Lecture 20 -- Model Evaluation

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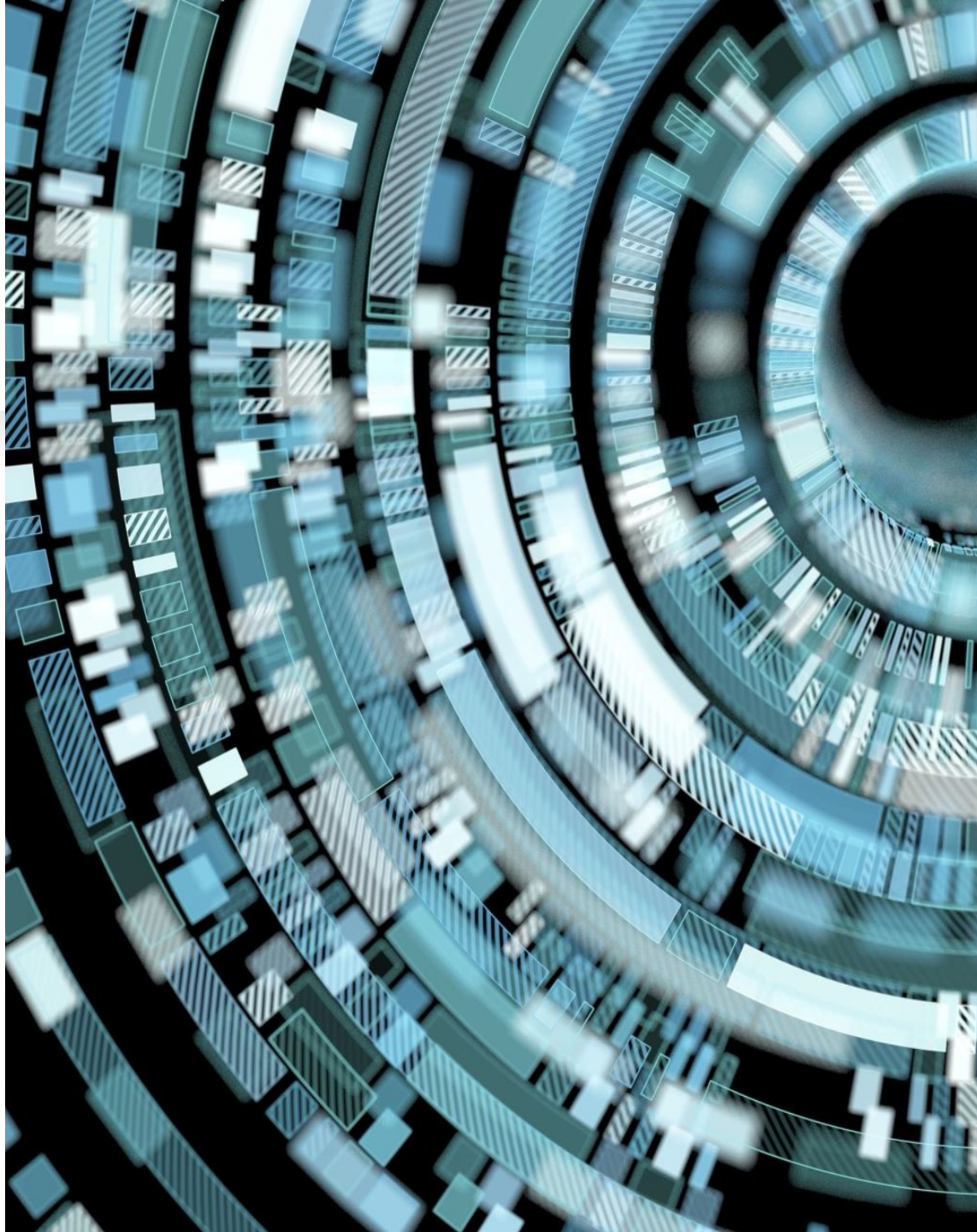
Up to now,

- Four traditional machine learning algorithms
- Adversarial attack and defence
- Deep learning
  - Introduction to Deep Learning
  - Functional view and features
  - Backward and forward computation
  - CNNs



Today's Topics

- Test sets revisited
- Learning curves

Accuracy

- Multiple training/test partitions
  - Stratified sampling
  - Cross validation

How about when data is not large enough?

- Confusion matrices
  - TP, FP, TN, FN

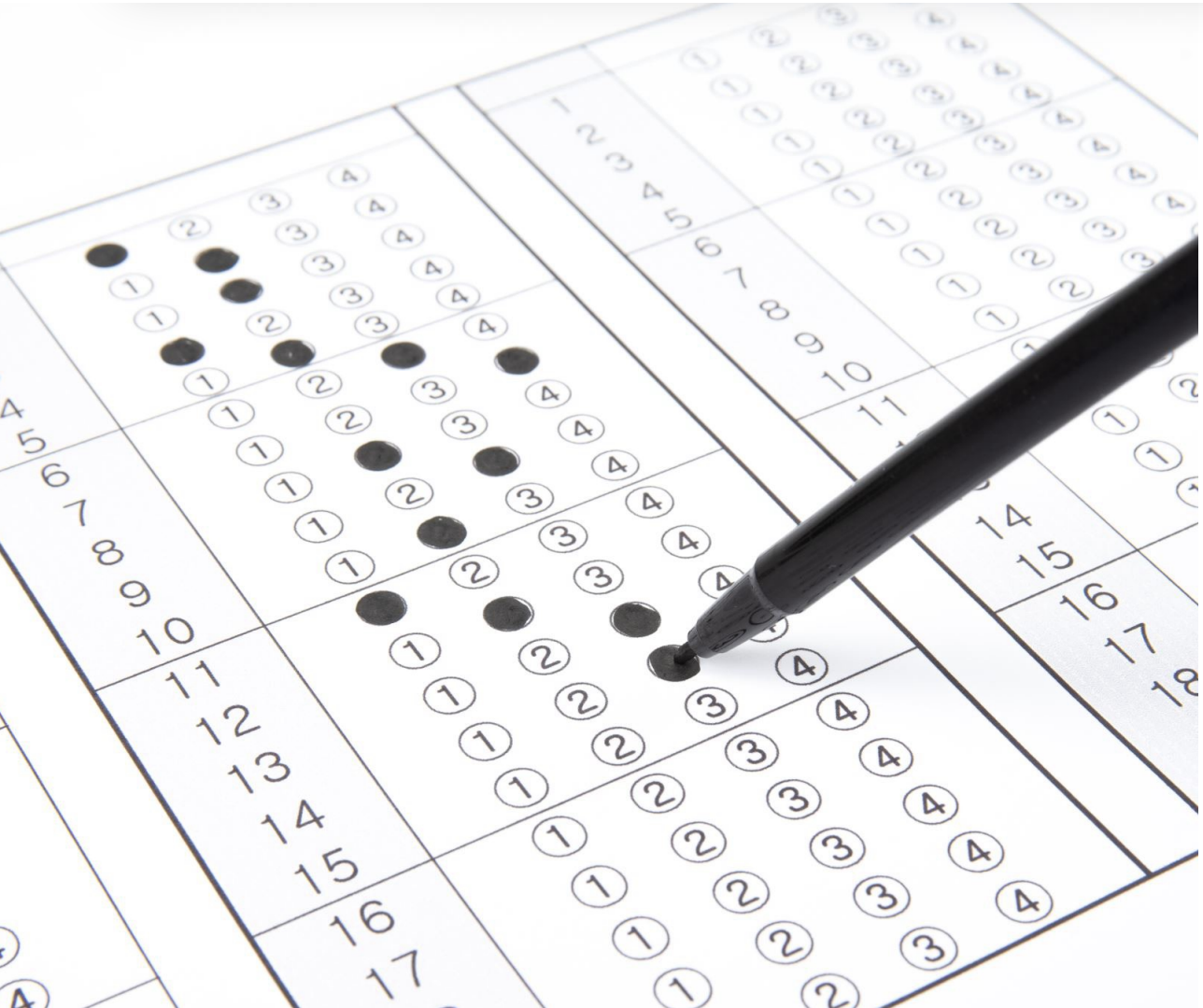
Going beyond a single accuracy

- ROC curves

Closer look at one class

- PR curves

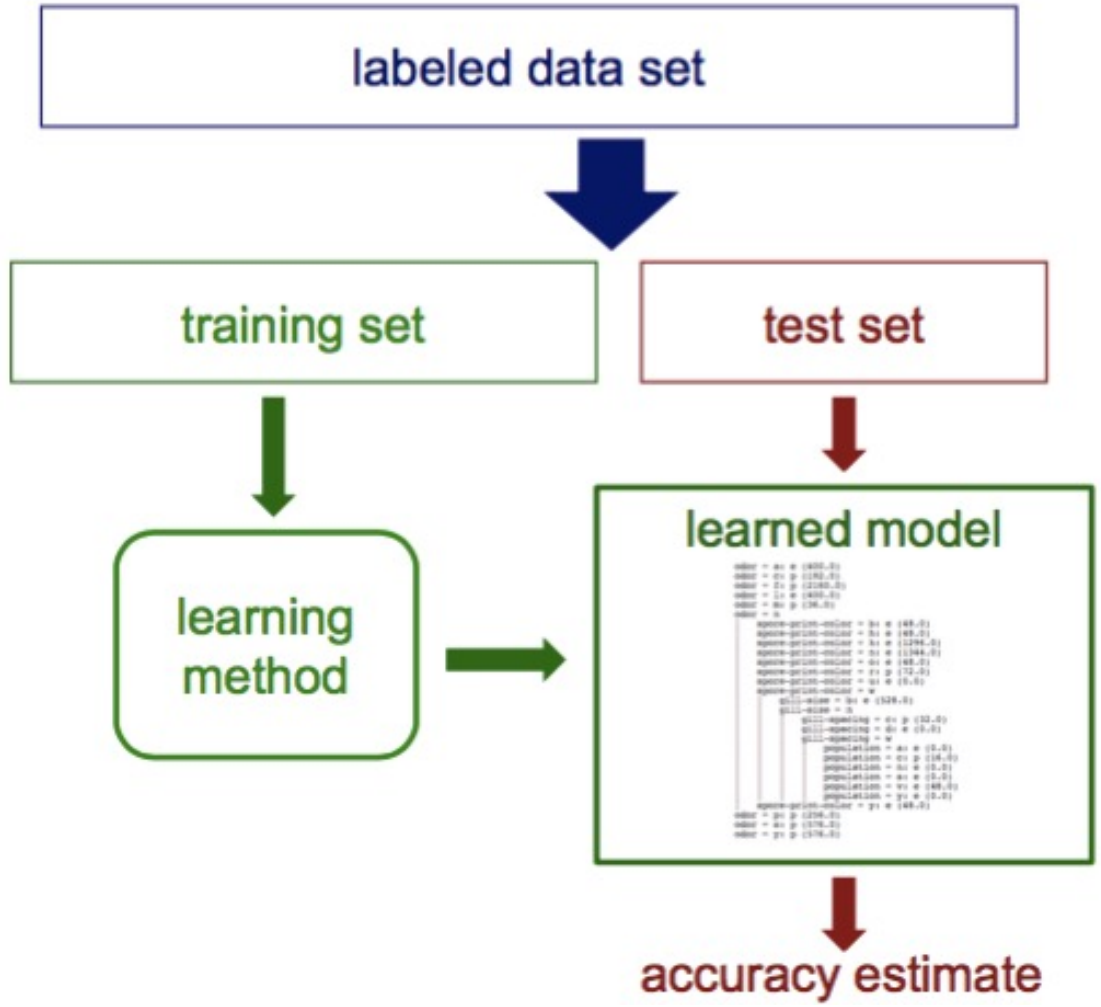
What if the one class is an unbalanced class



Test sets revisited

Test sets revisited

- How can we get an unbiased estimate of the accuracy of a learned model?



Test sets revisited

- How can we get an unbiased estimate of the accuracy of a learned model?
  - when learning a model, you should pretend that you don't have the test data yet (it is "in the mail")* during training
  - if the test-set labels influence the learned model in any way, accuracy estimates will be biased

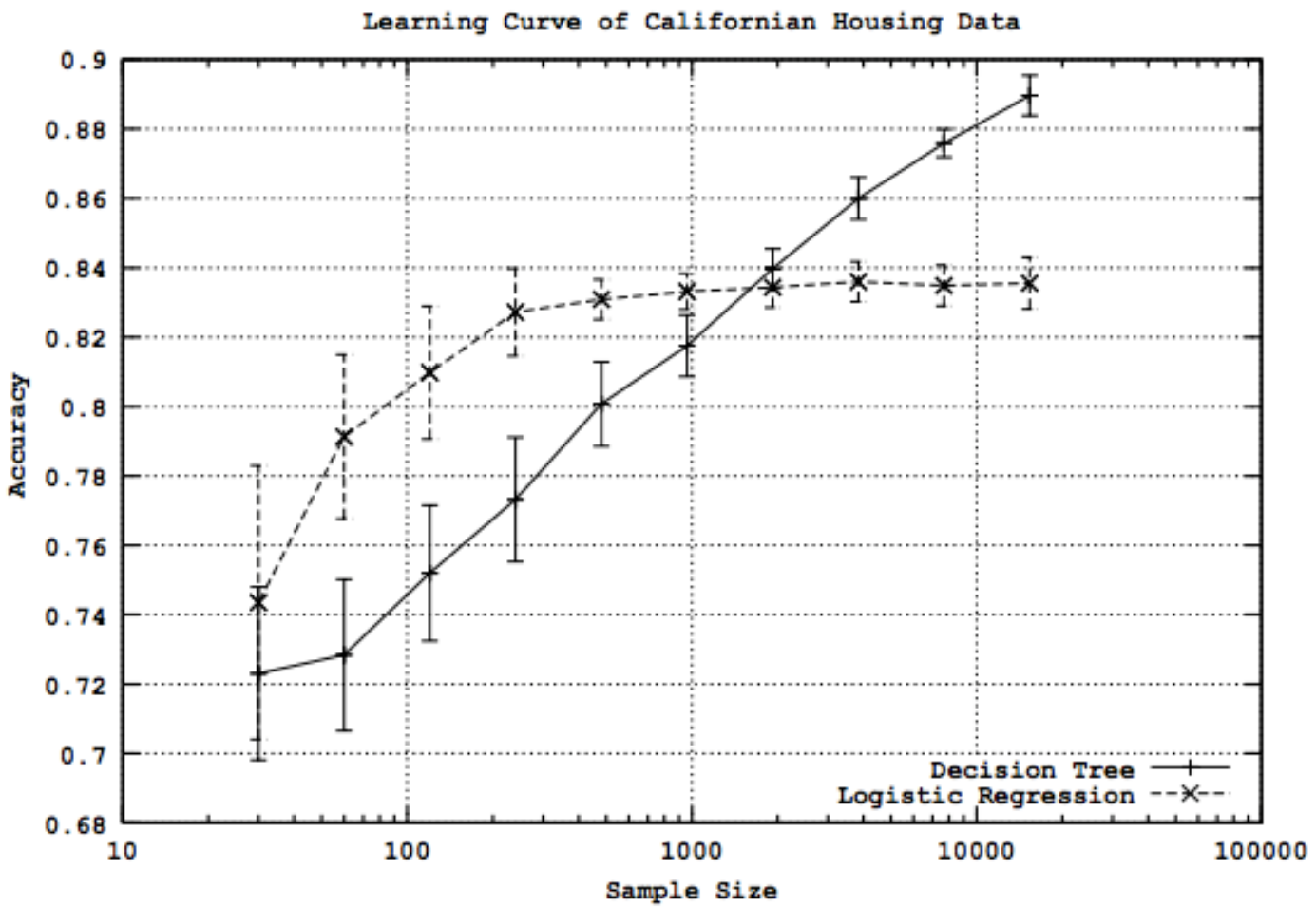
* In some applications it is reasonable to assume that you have access to the feature vector (i.e. x) but not the labelling (i.e., y) part of each test instance.

Semi-supervised learning

Learning Curve

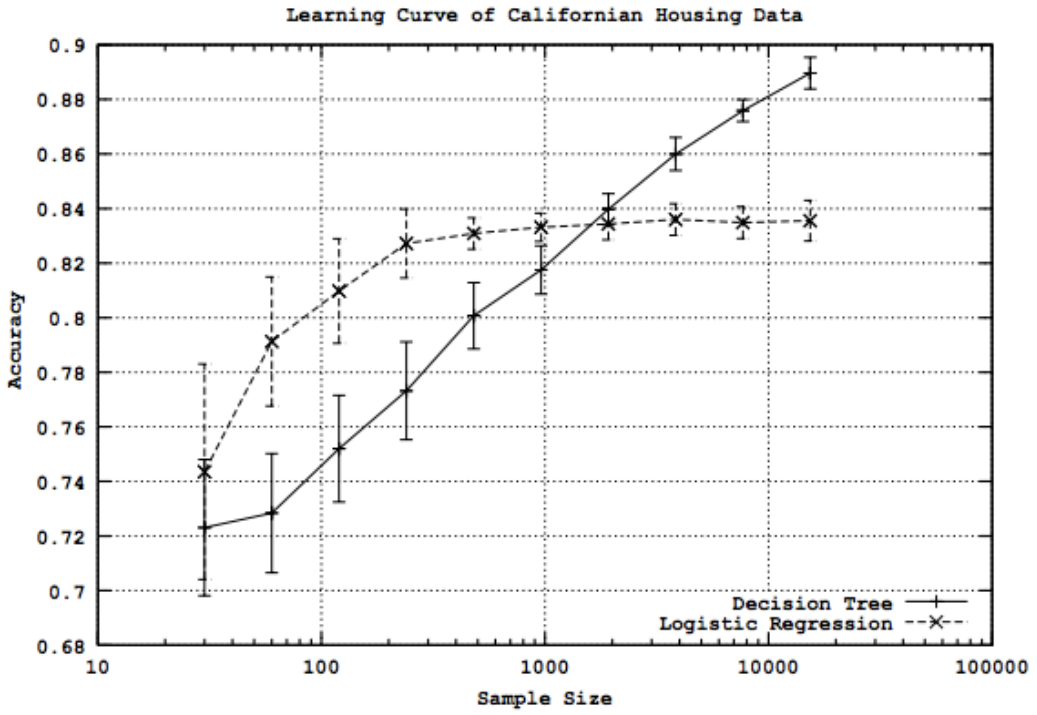
Learning curves

- How does the accuracy of a learning method change as a function of the training-set size?
  - this can be assessed by plotting *learning curves*



Learning curves

- given training/test set partition
  - for each sample size s on learning curve
    - repeat n times
      - randomly select s instances from training set
      - learn model
      - evaluate model on test set to determine accuracy a
    - plot (s, avg. accuracy and error bars)



multiple training/test partitions

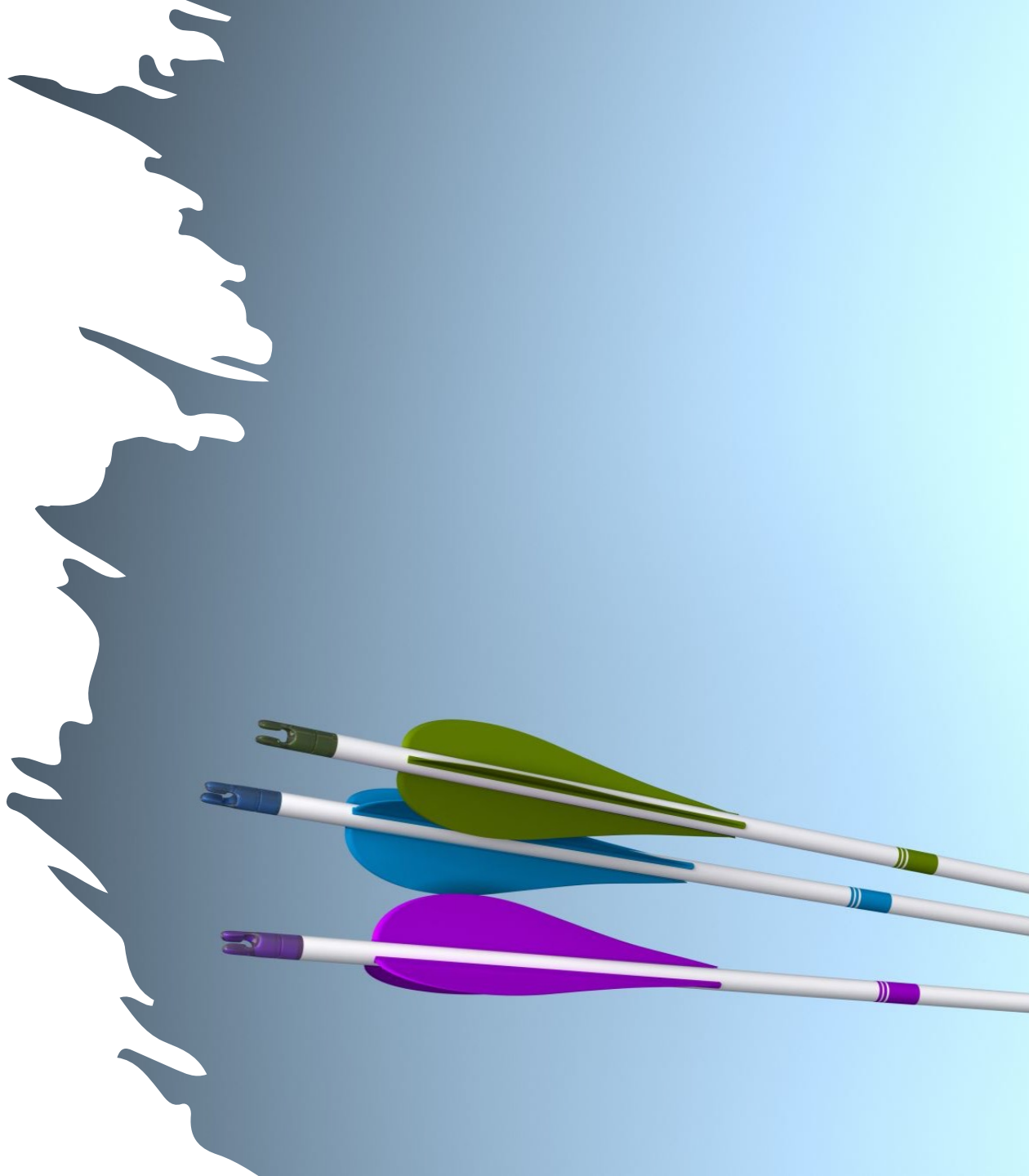
Limitations of using a single training/test partition

- we may not have enough data to make sufficiently large training and test sets
  - a larger test set gives us more reliable estimate of accuracy (i.e. a lower variance estimate)
  - but... a larger training set will be more representative of how much data we actually have for learning process

- a single training set doesn't tell us how sensitive accuracy is to a particular training sample

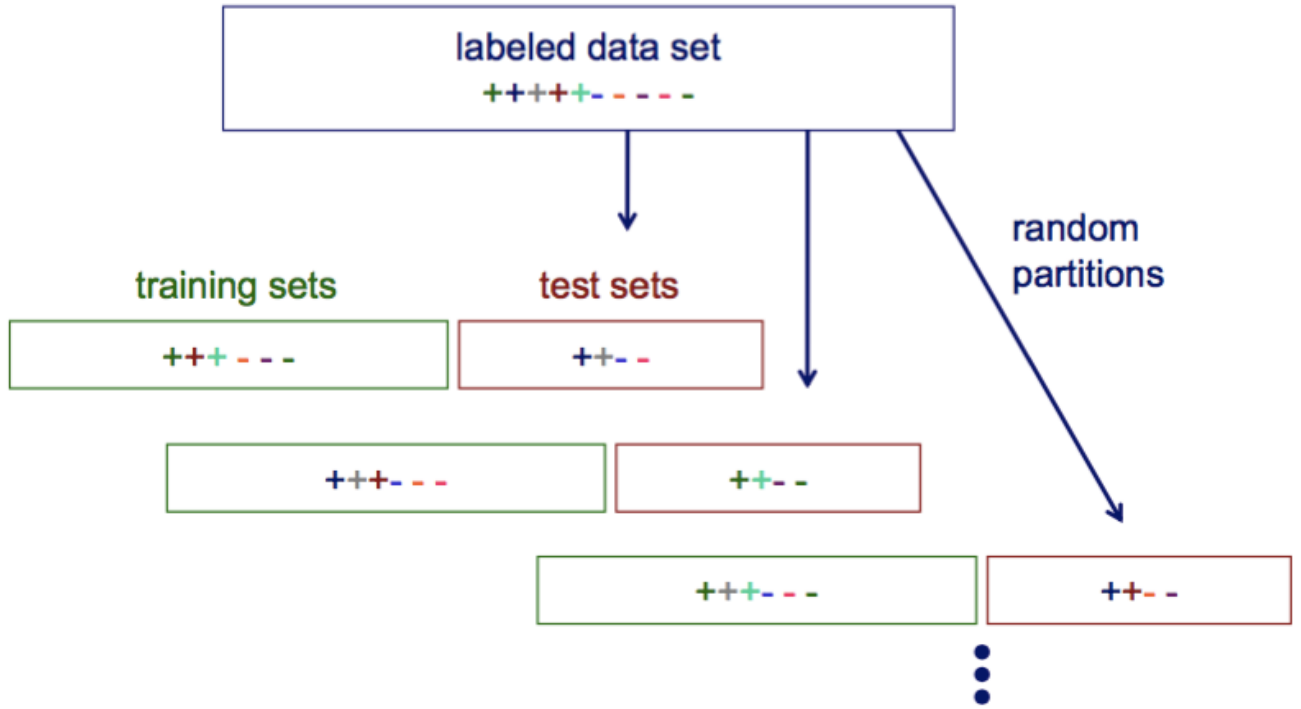
Using multiple training/test partitions

- Two general approaches for doing this
  - random resampling
  - cross validation



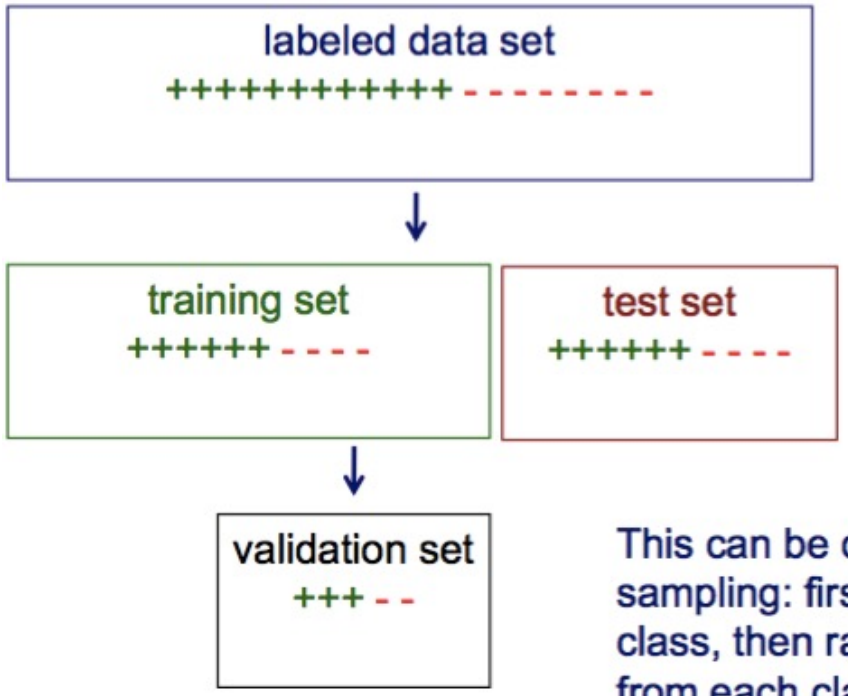
Random resampling

- We can address the second issue by repeatedly randomly partitioning the available data into training and test sets.



Stratified sampling

- When randomly selecting training or validation sets, we may want to ensure that class proportions are maintained in each selected set



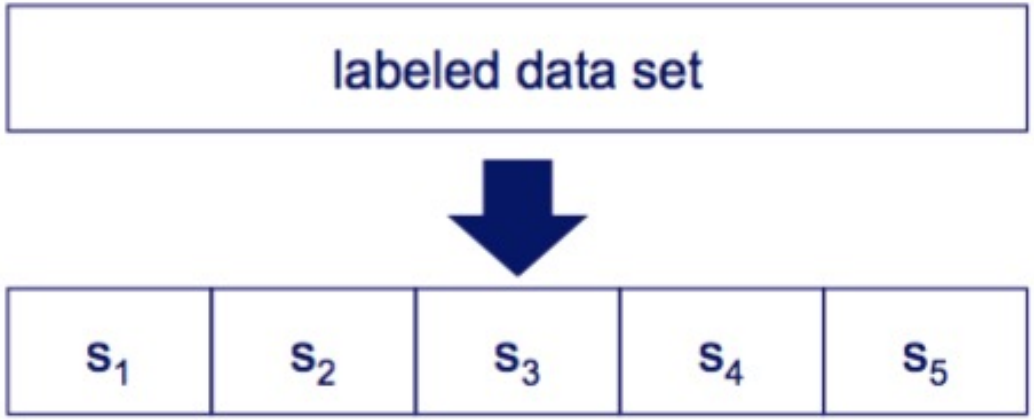
This can be done via stratified sampling: first stratify instances by class, then randomly select instances from each class proportionally.

Recall: a *validation set* (a.k.a. *tuning set*) is a subset of the training set that is held aside

Validation datasets can be used for regularization by early stopping: stop training when the error on the validation dataset increases, as this is a sign of overfitting to the training dataset

Cross validation

partition data into *n* subsamples



iteratively leave one subsample out for the test set, train on the rest

iteration	train on	test on
1	s_2 s_3 s_4 s_5	s_1
2	s_1 s_3 s_4 s_5	s_2
3	s_1 s_2 s_4 s_5	s_3
4	s_1 s_2 s_3 s_5	s_4
5	s_1 s_2 s_3 s_4	s_5

Cross validation example

- Suppose we have 100 instances, and we want to estimate accuracy with cross validation

iteration	train on	test on	correct
1	S_2 S_3 S_4 S_5	S_1	11 / 20
2	S_1 S_3 S_4 S_5	S_2	17 / 20
3	S_1 S_2 S_4 S_5	S_3	16 / 20
4	S_1 S_2 S_3 S_5	S_4	13 / 20
5	S_1 S_2 S_3 S_4	S_5	16 / 20

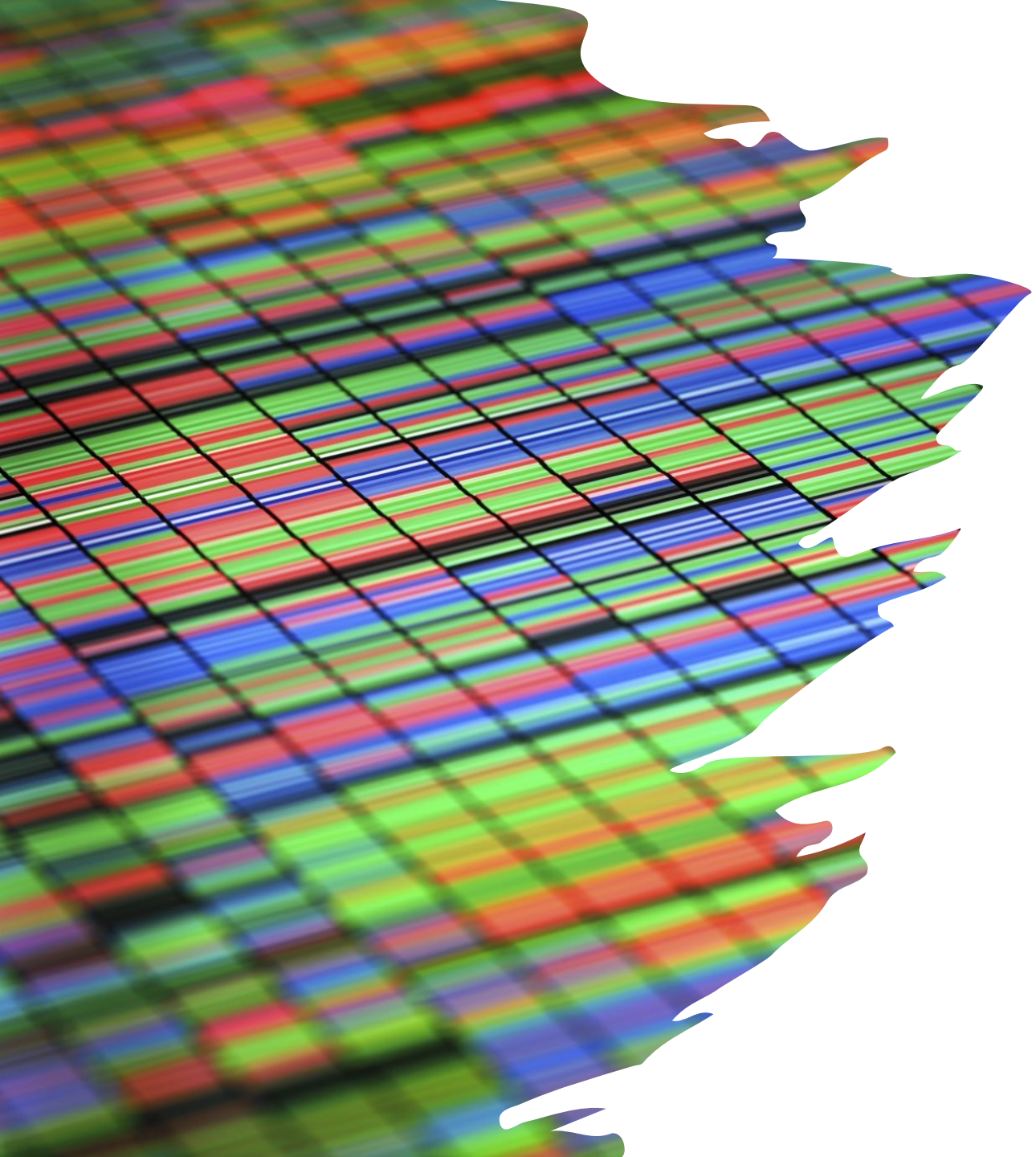
Too pessimistic if only use this split

Too optimistic if only use this split

accuracy = 73/100 = 73%

Cross validation

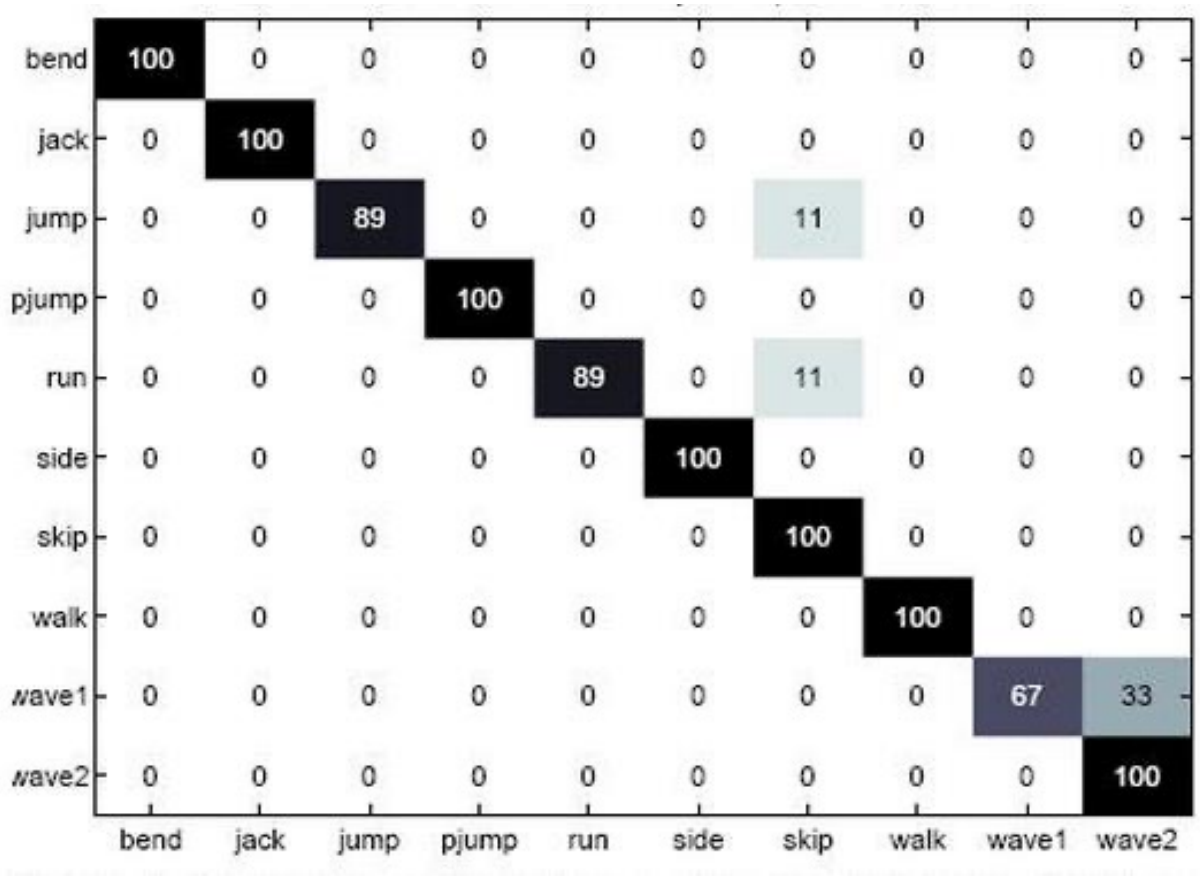
- 10-fold cross validation is common, but smaller values of *n* are often used when learning takes a lot of time
- in *leave-one-out* cross validation, *n* = # instances
- in *stratified* cross validation, stratified sampling is used when partitioning the data
- Cross validation makes efficient use of the available data for testing



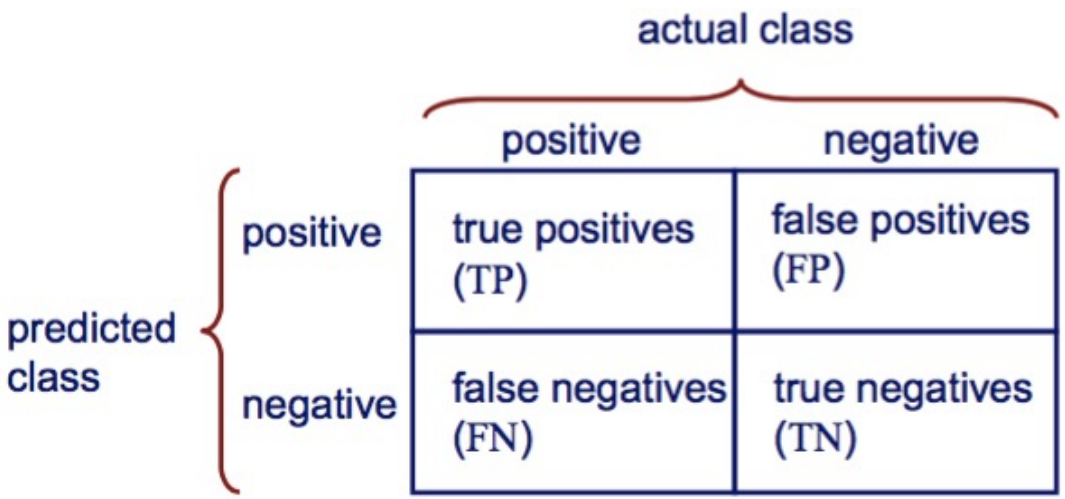
Confusion matrices

Confusion matrices

- How can we understand what types of mistakes a learned model makes?



Confusion matrix for 2-class problems



$$\text{accuracy} = \frac{TP + TN}{TP + FP + FN + TN}$$

$$\text{error} = 1 - \text{accuracy} = \frac{FP + FN}{TP + FP + FN + TN}$$

Some ML algorithms output not only a prediction, but also the confidence of the prediction.

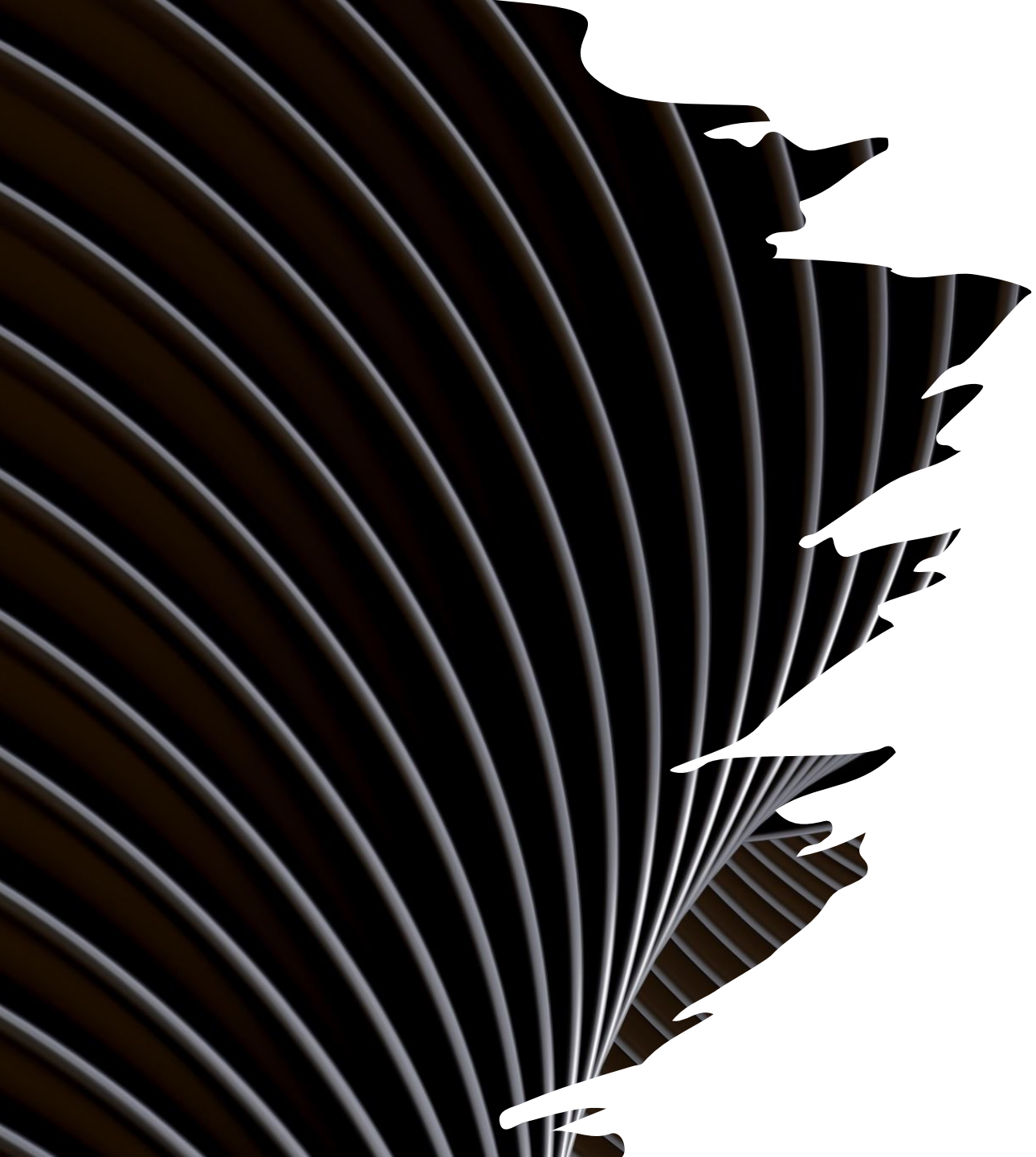
This table changes when the threshold on the confidence of an instance being positive is varied.

Is accuracy an adequate measure of predictive performance?

- accuracy may not be a useful measure in cases where
  - there is a large class skew
    - Is 98% accuracy good when 97% of the instances are negative?
  - there are different misclassification costs – say, getting a positive wrong costs more than getting a negative wrong
    - Consider a medical domain in which a false positive results in an extraneous test but a false negative results in a failure to treat a disease

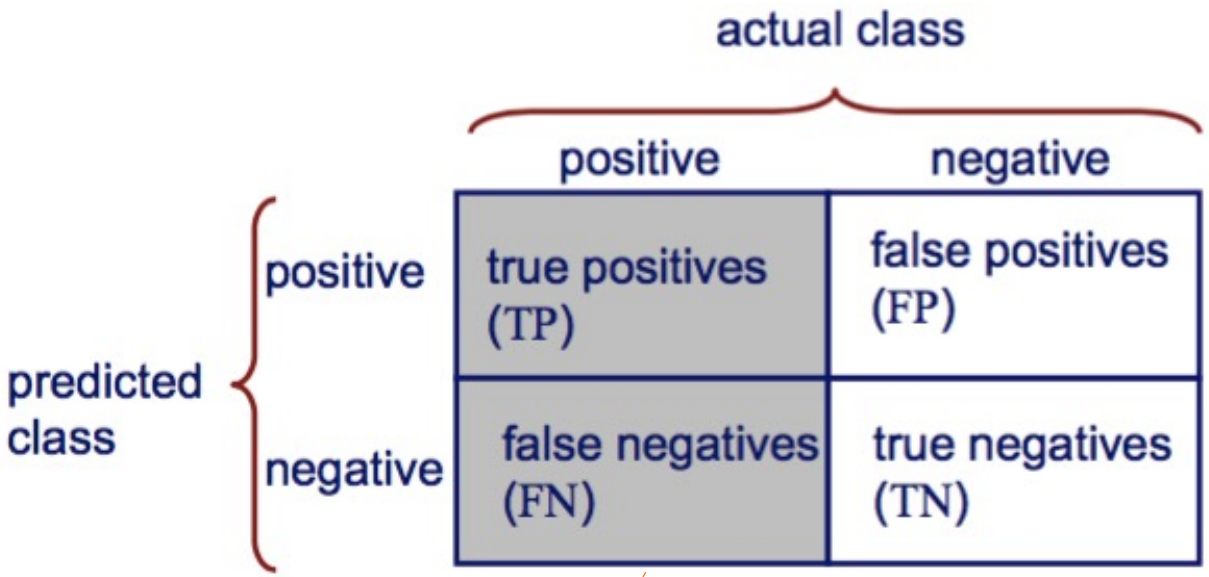
Data/class imbalance

- we are most interested in a subset of high-confidence predictions



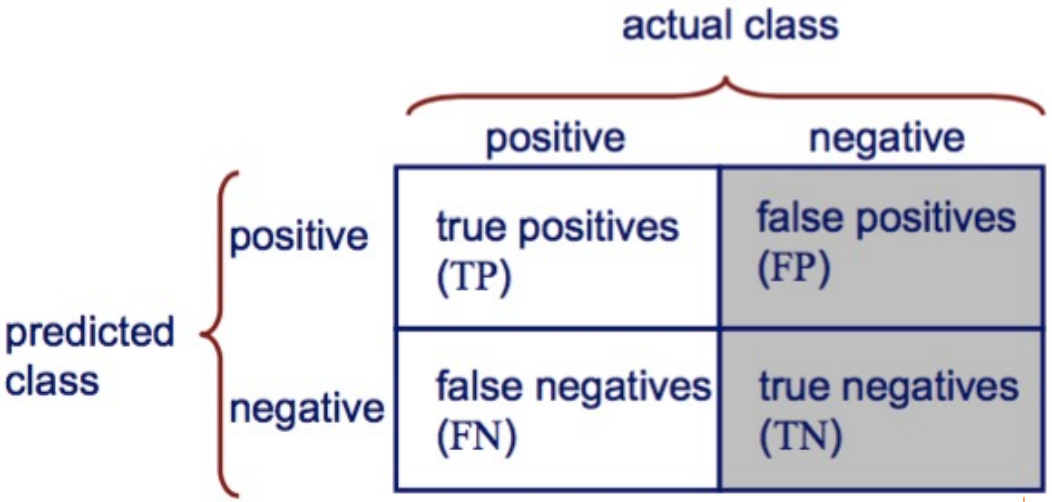
ROC curves

Other accuracy metrics



$$\text{true positive rate (recall)} = \frac{TP}{\text{actual pos}} = \frac{TP}{TP + FN}$$

Other accuracy metrics



$$\text{true positive rate (recall)} = \frac{TP}{\text{actual pos}} = \frac{TP}{TP + FN}$$

$$\text{false positive rate} = \frac{FP}{\text{actual neg}} = \frac{FP}{TN + FP}$$

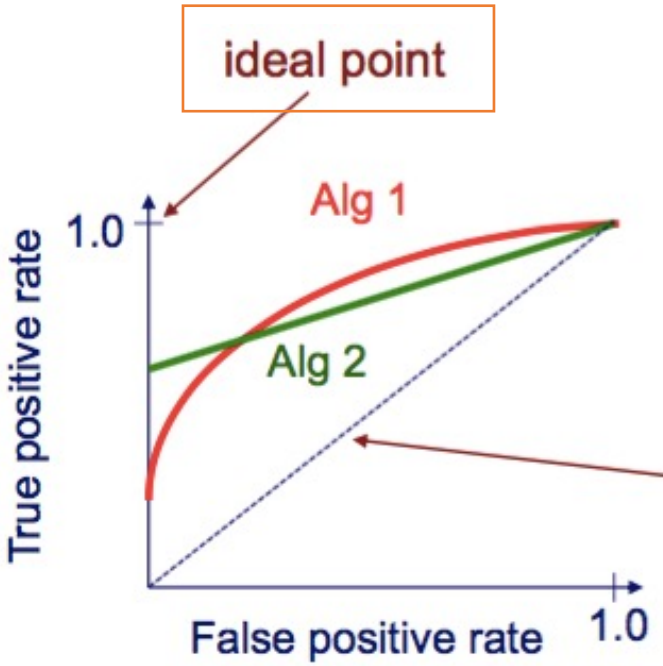
Confidence threshold changes

Confusion matrix changes

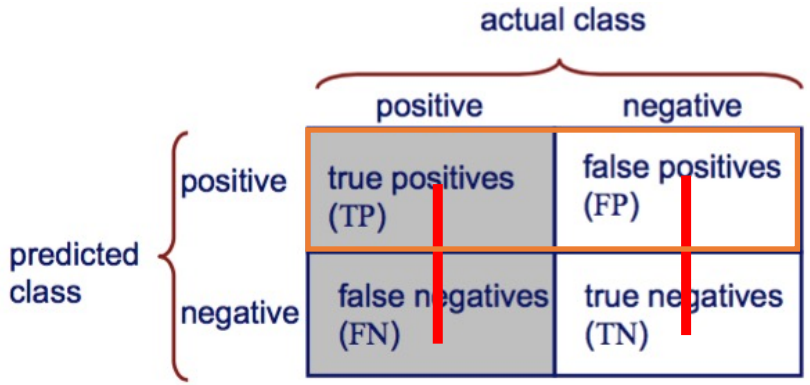
These metrics changes

ROC curves

- A *Receiver Operating Characteristic* (*ROC*) curve plots the TP-rate vs. the FP-rate as a threshold on the confidence of an instance being positive is varied



Different methods can work better in different parts of ROC space.



expected curve for random guessing

Why? Because among all groundtruth positives, half of them will be predicted as positive and another half as negative

Algorithm for creating an ROC curve

let $\left(\left(y^{(1)}, c^{(1)}\right)\ldots\left(y^{(m)}, c^{(m)}\right)\right)$ be the test-set instances sorted according to predicted confidence $c^{(i)}$ that each instance is positive

let *num_neg, num_pos* be the number of negative/positive instances in the test set

$TP = 0,\ FP = 0$

$last\_TP = 0$

for $i = 1$ to m

    // find thresholds where there is a pos instance on high side, neg instance on low side

    if $(i > 1)$ and $(c^{(i)} \neq c^{(i-1)})$ and $(y^{(i)} ==$ neg $)$ and $(TP > last\_TP)$

        $FPR = FP / num\_neg,\quad TPR = TP / num\_pos$

        output (FPR, TPR) coordinate

        $last\_TP = TP$

    if $y^{(i)} ==$ pos

        $++TP$

    else

        $++FP$

$FPR = FP / num\_neg,\ TPR = TP / num\_pos$

output (FPR, TPR) coordinate

General Idea:

(1) Sort the samples according to prediction confidence;

(2) Notice that every confidence threshold leads to a (TPR,FPR) pair;

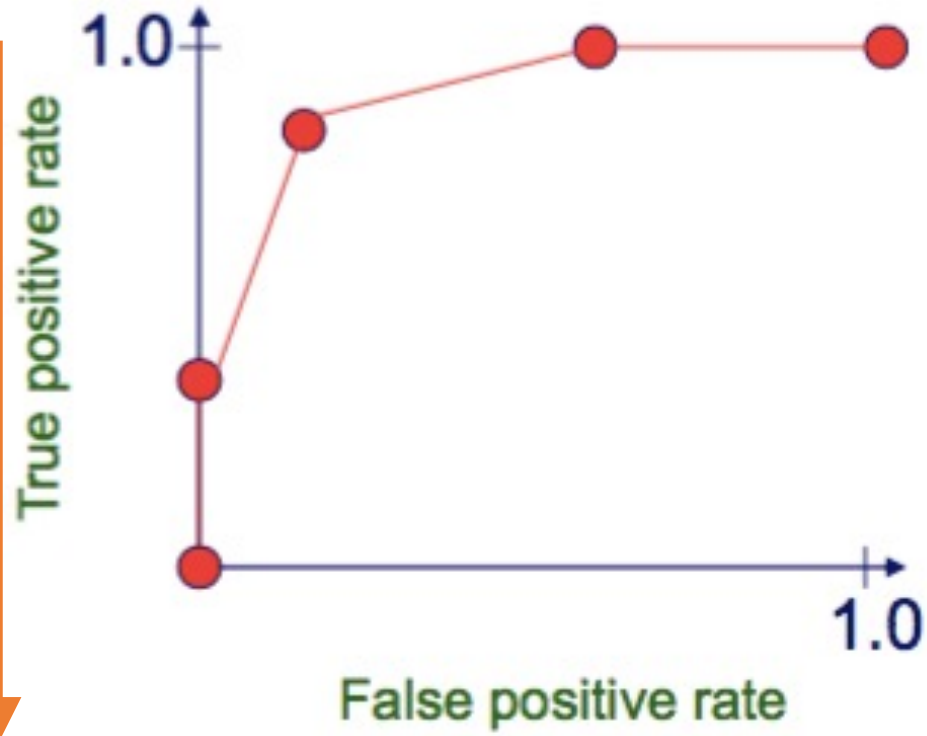
(3) Gradually lower the confidence threshold to obtain multiple(TPR, FPR) pairs for plotting.

Step 1: Sort the samples according to prediction confidence;

Plotting an ROC curve

instance	confidence positive		correct class
Ex 9	.99		+
Ex 7	.98	TPR= 2/5, FPR= 0/5	+
Ex 1	.72		-
Ex 2	.70		+
Ex 6	.65	TPR= 4/5, FPR= 1/5	+
Ex 10	.51		-
Ex 3	.39		-
Ex 5	.24	TPR= 5/5, FPR= 3/5	+
Ex 4	.11		-
Ex 8	.01	TPR= 5/5, FPR= 5/5	-

Step 2: Notice that every confidence threshold leads to a (TPR,FPR) pair



Step 3: Gradually lower the confidence threshold to obtain multiple(TPR, FPR) pairs for plotting

ROC curve example

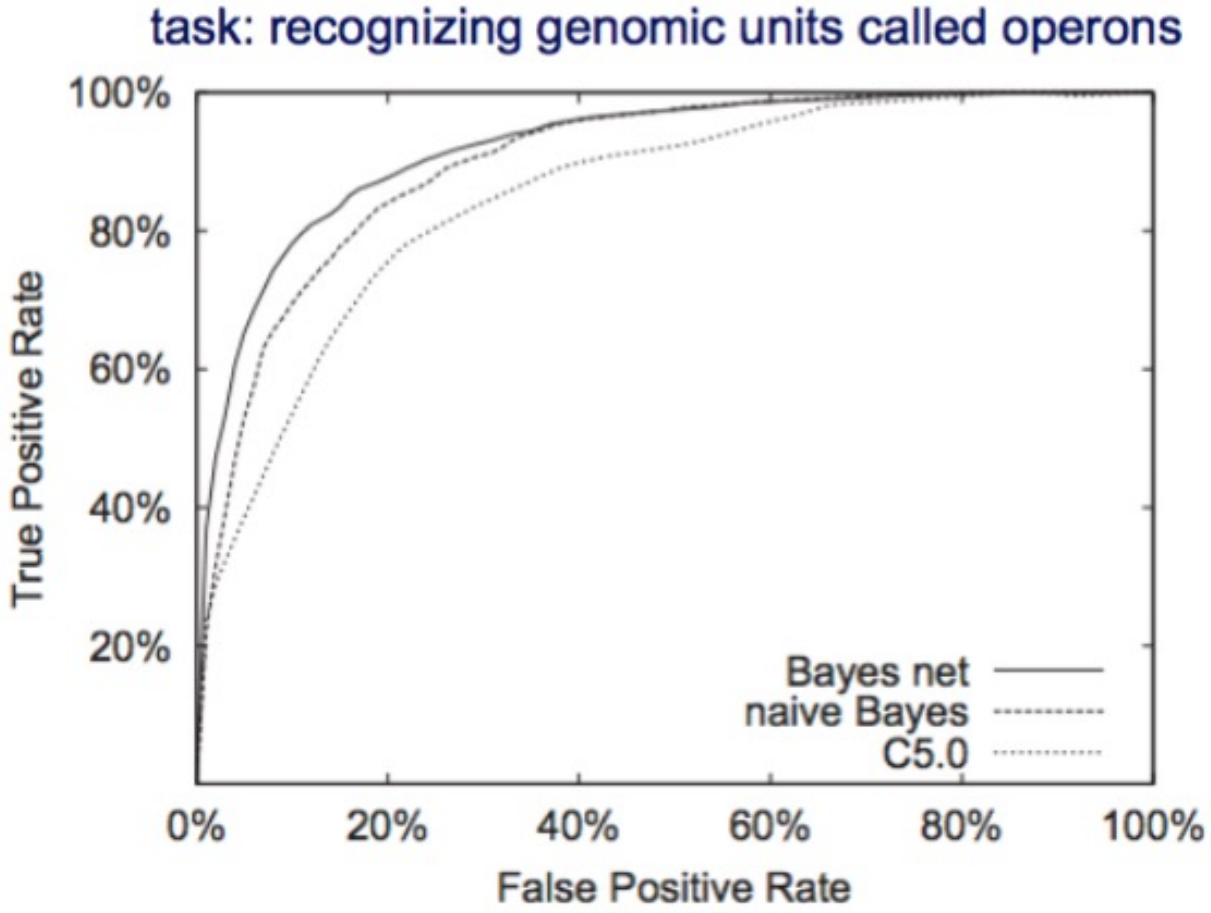


figure from Bockhorst et al., *Bioinformatics* 2003

•The area under the curve (AUC) can be used as a summary of the model skill.

How to read the ROC curves

- A skilful model will assign a higher probability to a randomly chosen real positive occurrence than a negative occurrence on average. This is what we mean when we say that the model has skill. Generally, skilful models are represented by curves that bow up to the top left of the plot.
- A model with no skill is represented at the point (0.5, 0.5). A model with no skill at each threshold is represented by a diagonal line from the bottom left of the plot to the top right and has an AUC of 0.5.
- A model with perfect skill is represented at a point (0,1). A model with perfect skill is represented by a line that travels from the bottom left of the plot to the top left and then across the top to the top right.

https://machinelearningmastery.com/roc-curves-and-precision-recall-curves-for-classification-in-python/

PR curves

ROC curves

- Does a low false positive rate indicate that most positive predictions (i.e., prediction with confidence > some threshold) are correct?

suppose our TPR is 0.9, and FPR is 0.01

fraction of instances that are positive	fraction of positive predictions that are correct
0.5	0.989
0.1	0.909
0.01	0.476
0.001	0.083

Let's do this exercise

$$TPR = \frac{TP}{TP + FN} = 0.9$$

$$FPR = \frac{FP}{TN + FP} = 0.01$$

$$TP + FN = 0.1 * n$$

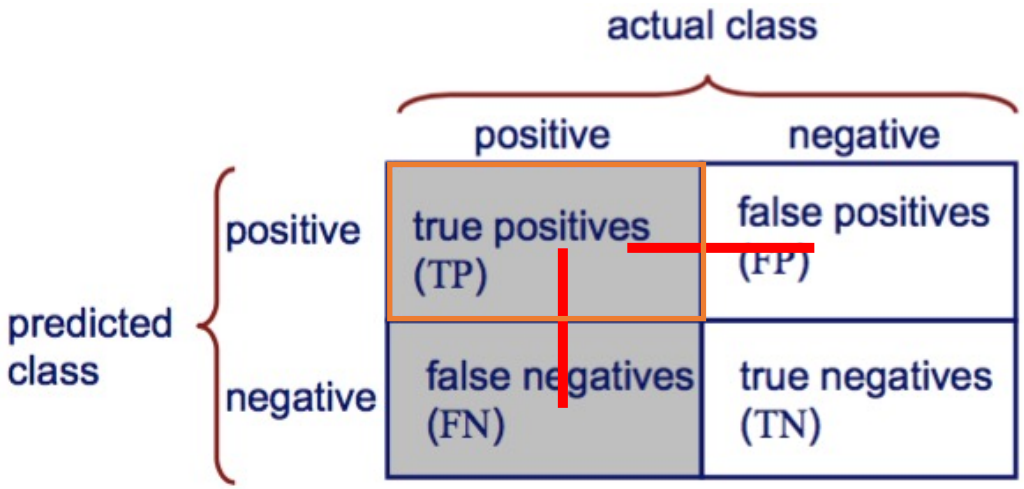
$$TP = 0.9 * 0.1 * n$$

$$FP = 0.01 * 0.9 * n$$

$$\frac{TP}{TP + FP} = \frac{0.9 * 0.1}{0.9 * 0.1 + 0.01 * 0.9} = 0.909$$

This is unacceptable if correct predictions on positive samples are very important.

Other accuracy metrics



$$\text{recall (TP rate)} = \frac{\text{TP}}{\text{actual pos}} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

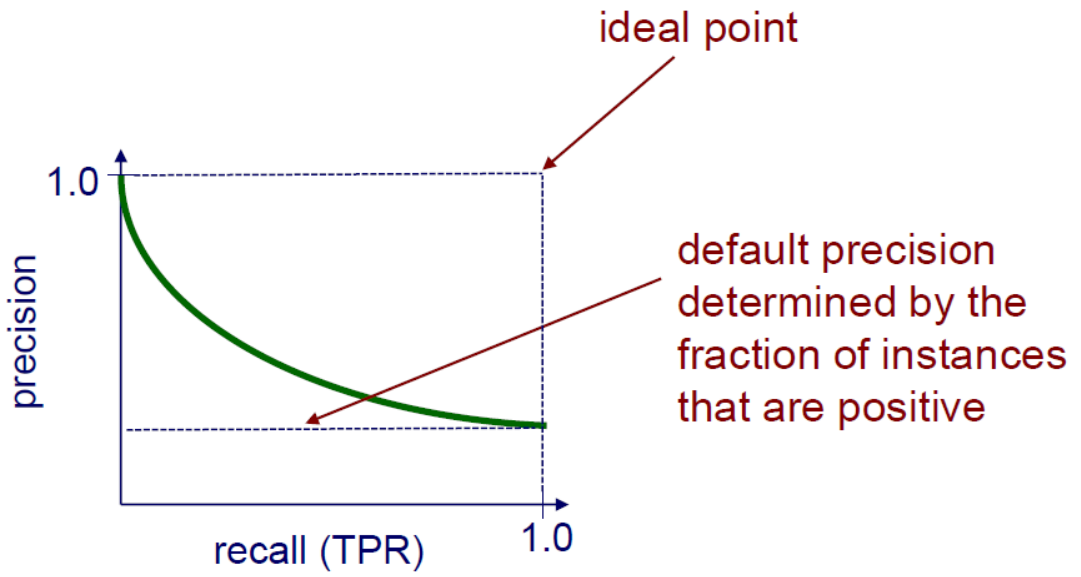
We like this to be as high as possible

$$\text{precision (positive predictive value)} = \frac{\text{TP}}{\text{predicted pos}} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

When correct predictions on positive samples are very important

Precision/recall curves

- A precision/recall curve plots the precision vs. recall (TP-rate) as a threshold on the confidence of an instance being positive is varied.



Precision/recall curve example

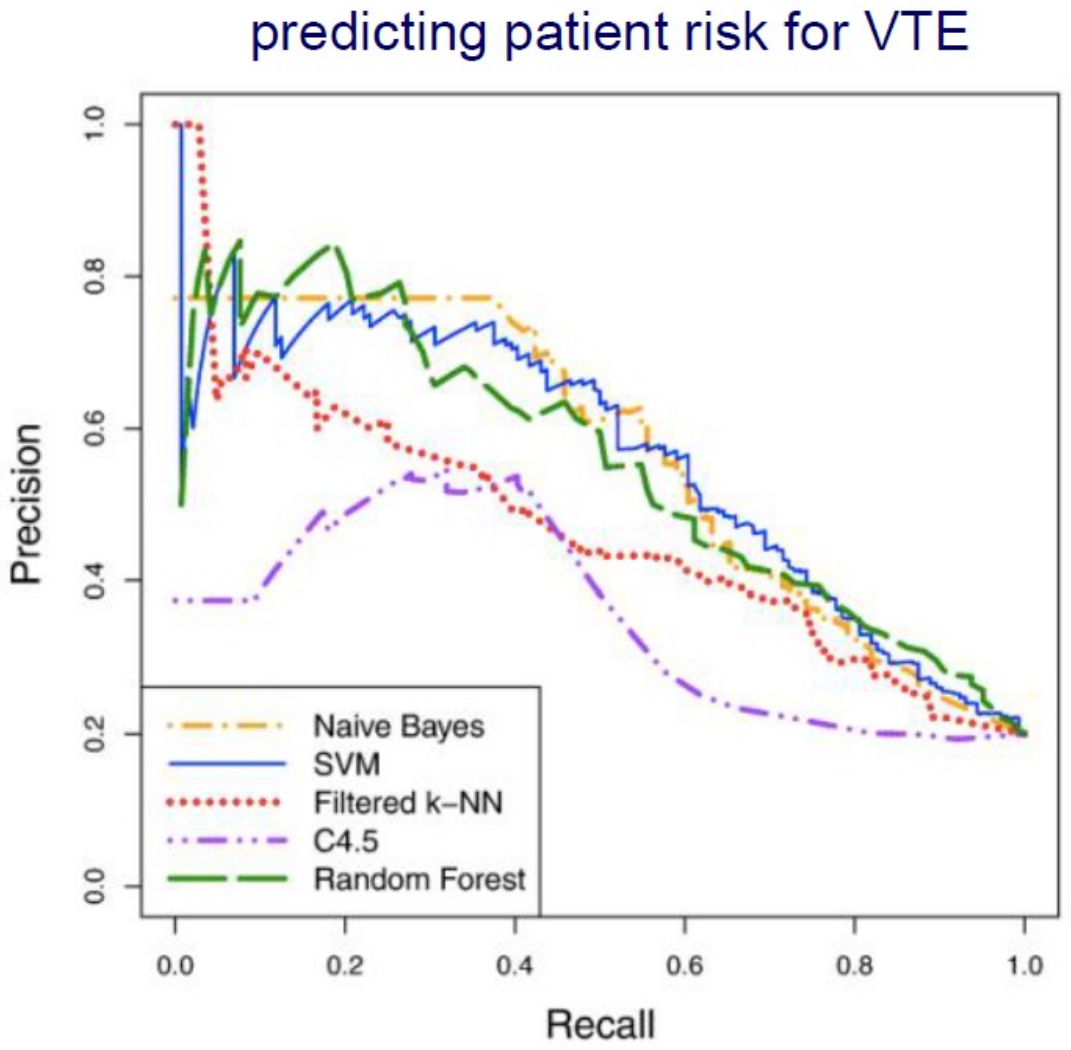
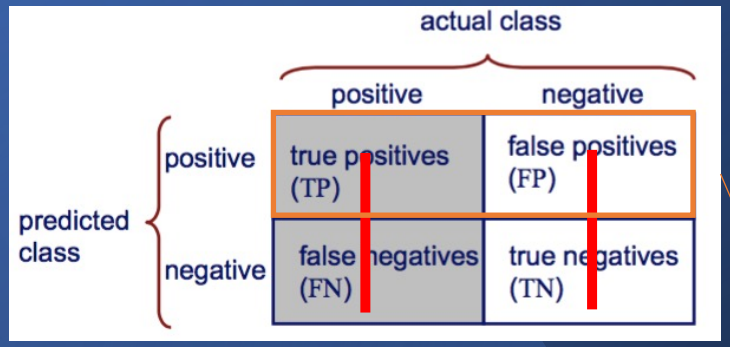
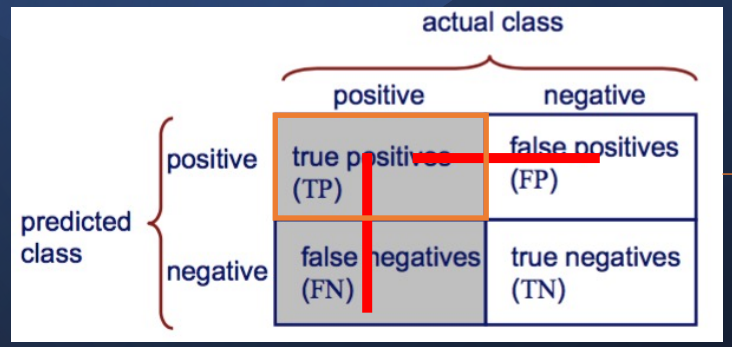


figure from Kawaler et al., *Proc. of AMIA Annual Symosium,* 2012



Comments on ROC and PR curves



Both

- Allow predictive performance to be assessed at various levels of confidence
- Assume binary classification tasks
- Sometimes summarized by calculating area under the curve

ROC curves

- Insensitive to changes in class distribution (ROC does not change if the proportion of positive and negative instances in the test set are varied)
- Can identify optimal classification thresholds for tasks with differential misclassification costs

PR curves

- Show the fraction of predictions that are false positives
- Well suited for tasks with lots of negative instances