(y^{(i)}(w^T x^{(i)} + b) - 1)$
$\frac{\partial L_p}{\partial\omega} = \omega - \sum\alpha_i y^{(i)}x^{(i)} = 0 \implies \omega = \sum\alpha_i y^{(i)}x^{(i)}$
$\frac{\partial L_p}{\partial b} = -\sum\alpha_i y^{(i)} = 0,\quad$ Note: $\alpha_i \neq 0$ only for support vectors.
Substitute the derivatives into the primal to get the dual.
Dual: $L_d(\alpha) = \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m} y^{(i)}y^{(j)}\alpha_i\alpha_j(x^{(i)})^T x^{(j)}$

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

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

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

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 $< x_i, f(x_i) >$
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.
K-d trees increase the efficiency of nearest neighbor lookup.

Gradients

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

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

Generative vs. Discriminative Model

Generative: Model class conditional density $p(x|y)$ and find $p(y|x) \propto p(x|y)p(y)$ or model joint density $p(x,y)$ and marginalize to find $p(y = k|x) = \int_x p(x, y = k)dx$
Discriminative: Model conditional $p(y|x)$.

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$(D|X_j)$

$$\max_j \quad \mathrm{H}(D) \; - \sum_{x_j \in X_j} P(X_j = x_j) \cdot \mathrm{H}(D|X_j = x_j)$$

   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

Optimal Split:

Random Forests

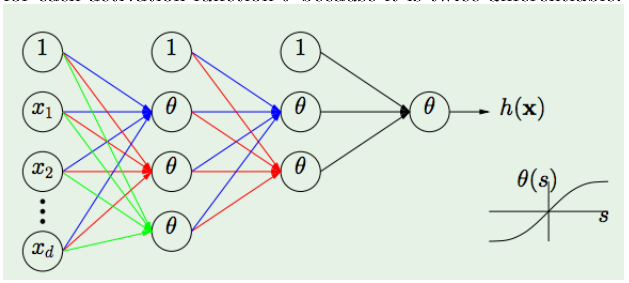
Problem: Decision trees are unstable: small changes in the input data have large effect on tree structure $\implies$ decision trees are high-variance estimators.
Solution: Random Forests train M different trees with randomly sampled subsets of the data (and sometimes with randomly sampled subsets of the features to decorrelate the trees). A new point is tested on all M trees and we take the majority as our output class (for regression we take the average of the output).

K means

Partition your data into a predetermined number of groups k. Randomly pick points to initialize the centers of the k clusters. Calculate the center (mean) of each of the k centroids. Re-assign objects to closest centroids. Stop when no re-assignments occur.

Neural Networks

Neural Nets explore what you can do by combining perceptrons, each of which is a simple linear classifier. We use a soft threshold for each activation function θ because it is twice differentiable.



Activation Functions:

$$\theta(s) = \tanh(s) = \frac{e^s - e^{-s}}{e^s + e^{-s}} \implies \theta'(s) = 1 - \theta^2(s)$$

$$\theta(s) = \sigma(s) \implies \theta'(s) = \sigma(s)(1 - \sigma(s))$$

Notation: $w_{ij}^{(l)}$ is the weight from neuron i in layer $l - 1$ to neuron j in layer l.
Back-propagation: We want to compute gradient descent on a neural network in an efficient manner. Start with the highest node and calculate: $\delta_1^L = \frac{\partial e(w)}{\partial s_i^L}$ Then we recursively calculate down: $\delta_i^{(l-1)} = \frac{\partial e(w)}{\partial s_i^{(l-1)}} = \sum_j \delta_j^{(l)} \cdot w_{ij}^{(l)} \cdot \theta'(s_i^{(l-1)})$. Then this allows us to compute the gradient quickly over the entire network.