Classification problems
Thus far in our study of prediction, we have focused on the *regression* problem: Predict *continuous* outcomes.

In this lecture we (briefly) cover the *classification* problem: Predict *discrete* outcomes.

Specifically, we will focus on *binary classification*, where the outcome is zero or one.
Example: Spam filtering

Suppose that you are running a mail server.

Given an incoming message your goal is to decide: Is this spam or not?

Typical covariates:

- Counts of key words, phrases, etc.
- Indicator for origin domain of e-mail
- Indicators for links/domains present in the e-mail
- Indicator for whether sender is in your address book
Example: Medical diagnostics

Suppose that given a patient, your goal is to determine whether this person is likely to suffer an adverse medical event (e.g., a heart attack).

Typical covariates:
- Weight, body mass index, obesity indicator
- Age
- Gender
- Cholesterol levels
- Indicator for family history
- Results of medical tests (blood tests, imaging, etc.)
Example: Hiring in a labor market

Suppose that, given a job opening and an applicant, your goal is to determine whether the applicant will be hired for the job opening.

Typical covariates:

- Indicators for skills of the applicant
- Indicators for skills required on the job
- Years of education, work experience of the applicant
- Years of education, work experience required in the job opening
- *Interactions* between the preceding covariates
- Detail in applicant’s profile
- Who made the first contact: applicant or employer
Classification: Formalism

Formally, classification problems look a lot like what we’ve studied so far:

- There is a dataset with $n$ observations; $Y_i$ is the outcome in the $i$’th observation, and $X_i$ is the covariate vector corresponding to the $i$’th observation.
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- For each \( i \), \( Y_i \in \{0, 1\} \) (or some other binary set). We refer to zeroes as “negative” outcomes, and ones as “positive” outcomes.
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- For each \( i \), \( Y_i \in \{0, 1\} \) (or some other binary set). We refer to zeroes as “negative” outcomes, and ones as “positive” outcomes.

- Using the data, fit a model \( \hat{f} \) (a “classifier”). Given a covariate vector \( \vec{X} \), \( \hat{f}(\vec{X}) \in \{0, 1\} \).

- The model is evaluated through some measure of its prediction error on new data (generalization error). Common example is expected 0-1 loss on a new sample:

\[
\mathbb{E}_Y[\mathbb{I}\{Y \neq \hat{f}(\vec{X})\}|X, Y, \vec{X}] = \mathbb{P}_Y(Y \neq \hat{f}(\vec{X})|X, Y, \vec{X}).
\]
0-1 loss and “accuracy”

The 0-1 loss function is a measure of accuracy: How well, on average, does the classifier make predictions?

Another way to say it: A good classifier minimizes the number of samples on which the classifier makes a classification mistake.

Is this always what we want?
Train-validate-test

The train-validate-test methodology carries over to classification in a straightforward way:

Given a dataset, split it into *training*, *validation*, and *test* sets.

- **Training**: Use the training data to build different candidate classifiers $\hat{f}^{(1)}, \ldots, \hat{f}^{(L)}$.

- **Validation**: Compute the average 0-1 loss of each of the $L$ classifiers on the validation data. Choose the classifier $\hat{f}^*$ with the lowest loss (i.e., lowest misclassification rate, or highest accuracy).

- **Test**: Make predictions using $\hat{f}^*$ on the test set to get an unbiased estimate of the generalization error.
False positives and false negatives
Example: Fraud detection

Suppose that you are asked to build a fraud detection algorithm for PayPal.

Data: Transactions, including account info, profile info, etc. of both parties, as well as amount and type of transaction

Outcomes: For each transaction, either zero (not fraud) or one (fraud)

Suppose: 0.3% of transactions are fraud.

Your job: build a “good” classifier. Is accuracy the right objective?
Beyond accuracy

Because of the issue identified in the preceding example, we should distinguish between misclassification of positive samples and negative samples.

For this purpose we typically use the confusion matrix of a classifier on a test set.\(^1\)

\[
\begin{array}{c|cc|c}
& 0 & 1 & \text{Total} \\
\text{Actual} & \text{TN} & \text{FP} & \text{TN} + \text{FP} \\
0 & & & \\
1 & \text{FN} & \text{TP} & \text{FN} + \text{TP} \\
\text{Total} & \text{TN} + \text{FN} & \text{TP} + \text{FP} & n \\
\end{array}
\]

Here:

- TN = \# of true negatives; FP = \# of false positives
- FN = \# of false negatives; TP = \# of true positives

\(^1\)Be careful! One source of “confusion” about confusion matrices is that sometimes the truth indexes the rows, and sometimes the truth indexes the columns.
Confusion matrices

How to interpret confusion matrices:
Other metrics

Nearly every metric of interest in binary classification can be derived from confusion matrices:

- **Accuracy** = (TP + TN)/n.
- **Mean 0-1 loss** = (FP + FN)/n = 1 − accuracy.
- **True positive rate (TPR)** = TP/(FN + TP).
- **False positive rate (FPR)** = FP/(TN + FP).
- **True negative rate (TNR)** = TN/(TN + FP).
- **False negative rate (FNR)** = FN/(FN + TP).
- **Sensitivity** = TPR.
- **Specificity** = TNR.
- **Precision** = TP/(TP + FP).
- **Recall** = sensitivity = TPR.
- **Type I error rate** = FPR.
- **Type II error rate** = FNR.
- **False discovery rate** = FP/(TP + FP)
False positives and false negatives

Except for accuracy and 0-1 loss, all these metrics are just different ways of measuring the two kinds of error that can be made by the classifier:

1. Misclassifying a true negative example as a positive (false positive, or Type I error).
2. Misclassifying a true positive example as a negative (false negative, or Type II error).
A tradeoff

Note that:

1. It is easy to design a classifier with no false positives. (How?)
2. It is easy to design a classifier with no false negatives. (How?)

On the other hand, in general there is “no free lunch”: it is generally not possible to ensure both no false positives and no false negatives.

In general, for “good” classifiers, reducing false positives comes at the expense of increasing false negatives.

Therefore in designing a classifier it is important to consider which type of error is more consequential to you.²

²Note that this sometimes leads to objectives that are weighted sums of the entries of the confusion matrix.
Example: Fraud detection

As an example, suppose that you build a classifier for fraud detection on a dataset with \( n = 50,000 \) with the following confusion matrix:

<table>
<thead>
<tr>
<th>Actual</th>
<th>Predicted</th>
<th>Not Fraud</th>
<th>Fraud</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Not Fraud</td>
<td>49,603</td>
<td>247</td>
<td>49,850</td>
<td></td>
</tr>
<tr>
<td>Fraud</td>
<td>22</td>
<td>128</td>
<td>150</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>49,625</td>
<td>375</td>
<td>50,000</td>
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Note that this classifier has lower accuracy than one that just always predicts "Not Fraud." Would you use this classifier? What if reducing the false negatives to zero also meant increasing false positives to \( \geq 1000 \)?
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- Note that this classifier has lower accuracy than one that just always predicts “Not Fraud.”
- Would you use this classifier? What if reducing the false negatives to zero also meant increasing false positives to \( \approx 1000 \)?
Example: Fraud detection

Analysis:
Building a classifier
In regression, we saw that if we knew the population model, then:

- Given a new covariate vector $\tilde{X}$, the best prediction we could make (in terms of squared error) was the conditional expectation $f(\tilde{X}) = \mathbb{E}[Y|\tilde{X}]$.

- Even if we did so, there is still some error remaining in our predictions: the *irreducible error*.

What is the analogue of conditional expectation for classification with 0-1 loss?
The Bayes classifier

Suppose we want to minimize 0-1 loss (i.e., maximize accuracy). Note that:

\[ \mathbb{E}_Y [\mathbb{I}\{Y \neq \hat{f}(\vec{X})\} | \vec{X}] = \mathbb{P}_Y (Y \neq \hat{f}(\vec{X}) | \vec{X}). \]

How do we minimize this?

- If \( Y \) is more likely to be 0 than 1 (given \( \vec{X} \)), then we should set \( \hat{f}(\vec{X}) = 0 \); and vice versa.

- In other words: If \( \mathbb{P}_Y (Y = 0 | \vec{X}) > 1/2 \), set \( \hat{f}(\vec{X}) = 0 \); otherwise if \( \mathbb{P}_Y (Y = 1 | \vec{X}) > 1/2 \), set \( \hat{f}(\vec{X}) = 1 \).

This is called the Bayes classifier.
Approximating the Bayes classifier

The Bayes classifier is unattainable as a predictive model, for the same reason the conditional expectation is unattainable: we don’t know the population model.

In general, good classification models (with respect to 0-1 loss) are those that approximate the Bayes classifier well.

One example we explore: $k$-nearest-neighbor classification.
An example: $k$-nearest-neighbor classification
Basic version:

- Given a covariate vector $\vec{X}$, find the $k$ nearest neighbors.
- Take a *majority vote* to determine the classification.\(^3\)

This approximates the Bayes classifier by *local averaging*.

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\(^3\)Ties are typically broken at random among the furthest neighbors, or just by choosing $k$ odd.
Adding a threshold

More generally, let $\text{NN}(k, L)$ denote the $k$-nearest neighbor algorithm with a threshold $L$:

- Require at least $L$ of the $k$ nearest neighbors to have label 1 to assign label 1; otherwise assign label 0.
- Basic algorithm corresponds to $\text{NN}(k, k/2)$.
- What happens if $L = 0$?
- What happens if $L > k$?
Example: The CORIS dataset

462 South African males evaluated for heart disease.

Outcome variable: Coronary heart disease (chd).

Covariates:
- Systolic blood pressure (sbp)
- Cumulative tobacco use (tobacco)
- LDL cholesterol (ldl)
- Adiposity (adiposity)
- Family history of heart disease (famhist)
- Type A behavior (typea)
- Obesity (obesity)
- Current alcohol consumption (alcohol)
- Age (age)
Example: The CORIS dataset

Steps:

- Import the data
- (Random) split into train and test
- Train $\text{NN}(k, L)$ for range of $k$, and for $L = ak$, $a \in [0, 1.05]$
- Record TP, FP, TN, FN on test set.
Example: The CORIS dataset

Prediction error (0-1 loss) on test set:
Example: The CORIS dataset

FPR vs. TPR for the choice $k = 10$, as threshold $L/k$ varies:
The ROC curve

The graph of FPR vs. TPR as the classifier’s threshold is varied is called the *ROC curve* (for “receiver operating characteristic”).

The *area under the curve (AUC)* is often reported as a measure of the quality of the classifier:

- Better classifiers are further “up and to the left” in the graph.
- A perfect classifier would have zero FPR and unit TPR ≡ top left corner.
- Therefore a perfect classifier should have AUC 1.
- The closer the AUC is to 1, the better the classifier is on *both* types of errors.
More on ROC curves
Model scoring and selection for classification
As noted previously, cross validation is a completely general technique that can be applied regardless of the model class or loss function being used.

In particular, $K$-fold CV can be used in exactly the same way for evaluation and selection of classifiers with 0-1 loss (or any other objective derived from the confusion matrix).
Model complexity scores

The scores we developed ($C_p$, AIC, BIC) are also developed only for squared error loss.

In practice, AIC and BIC are often used even in the case of 0-1 loss. There is no formal justification for this practice, except that both scores provide a heuristic penalty for excessive model complexity.
Bias, variance, and model complexity

Note that the bias-variance decomposition we computed only applies for squared error loss.

There are versions of this decomposition that have been developed for 0-1 loss as well, though one has to be careful in interpreting them.\(^4\)

In general, just as there is often a “bias-variance tradeoff” in regression, something similar is true in classification:

- More “complex” models (e.g., lower \(k\) in \(k\)-NN classification) tend to overfit the training data, and thus have higher variance, but have lower bias.
- Less “complex” models (e.g., higher \(k\) in \(k\)-NN classification) tend to underfit the training data, and thus have lower variance, but have higher bias.