Carnegie Mellon University
Heinz College

95-865 Unstructured Data Analytics

Recitation: More on Hyperparameter Tuning and Model Evaluation

Slides by George H. Chen

(Flashback) Hyperparameter Tuning in General (Not Just for *k*-NN Classifier)

Suppose that we have a classifier with hyperparameter setting θ

could consist of multiple hyperparameters
(think of θ as a tuple)

For each hyperparameter setting θ (in a list of hyperparameter settings we are willing to try):

1. Train classifier on proper training data using hyperparameter setting θ
2. Use a score function to evaluate how well the trained model predicts on validation data

Use classifier corresponding to whichever value of θ achieves the best score

⚠ How we randomly split the training data into proper training/validation sets affects the scores we get

⚠ If the classifier's training procedure is random, then using different random seeds could also change the scores we get

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Which score function is used for measuring accuracy matters!

Score Functions for Accuracy

What we already saw:

- **Raw accuracy:** fraction of predicted labels that are correct

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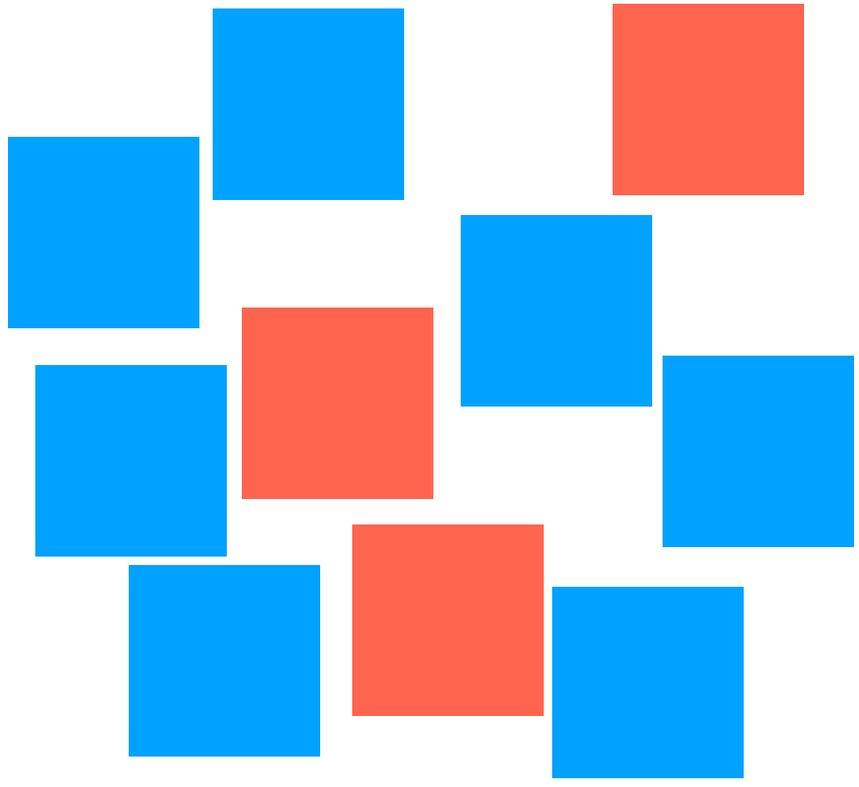

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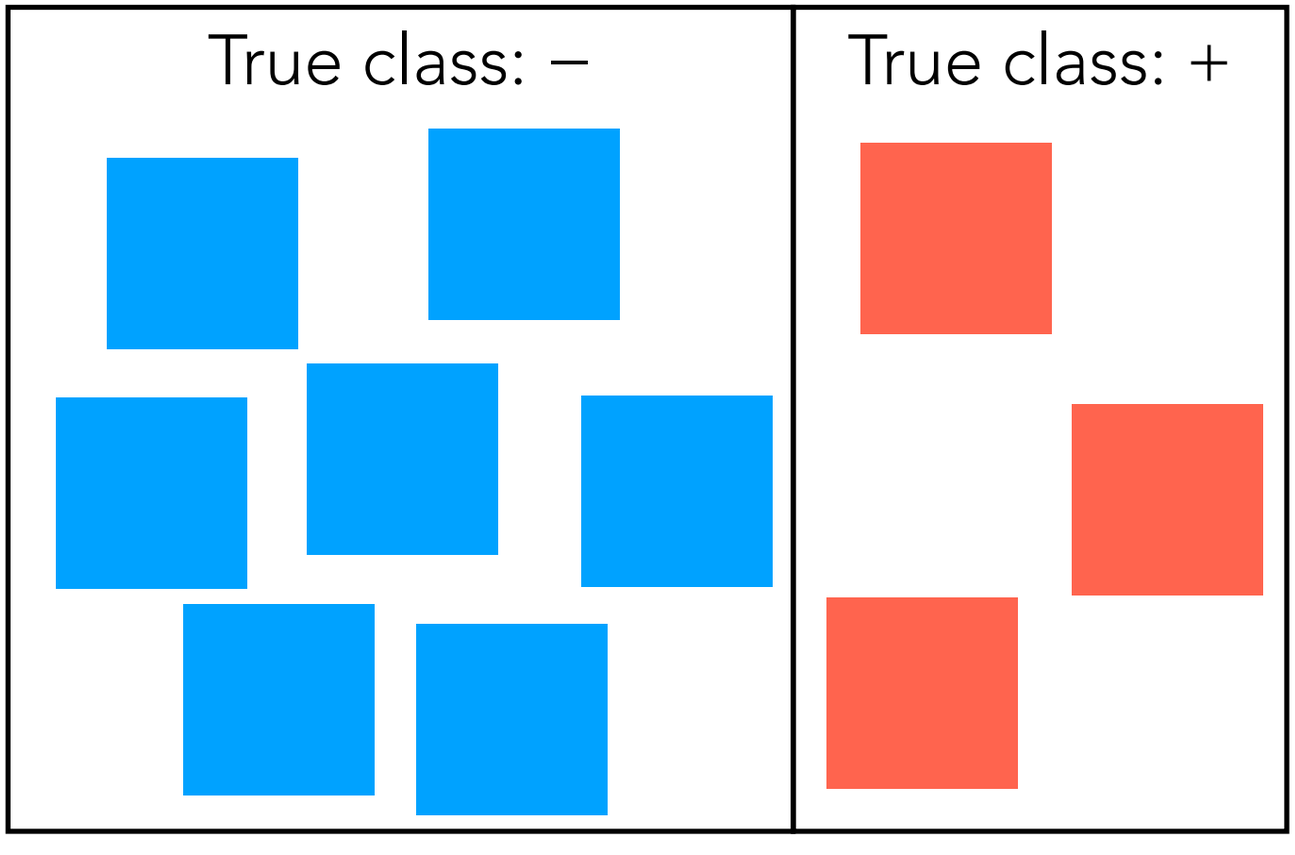

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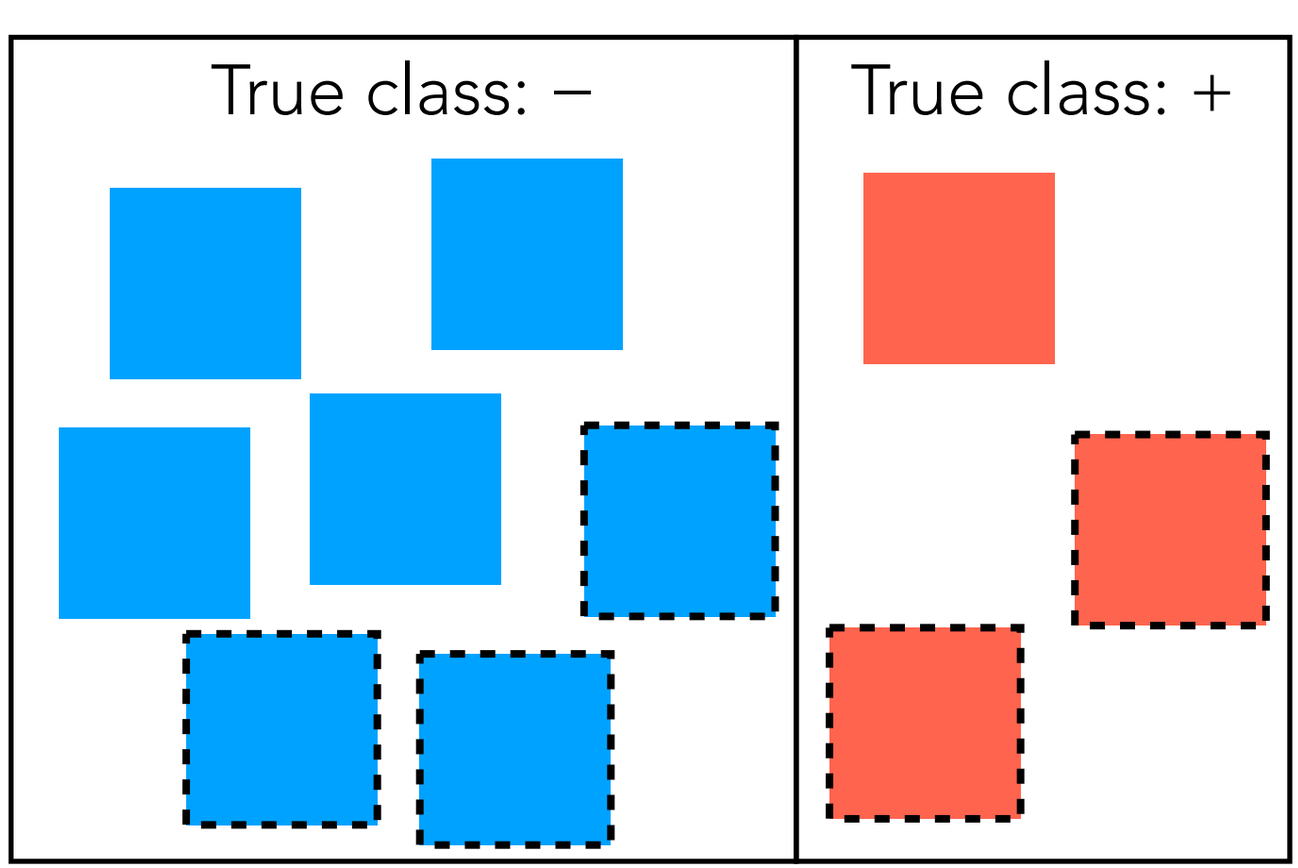

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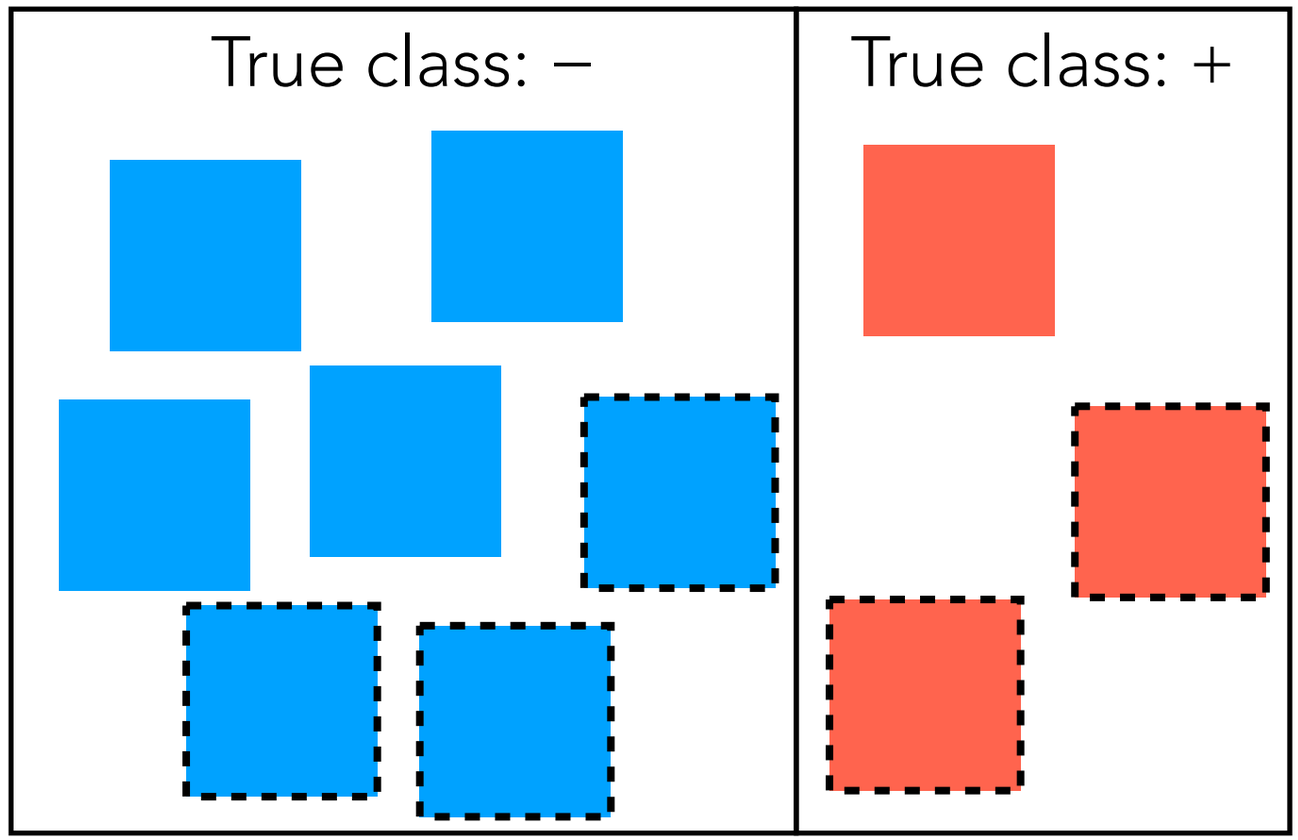


Recall/True Positive Rate: fraction of red points correctly predicted = 2/3

Precision: fraction of dotted points correctly predicted

False Positive Rate: fraction of blue points incorrectly predicted = 3/7

F1 score: $\dfrac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}} = 1/2$

Generalizing F1 Score to More Than 2 Classes

For each class $c \in \mathcal{C}$: ($\mathcal{C}$: set of possible classes)

- Treat class c as the positive class and compute the F1 score

  Denote the resulting F1 score as: $F_1^{(c)}$

How do we aggregate across the different classes' F1 scores to produce a single number as an overall score?

Option #1: report an equally weighted average across classes

$$F_1^{\text{equally weighted}} = \frac{1}{|\mathcal{C}|} \sum_{c \in \mathcal{C}} F_1^{(c)}$$

Option #2: weight each class by how often it appears in the data that we're evaluating the F1 score for

$$F_1^{\text{weighted}} = \sum_{c \in \mathcal{C}} [\text{fraction of points in class } c] \times F_1^{(c)}$$

“Receiver Operating Characteristic” (ROC) Curves

Probability Thresholding

Recall that logistic regression predicts the probability of each class for any test feature vector ***x***

(MNIST: for any test image, we predict probabilities for all 10 digits)

To get final predicted class of test feature vector ***x***:
pick whichever class has the highest probability

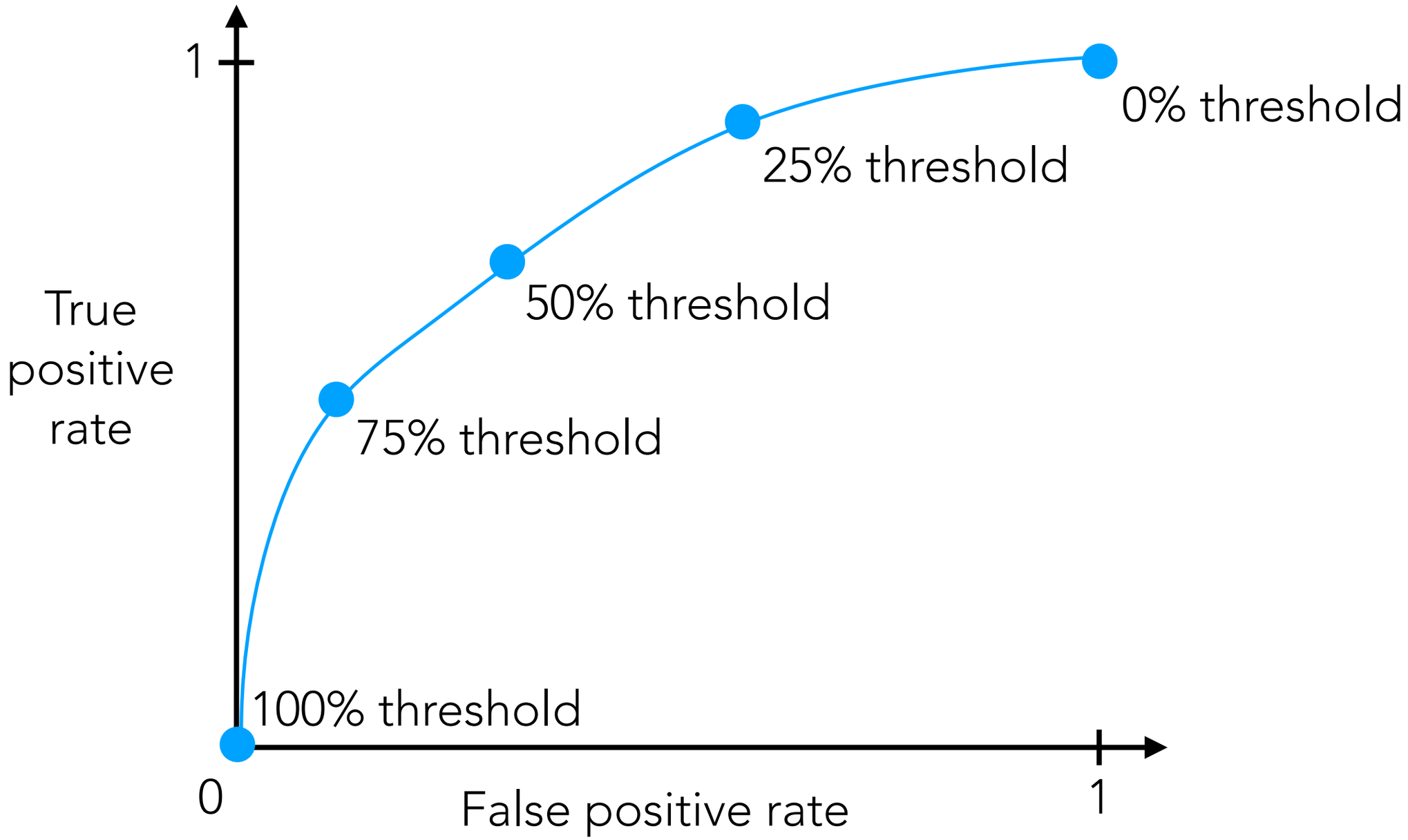
When there are 2 classes positive and negative

Predict positive if P(positive | test feature vector ***x***) ≥ 0.5

Predict negative otherwise

We can vary this 50% threshold!

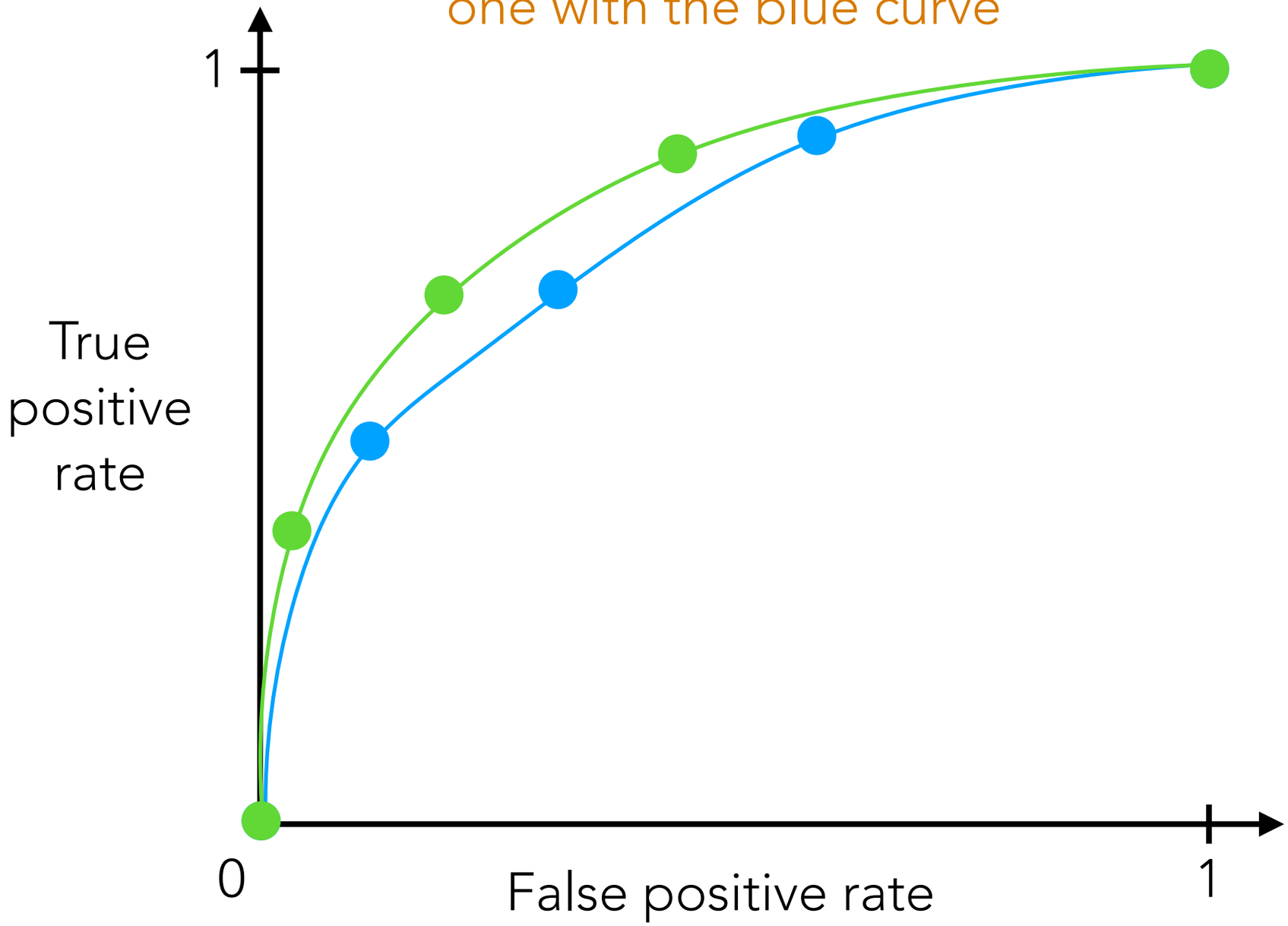
Binary Classification: ROC Curves



TPR and FPR are computed using test data

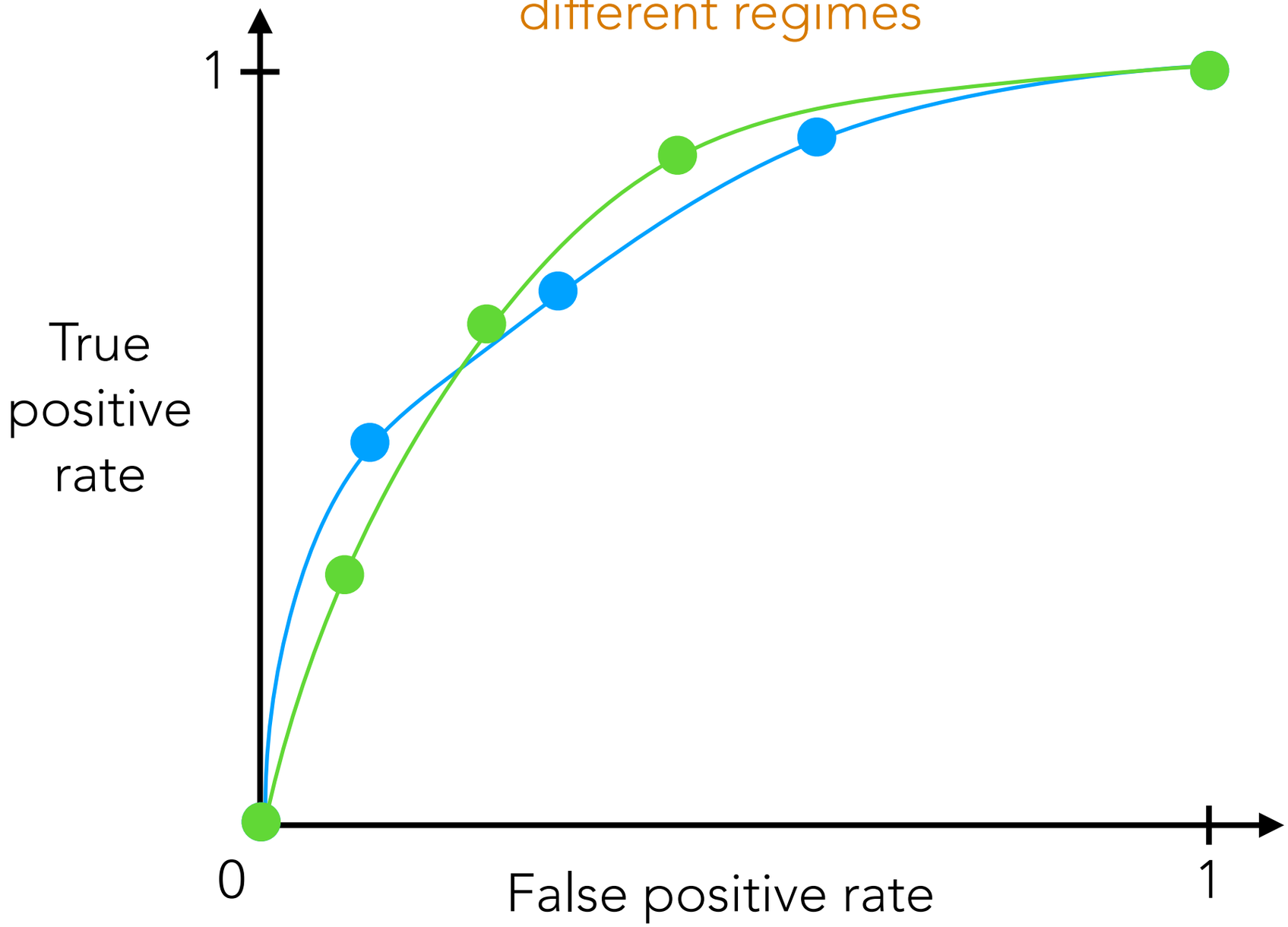
Binary Classification: ROC Curves

A classifier with the green curve is better than the one with the blue curve



Binary Classification: ROC Curves

It's possible that different models are better in different regimes



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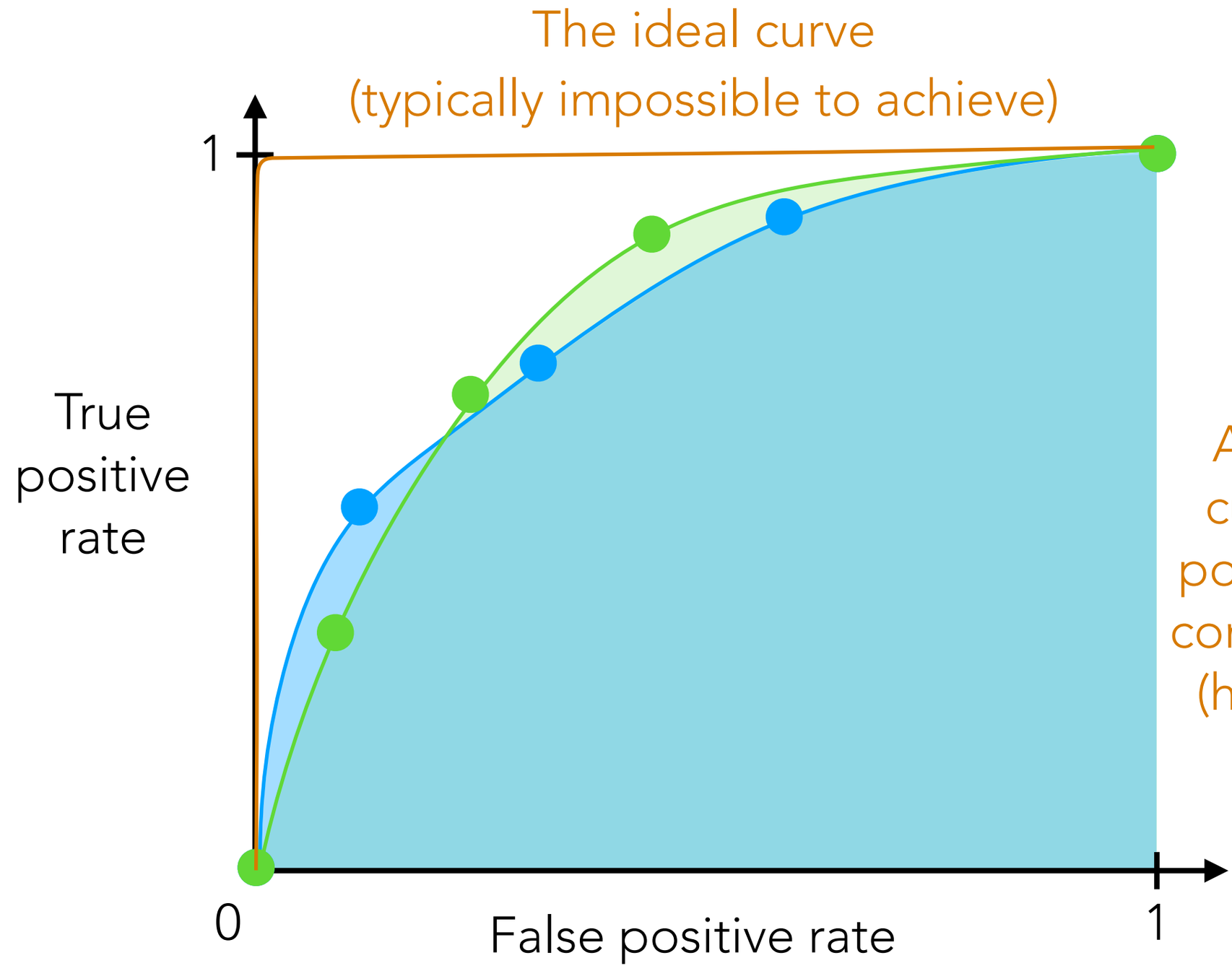


Area under the curve (AUC) is a popular metric for comparing models (higher is better)

Binary Classification: ROC Curves

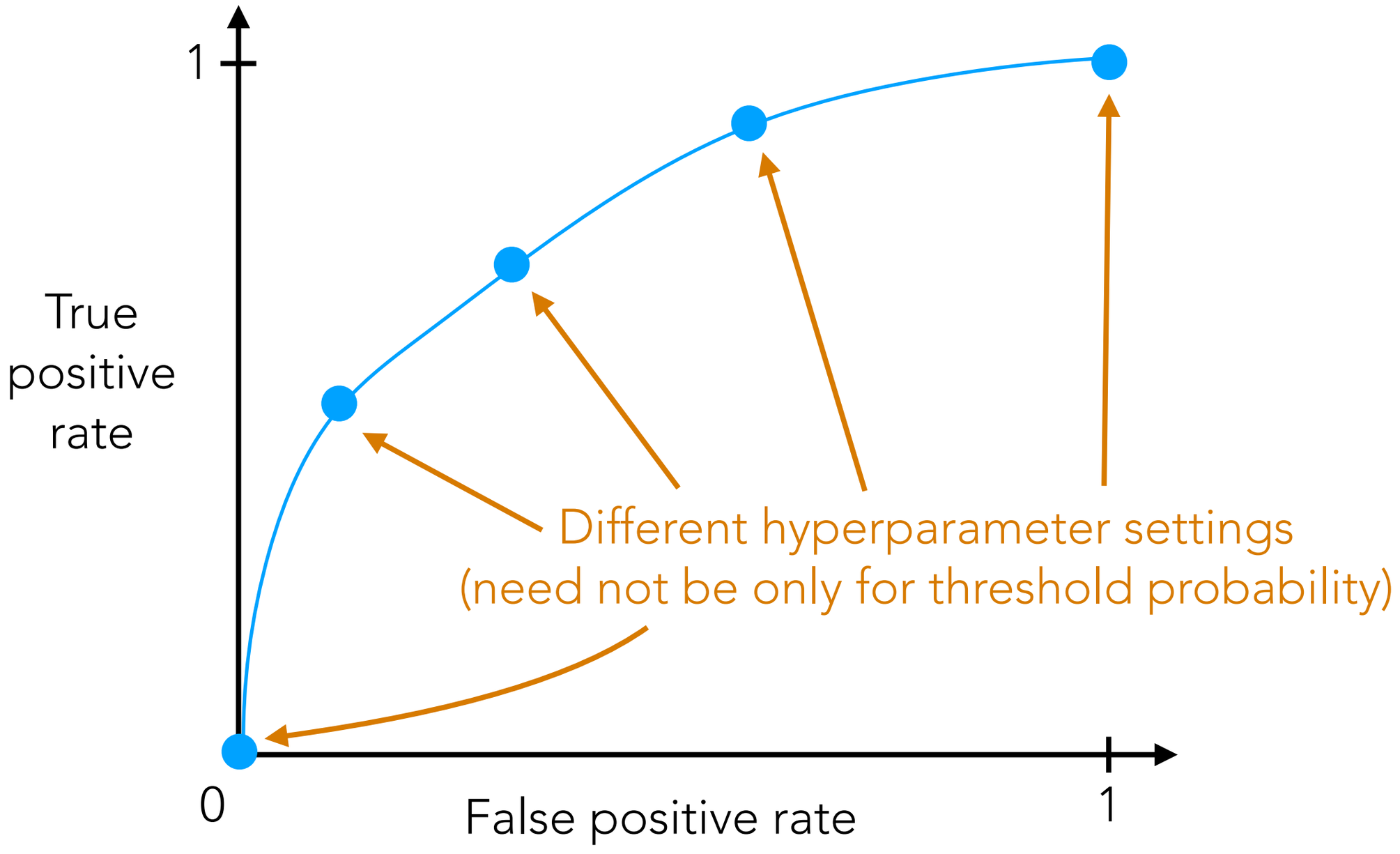
What we just saw:

- For a classifier that we can set the threshold probability to different values, we can plot an ROC curve
- True positive rate (TPR) and false positive rate (FPR) are evaluated on test data

Other variants are possible:

- Plot precision vs recall instead of TPR vs FPR
- Can actually plot ROC/precision-recall curves sweeping over hyperparameters *aside from threshold probability*!
- For ROC/precision-recall, rather than evaluating on test data, can evaluate on validation data during training *to help choose hyperparameters*

Binary Classification: ROC Curves



Can also be computed on validation data instead of test data!