


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

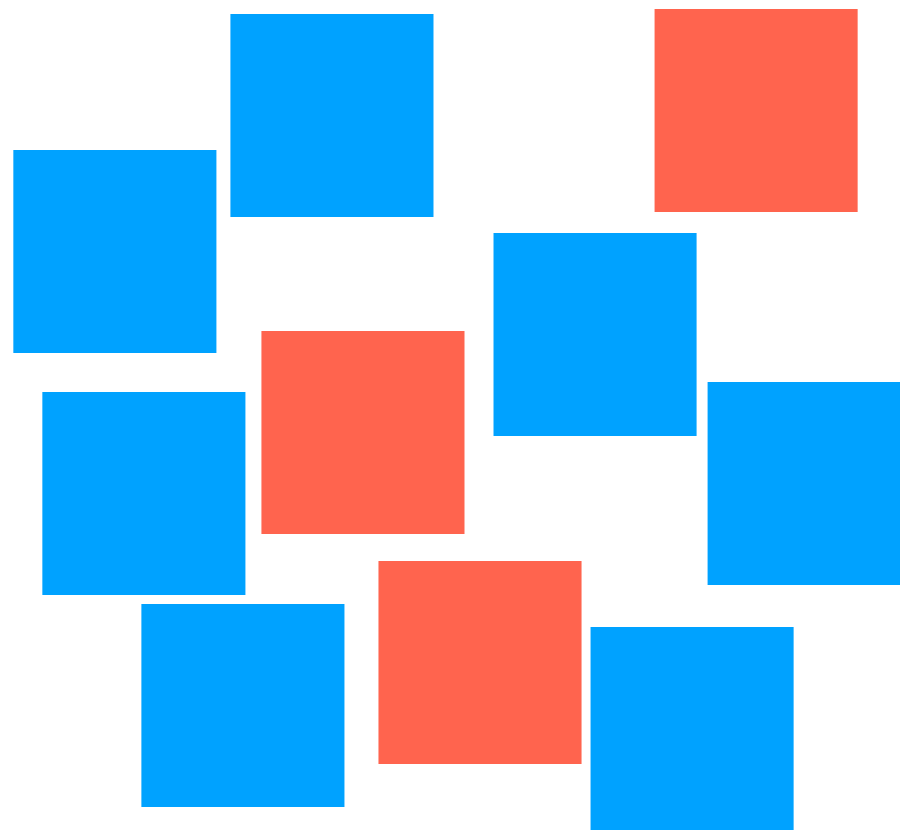
In “binary” classification (there are 2 classes such as spam/ham) when 1 class is considered “positive” and the other “negative”:

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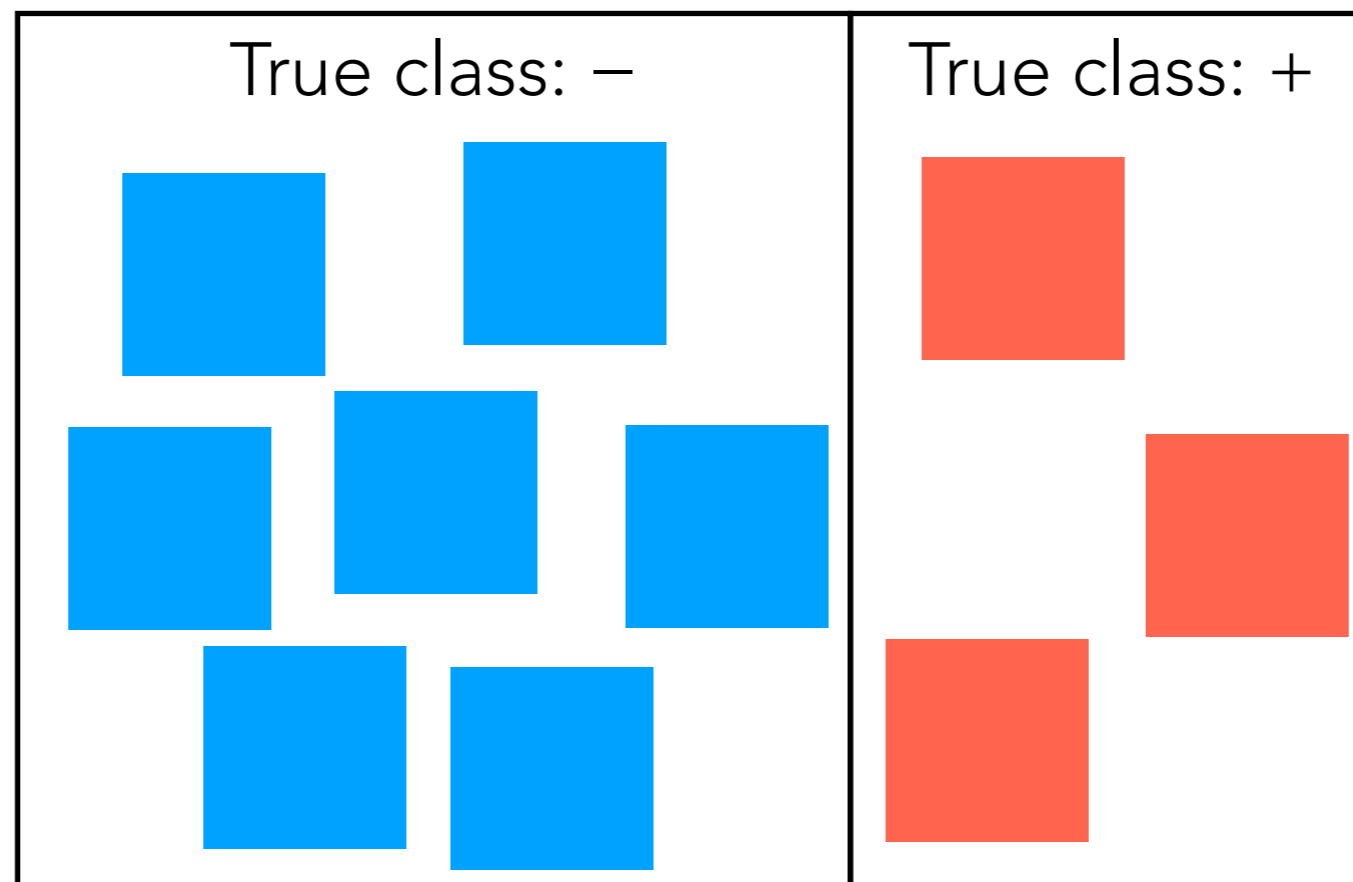


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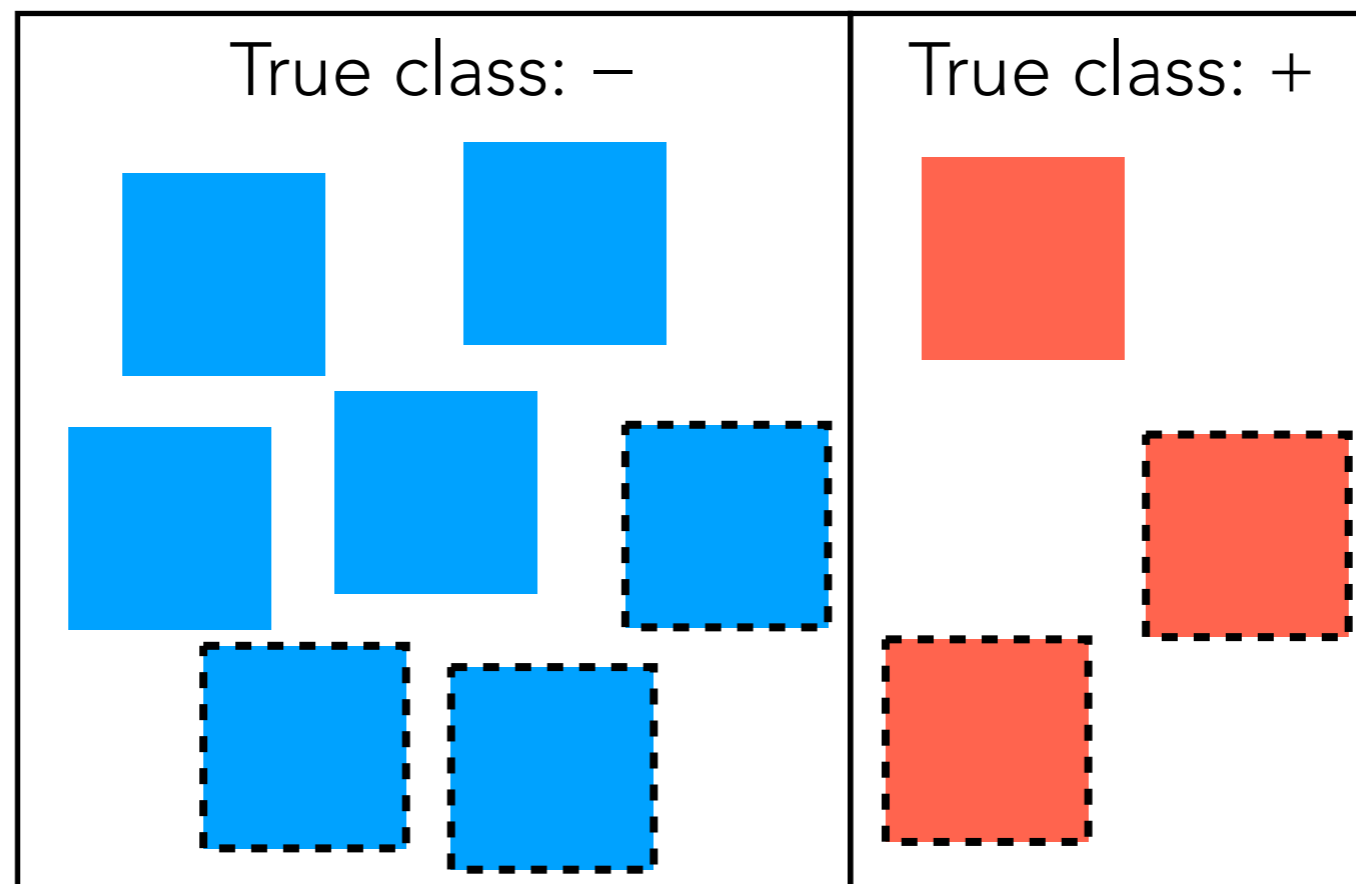


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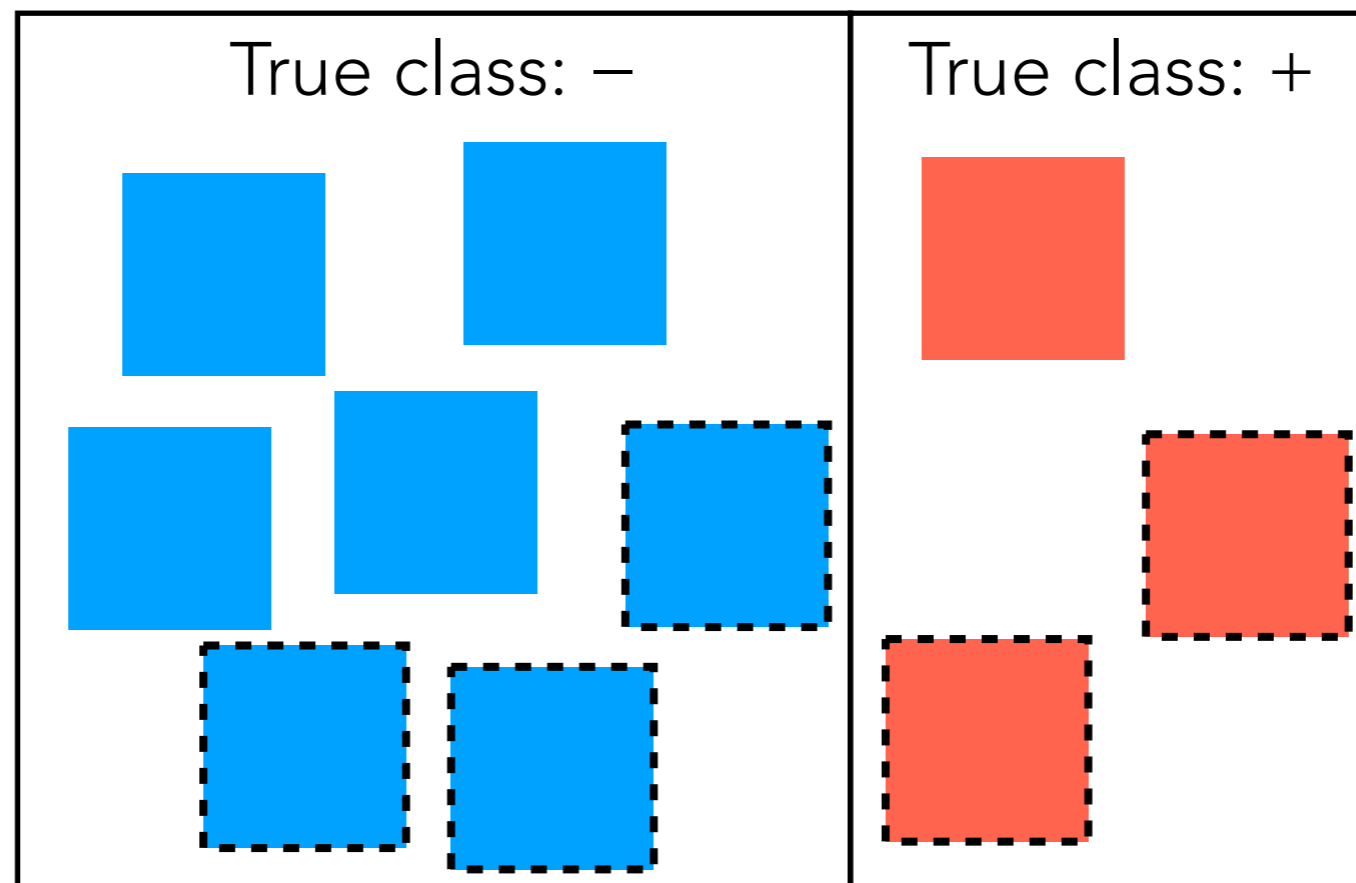


Outlined in dotted black: predicted label +
(all other points predicted to be -)

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

Score Functions for Accuracy

In "binary" classification (there are 2 classes such as spam/ham) when 1 class is considered "positive" and the other "negative":



Outlined in dotted black: predicted label +
(all other points predicted to be -)

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:
$$\frac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}} = 1/2$$

Generalizing F1 Score to More Than 2 Classes

For each class $c \in \mathcal{C}$:  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

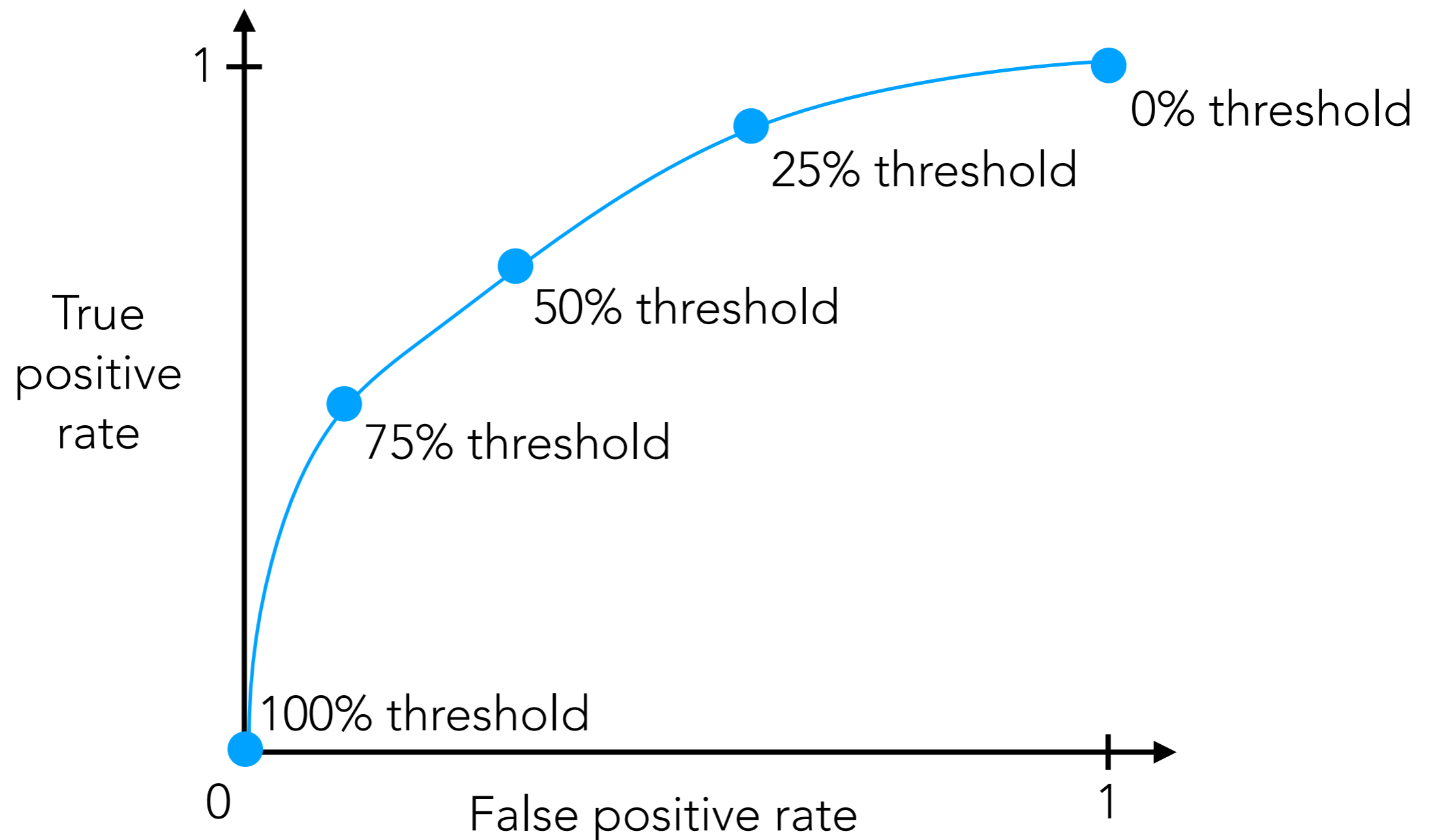
When there are 2 classes **positive** and **negative**

Predict **positive** if $P(\text{positive} \mid \text{test feature vector } x) \geq 0.5$

Predict **negative** otherwise

We can vary this 50% threshold!

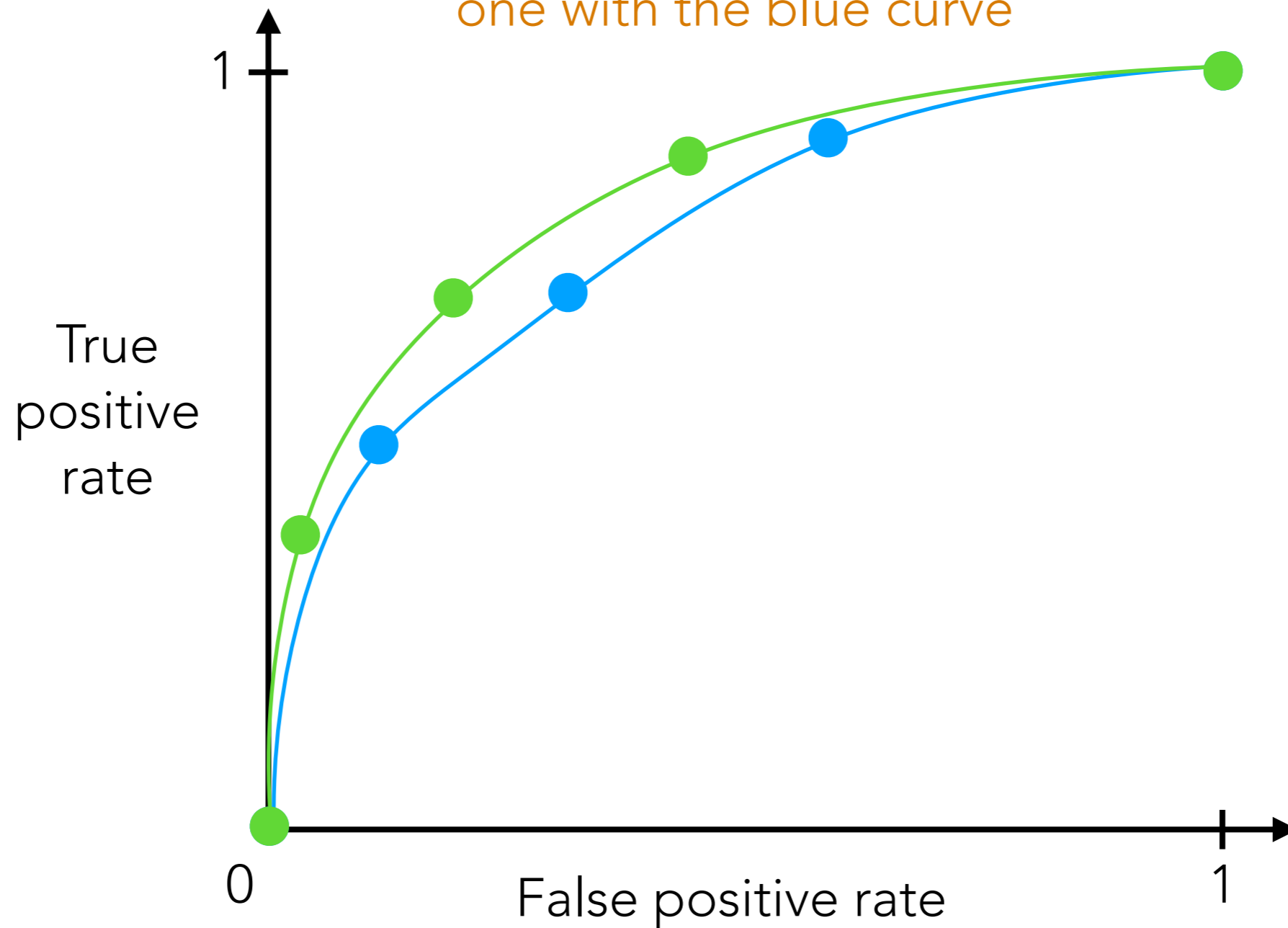
Binary Classification: ROC Curves



TPR and FPR are computed using test data

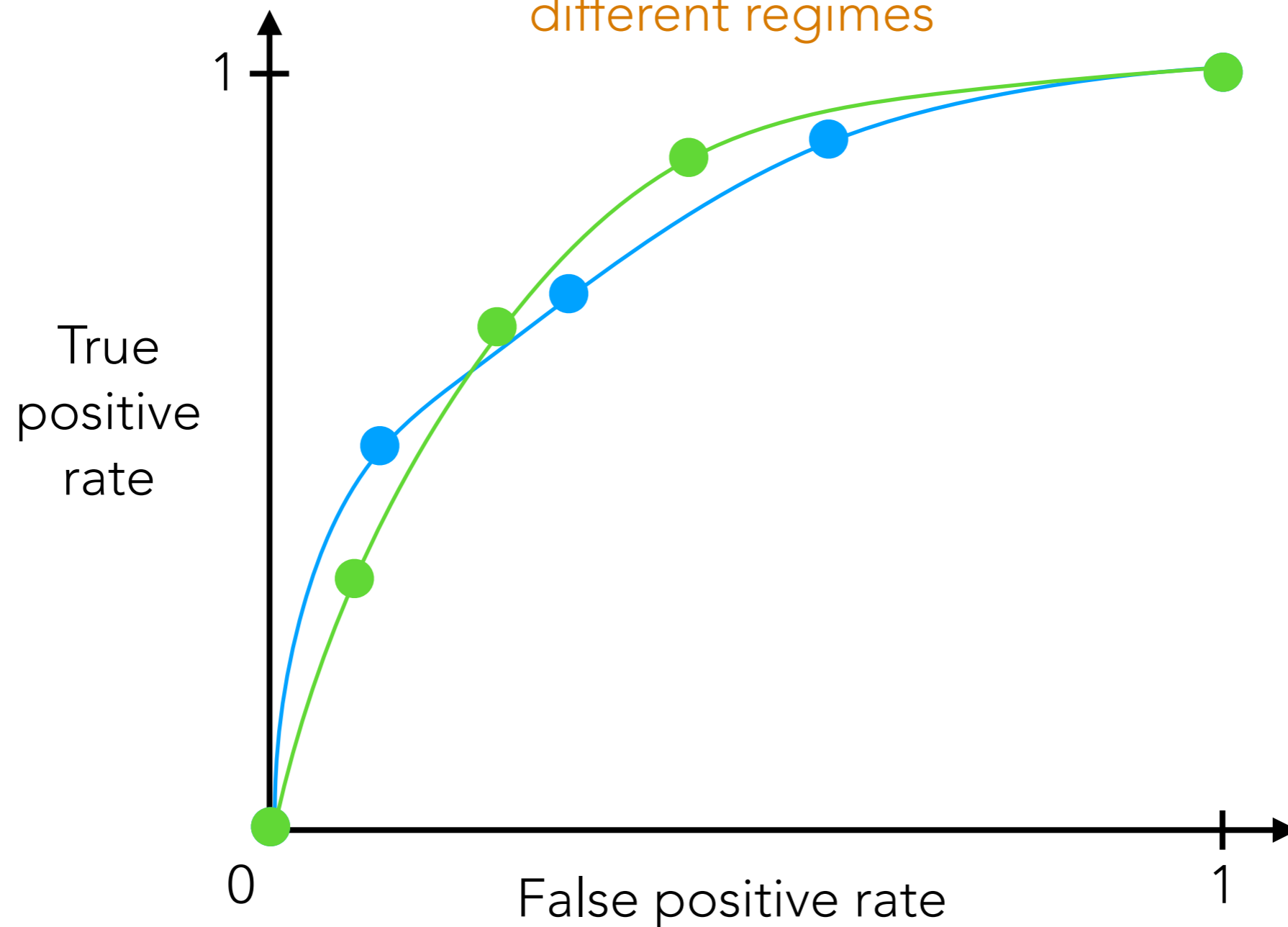
Binary Classification: ROC Curves

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

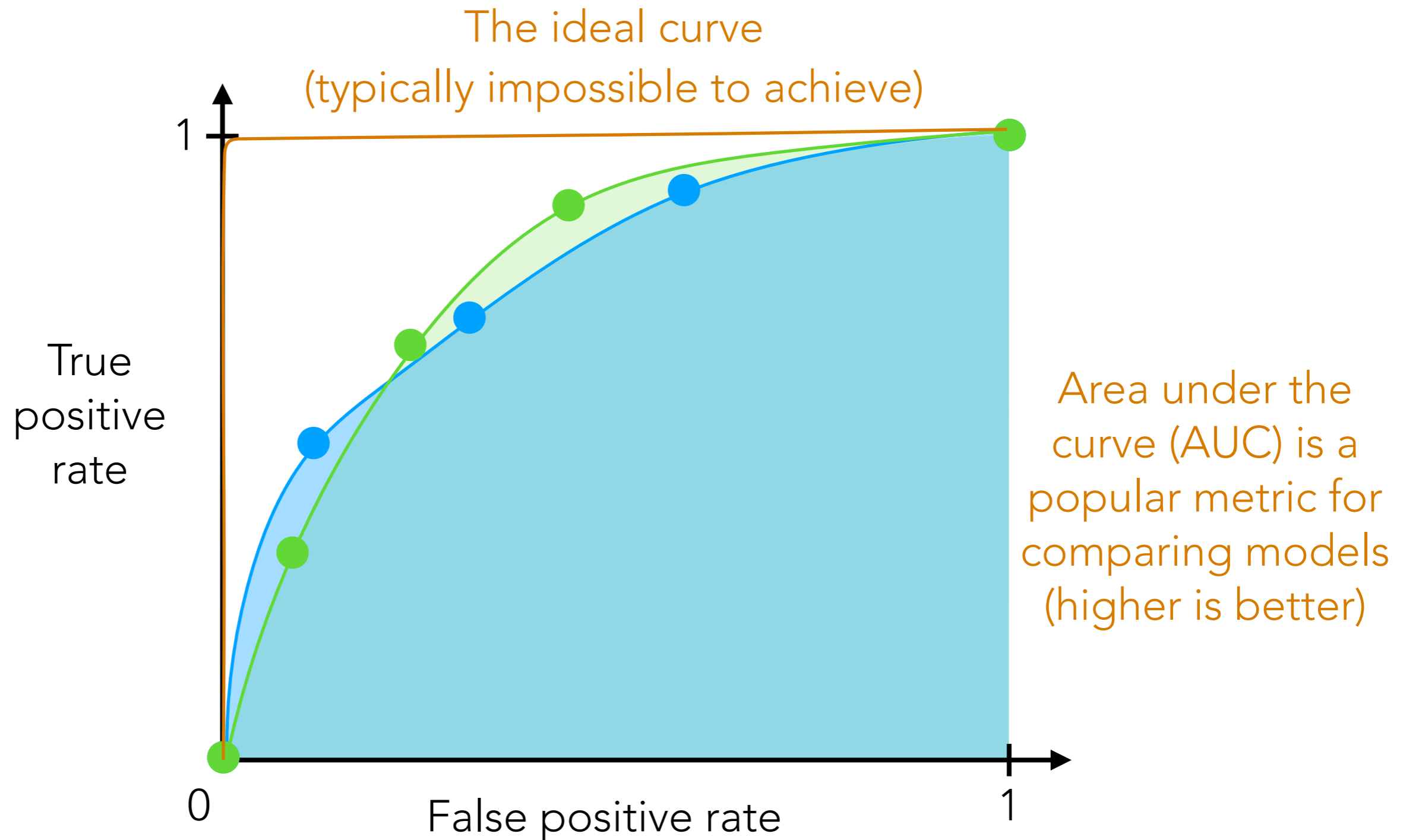


Binary Classification: ROC Curves

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



Binary Classification: ROC Curves



Binary Classification: ROC Curves

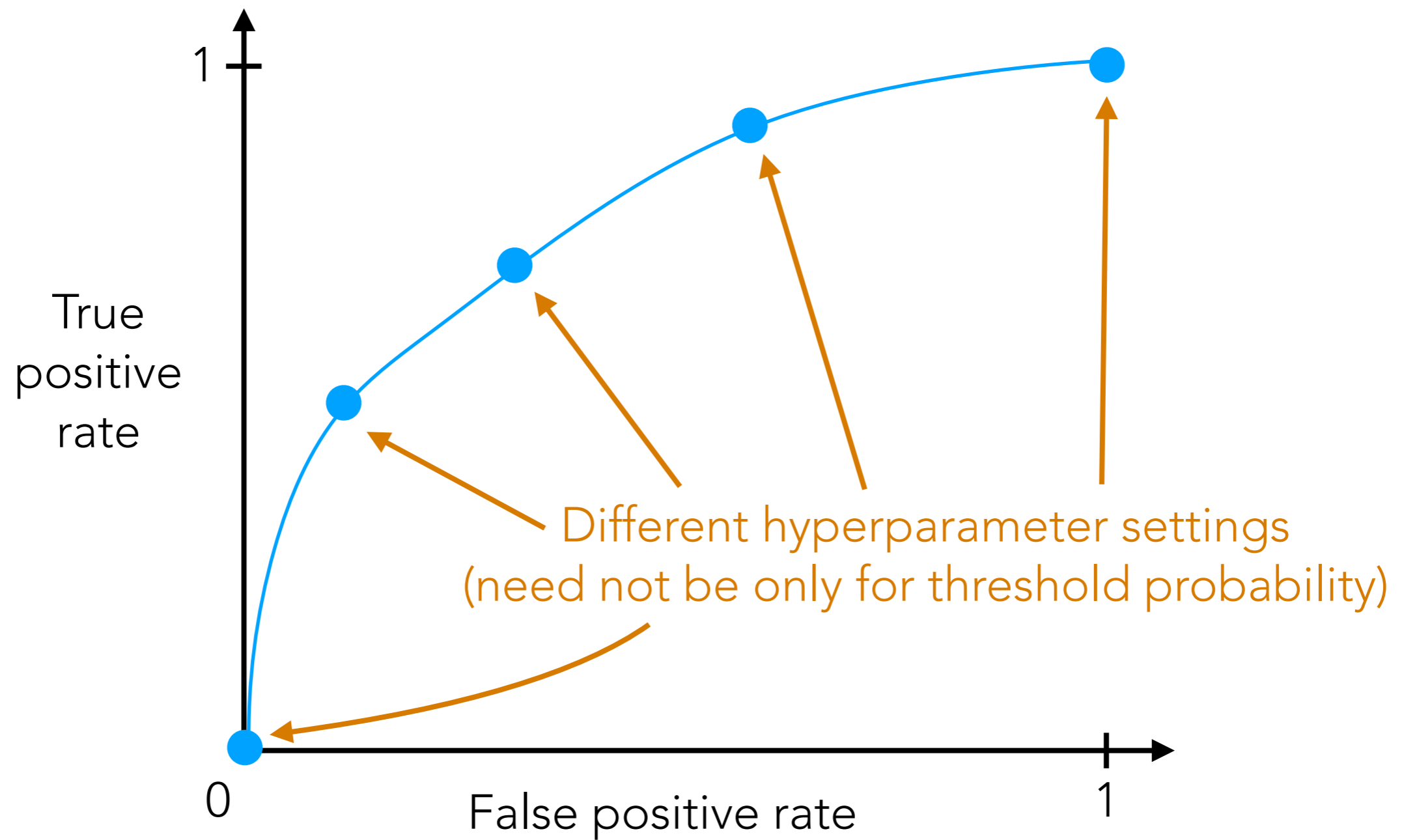
What we just saw:

- 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!

One more PyTorch thing...

Constructing PyTorch Models with `nn.Module`

```
deeper_model = nn.Sequential(nn.Flatten(),
                             nn.Linear(in_features=784, out_features=512),
                             nn.ReLU(),
                             nn.Linear(in_features=512, out_features=10))
```

Another way to write this (we'll need this level of detail for next lecture):

```
class DeeperModel(nn.Module):
    def __init__(self, num_in_features, num_intermediate_features, num_out_features):
        super().__init__()
        self.flatten = nn.Flatten()
        self.linear1 = nn.Linear(num_in_features, num_intermediate_features)
        self.relu = nn.ReLU()
        self.linear2 = nn.Linear(num_intermediate_features, num_out_features)

    def forward(self, inputs):
        flatten_output = self.flatten(inputs)
        linear1_output = self.linear1(flatten_output)
        relu_output = self.relu(linear1_output)
        linear2_output = self.linear2(relu_output)
        return linear2_output

deeper_model = DeeperModel(784, 512, 10)
```