Your name: ____

Your SUNet ID: ____________________________________

Exam rules:

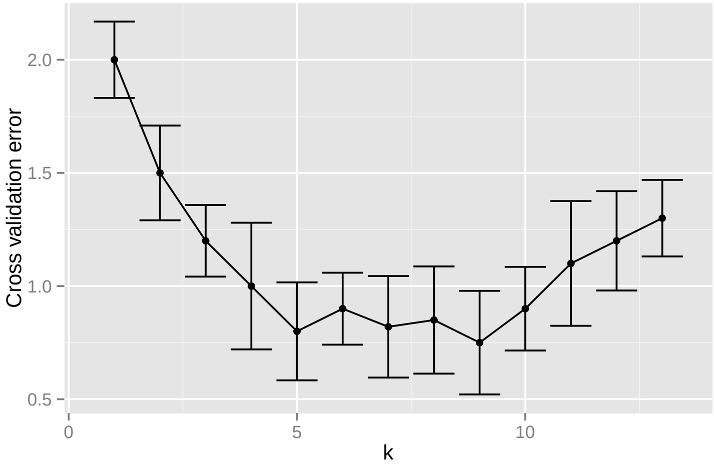
- You have 75 minutes to complete the exam.
- You are not allowed to consult books or notes, or to use calculator or cell phone. If you must use a computer to type your solutions, you are not allowed to use any software aside from a Word processor or LaTeX.
- A Cheat Sheet is provided at the end of the exam.
- Please show your work and justify your answers.
- **SCPD students:** If you are taking the exam remotely, please return your solutions along with a routing form, signed by your proctor, by 5:50 pm PST on Thursday, July 20. You can email a PDF to scpd-distribution@lists.stanford.edu.

Problem	Points
1	
2	
3	
4	
5	
6	
Total	

1. **[10 points]** Explain what a *ROC curve* is and how it is used.

   The Receiver Operating Characteristic (ROC) curve displays the relationship between the True Positive Rate (TPR) and the False Positive Rate (FPR) for a given binary classifier, under every discrimination threshold. ROC analysis provides a way to select possibly optimal models (as defined by TPR or FPR) and to discard suboptimal ones independently from (and prior to specifying) the cost context or the class distribution.

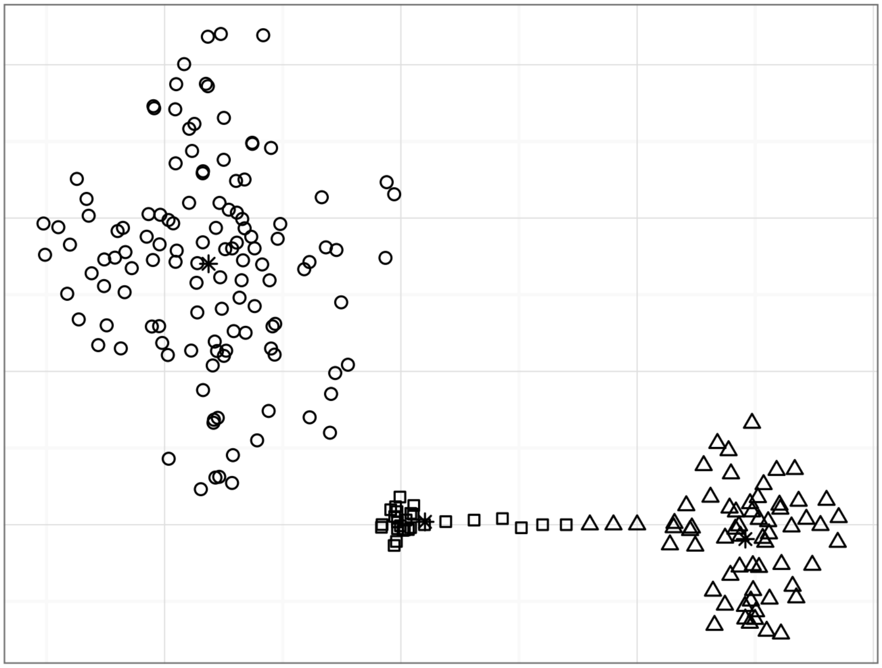
2. **[10 points]** State and explain the one standard error rule for model selection using 10-fold cross validation. Apply it to select the optimal number of nearest neighbors in the plot below, which shows the cross-validation error and one standard error intervals as a function of k.



   The one-standard error rule states we should choose the simplest model whose error lies within a standard error of the minimum error. The minimum error in the plot above is achieved at $k = 9$. The flexibility or variance of k-nearest neighbors decreases with k, so we would have to choose a model with $k \geq 9$. The model with $k = 10$ is the only model whose error lies within a standard error of the minimum error, so we would pick $k = 10$.

3. **[20 points]** Determine which of the following methods produced the clustering shown below and explain your reasoning. The centroid of each cluster is shown as an asterisk.

   - k-means clustering with $k = 3$.
   - Single linkage hierarchical clustering (dendogram cut at the level where there are 3 clusters).
   - Complete linkage hierarchical clustering (dendogram cut at the level where there are 3 clusters).



The method used was complete linkage hierarchical clustering. We can eliminate 3-means clustering, because it is clear that some of the circles are closer to the centroid of the squares than to the centroid of the circles. Similarly, we can eliminate single-linkage hierarchical clustering because several circles are farther away from all other circles than the square and triangle that are closest to each other.

4. We define a new kind of discriminant analysis for a classification problem with a binary response. The classes have prior probabilities π_0 and π_1. Given the class, k, the conditional probability of the inputs $X_1, \dots, X_p$ is multivariate normal with a class-dependent mean μ_k and covariance matrix $\sigma_k \boldsymbol{\Sigma}$. The matrix $\boldsymbol{\Sigma}$ is common to both classes and σ_k is a class-dependent constant. All parameters, π_k, μ_k, σ_k, for each class, as well as Σ, are set to their Maximum Likelihood estimates.

   (a) **[10 points]** Provide an equation describing the classifier's decision boundary or discriminant. What would the boundary look like?

   Note that this is a special case of Quadratic Discriminant Analysis. The covariance matrix for the inputs in each class may be different, but they are constrained to be related by scaling by a constant. The discriminant is the same as in QDA, but with this additional constraint. It is described by equating the objective functions for the two classes $\delta_1(x) = \delta_0(x)$, in this case

$$\log \pi_1 - \frac{1}{2}\sigma_1^{-1}\mu_1^T \boldsymbol{\Sigma}^{-1}\mu_1 + \sigma_1^{-1} x^T \boldsymbol{\Sigma}^{-1}\mu_1 - \frac{1}{2}\sigma_1^{-1} x^T \boldsymbol{\Sigma}^{-1} x - \frac{1}{2}\log|\sigma_1 \boldsymbol{\Sigma}| =$$

$$\log \pi_0 - \frac{1}{2}\sigma_0^{-1}\mu_0^T \boldsymbol{\Sigma}^{-1}\mu_0 + \sigma_0^{-1} x^T \boldsymbol{\Sigma}^{-1}\mu_0 - \frac{1}{2}\sigma_0^{-1} x^T \boldsymbol{\Sigma}^{-1} x - \frac{1}{2}\log|\sigma_0 \boldsymbol{\Sigma}|.$$

   This is still a quadratic equation in x.

   (b) **[10 points]** Why might this classifier be preferable to Linear Discriminant Analysis?

   The quadratic boundaries are more flexible than linear boundaries. This model allows you to fit cases in which different classes have different spreads.

   (c) **[10 points]** Why might this classifier be preferable to Quadratic Discriminant Analysis?

   By constraining the relationship between the covariance matrices for different classes, we have to estimate much fewer parameters from the data. This reduces the variance of the classification, which could lower the test error.

5. Two distances, d and d', are related by a monotone transformation:

$$d'(a,b) = f(d(a,b))$$

which satisfies $f(x) \geq f(y)$ if $x \geq y$.

(a) **[10 points]** Prove that the single linkage hierarchical clustering with k clusters is the same under d and d'.

At each step of an agglomerative clustering algorithm, we join the two clusters that are closest together. Suppose at some level in the dendrogram, the clusters are the same under d and d'. Let A and B be two clusters, and (a,b) be the pair of samples that are closest together under d, with $a \in A$ and $b \in B$. Since d' is a monotone transformation of d, the pair of points in A and B that are closest together under d' will also be (a,b). The single-linkage distance between clusters A and B is then $d(a,b)$ in the first case, and $d'(a,b)$ in the second case.

Now, suppose that A^* and B^* are the two clusters that are closest together under d. By monotonocity again, A^* and B^* will be the most proximal clusters under d'. This implies that the next pair of clusters to be joined in the dendrogram is the same under both distances. By induction, the two dendrograms have the same structure, and the clustering with k clusters will be identical.

(b) **[10 points]** Prove that the complete linkage hierarchical clustering with k clusters is the same under d and d'.

The proof follows the same argument as above. The complete-linkage distance between clusters A and B is just the distance between two samples a and b, and by monotonicity, these will be the same two samples under d and d'. Then, at every step of the agglomerative algorithm we join the two closest clusters, and because of the previous fact and monotonicity, this pair of clusters is always the same under d' and d. Hence, the dendrograms have the same structure and the clusterings with k clusters are identical.

6. **[10 points]** Let $(X_1, Y_1), ..., (X_n, Y_n) \overset{iid}{\sim} P_0$ and assume we fit a logistic regression to our data with no intercept. Specifically, we fit the following model

$$\log\left[\frac{\mathbb{P}[Y=1|\mathbf{X}]}{\mathbb{P}[Y=0|\mathbf{X}]}\right] = \beta_1 X_1, \tag{1}$$

Derive the gradient for β_1.

Using the negative log likelihood $-\ell(\beta)$ as our loss, we can apply the chain rule, i.e.

$$\begin{aligned}
-\frac{\partial\ell(\beta)}{\partial\beta} &= -\frac{\partial\ell(\beta)}{\partial p}\frac{\partial p}{\partial Z}\frac{\partial Z}{\partial\beta} \\
&= \left(-\frac{\mathbf{y}}{\mathbf{p}} + \frac{1-\mathbf{y}}{1-\mathbf{p}}\right)(\mathbf{p})(1-\mathbf{p})\mathbf{X} \\
&= (\mathbf{p}-\mathbf{y})\mathbf{X}
\end{aligned}$$

n.b. This is the same formula that was derived in class. The only difference is that $\mathbf{X}$ does not include a column of $\mathbf{1}$'s.

Cheat sheet

The sample variance of $x_1, \dots, x_n$ is:

$$\hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2,$$

The residual sum of squares for a regression model is:

$$RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

t-test:

The t-statistic for hypothesis $H_0 : \beta_i = 0$ is

$$t = \frac{\hat{\beta}_i}{\text{SE}(\hat{\beta}_i)}$$

F-test:

The F-statistic for hypothesis $H_0 : \beta_{p-q+1} = \beta_{p-q+2} = \cdots = \beta_p = 0$ is

$$F = \frac{(RSS_0 - RSS)/q}{RSS/(n-p-1)},$$

where RSS_0 is the residual sum of squares for the null model H_0, and RSS is the residual sum of squares for the full model with all predictors. Asymptotically, the F-statistic has the F-distribution with degrees of freedom $d_1 = q$ and $d_2 = n - p - 1$.

Minimum F-statistic to reject H_0 at a significance level $\alpha = 0.01$

		d_1			
		1	2	3	4
d_2	1	4052.181	4999.500	5403.352	5624.583
	10	10.044	7.559	6.552	5.994
	20	8.096	5.849	4.938	4.431
	30	7.562	5.390	4.510	4.018
	120	6.851	4.787	3.949	3.480

Logistic regression:

Logistic regression assigns to positive if the estimated conditional probability

$$\hat{P}(Y = +|X = x) = \frac{e^{X\cdot\hat{\beta}}}{1 + e^{X\cdot\hat{\beta}}}$$

LDA:

The log-posterior of class k given an input x is:

$$C + \log \pi_k - \frac{1}{2}\mu_k^T \mathbf{\Sigma}^{-1}\mu_k + x^T \mathbf{\Sigma}^{-1}\mu_k$$

where C is a constant which does not depend on k.

QDA:

The log-posterior of class k given an input x in QDA is:

$$C + \log \pi_k - \frac{1}{2}\mu_k^T \mathbf{\Sigma}_k^{-1}\mu_k + x^T \mathbf{\Sigma}_k^{-1}\mu_k - \frac{1}{2}x^T \mathbf{\Sigma}_k^{-1}x - \frac{1}{2}\log|\mathbf{\Sigma}_k|$$

where C is a constant which does not depend on k.