Mudcard

- **We discussed about feature engineering in this class. In a problem like household power consumption prediction, we might wanna incorporate outside information such as weather data in the original dataset. Is this some aspect of feature engineering?**
  - Not really. That would be brining in external data so more in the realm of merging and appending multiple datasets together.
- **I am wondering about how you choose a p_crit and if there are commonly accepted values. I am also wondering how you'd choose one with multiple classes.**
  - Most commonly p_crit = 0.5 is used but we will discuss today why and how to tune it.
- **I understand how the evaluation metric works, but are we supposed to convert our data into 1 and 0 before doing evaluation metric? I'm confused about why we only use 1 and 0 as examples in the lecture.**
  - We considered classification problems today so the target variable contained either 0s and 1s (binary classification) or 0s, 1s, 2s (multiclass classification)

Evaluation metrics in supervised ML, part 2, predicted probabilities and regression metrics

By the end of this lecture, you will be able to

- Summarize the ROC and precision-recall curves, and the logloss metric
- Describe the most commonly used regression metrics

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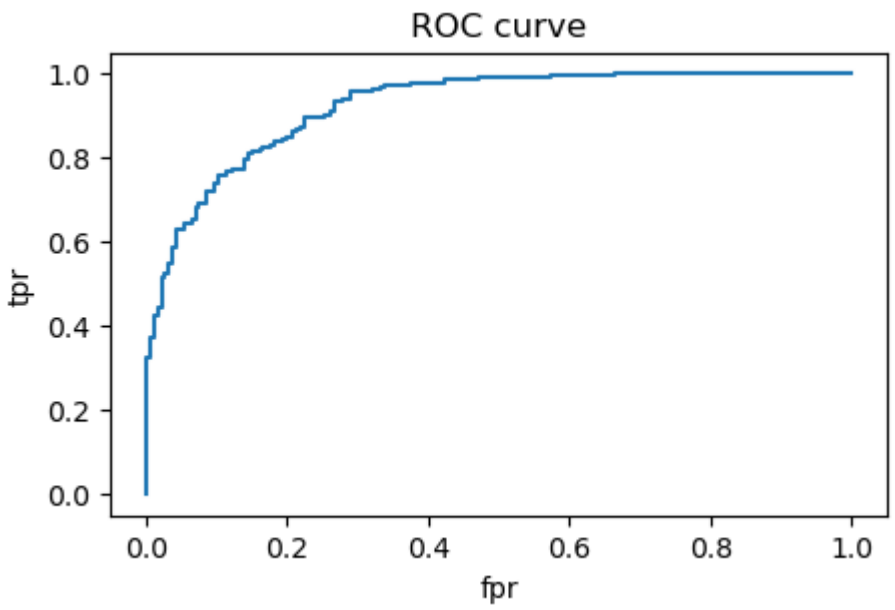
The ROC curve

- 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 [1]:
```
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']
pred_prob_class0 = df['pred_prob_class0']

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 [2]:
```
plt.figure(figsize=(5,3))
plt.plot(fpr,tpr)
```

```
plt.xlabel('fpr')
plt.ylabel('tpr')
plt.title('ROC curve')
plt.show()
```



Quiz 1

What's the (fpr,tpr) coordinate on the ROC curve if p_crit = 1?

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)
- 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
  - AUC < 0.5 is a bad predictor
  - AUC = 0 classifies all points incorrectly

In [3]:
```
from sklearn.metrics import roc_auc_score
print(roc_auc_score(y_true,pred_prob_class1))
```

```
0.9236524315231854
```

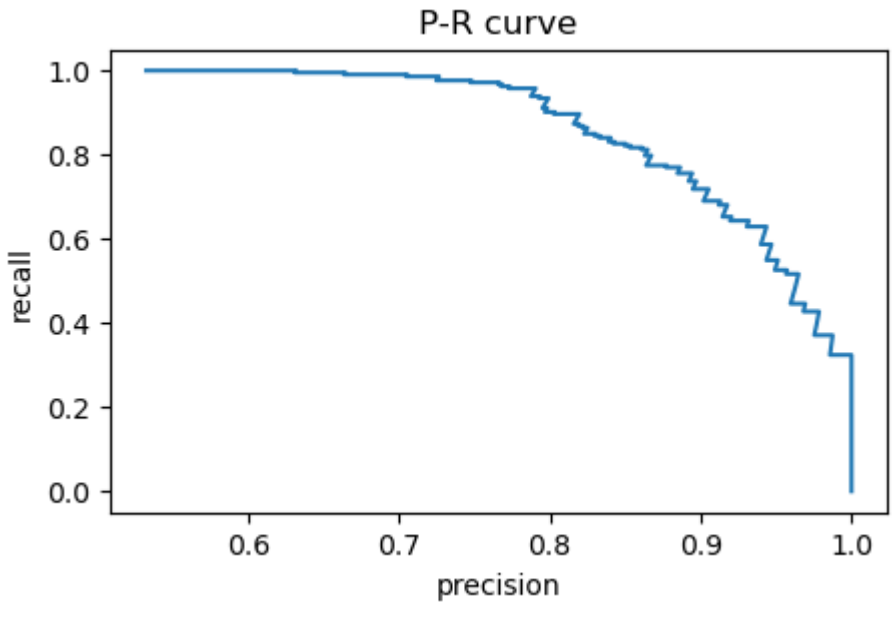
Precision-recall curve

- 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 [4]:
```
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))
```

```
0.9315588971251672
```

In [5]:
```
plt.figure(figsize=(5,3))
plt.plot(p,r)
plt.xlabel('precision')
plt.ylabel('recall')
plt.title('P-R curve')
plt.show()
```



Quiz 2

What's the (p,r) coordinate on the curve if p_crit = 0?

The logloss metric

$$logloss = -\frac{1}{m}\sum_{i=0}^{m-1}(y_{i,true}\ln(p_{i,pred}) + (1-y_{i,true})\ln(1-p_{i,pred}))$$

- 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

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

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

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

In [6]:
```
from sklearn.metrics import log_loss
print(log_loss(y_true,pred_prob_class1))
help(log_loss)
```

```
0.3501519054532857
Help on function log_loss in module sklearn.metrics._classification:

log_loss(y_true, y_pred, *, normalize=True, sample_weight=None, 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 negative
    log-likelihood of a logistic model that returns ``y_pred`` probabilities
    for its training data ``y_true``.
    The log loss is only defined for two or more labels.
    For a single sample with true label :math:`y \in \{0,1\}` and
    a probability estimate :math:`p = \operatorname{Pr}(y = 1)`, the log
    loss is:

    .. math::
        L_{\log}(y, p) = -(y \log (p) + (1 - y) \log (1 - p))

    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:`~sklearn.preprocessing.LabelBinarizer`.

        `y_pred` values are clipped to `[eps, 1-eps]` where `eps` is the machine
        precision for `y_pred`'s dtype.

    normalize : bool, 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, default=None
        If not provided, labels will be inferred from y_true. If ``labels``
        is ``None`` and ``y_pred`` has shape (n_samples,) the labels are
        assumed to be binary and are inferred from ``y_true``.

        .. versionadded:: 0.18

    Returns
    -------
    loss : float
        Log loss, aka logistic loss or cross-entropy loss.

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

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

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

Evaluation metrics in supervised ML, part 2, predicted probabilities and regression

By the end of this lecture, you will be able to

- Summarize the ROC and precision-recall curves, and the logloss metric
- **Describe the most commonly used regression metrics**

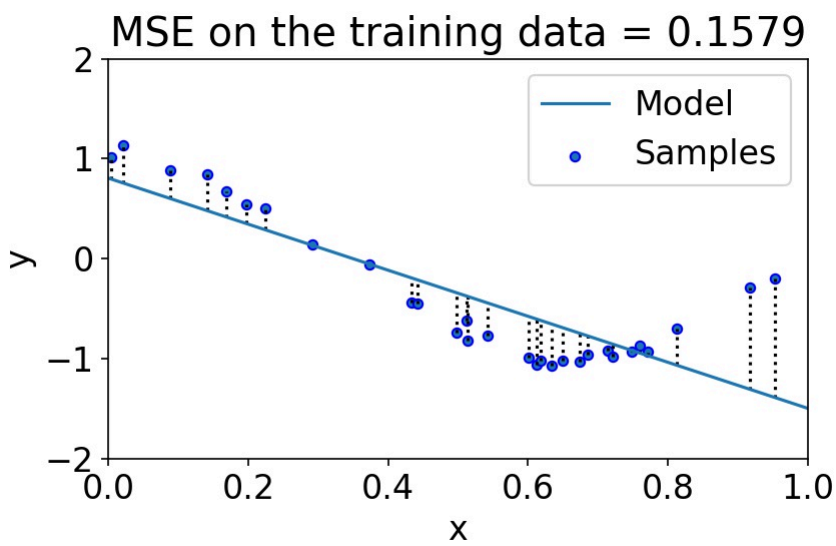
Regression metrics

- 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

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



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

Root Mean Square Error

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

Mean Absolute Error

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

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

R2 score - coefficient of determination

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

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 ($\bar{y}$)
- R2 < 0 is a bad regression model

R2 is dimensionless.

In [7]:
```
from sklearn.metrics import mean_squared_error
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import r2_score
help(mean_squared_error)
```

```
Help on function mean_squared_error in module sklearn.metrics._regression:

mean_squared_error(y_true, y_pred, *, sample_weight=None, multioutput='uniform_average', squared='deprecated')
    Mean squared error regression loss.

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

    Parameters
    ----------
    y_true : array-like of shape (n_samples,) or (n_samples, n_outputs)
        Ground truth (correct) target values.

    y_pred : array-like of shape (n_samples,) or (n_samples, n_outputs)
        Estimated target values.

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

    multioutput : {'raw_values', 'uniform_average'} or array-like of shape             (n_outputs,), default='unifor
m_average'
        Defines aggregating of multiple output values.
        Array-like value defines weights used to average errors.

        'raw_values' :
            Returns a full set of errors in case of multioutput input.

        'uniform_average' :
            Errors of all outputs are averaged with uniform weight.

    squared : bool, default=True
        If True returns MSE value, if False returns RMSE value.

        .. deprecated:: 1.4
           `squared` is deprecated in 1.4 and will be removed in 1.6.
           Use :func:`~sklearn.metrics.root_mean_squared_error`
           instead to calculate the root mean squared error.

    Returns
    -------
    loss : float or ndarray of floats
        A non-negative floating point value (the best value is 0.0), or an
        array of floating point values, one for each individual target.

    Examples
    --------
    >>> from sklearn.metrics import mean_squared_error
    >>> y_true = [3, -0.5, 2, 7]
    >>> y_pred = [2.5, 0.0, 2, 8]
    >>> mean_squared_error(y_true, y_pred)
    0.375
    >>> y_true = [[0.5, 1],[-1, 1],[7, -6]]
    >>> y_pred = [[0, 2],[-1, 2],[8, -5]]
    >>> mean_squared_error(y_true, y_pred)
    0.708...
    >>> mean_squared_error(y_true, y_pred, multioutput='raw_values')
    array([0.41666667, 1.        ])
    >>> mean_squared_error(y_true, y_pred, multioutput=[0.3, 0.7])
    0.825...
```

- RMSE is not implemented in sklearn, but you can calculate it as `np.sqrt(mean_squared_error(y_true,y_pred))`
- you can find more on regression metrics here

Quiz 3

Read in `data/reg_preds.csv`. It contains two columns:

- y_true: value of owner-occupied homes in $1000's in Boston
- y_pred: predictions of a regression model

What's the ratio between the MSE and the variance of the home values? How does this ratio relate to the R2 score?

In [ ]:

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