Mudcard

- **how is this related to the datasets that we use for our projects?**
  - you will train several ML models using your project dataset so you'll need to choose an evaluation metric
- **I'm just wondering why we don't use Pearson correlation to calculate the linear correlation. Is it positively correlated to F-test?**
  - the pearson correlation coefficient can only be calculated between two continuous variables
  - if your target variable or the feature is categorical, it shouldn't be used
  - the f test is more general
- **how do we determine p_critical?**
  - you will see in the next problem set
  - you choose an evaluation metric (e.g., accuracy), you loop through various p_crit values, and you select the p_crit which maximizes accuracy
- **"When using a real dataset in and trying to find the best evaluation metric through the confusion matrix, how to we find the y_pred that was utilized throughout the python coding? In the examples in class, the y_pred was provided but I am not sure how to do that in real data examples.**
  - after you train an ML model, you can use it to generate predictions
  - we will put together our first ML pipeline in a week and I hope everything we covered so far will fall into place then
- **what is imbalanced dataset?**
  - a classification dataset in which most of the data points belong to one class
  - e.g., fraud detection in credit card transactions is imbalanced because 99.9% of transactions are not fraudulant, and only 0.1% of transactions are

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

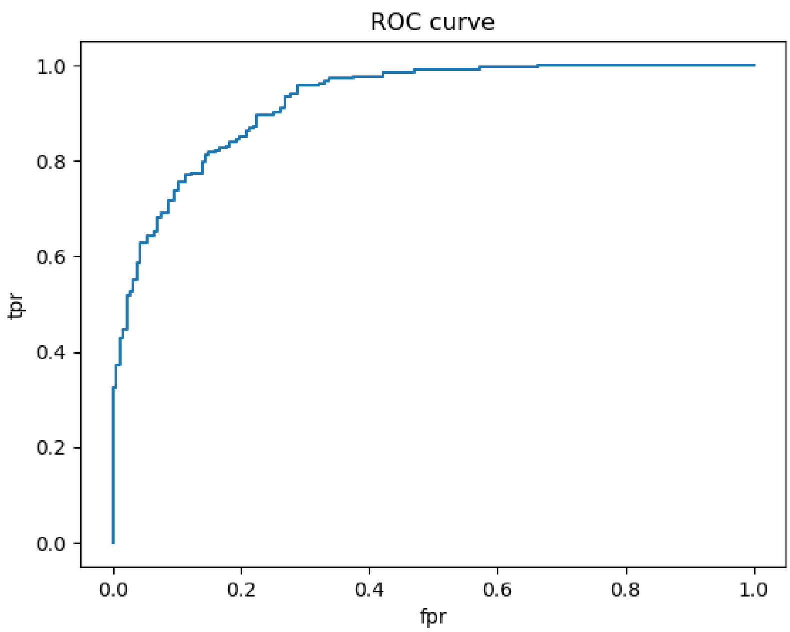
- Receiver Operating Characteristic
  - x axis: false positive rate (fpr = FP / (FP + TN))
  - y axis: true positive rate (R = TP / (TP + FN))
  - the curve shows fpr and R value pairs for various class 1 critical probabilities
- upper left corner: perfect predictor
- diagonal point: chance level predictions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

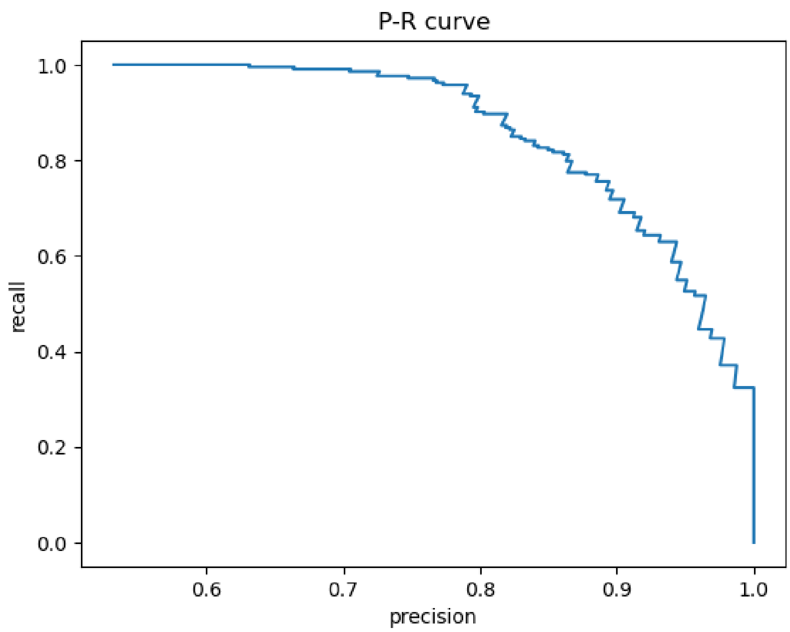
Precision-recall curve

- 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.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

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

- 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 [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, *, eps='auto', 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:`preprocessing.LabelBinarizer`.

    eps : float or "auto", default="auto"
        Log loss is undefined for p=0 or p=1, so probabilities are
        clipped to `max(eps, min(1 - eps, p))`. The default will depend on the
        data type of `y_pred` and is set to `np.finfo(y_pred.dtype).eps`.

        .. versionadded:: 1.2

        .. versionchanged:: 1.2
           The default value changed from `1e-15` to `"auto"` that is
           equivalent to `np.finfo(y_pred.dtype).eps`.

        .. deprecated:: 1.3
           `eps` is deprecated in 1.3 and will be removed in 1.5.

    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

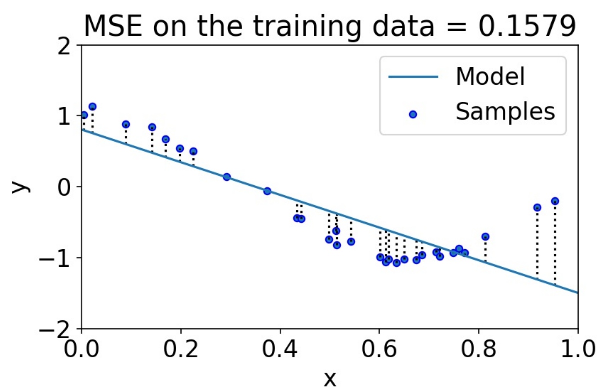
- Summarize the ROC and precision-recall curves, and the logloss metric
- **Describe the most commonly used regression metrics**

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

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



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 ($\bar{y}$)
- 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
```

- 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 [ ]:
```

Mudcard