AI200: APPLIED MACHINE LEARNING

MODEL EVALUATION FOR CLASSIFICATION MODELS

MODEL EVALUATION METRICS: CONFUSION MATRIX

- For classification models, we use the **Confusion Matrix**, which helps us produce **a suite of model evaluation metrics** to evaluate model performance.
- For example, we may build a classifier to predict whether 10 people would have diabetes or not, and the results can be collated into a **Confusion Matrix** as shown below.

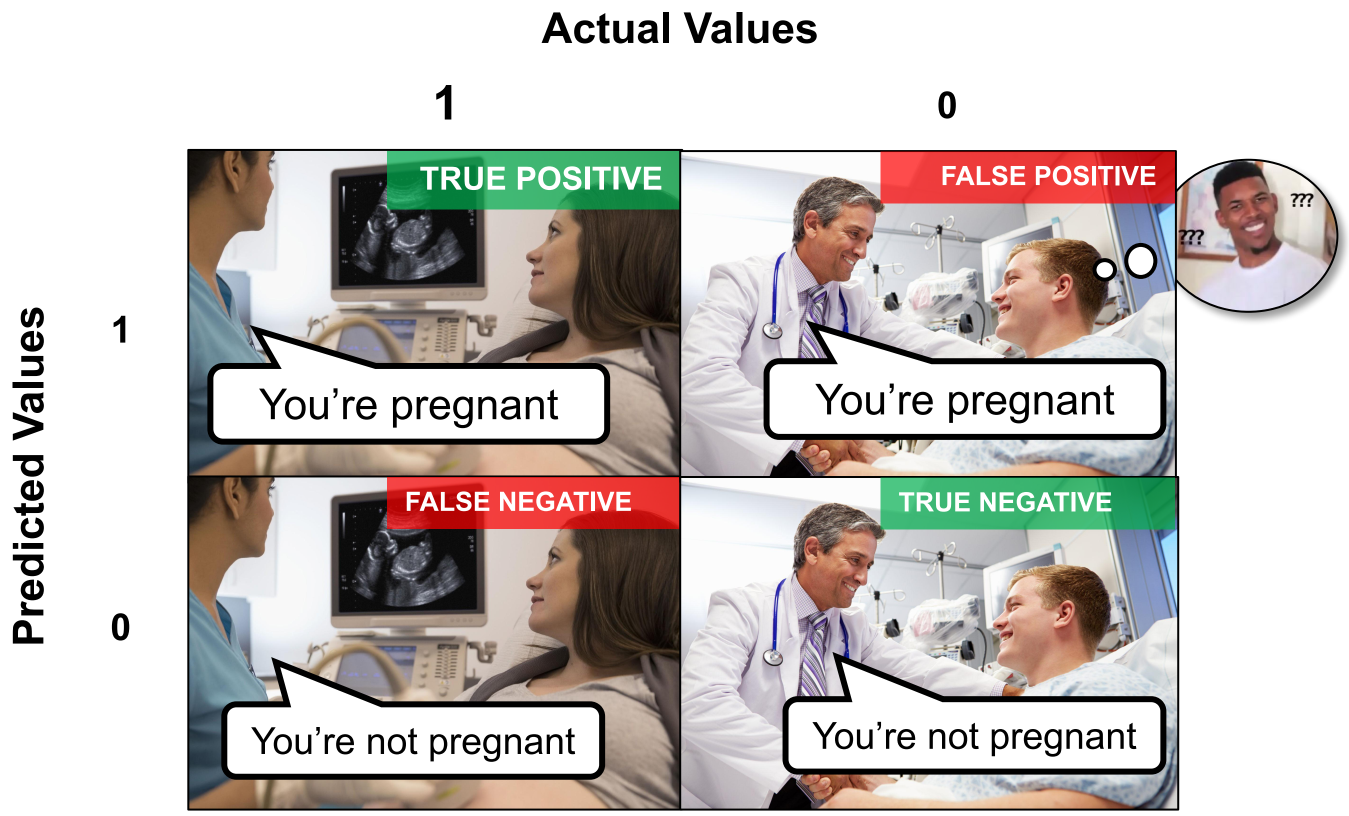
Predicted by ML Models

S/N	Glucose	BMI	Actual Values	Predicted Values
1	148	33.6	1	1
2	85	26.6	0	0
3	183	23.3	1	1
4	89	28.1	0	0
5	137	43.1	1	1
6	116	25.6	0	0
7	78	31.0	1	1
8	115	35.3	0	1
9	197	30.5	1	1
10	125	0.0	1	0

		Actual Values	
		Positive (1)	Negative (0)
Predicted Values	Positive (1)	**True Positive** 5	**False Positive** 1
	Negative (0)	**False Negative** 1	**True Negative** 3

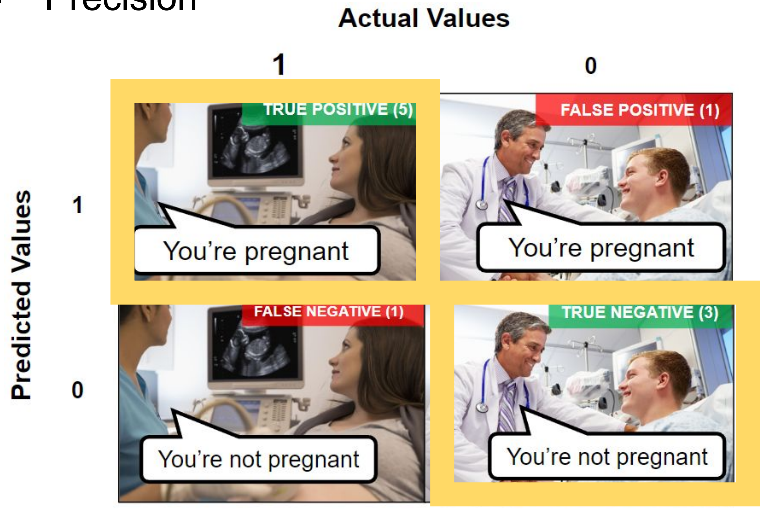
MODEL EVALUATION METRICS: CONFUSION MATRIX (ANALOGY)

- Let’s use a memorable analogy to help us grasp the intuition of the confusion matrix.
- Imagine we created a classification model to predict whether 10 people are pregnant or not, and after the model churned out its predictions, we see how well the model performed:



MODEL EVALUATION METRICS: ACCURACY

- Using the confusion matrix, we can compute metrics to evaluate the performance of classification models:
  - Accuracy
  - Error Rate
  - Sensitivity / Recall
  - Specificity
  - Precision



True Negative (TN):
- The model predicted that the person is not pregnant
- The person indeed is not pregnant
- Therefore, the model's **prediction of a negative outcome was true**

True Positive (TP):
- The model predicted that the person is pregnant
- The person is indeed pregnant
- Therefore, the model's **prediction of a positive outcome was true**

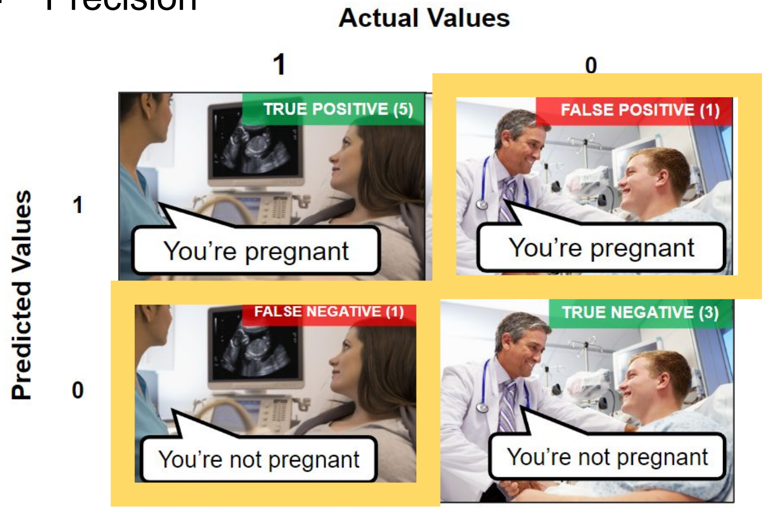
Accuracy of model: Overall, how often is the classifier correct?

$$\frac{TN+TP}{Number\ of\ Predictions\ Generated} = \frac{TN+TP}{TN+TP+FN+FP}$$
$$= \frac{3+5}{3+5+1+1}$$
$$= 0.8$$

This is actually very intuitive. If you think about it, we are just dividing the total number of instances our model was correct, by the total number of predictions. In this example, the accuracy rate of our diabetes prediction model is 80%.

MODEL EVALUATION METRICS: ERROR RATE

- Using the confusion matrix, we can compute metrics to evaluate the performance of classification models:
  - Accuracy
  - Error Rate
  - Sensitivity / Recall
  - Specificity
  - Precision



Error Rate = 1 – Accuracy

False Negative (FN), aka Type II Error:
- The model predicted that the person is not pregnant
- But the person is actually pregnant
- Therefore, the model's **prediction of a negative outcome was false**

False Positive (FP), aka Type I Error:
- The model predicted that the person is pregnant
- But the person is not pregnant (c'mon, he is a guy) ☹
- Therefore, the model's **prediction of a positive outcome was false**

Error Rate of model: Overall, how often is the classifier wrong?

$$\frac{FN+FP}{Number\ of\ Predictions\ Generated} = \frac{FN+FP}{TN+TP+FN+FP} = \frac{1+1}{3+5+1+1} = 0.2$$

This is actually very intuitive. If you think about it, we are just dividing the total number of instances our model was wrong, by the total number of predictions. In this example, the classification error rate of our diabetes prediction model is 20%.

MODEL EVALUATION METRICS: SENSITIVITY

- Using the confusion matrix, we can compute metrics to evaluate the performance of classification models:
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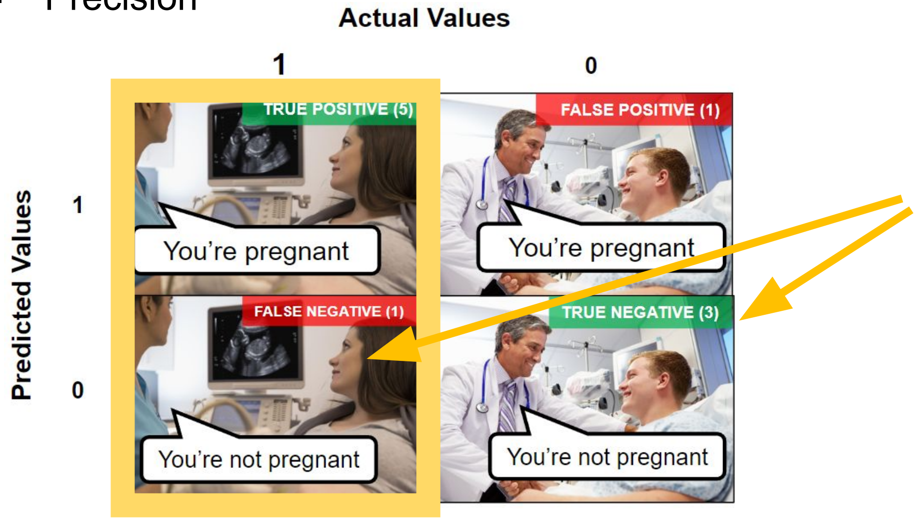
  - Sensitivity / Recall
  - Specificity
  - Precision



Say we build a model that only predicts zeros, all data points would either be **False Negatives** or True Negatives.

Thus, Sensitivity: TP / (TP + FN)
= 0 / (0 + FN) = 0 if there are false negatives.

Unlike accuracy which cannot distinguish between Type I & II errors, the Sensitivity metric provides more specific information:

Lower count of False Negatives => Higher Sensitivity.

Sensitivity / Recall of model: When the actual outcome is positive, how often is the prediction correct?

$$\frac{TP}{Number\ of\ Actual\ Positive\ Outcomes} = \frac{TP}{TP+FN} = \frac{5}{5+1} = 0.83333$$

Sensitivity measures how effective is the classifier in detecting positive instances, also known as **"True Positive Rate" or "Recall".**

For **use cases like cancer diagnosis**, this metric is very important, because any patient you falsely diagnose as benign is a potential life lost.

MODEL EVALUATION METRICS: SPECIFICITY

- Using the confusion matrix, we can compute metrics to evaluate the performance of classification models:
  - Accuracy
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  - Sensitivity / Recall
  - Specificity
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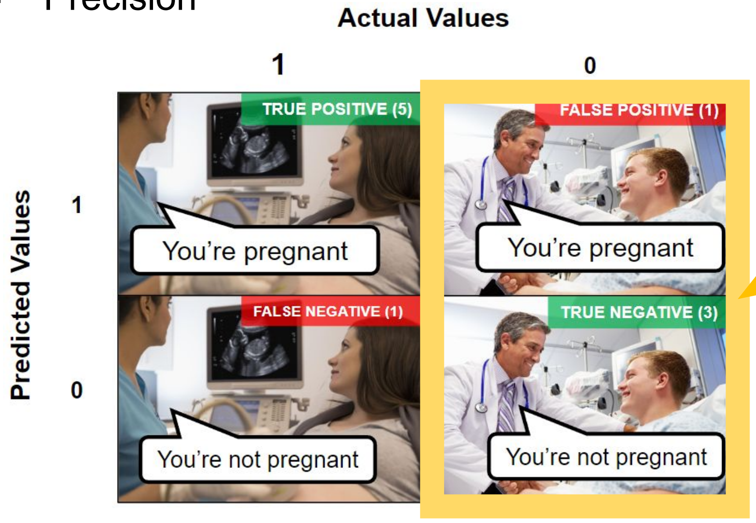


On the other hand, **Specificity** looks at a different half of the quadrant.

Specificity = TN / (TN + FP)

Lower count of False Positives => Higher Specificity.

NOTE: Like Sensitivity, Specificity ranges between 0 and 1.
The higher the metric, the better!

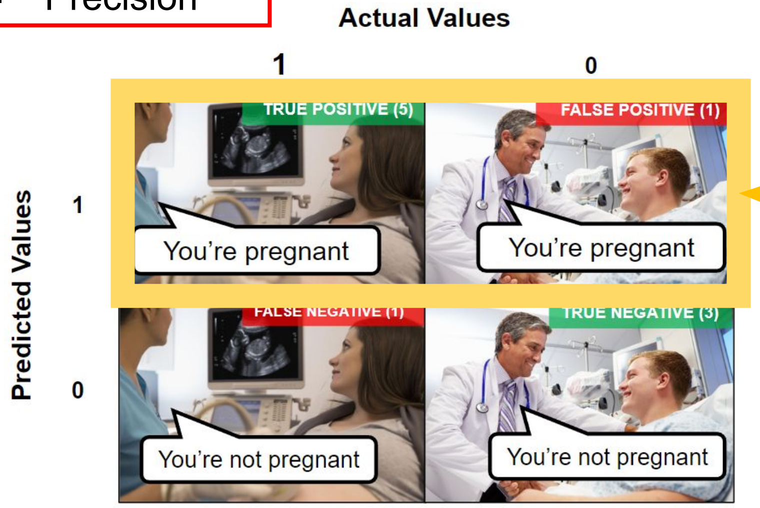
Specificity of model: When the actual outcome is negative, how often is the prediction correct?

$$\frac{TN}{Number\ of\ Actual\ Negative\ Outcomes} = \frac{TN}{TN+FP} = \frac{3}{3+1} = 0.75$$

Specificity measures how effective the classifier is in detecting negative cases.

MODEL EVALUATION METRICS: PRECISION

- Using the confusion matrix, we can compute metrics to evaluate the performance of classification models:
  - Accuracy
  - Error Rate
  - Sensitivity / Recall
  - Specificity
  - Precision



Precision focuses on the relevance of positive instances flagged by the classifier. (Are they ***True Positives***, or ***False Positives***?)

Precision = TP / (TP + FP)

Lower count of False Positives => Higher Precision.

*NOTE: Precision is often used together with "Recall" (aka Sensitivity). You might also be interested in **F1 Score**,which combines precision with recall.*

Precision of model: When the predicted outcome is positive, how often is the prediction correct?

$$\frac{TP}{Number\ of\ Actual\ Negative\ Outcomes} = \frac{TP}{TP+FP}$$

$$= \frac{5}{5+1}$$

$$=0.83333$$

MODEL EVALUATION METRICS: HOW TO COLLECT THEM?

- Similar to RMSE, we **use one of these two methods** covered during our previous lesson on Regression:
  - Train-test split
  - Cross Validation
- The only difference is that **instead of RMSE, we calculate accuracy (or other metrics)** on the validation dataset.

LOGISTIC REGRESSION

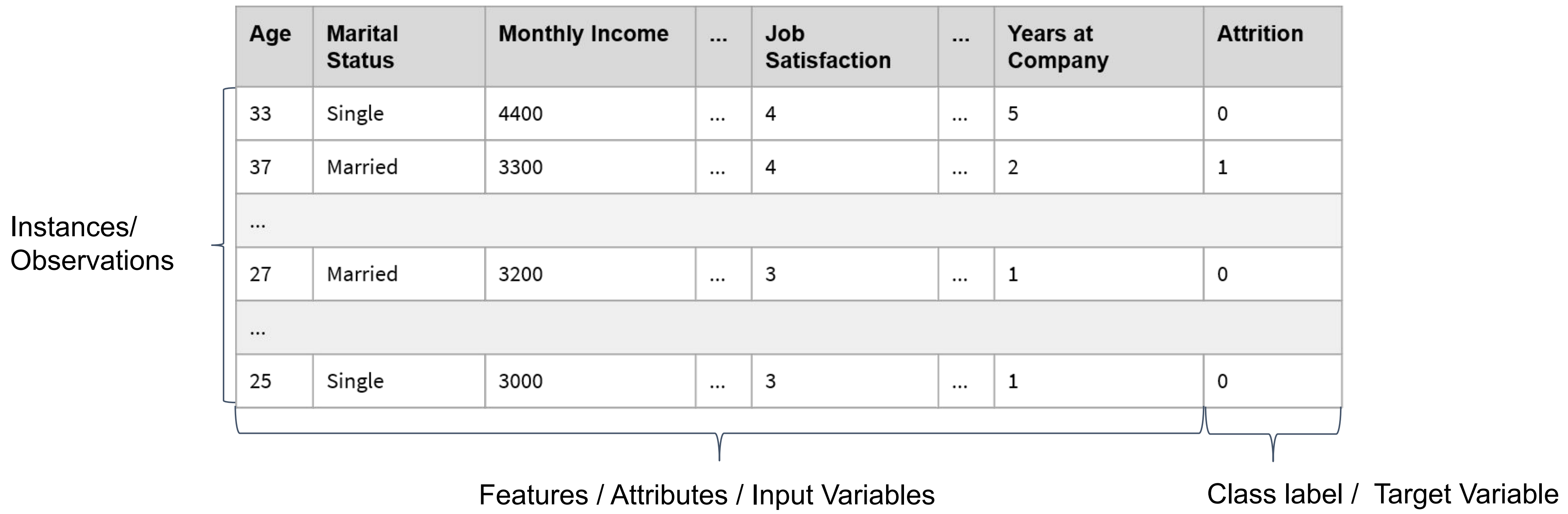
MODEL EVALUATION PROCEDURE (SELF-READING)

** This section was already covered in Lesson 3, but is added here explicitly so that you understand that the same techniques apply to classification problems as well.*

MODEL EVALUATION / ASSESSING MODEL ACCURACY: TRAIN-TEST SPLIT

- Train-test split is a technique that estimates a model's test error by leaving out a subset of provided data during training / fitting process and using this subset as a test dataset. The specific steps are:

  - **Step 1**: Randomly divide available data into two parts (usual norm for splitting is 70-30):
    - **Training** set
    - **Validation** set
  - **Step 2**: Use the **training set** to fit the model
  - **Step 3**: Generate predictions for the **validation set** with the model
  - **Step 4**: Calculate the accuracy for the model based on the **validation set**


Instances/ Observations
Features / Attributes / Input Variables
Class label / Target Variable

Age	Marital Status	Monthly Income	...	Job Satisfaction	...	Years at Company	Attrition
33	Single	4400	...	4	...	5	0
37	Married	3300	...	4	...	2	1
...							
27	Married	3200	...	3	...	1	0
...							
25	Single	3000	...	3	...	1	0

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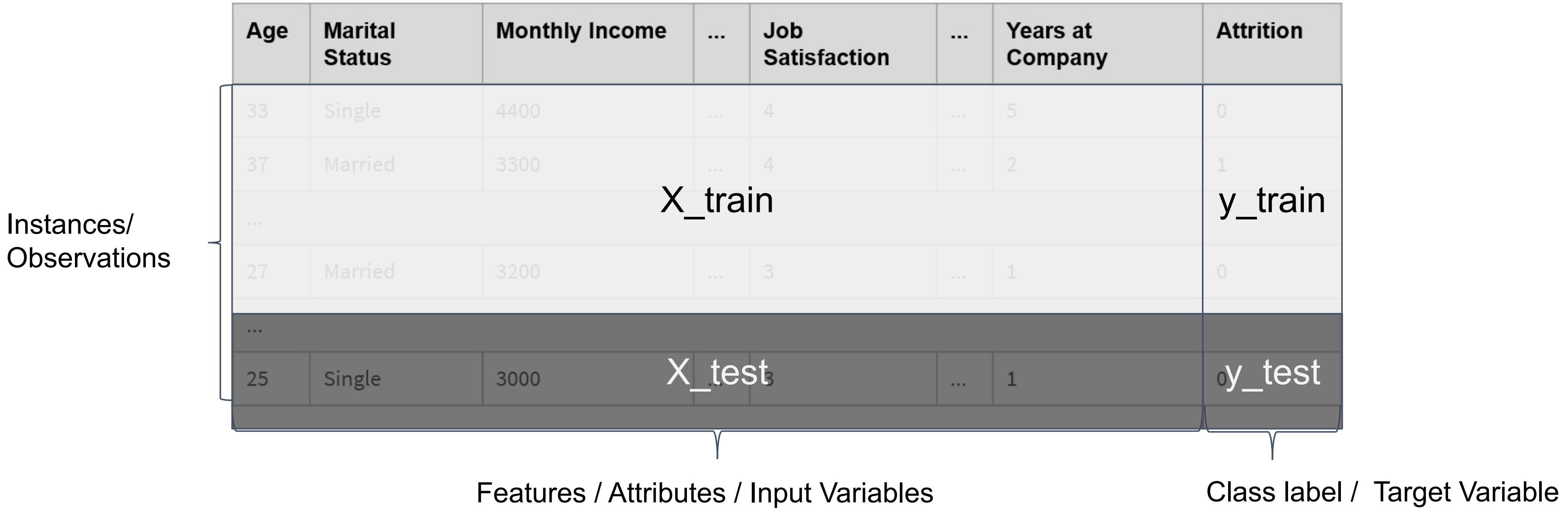
Instances/ Observations
X_train
y_train
X_test
y_test
Features / Attributes / Input Variables
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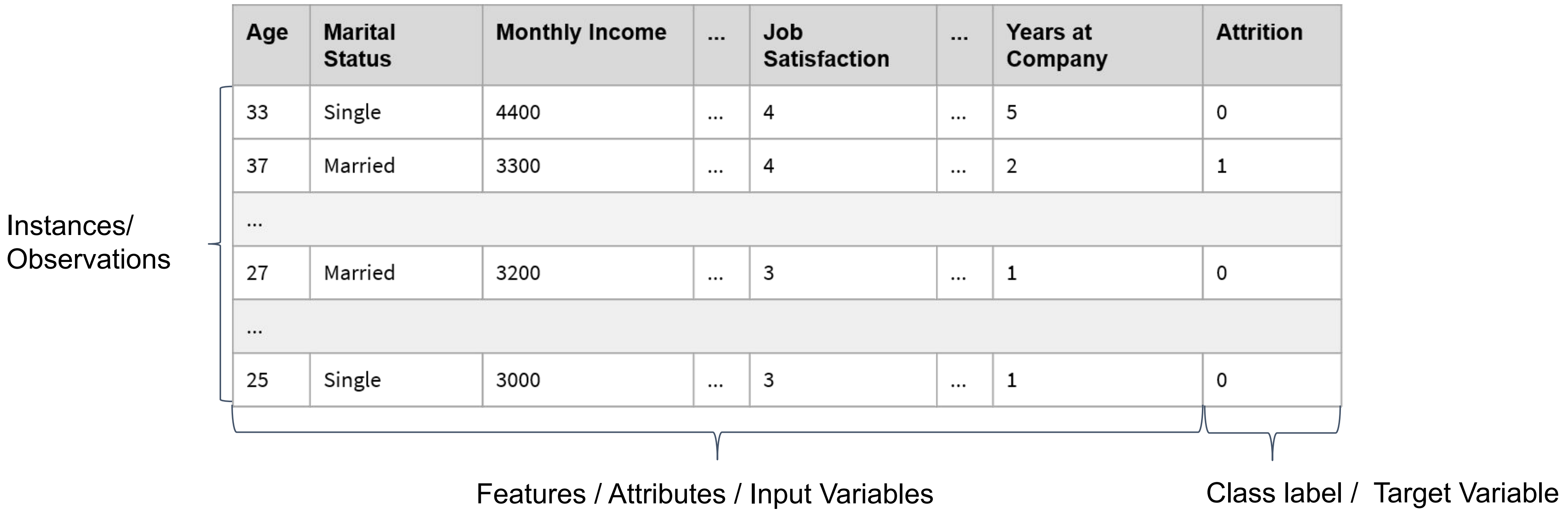
MODEL EVALUATION / ASSESSING MODEL ACCURACY: CROSS VALIDATION

- Cross Validation is a is a resampling procedure used to evaluate machine learning models on a limited data sample. The procedure has a single parameter called k that refers to the number of groups that a given data sample is to be split into. As such, the procedure is often called k-fold **cross-validation.** The specific steps are:
  - **Step 1**: Randomly split the dataset into K equal partitions or 'folds'
  - **Step 2**: Use **Fold 1 as validation set**, and the rest of the **other folds as training data**
  - **Step 3**: Fit the model on the **training set** and estimate the model's accuracy using the **validation set**
  - **Step 4**: Repeat step 2-3 **using a different fold as validation set** at each iteration
  - **Step 5**: Take the average error as the estimate of test error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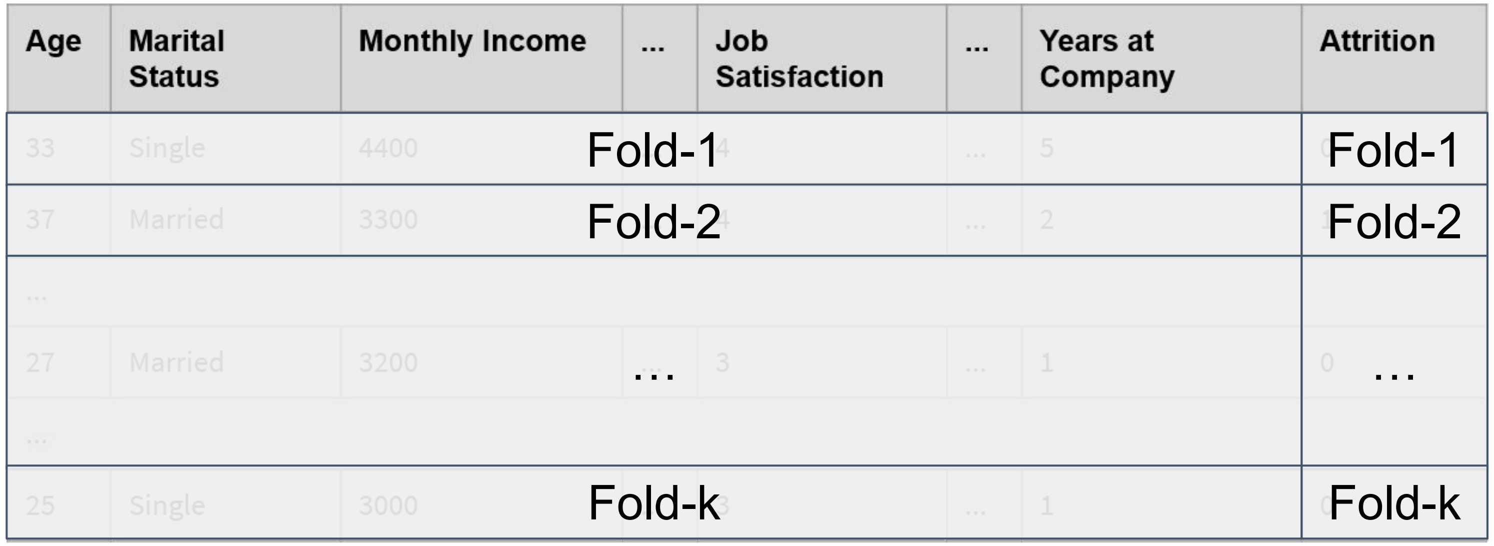

If k = 10, that means each fold contains 10% of the data, where the entire dataset is split into 10 equal parts

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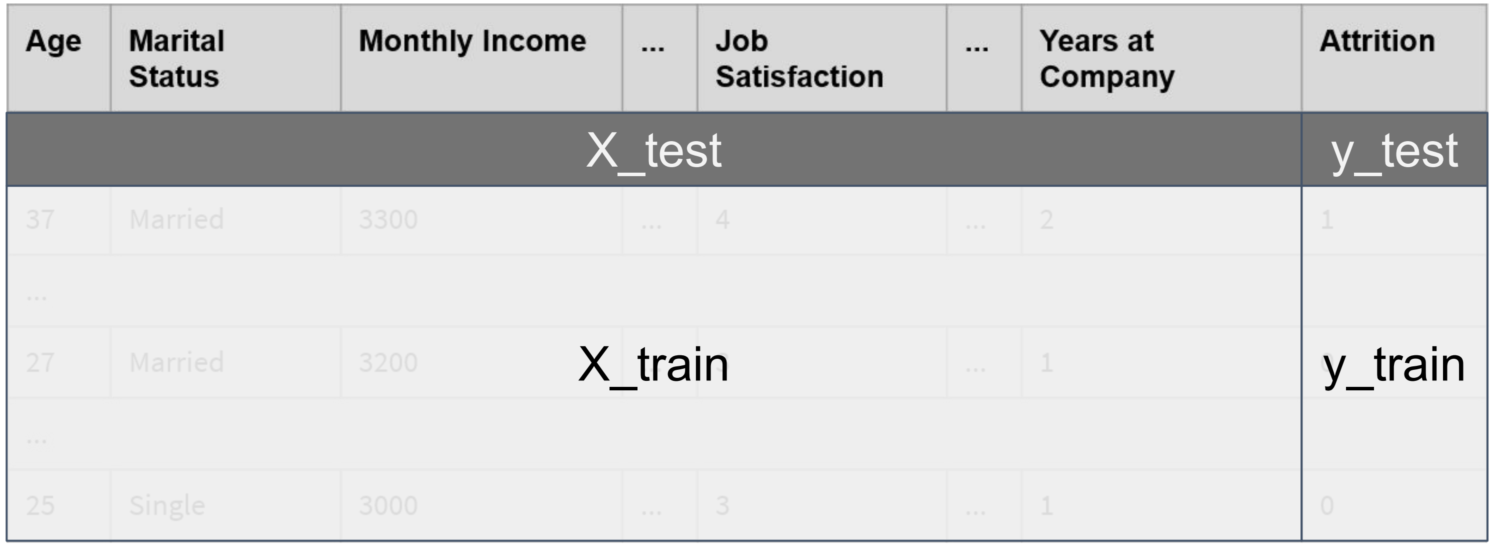

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...							
27	Married	3200	[illegible]	[illegible]	...	1	[illegible]
...							
25	Single	3000	...	3	...	1	0

X_test
y_test
X_train
y_train

We would use fold-1 as the test data set, and calculate the RSME based on it

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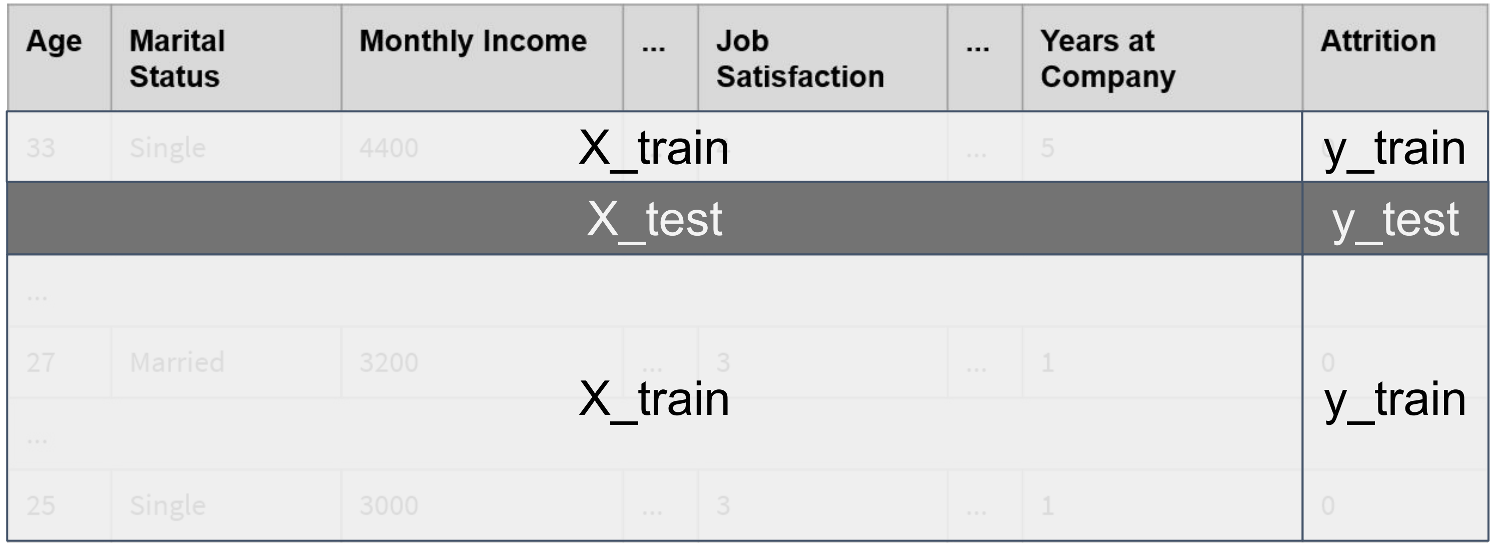

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...							
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We repeat this with the subsequent fold.

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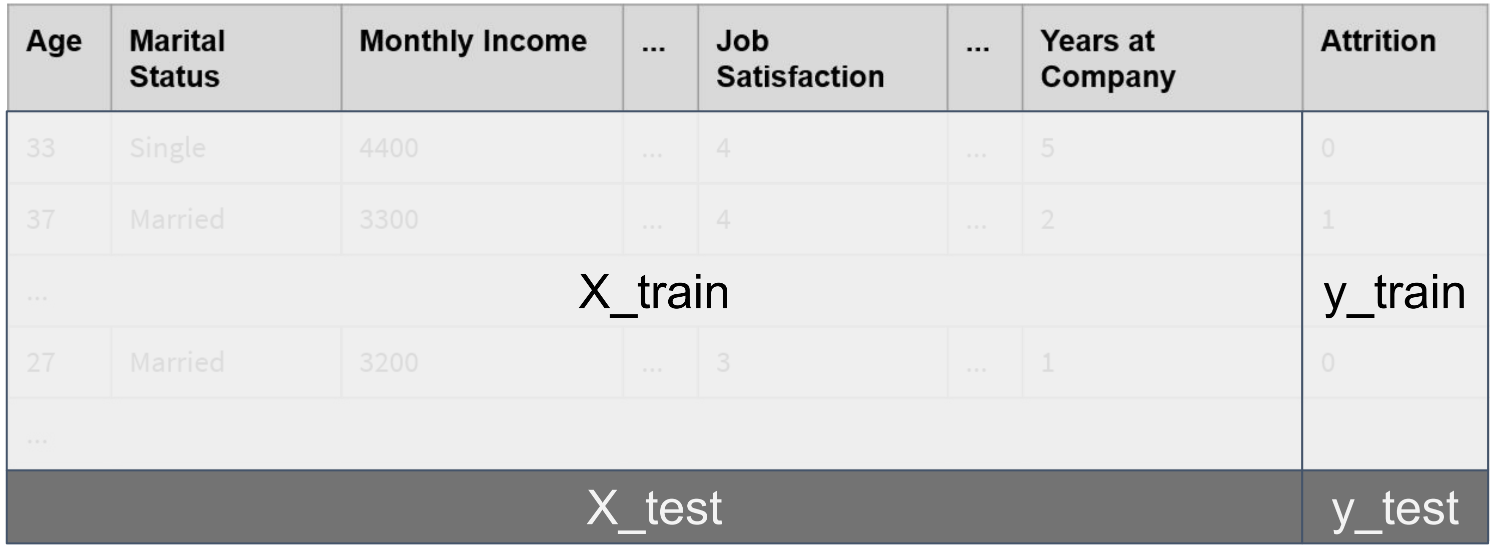

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...							
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...							

X_train
y_train
X_test
y_test

And we keep doing this until each fold has served as the validation dataset

MODEL EVALUATION / ASSESSING MODEL ACCURACY: CROSS VALIDATION

- Pros: Cross Validation / K-Fold Cross Validation provides a **more accurate estimate of test error**. It **uses the dataset more efficiently** than just a single train-test split

- Cons: However, the **tradeoff is the computational cost**. A k-fold cross validation takes **k times longer** than the train-split test approach.