Welcome to Supervised Learning

Part 3: Evaluation metrics in supervised machine learning

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[https://github.com/azsom/Supervised-Learning (https://github.com/azsom/Supervised-Learning)](https://github.com/azsom/Supervised-Learning)

The topic of the course series: supervised Machine Learning (ML)

- how to build an ML pipeline from beginning to deployment
- we assume you already performed data cleaning
- this is the third course out of 6 courses
  - Part 1: Introduction to machine learning and the bias-variance tradeoff
  - Part 2: How to prepare your data for supervised machine learning
  - **Part 3: Evaluation metrics in supervised machine learning**
  - Part 4: Non-linear supervised machine learning algorithms
  - Part 5: Missing data in supervised ML
  - Part 6: Interpretability
- you can complete the courses in sequence or complete individual courses based on your interest

Structured data

X	feature_1	feature_2	...	feature_j	...	feature_m	Y
data_point_1	x_11	x_12	...	x_1j	...	x_1m	**y_1**
data_point_2	x_21	x_22	...	x_2j	...	x_2m	**y_2**
...	...	...	...	...	...	...	**...**
data_point_i	x_i1	x_i2	...	x_ij	...	x_im	**y_i**
...	...	...	...	...	...	...	**...**
data_point_n	x_n1	x_n2	...	x_nj	...	x_nm	**y_n**

We focus on the target variable (y) in this course.

Learning objectives of this course

- Describe the elements of the confusion matrix
- Describe metrics derived from the confusion matrix such as accuracy, precision, recall, and the f_beta score
- Summarize what the ROC and precision-recall curves and AUC are
- Review the logloss metric and its properties
- Outline metrics often used in regression (MSE, RMSE, MAE, R2 score)
- Calculate the value of each metric given a set’s target variable and predictions from an ML model
- Calculate the baseline of each metric given a set’s target variable
- Choose an appropriate evaluation metric given your ML problem

Module 1: Hard predictions in classification

Learning objectives of this module:

- Describe the elements of the confusion matrix
- Describe metrics derived from the confusion matrix such as accuracy, precision, recall, and the f_beta score
- Calculate the value of each metric given a set’s target variable and predictions from an ML model
- Calculate the baseline of each metric given a set’s target variable

Let's start

- decide what metric we will use to evaluate the supervised ML model
    - this is necessary even before we train the model
    - we need to know what single number metric we will use to compare models and to select the best one
    - need to understand the metrics and our needs
    - we also need a baseline to compare the scores againts - more on this at the end of the module
- sklearn classifiers have two methods to return predictions
    - .predict_proba which returns the probability that the point belongs to each class with shape (n_samples, n_classes)
    - .predict which returns the predicted class for each point with shape (n_samples)

.predict_proba vs. .predict

```
y_true = [1 0 1 1 0] # the true labels

pred_probs =
[[0.02796171 0.97203829]
 [0.89682444 0.10317556]
 [0.50104129 0.49895871]
 [0.13713222 0.86286778]
 [0.95707434 0.04292566]] # predicted probabilities show the model's confidence

y_pred = [1 0 0 1 0] # predicted class
```

- pred_probs
  - first column is the probability that the point belongs to class 0
  - second column is the probability that the point belings to class 1
  - the rows sum to 1
- y_pred
  - 0 if class 0 probability is equal or larger than 50% (or equivalently if class 1 probability is less than 50%)
  - 1 if class 0 probability is less than 50% (or equivalently of class 1 probability is equal or larger than 50%)

How to transform predicted probabilities to predicted class?

In [1]:
```python
import numpy as np
y_true = np.array([0,0,1,0,1,1,0,1,0,1]) # the true classification label
s of the dataset
# pred_probs_class1 is the second column of pred_probs
pred_probs_class1 = np.array([0.3, 0.7,  0.55, 0.12, 0.45, 0.89, 0.41,
0.02, 0.29, 0.85])
p_crit =  0.5

# If predicted probability is < p_crit (by default 0.5), predicted class
is 0, otherwise it is 1.
y_pred = np.zeros(len(pred_probs_class1),dtype=int)
y_pred[pred_probs_class1 < p_crit] = 0
y_pred[pred_probs_class1 >= p_crit] = 1

print(y_true)
print(y_pred) # the predicted classification labels
```

```
[0 0 1 0 1 1 0 1 0 1]
[0 1 1 0 0 1 0 0 0 1]
```

For now, we focus on evaluation metrics applicable to predicted classes!

We work with y_true and y_pred arrays.

We will work with metrics applicable to pred_probs in module 2 and regression metrics in module 3.

The confusion matrix

```
y_true = [0, 0, 1, 0, 1, 1, 0, 1, 0, 1] # the true classification labels of the dataset
```

```
y_pred = [0, 1, 1, 0, 0, 1, 0, 0, 0, 1] # the predicted classification labels
```

Let's count how many points we have in four categories:

- true label is 0, predicted label is 0 - **True Negatives**
- true label is 1, predicted label is 1 - **True Positives**
- true label is 0, predicted label is 1 - **False Positive**
- true label is 1, predicted label is 0 - **False Negative**

Generally, the confusion matrix C is such that $C_{i,j}$ is equal to the number of observations known to be in group i but predicted to be in group j.

Back to our example:

```
y_true = [0, 0, 1, 0, 1, 1, 0, 1, 0, 1] # the true classification labels of the dataset
```

```
y_pred = [0, 1, 1, 0, 0, 1, 0, 0, 0, 1] # the predicted classification labels
```

			Predicted class
		Predicted Negative (0)	Predicted Positive (1)
Actual class	Condition Negative (0)	**True Negative (TN): 4**	**False Positive (FP): 1**
	Condition Positive (1)	**False Negative (FN): 2**	**True Positive (TP): 3**

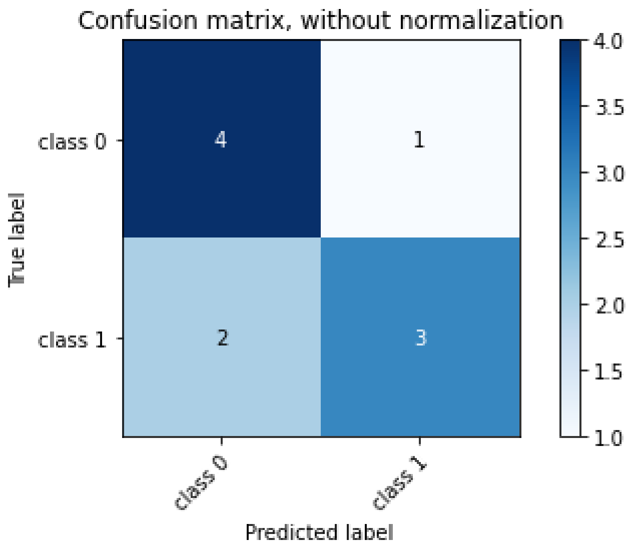
In sklearn

```
In [2]: from sklearn.metrics import confusion_matrix

        y_true = [0,0,1,0,1,1,0,1,0,1]
        y_pred = [0,1,1,0,0,1,0,0,0,1]
        print(confusion_matrix(y_true,y_pred))
```

```
[[4 1]
 [2 3]]
```

In [3]:
```
# https://scikit-learn.org/stable/modules/generated/sklearn.metrics.plot
_confusion_matrix.html
# the function above requires a trained classifier, a feature matrix, an
d a true target variable
# the function below in this cell requires the true and predicted target
variable
import numpy as np
import matplotlib.pyplot as plt
from sklearn.utils.multiclass import unique_labels

def plot_confusion_matrix(y_true, y_pred, classes,
                          normalize=False,
                          title=None,
                          cmap=plt.cm.Blues):
    """
    This function prints and plots the confusion matrix.
    Normalization can be applied by setting `normalize=True`.
    """
    if not title:
        if normalize:
            title = 'Normalized confusion matrix'
        else:
            title = 'Confusion matrix, without normalization'

    # Compute confusion matrix
    cm = confusion_matrix(y_true, y_pred)
    # Only use the labels that appear in the data
    classes = np.array(classes)
    classes = classes[unique_labels(y_true, y_pred)]
    if normalize:
        cm = cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]

    fig, ax = plt.subplots()
    im = ax.imshow(cm, interpolation='nearest', cmap=cmap)
    ax.figure.colorbar(im, ax=ax)
    # We want to show all ticks...
    ax.set(xticks=np.arange(cm.shape[1]),
           yticks=np.arange(cm.shape[0]),
           # ... and label them with the respective list entries
           xticklabels=classes, yticklabels=classes,
           title=title,
           ylabel='True label',
           xlabel='Predicted label')

    # Rotate the tick labels and set their alignment.
    plt.setp(ax.get_xticklabels(), rotation=45, ha="right",
             rotation_mode="anchor")

    # Loop over data dimensions and create text annotations.
    fmt = '.2f' if normalize else 'd'
    thresh = cm.max() / 2.
    for i in range(cm.shape[0]):
        for j in range(cm.shape[1]):
            ax.text(j, i, format(cm[i, j], fmt),
                    ha="center", va="center",
                    color="white" if cm[i, j] > thresh else "black")
    fig.tight_layout()
    return ax
```

In [4]:
```
plot_confusion_matrix(y_true,y_pred,classes=['class 0','class 1'])
plt.show()
```



Metrics derived from C

C contains $n_{classes}^2$ elements but we need a single number metric to easily compare various models.

For two classes:

		Predicted class	
		Predicted Negative (0)	Predicted Positive (1)
Actual class	Condition Negative (0)	**True Negative (TN)**	**False Positive (FP)**
	Condition Positive (1)	**False Negative (FN)**	**True Positive (TP)**

Some single number metrics derived from C:

- accuracy: fraction of data points correctly classified
  - $a = \sum_i C_{i,i} / \sum C$ = (TP + TN) / (TP + TN + FP + FN)
- recall: what fraction of the condition positive samples are true positives?
  - it measures the ability of the classifier to identify all positive samples
  - in binary classification: R = TP / (TP + FN)
- precision: what fraction of the predicted positive points are true positives?
  - it measures the ability of the classifier to not predict a negative sample to be positive
  - in binary classification: P = TP / (TP + FP)

		Predicted class	
		Predicted Negative (0)	Predicted Positive (1)
Actual class	Condition Negative (0)	**True Negative (TN)**	**False Positive (FP)**
	Condition Positive (1)	**False Negative (FN)**	**True Positive (TP)**

A = (TP + TN) / (TP + TN + FP + FN)

R = TP / (TP + FN) = TP / CP

P = TP / (TP + FP) = TP / PP

The f_beta score

Weighted harmonic mean of P and R:

$$f_\beta = (1 + \beta^2)\frac{PR}{\beta^2 P + R}$$

If $\beta = 1$, we have the f1 score:

$$f_1 = 2\frac{PR}{P + R}$$

If $\beta < 1$, more weight to precision.

If $\beta > 1$, more weight to recall.

The scores are a function of p_crit

In [5]:
```
from sklearn.metrics import precision_score, recall_score, accuracy_scor
e, fbeta_score

y_true = np.array([0,0,1,0,1,1,0,1,0,1]) # the true classification label
s of the dataset
y_pred_proba = np.array([0.3, 0.7,  0.55, 0.12, 0.45, 0.89, 0.41, 0.02,
0.29, 0.85])

p_crit = 0.5

y_pred = np.zeros(len(y_pred_proba),dtype=int)
y_pred[y_pred_proba < p_crit] = 0
y_pred[y_pred_proba >= p_crit] = 1

print(y_true)
print(y_pred) # the predicted classification labels
print('accuracy',accuracy_score(y_true,y_pred))
print('recall',recall_score(y_true,y_pred))
print('precision',precision_score(y_true,y_pred))
print('f1',fbeta_score(y_true,y_pred,1))
```

```
[0 0 1 0 1 1 0 1 0 1]
[0 1 1 0 0 1 0 0 0 1]
accuracy 0.7
recall 0.6
precision 0.75
f1 0.6666666666666665

/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.7/site-packages/sk
learn/utils/validation.py:71: FutureWarning: Pass beta=1 as keyword arg
s. From version 0.25 passing these as positional arguments will result
in an error
  FutureWarning)
```

Why and how to calculate a baseline score?

- if you calculate a model's score, it is meaningless without a baseline
  - if a binary classification model has 90% accuracy, is that good or bad? what does it mean that the accuracy is 90%?
  - if the problem is balanced (class 0 and class 1 both contain roughly 50% of the points), 90% is good.
  - if the problem is imbalanced (99% of points belong to class 0), 90% is bad.
- a baseline is a score calculated based on the statistical properties of the true target variable
- we will cover the baseline accuracy and the baseline f1 score
- you need to work out the baseline of other scores on 'pen and paper' similarly

Baseline accuracy

- the most accurate predictions you can make if you only use the target variable (no features, no ML model) is to predict that all points belong to the most populous class
- calculate what fraction of points belong to each class in your set
- the largest fraction is your baseline score
- example:
    - let's assume 70% of points belong to class 0 and 30% of points belong to class 1
        - if you predict class 0 for all points, you will be accurate 70% of the time
        - the baseline is 0.7
    - let's assume 10% of points belong to class 0, 30% of points belong to class 1, 40% of points belong to class 2, and 20% of points belong to class 3
        - if you predict class 2 for each point, you will be accurate 40% of the time
        - the baseline is 0.4

Baseline f1 score

- Let's assume n_0 points are in class 0 and $n_1 = n - n_0$ points are in class 1 where n is the number of points in your dataset
- a little cheat sheet:

P = TP / (TP + FP) = TP / PP

R = TP / (TP + FN) = TP / CP

F1 = 2PR/(P+R)

- if all points are predicted to be class 0, fp = tp = 0 and precision is undefined (0/0), the f1 score cannot be calculated
- the good way to go is to predict all points to be class 1
- then tp = n1/n, fp = n0/n, fn = 0. Let's add these to the equations of P and R:

P = n1/n / (n1/n + n0/n) = n1 / (n1 + n0) = n1/n

R = n1/n / (n1/n + 0) = 1

- finally, the F1 score becomes

F1 = (2 n1/n * 1) / (n1/n + 1) = 2 P / (P + 1)

Notes on the baseline score

- it can be a bit involved to calculate it for certain evaulation metrics
- it is definitely worth it though
    - you'll gain a deeper understanding of the metric and your dataset
- once you choose an evaluation metric, calculate the baseline even before you train the first ML model

Module 2: Working with predicted probabilities in classification

Learning objectives of this module:

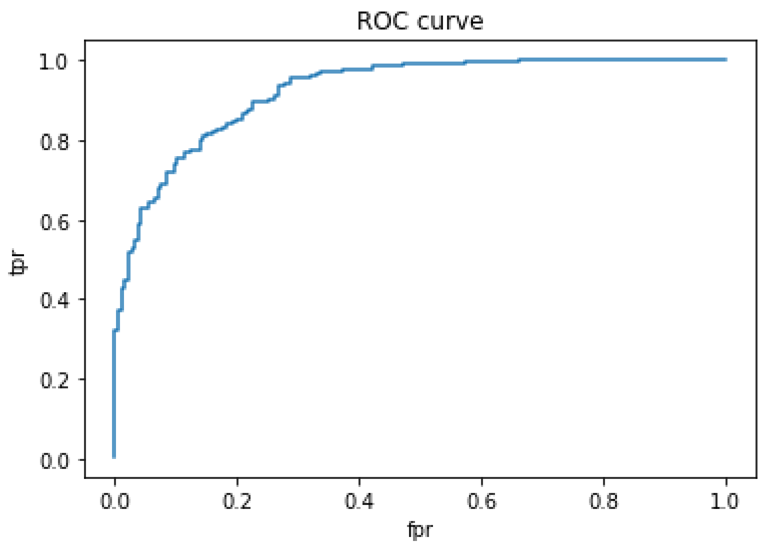
- Summarize what the ROC and precision-recall curves and AUC are
- Review the logloss metric and its properties
- Calculate the value of each metric given a set’s target variable and predictions from an ML model
- Calculate the baseline of each metric given a set’s target variable
- Choose an appropriate evaluation metric given your ML problem

The ROC curve

- Receiver Operating Characteristic
    - x axis: false positive rate (fpr = FP / (FP + TN))
    - y axis: true positive rate (R = TP / (TP + FN))
    - the curve shows fpr and R value pairs for various class 1 critical probabilities
- upper left corner: perfect predictor
- diagonal point: chance level predictions
- lower right corner: worst predictor

In [6]:
```
import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
from sklearn.metrics import confusion_matrix
df = pd.read_csv('data/true_labels_pred_probs.csv')

y_true = df['y_true']
pred_prob_class1 = df['pred_prob_class1']

fpr = np.zeros(len(y_true))
tpr = np.zeros(len(y_true))

p_crits = np.sort(pred_prob_class1) # the sorted predicted probabilities
serve as critical probabilities

for i in range(len(p_crits)):
    p_crit = p_crits[i]

    y_pred = np.zeros(len(y_true))
    y_pred[pred_prob_class1 < p_crit] = 0
    y_pred[pred_prob_class1 >= p_crit] = 1

    C = confusion_matrix(y_true,y_pred)

    tpr[i] = C[1,1]/(C[1,0]+C[1,1])
    fpr[i] = C[0,1]/(C[0,0]+C[0,1])

# from sklearn.metrics import roc_curve
# # the roc_curve function performs the same calculation
# fpr,tpr,p_crits = roc_curve(y_true,pred_prob_class1)
```

In [7]:
```
plt.plot(fpr,tpr)
plt.xlabel('fpr')
plt.ylabel('tpr')
plt.title('ROC curve')
plt.show()
```



ROC AUC

- ROC is useful but it is not a single number metric
  - it cannot be directly used to compare various classification models
- summary statistics based on the ROC curve (for a complete list, see here (https://en.wikipedia.org/wiki/Receiver_operating_characteristic#Further_interpretations))
- most commonly used metric is ROC AUC - ROC Area Under the Curve
  - AUC = 1 is a perfect classifier
  - AUC > 0.5 is above chance-level predictor
  - AUC = 0.5 is a chance-level classifier - the baseline!
  - AUC < 0.5 is a bad predictor
  - AUC = 0 classifies all points incorrectly

In [8]:
```
from sklearn.metrics import roc_auc_score
print(roc_auc_score(y_true,pred_prob_class1))
```

```
0.9236524315231854
```

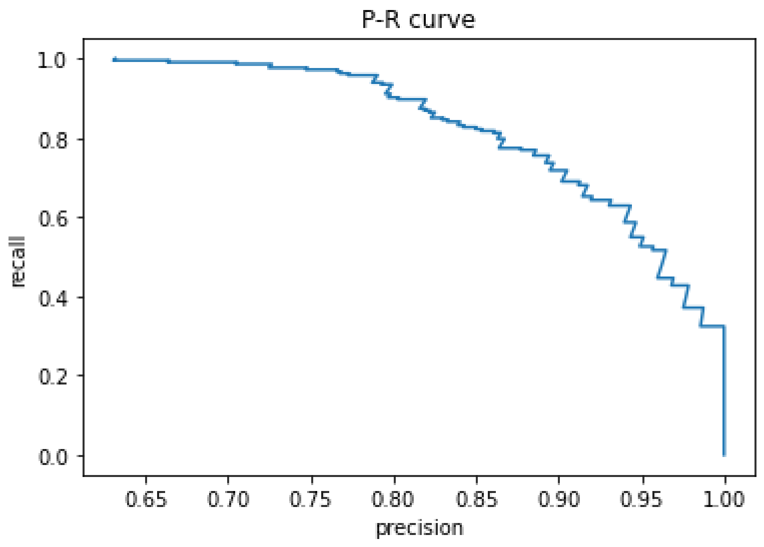
Precision-recall curve

- the drawback of ROC is that it uses TN, not good for imbalanced problems.
- the precision-recall curve doesn't use TN, ideal for imbalanced problems.

In [9]:
```
from sklearn.metrics import precision_recall_curve
from sklearn.metrics import average_precision_score # the AUC of the P-R
curve

p,r,p_crits = precision_recall_curve(y_true,pred_prob_class1)

print(average_precision_score(y_true,pred_prob_class1))
```

```
0.9315588971251673
```

```
In [10]: plt.plot(p,r)
         plt.xlabel('precision')
         plt.ylabel('recall')
         plt.title('P-R curve')
         plt.show()
```



The logloss metric

$$logloss = -\frac{1}{N} \sum(y_{true} \ln(p_{pred}) + (1 - y_{true})(1 - \ln(1 - p_{pred})))$$

- p_{pred} is the predicted probability of the **positive class**
- the predicted probabilities are not converted into predicted classes
- excellent choice if you need accurate probabilities (e.g., when it is expensive/costly to act due to limited resources so you need to rank your points based on probabilities)
- two scenarios:
  - y_true = 0 - left term disappears
  - y_true = 1 - right term disappears
- log(0) is undefined
  - p_{pred} is replaced with $\max(\min(p, 1 - 10^{-15}), 10^{-15})$ to avoid this issue

The extreme cases

- the classifier is confidently wrong
  - $p_{pred} = 10^{-15}$ for points in class 1
  - $p_{pred} = 1 - 10^{-15}$ for points in class 0

$$logloss = -\frac{1}{N}\sum \ln(10^{-15}) = -\ln(10^{-15})$$
$$logloss \sim 34.5$$

- the classifier is correct
  - $p_{pred} = 10^{-15}$ for points in class 0
  - $p_{pred} = 1 - 10^{-15}$ for points in class 1

$$logloss = -\frac{1}{N}\sum(1-0)(1-\ln(1-10^{-15})) = 10^{-15} \text{ for class 0}$$
$$logloss = -\frac{1}{N}\sum 1 * \ln(1-10^{-15}) = 10^{-15} \text{ for class 1}$$
$$logloss \sim 0$$

In [11]:
```
from sklearn.metrics import log_loss
print(log_loss(y_true,pred_prob_class1))
help(log_loss)
```

```
0.35015190545328556
Help on function log_loss in module sklearn.metrics._classification:

log_loss(y_true, y_pred, *, eps=1e-15, normalize=True, sample_weight=No
ne, labels=None)
    Log loss, aka logistic loss or cross-entropy loss.

    This is the loss function used in (multinomial) logistic regression
    and extensions of it such as neural networks, defined as the negati
ve
    log-likelihood of a logistic model that returns ``y_pred`` probabil
ities
    for its training data ``y_true``.
    The log loss is only defined for two or more labels.
    For a single sample with true label yt in {0,1} and
    estimated probability yp that yt = 1, the log loss is

        -log P(yt|yp) = -(yt log(yp) + (1 - yt) log(1 - yp))

    Read more in the :ref:`User Guide <log_loss>`.

    Parameters
    ----------
    y_true : array-like or label indicator matrix
        Ground truth (correct) labels for n_samples samples.

    y_pred : array-like of float, shape = (n_samples, n_classes) or (n_
samples,)
        Predicted probabilities, as returned by a classifier's
        predict_proba method. If ``y_pred.shape = (n_samples,)``
        the probabilities provided are assumed to be that of the
        positive class. The labels in ``y_pred`` are assumed to be
        ordered alphabetically, as done by
        :class:`preprocessing.LabelBinarizer`.

    eps : float
        Log loss is undefined for p=0 or p=1, so probabilities are
        clipped to max(eps, min(1 - eps, p)).

    normalize : bool, optional (default=True)
        If true, return the mean loss per sample.
        Otherwise, return the sum of the per-sample losses.

    sample_weight : array-like of shape (n_samples,), default=None
        Sample weights.

    labels : array-like, optional (default=None)
        If not provided, labels will be inferred from y_true. If ``labe
ls``
        is ``None`` and ``y_pred`` has shape (n_samples,) the labels ar
e
        assumed to be binary and are inferred from ``y_true``.

        .. versionadded:: 0.18

    Returns
    -------
```

```
        loss : float

        Examples
        --------
        >>> from sklearn.metrics import log_loss
        >>> log_loss(["spam", "ham", "ham", "spam"],
        ...          [[.1, .9], [.9, .1], [.8, .2], [.35, .65]])
        0.21616...

        References
        ----------
        C.M. Bishop (2006). Pattern Recognition and Machine Learning. Sprin
    ger,
        p. 209.

        Notes
        -----
        The logarithm used is the natural logarithm (base-e).
```

How should you choose a metric?

- What are the terms in the confusion matrix that you most (or least) care about?
    - In an imbalanced dataset, TNs are large so you should use a metric that doesn't include TN
    - no accuracy
    - f score is usually preferred if your dataset is imbalanced
- Will we act (intervene/apply treatment) on the model's prediction?
    - Is it cheap to act? (e.g., mass email)
        - we want to capture the largest fraction of the condition positive samples even if FPs will be large as a result
        - recall or fbeta with beta > 1 (f1.5 or f2 are often used)
    - Is it expensive to act? Do we have limited resources? Or treatment/action is costly?
        - we want to make sure that the resources are allocated the best way possible
        - want to make sure that a large fraction of the predicted positives are true positives
        - precision or fbeta with beta < 1 (f0.5 is often used)

Module 3: Regression metrics

Learning objectives of this module:

- Outline metrics often used in regression (MSE, RMSE, MAE, R2 score)
- Calculate the value of each metric given a set’s target variable and predictions from an ML model
- Calculate the baseline of each metric given a set’s target variable
- Choose an appropriate evaluation metric given your ML problem

Regression metrics

- the target variable is continuous
- the predicted values are also continuous
- regression metrics measure some type of difference between y (true values) and y' (predicted values)

Mean Squared Error

$$MSE(y, y') = \frac{1}{n} \sum_{i=1}^{n} (y_i - y_i')^2$$

The unit of MSE is not the same as the target variable.

Root Mean Square Error

$$RMSE(y, y') = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - y_i')^2}$$

Mean Absolute Error

$$MAE(y, y') = \frac{1}{n} \sum_{i=1}^{n} |y_i - y_i'|$$

Both RMSE and MAE have the same unit as the target variable.

R2 score - coefficient of determination

$$R^2(y, y') = 1 - \frac{\sum_{i=1}^{n} (y_i - y_i')^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2},$$

where $\bar{y}$ is the mean of y.

- R2 = 1 is the perfect regression model ($y == y'$)
- R2 = 0 is as good as a constant model that always predicts the expected value of y ($\bar{y}$) - the baseline
- R2 < 0 is a bad regression model

R2 is dimensionless.

In [12]:
```
from sklearn.metrics import mean_squared_error
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import r2_score
```

- RMSE is not implemented in sklearn, but you can calculate it as `np.sqrt(mean_squared_error(y_true,y_pred))` or `mean_squared_error(y_true,y_pred, squared = False)`
- you can find more on regression metrics here (https://scikit-learn.org/stable/modules/model_evaluation.html#regression-metrics)

The baseline of regression metrics

- replace y' with $\bar{y}$
- the MSE baseline is the variance of the target variable
- the RMSE baseline is the standard deviation of the target variable
- the MAE baseline is the average abolsute deviation of the target variable
- the R2 baseline is 0

How to choose a regression metric?

- as far as I know, the choice has little to no impact on the overall performance of the ML model
- personally I usually use either R2 or RMSE

In [ ]:
```

```