# 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 $\theta$
$\implies p(y^{(i)}|x^{(i)};\theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y^{(i)}-\theta^\intercal x^{(i)})^2}{2\sigma^2}\right)$
$\implies L(\theta) = \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y^{(i)}-\theta^\intercal x^{(i)})^2}{2\sigma^2}\right)$
$\implies l(\theta) = m\log\frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2}\sum_{i=1}^{m}(y^{(i)} - \theta^\intercal x^{(i)})^2$
$\implies \max_\theta l(\theta) \equiv \min_\theta \sum_{i=1}^{m}(y^{(i)} - h_\theta(x))^2$
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: $\min_x ||Ax - y||_2^2 + \lambda||x||_2^2 \implies x^* = (A^TA + \lambda I)^{-1}X^Ty$
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 $y \in \{0,1\} \implies$ 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 $X \sim \mathcal{N}(\mu, \Sigma)$

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

$\Sigma$ is PSD $\implies x^T\Sigma x \geq 0$, if inverse exists $\Sigma$ 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 $\Sigma^{-\frac{1}{2}} = U\Lambda^{-\frac{1}{2}}$

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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 $\Sigma$), 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 $\pi_k = p(y=k)$

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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 $\alpha$ and $\beta$

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

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

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

The dual for non-separable doesn't change much except that each $\alpha_i$ 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. How do deal with this curse:

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. Recursively split on the new subset of data. Growing the tree to max depth tends to overfit (training data gets cut quickly $\implies$ subtrees train on small sets), mistakes high up in the tree propagate to corresponding subtrees. To reduce overfitting, we can prune using a validation set, and we can limit the depth. DT's are prone to label noise. Building the correct tree is hard.
**Heurisitic**: For classification, maximize information gain

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

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 $c$.
For regression, minimize the variance. Same optimiation problem as above, except H is replaced with var. Pure leaves correspond to low variance, and the result is the mean of the current leaf.

## Random Forests

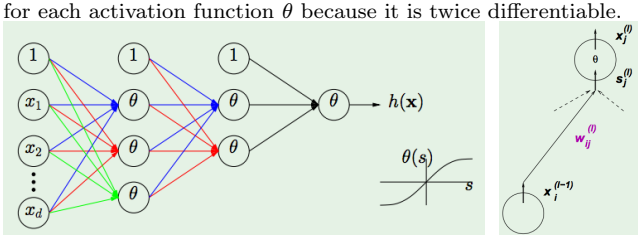
**Problem**: DT's are unstable: small changes in the input data have large effect on tree structure $\implies$ DT's are high-variance estimators.
**Solution**: Random Forests train $M$ different trees with randomly sampled subsets of the data (called bagging), and sometimes with randomly sampled subsets 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).

## Boosting

Weak Learner: Can classify with at least 50% accuracy.
Train weak learner to get a weak classifier. Test it on the training data, up-weigh misclassified data, down-weigh correctly classified data. Train a new weak learner on the weighted data. Repeat. A new point is classified by every weak learner and the output class is the sign of a weighted avg. of weak learner outputs. Boosting generally overfits. If there is label noise, boosting keeps upweighing the mislabeled data.
**AdaBoost** is a boosting algorithm. The weak learner weights are given by $\alpha_t = \frac{1}{2} \ln(\frac{1-\epsilon_t}{\epsilon_t})$ where $\epsilon_t = Pr_{D_t}(h_t(x_i) \neq y_i)$ (probability of misclassification). The weights are updated $D_{t+1}(i) = \frac{D_t(i) exp(-\alpha_t y_i h_t(x_i))}{Z_t}$ where $Z_t$ is a normalization factor.

## 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 $\theta$ because it is twice differentiable.







**Activation Functions:**

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

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

**Error Function**:

**Notation:**

$w_{ij}^{(l)}$ is the weight from neuron $i$ in layer $l-1$ to neuron $j$ in layer $l$.

1. $w_{ij}^{(l)}$ is the weight from neuron $i$ in layer $l-1$ to neuron $j$ in layer $l$
2. $l \in \{1, \ldots, L\}$ (there are L layers), $i \in \{1, \ldots, d^{(l-1)}\}, j \in \{1, \ldots, d^{(l)}\}$ (there are $d^{(l-1)}$ nodes in the previous layer that are fully connected to the $d^{(l)}$ nodes in the current layer)
3. $s_j^{(l)} = \sum_{i=1}^{d^{(l-1)}} w_{ij}^{(l)} x_i^{(l-1)}$ is the input signal for neuron $j$ at layer $l$ and is a weighted combination of the output signals $x_i^{(l-1)}$ of neurons previous layer.
4. $x_j^{(l)} = \theta(s_j^{(l)})$ is the output of a neuron which is the activation function applied to the input signal.
5. $e(w)$ is the error as a function of the weights

## Clustering

1) Agglomerative: Start with n clusters and recursively merge the two closest clusters.
2) Division: Start with 1 cluster and recursively divide one of the existing clusters into two daughter clusters.
3) Partitioning: Partition data into K non-overlapping clusters, iteratively reallocate data between the clusters until some loss is minimized.
The goal is to find the weights $w_{ij}^{(l)}$. Use stock gradient descent.

$$\nabla e(w) \to \frac{\partial e(w)}{\partial w_{ij}^{(l)}} = \frac{\partial e(w)}{\partial s_j^{(l)}} \frac{\partial s_j^{(l)}}{\partial w_{ij}^{(l)}} = \delta_j^{(l)} x_i^{(l-1)}$$

**Computing $\delta_j^{(l)}$**:

Final Layer: $\delta_1^{(L)} = \frac{\partial e(w)}{\partial s_j^{(l)}} = \frac{\partial e(w)}{\partial \theta(s_1^{(L)})} \frac{\partial \theta(s_1^{(L)})}{\partial s_1^{(L)}} = e'(x_1^{(L)}) \theta'(s_1^L)$

General:

$$\delta_i^{(l-1)} = \frac{\partial e(w)}{\partial s_j^{(l-1)}} = \sum_{i=1}^{d^{(l)}} \frac{\partial e(w)}{\partial s_j^{(l)}} \times \frac{\partial s_j^{(l)}}{\partial x_i^{(l-1)}} \times \frac{\partial x_i^{(l-1)}}{\partial s_i^{(l-1)}}$$

$$= \sum_{i=1}^{d^{(l)}} \delta_j^{(l)} \times w_{ij}^{(l)} \times \theta'(s_i^{(l-1)})$$

1. Initialize all weights $w_{ij}^{(l)}$ at random
2. for $t = 0, 1, 2, \ldots$ do
3. Pick $n \in \{1, 2, \cdots, N\}$
4. *Forward:* Compute all $x_j^{(l)}$
5. *Backward:* Compute all $\delta_j^{(l)}$
6. Update the weights: $w_{ij}^{(l)} \leftarrow w_{ij}^{(l)} - \eta\, x_i^{(l-1)} \delta_j^{(l)}$
7. Iterate to the next step until it is time to stop
8. Return the final weights $w_{ij}^{(l)}$

## Clustering

Unsupervised Learning (no labels). Two main types:

- **Hierarchical**:
  - Agglomerative: Start with n points, merge 2 closest clusters using some measure, such as: Single-link (closest pair), Complete-link (furthest pair), Average-link (average of all pairs), Centroid (centroid distance).
  - Divisive: Start with single cluster, recursively divide clusters. Less popular
- **Partitioning**: Partition the data into a K mutually exclusive exhaustive groups (i.e. encode k=C(i)). Iteratively reallocate to minimize loss function, like $W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')=k} d(x_i, x_i')$. We can't minimize over the entire loss function so just do greedy iterative descent. This ends up being **K-means**: Choose clusters at random, calculate centroid of each cluster, reallocate objects to nearest centroid, repeat. Finds local minimum of W(C), not global.

**Vector Quantization**: Use representative prototype vectors to simplify representations of signals. Use clustering to find prototype vectors.

**Parametric Discriminative Clustering (Mixture Models)**: Assume PDF is made up of multiple gaussians with different centers. Then use EM to compute this model.

E Step: $P(\mu_i | x_k) = \frac{P(\mu_i) P(x_k | mu_i)}{\sum_j P(\mu_j) P(x_j | mu_j)}$

M Step: $P(c_i) = \frac{1}{n_e} \sum_{k=1}^{n_e} P(\mu_i | x_k)$. Now update mu and sigma:

$\mu_i = \frac{\sum_k x_k P(\mu_i | x_k)}{\sum_k P(\mu_i | x_k)}$

$\sigma_i^2 = \frac{\sum_k (x_k - \mu_i)^2 P(\mu_i | x_k)}{\sum_k P(\mu_i | x_k)}$.

**Nonparametric Discriminative Clustering**: Histogram, Kernel Density Estimation.

Kernel: $P(x) = \frac{1}{n} \sum K(x - x_i)$, s.t. K is normalized, symmetric, and $\lim_{||x|| \to \infty} ||x||^d K(x) = 0$.

## 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.