

Spring 2022 Data 100/200 Final Reference Sheet

Principal Component Analysis

The i -th Principal Component of the matrix X is defined as the i -th column of $U\Sigma$ defined by Singular Value Decomposition (SVD).

$X = U\Sigma V^T$ is the SVD of X if U and V^T are orthonormal matrices and Σ is a diagonal matrix. The diagonal entries of Σ , $[s_1, \dots, s_r, 0, \dots, 0]$, are known as singular values of X , where $s_i > s_j$ for $i > j$ and $r = \text{rank}(X)$.

Define the design matrix $X \in \mathbb{R}^{n \times p}$. Define the total variance of X as the sum of individual variances of the p features. The amount of variance captured by the i -th principal component is equivalent to s_i^2/n , where n is the number of datapoints.

Logistic Regression and Classification

Logistic Regression Model: For input feature vector x , $\hat{P}_\theta(Y = 1|x) = \sigma(x^T\theta)$. The estimate $\hat{\theta}$ is the parameter θ that minimizes the average cross-entropy loss on training data. For a single datapoint, define cross-entropy loss as $-[y\log(p) + (1 - y)\log(1 - p)]$, where p is the probability that the response is 1.

Logistic Regression Classifier: For a given input x and trained logistic regression model with parameter θ , compute $p = \hat{P}(Y = 1|x) = \sigma(x^T\theta)$. predict response \hat{y} with classification threshold T as follows:

$$\hat{y} = \text{classify}(x) = \begin{cases} 1 & p \geq T \\ 0 & \text{otherwise} \end{cases}$$

Confusion Matrix

Columns are the predicted values \hat{y} and rows are the actual classes y .

	0	1
0	True negative (TN)	False Positive (FP)
1	False negative (FN)	True Positive (TP)

Classification Performance

Suppose you predict n datapoints.

Metric	Formula	Other Names	Visualization	Plot
Accuracy	$\frac{TP+TN}{n}$		Precision-Recall Curve	Precision vs. Recall for different thresholds T
Precision	$\frac{TP}{TP+FP}$		ROC Curve	TPR vs. FPR for different thresholds T
Recall	$\frac{TP}{TP+FN}$	True Positive Rate (TPR), Sensitivity		
FPR	$\frac{FP}{FP+TN}$	False Positive Rate, Specificity		

Scikit-Learn

Suppose `linear_model` is an imported `sklearn` package.

Class/Attribute	Description	Function	Description
<code>linear_model.LogisticRegression(fit_intercept=True, penalty='l2', C=1.0)</code>	Returns an ordinary least squares Linear Regression model. Hyperparameter C is inverse of regularization parameter, C = 1/λ.	<code>model.fit(X, y)</code>	Fits the scikit-learn <code>model</code> to the provided <code>X</code> and <code>y</code> .
<code>model.coef_</code>	Estimated coefficients for the model, not including the intercept term.	<code>model.predict_proba(X)</code>	Returns predicted probabilities for the <code>X</code> passed in according to the fitted <code>model</code> . If binary classes, will return probabilities for both class 0 and 1.
<code>model.intercept_</code>	Bias/intercept term of the model. Set to 0.0 if <code>fit_intercept=False</code> .	<code>model.predict(X)</code>	Returns predictions for the <code>X</code> passed in according to the fitted <code>model</code> .
		<code>model.score(X, y)</code>	Returns the average <code>model</code> accuracy on the given test data <code>X</code> and labels <code>y</code> .

Suppose `tree` and `ensemble` are imported `sklearn` packages.

Class/Function	Description
<code>tree.DecisionTreeClassifier(criterion='entropy', max_depth=None)</code>	Returns a decision tree model which uses <code>criterion</code> to measure the quality of a split. <code>max_depth</code> is the maximum depth of the tree; if <code>None</code> , then nodes are expanded until all leaves are pure.
<code>ensemble.RandomForestClassifier(n_estimators=100, criterion='entropy', max_depth=None)</code>	Fit <code>n_estimators</code> decision tree classifiers on sub-samples of the dataset.
<code>model.fit</code>	Decision tree: Fit a decision tree classifier to the provided <code>X</code> and <code>y</code> . Random forest classifier: Build a forest of decision trees fit to the provided <code>X</code> and <code>y</code> .
<code>model.predict</code>	Decision tree: Returns predicted class response for the <code>X</code> passed in according to the fitted <code>model</code> . Random forest classifier: Returns the predicted class by highest mean probability estimate according to the trees in the forest <code>model</code> .

Clustering

K-Means Clustering: Pick an arbitrary k , and randomly place k “centers”, each a different color. Then repeat until convergence:

1. Color points according to the closest center (defined as squared distance).
2. Move center for each color to center of points with that color.

K-Means minimizes inertia, defined as the sum of squared distances from each datapoint to its center.

Agglomerative Clustering: Assign each datapoint to its own cluster. Then, recursively merge pairs of clusters together until there are k clusters remaining.

A datapoint's **silhouette score** S is defined as $S = (B - A) / \max(A, B)$, where A is the mean distance to other points in its cluster, and B is the mean distance to points in its closest cluster.

Decision Trees and Random Forests

Suppose you have a **decision tree classifier** for k classes. For each node, define the probability for class $C \in \{1, \dots, k\}$ as $p_C = d_C/d$, where d_C is the number of datapoints in class C (of the d total in the node). Then the entropy of the node (in bits) is defined as $S = - \sum_C p_C \log_2 p_C$, and the weighted entropy of the node is its entropy scaled by the fraction of datapoints in that node.

Decision tree generation algorithm: All of the data starts in the root node. Repeat until every node is either pure or unsplittable:

- Pick the best feature x and best split value β , where β is picked to maximize the change in weighted entropy between the parent node and the child nodes.
- Split data into two nodes, one where $x < \beta$, and one where $x \geq \beta$.

A node that has only one samples from one class is called a “pure” node. A node that has overlapping data points from different classes and thus that cannot be split is called “unsplittable”.

A **random forest** is a collection of many decision trees fit to variations of the same training data (e.g., bootstrapped samples, also called bagging; or random subsets of features). It is an ensemble method.