Carnegie Mellon University
Heinz College

95-865: Introduction to Predictive Data Analytics

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Disclaimer: unfortunately “*k*” means many things

Announcements

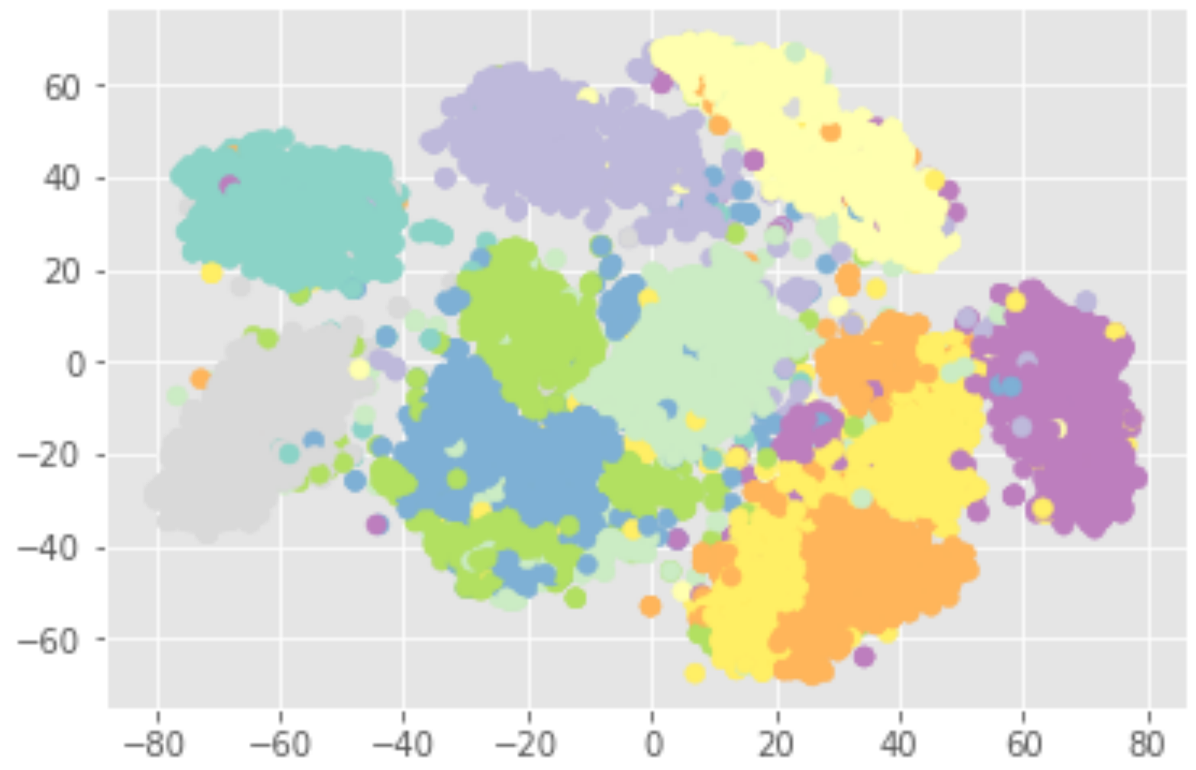
- Due **tomorrow**: taxes
- Due Wednesday 10:30am: HW2
- Final exam: **Tuesday May 8, 1pm, $\boxed{\textbf{HBH 1002}}$** different room!
  - Similar format to the quiz (but you'll get 3 hours)
- My office hours are back to the usual time (Wednesday 3pm-5pm, HBH 2216)

Previous Lecture: Topic Modeling

- There are actually *many* topic models, not just LDA & HDP
    - Correlated topic models, Pachinko allocation,
      biterm topic models, anchor word topic models, …

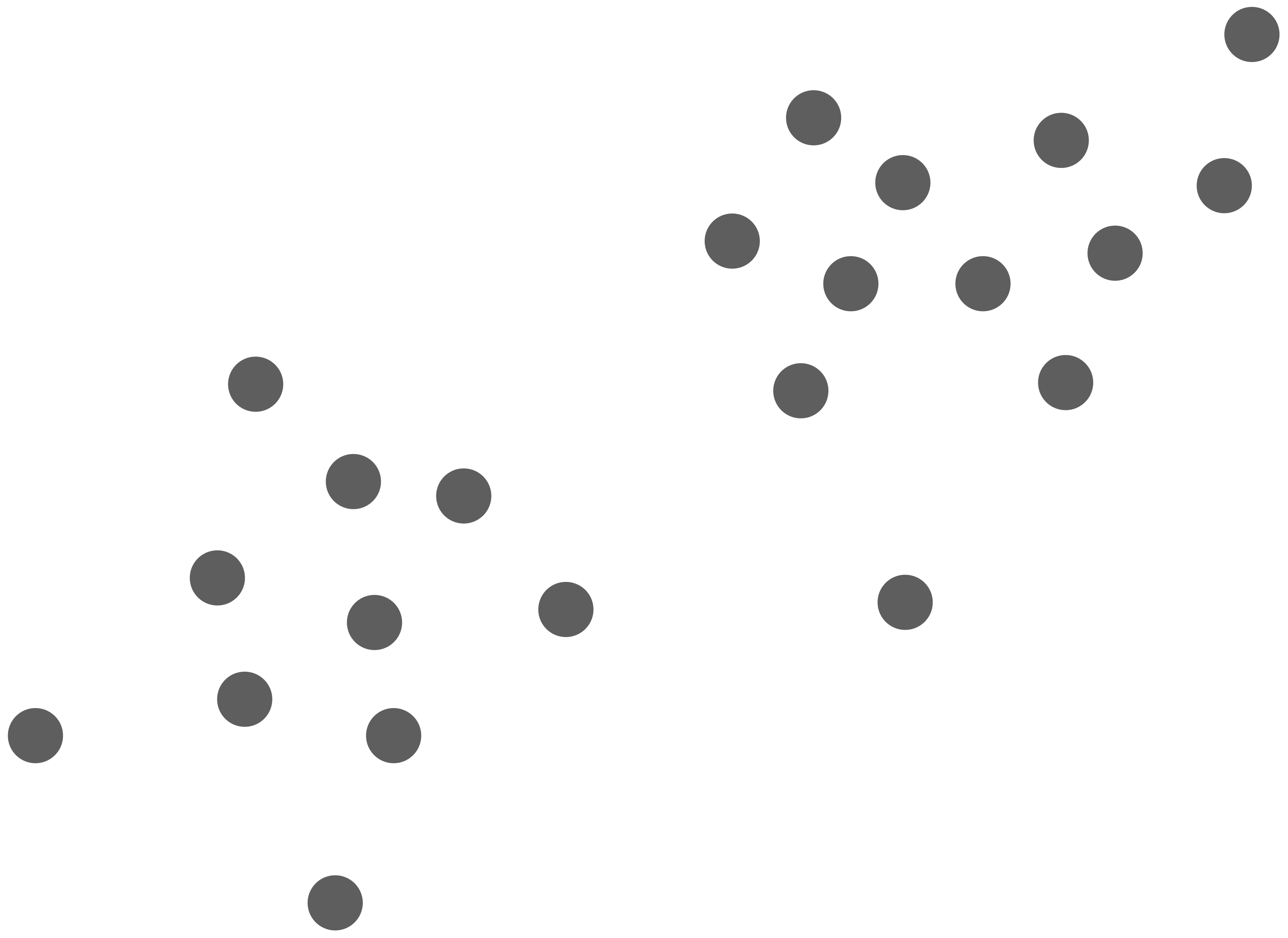
- Dynamic topic models: tracks how topics change *over time*
    - This sort of idea could be used to figure out how user tastes change over time in a recommendation system
        - Could try to see if there are existing patterns for how certain topics become really popular

What if we have labels?



Example: MNIST handwritten digits have known labels

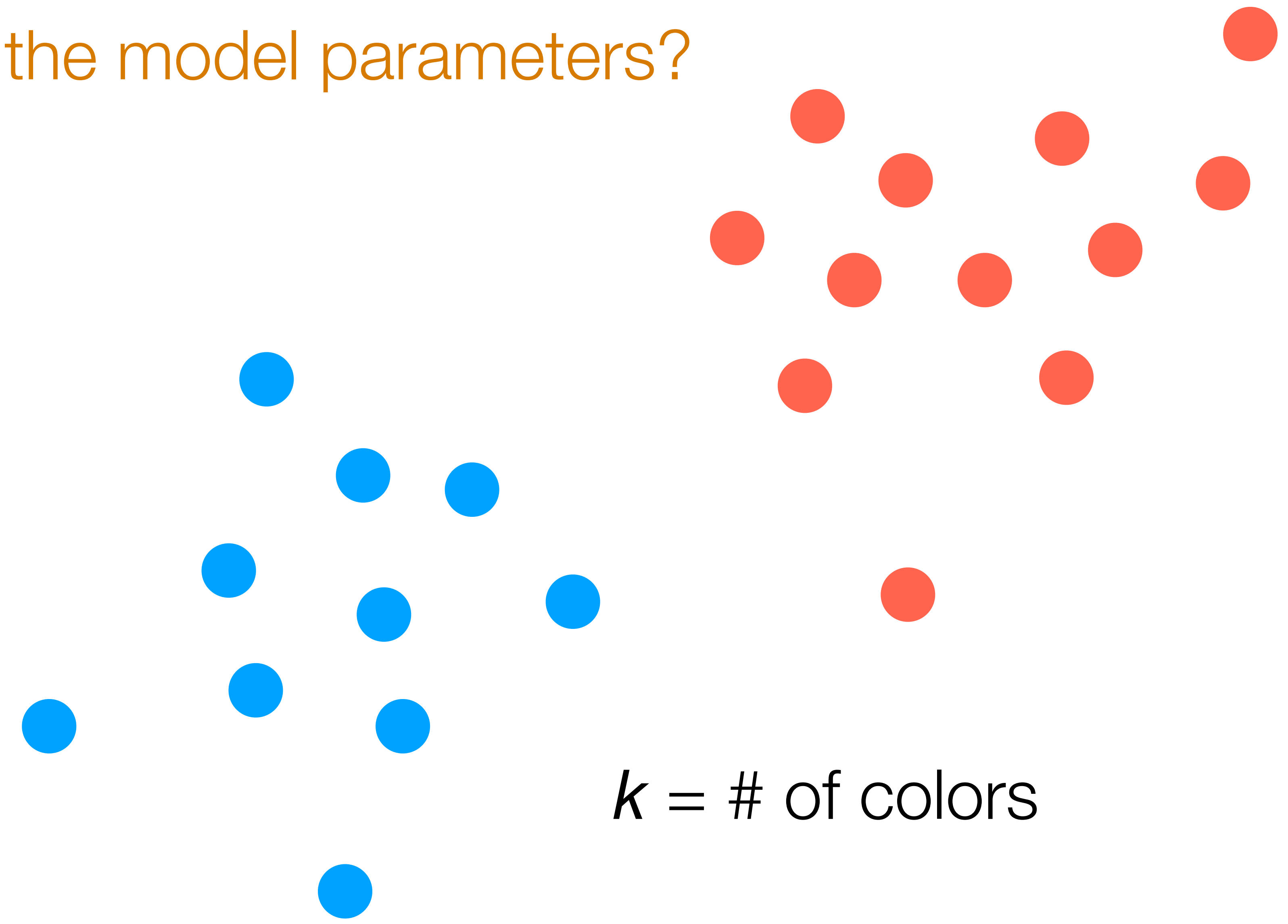
If the labels are known…



If the labels are known…

And we assume data generated by GMM…

What are the model parameters?



k = # of colors

We can directly estimate cluster means, covariances

Flashback: Learning a GMM

Don’t need this top part if we know the labels!

~~Step 0: Pick *k*~~

~~Step 1: Pick guesses for **cluster means and covariances**~~

~~**Repeat until convergence:**~~

~~Step 2: Compute probability of each point belonging to each of the *k* clusters~~

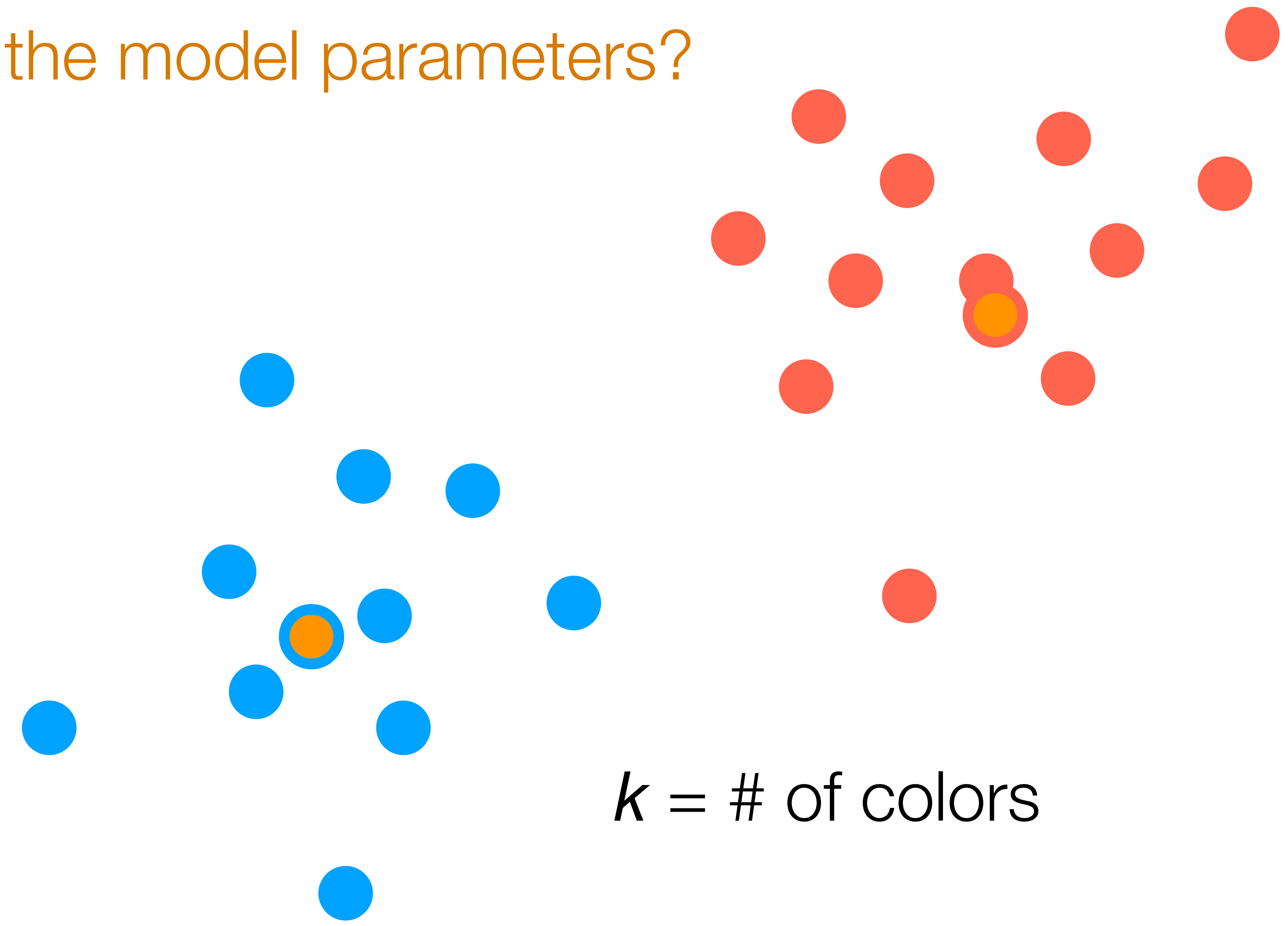
Step 3: Update **cluster means and covariances** carefully accounting for probabilities of each point belonging to each of the clusters

We don’t need to repeat until convergence

If the labels are known…

And we assume data generated by GMM…

What are the model parameters?



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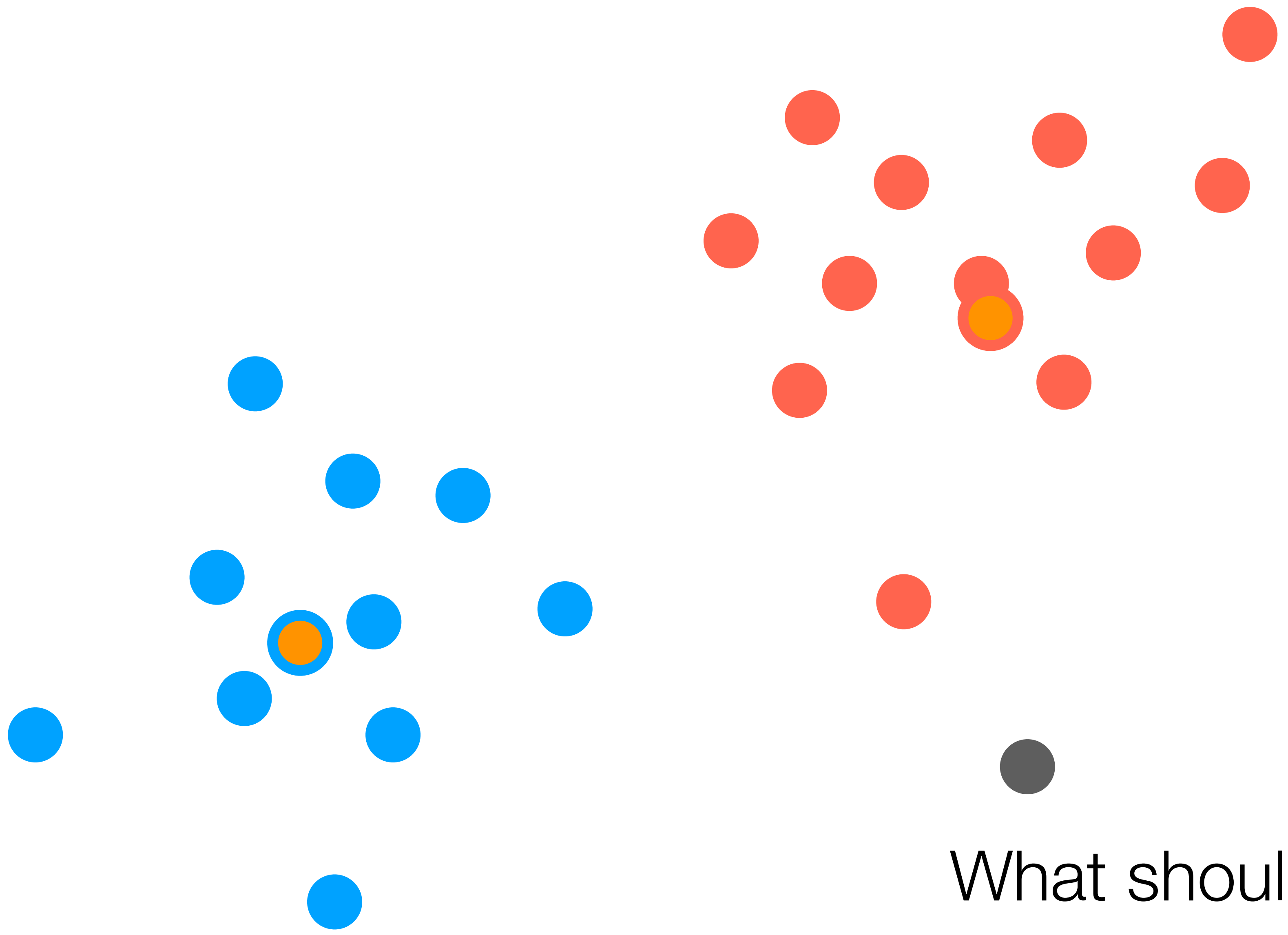
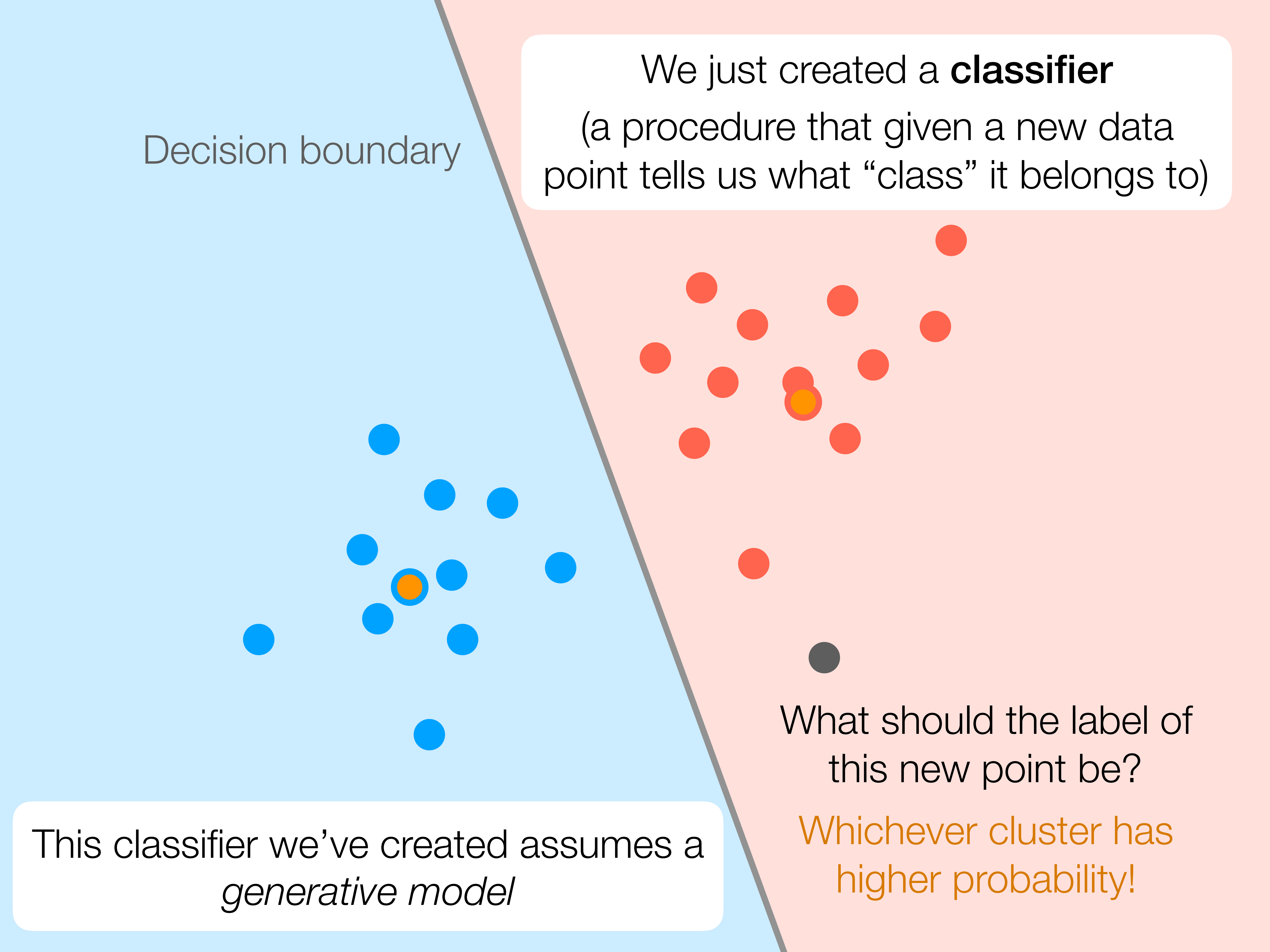


What should the label of this new point be?

Whichever cluster has higher probability!



We just created a **classifier**

(a procedure that given a new data point tells us what "class" it belongs to)

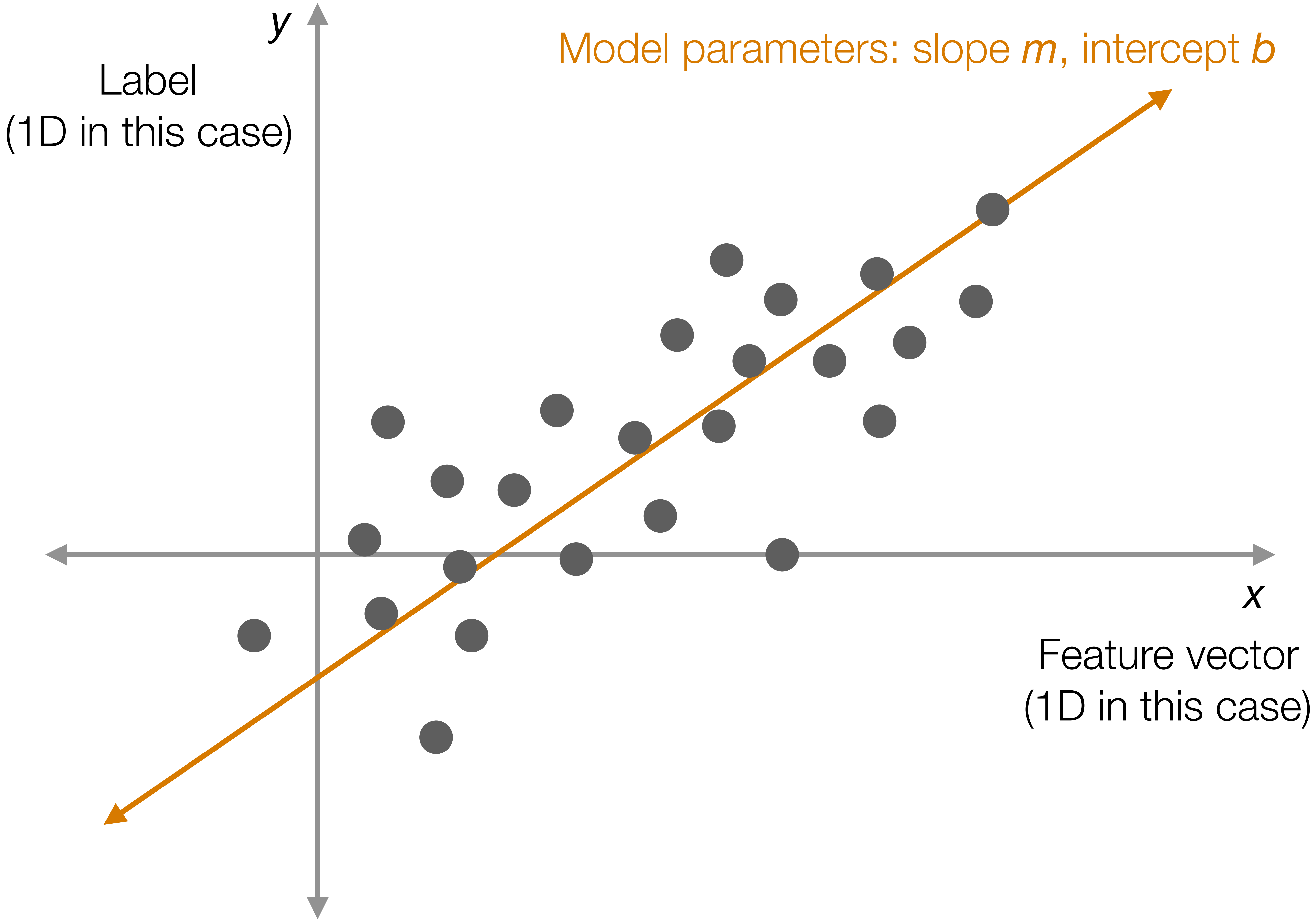
What should the label of this new point be?

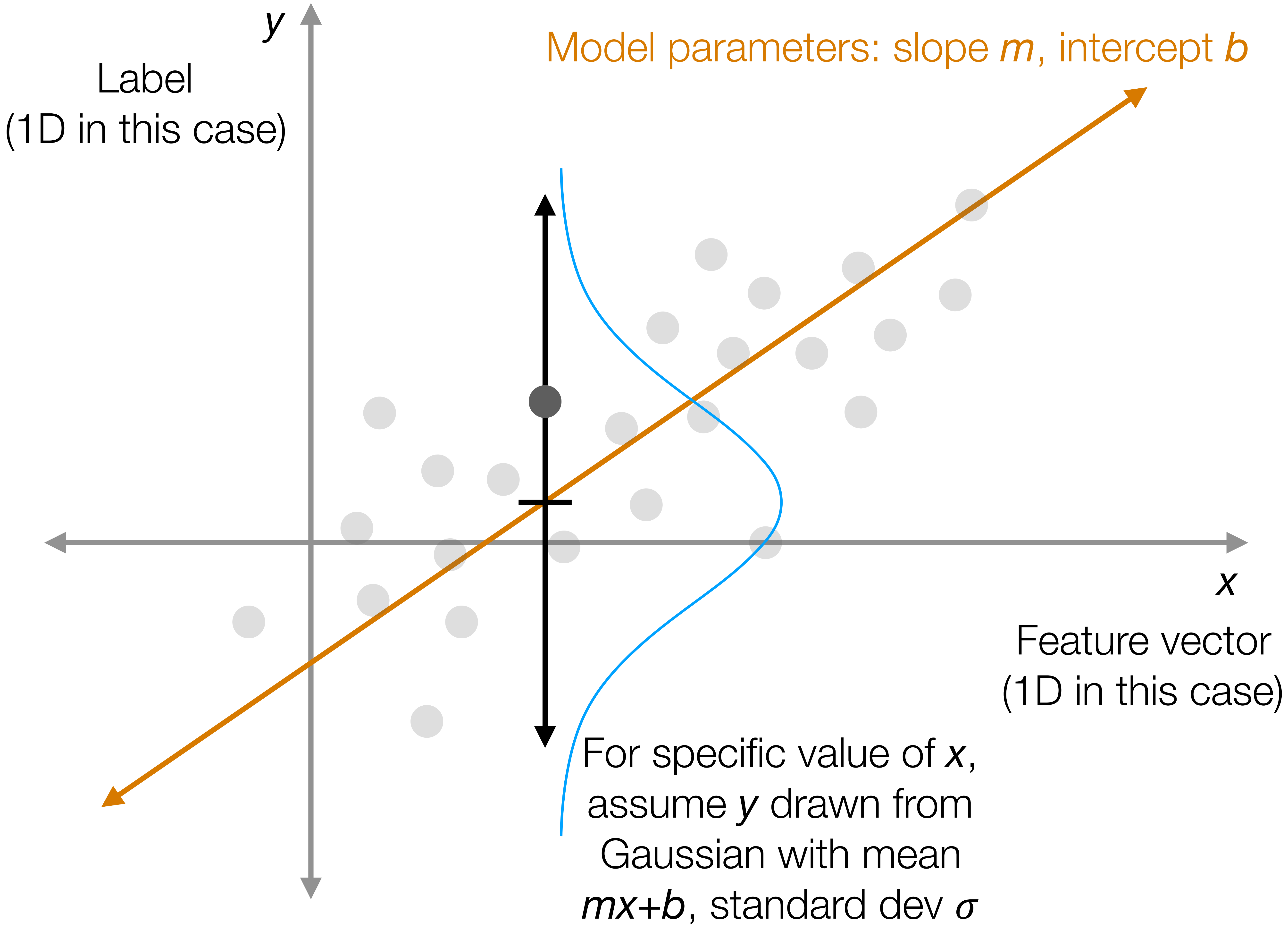
Whichever cluster has higher probability!

This classifier we've created assumes a *generative model*

You’ve seen generative models before for prediction

Linear regression!


y
Label
(1D in this case)
Model parameters: slope m, intercept b
x
Feature vector
(1D in this case)


y
Label
(1D in this case)
Model parameters: slope *m*, intercept *b*
x
Feature vector
(1D in this case)
For specific value of *x*,
assume *y* drawn from
Gaussian with mean
mx+*b*, standard dev *σ*

Predictive Data Analysis

Training data

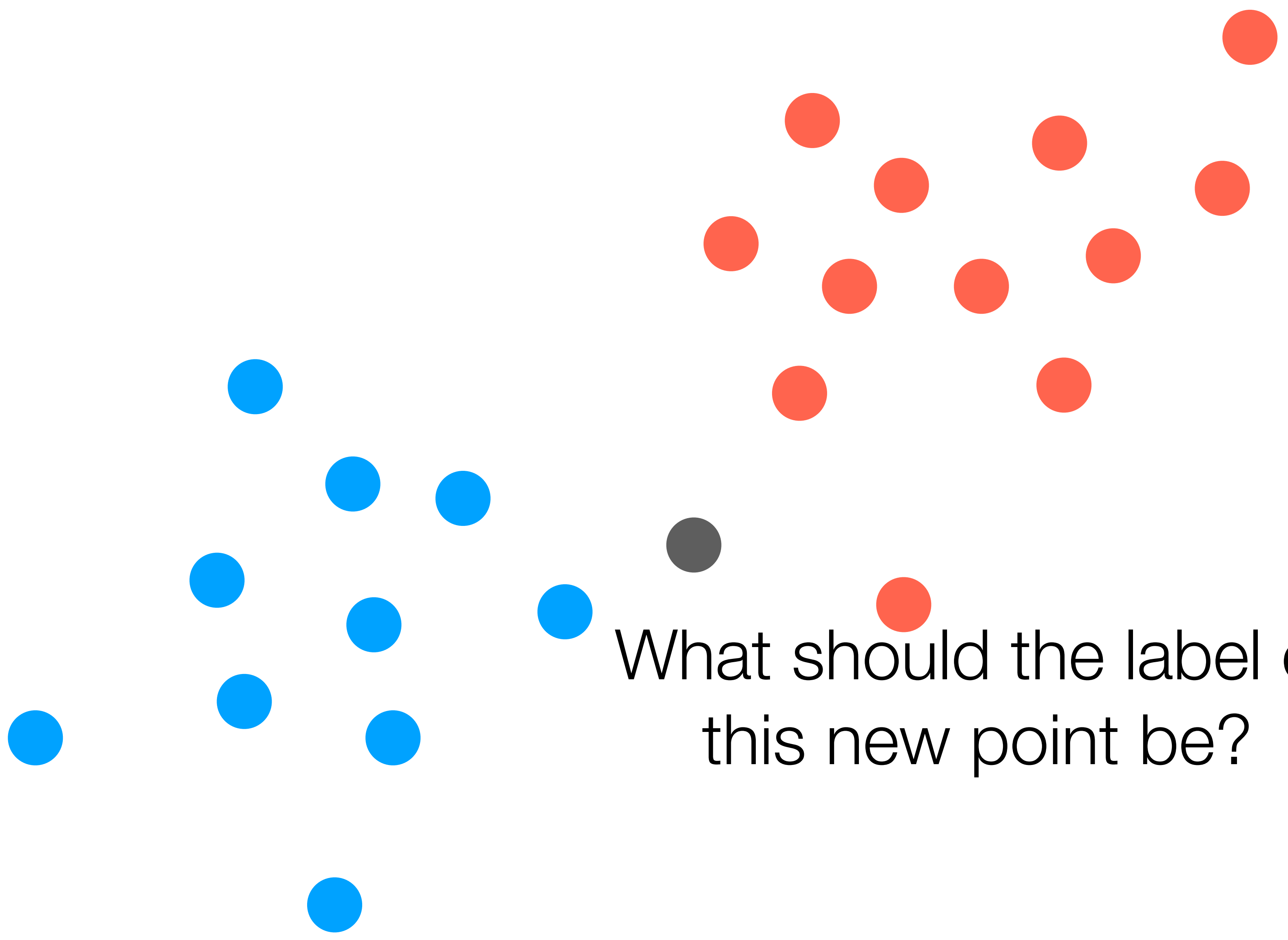
$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$$

Goal: Given new feature vector *x*, predict label *y*

- *y* is discrete (such as colors red and blue)
  ➔ prediction method is called a **classifier**
- *y* is continuous (such as a real number)
  ➔ prediction method is called a **regressor**

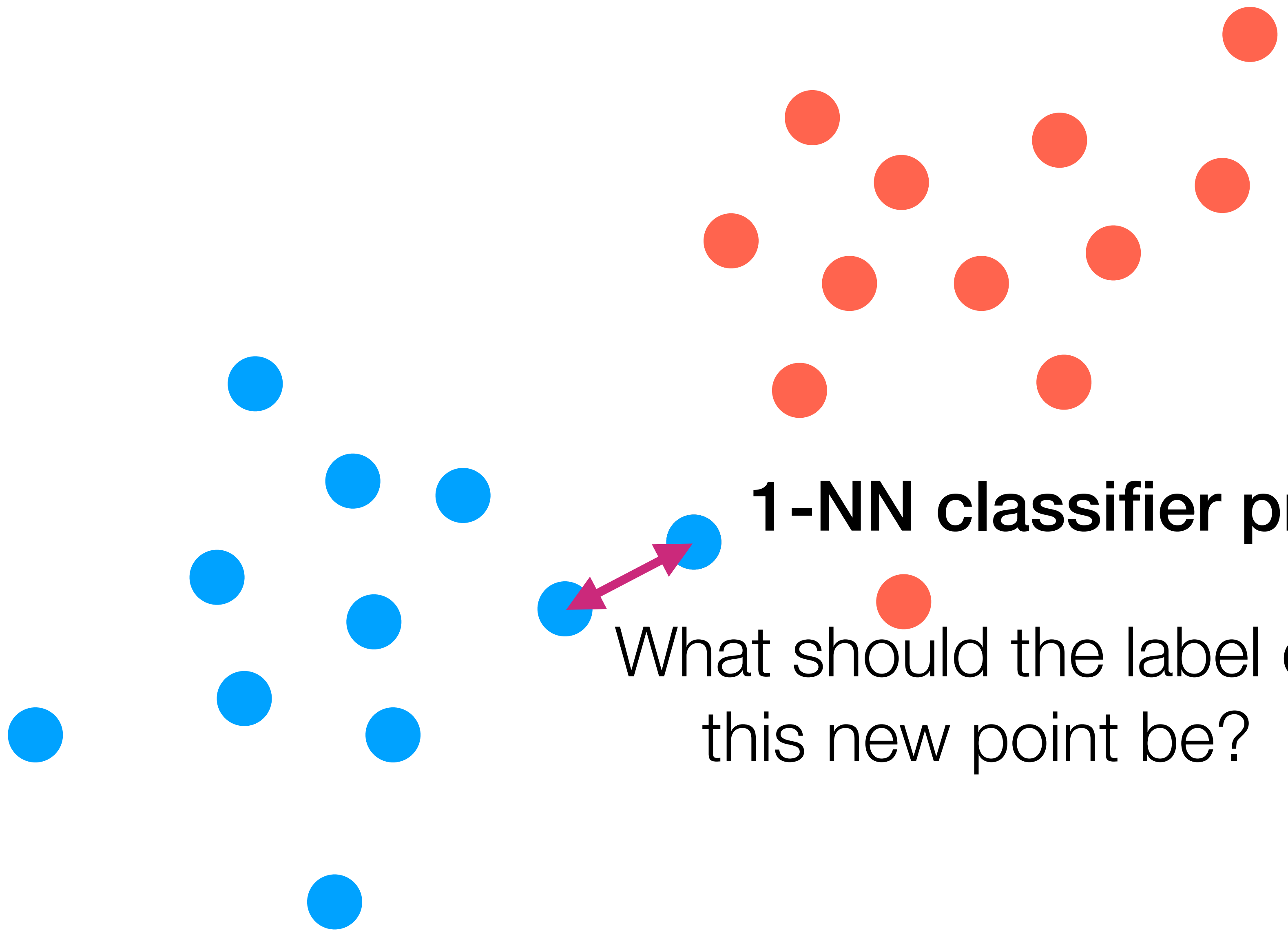
A giant zoo of methods

Example: *k*-NN Classification

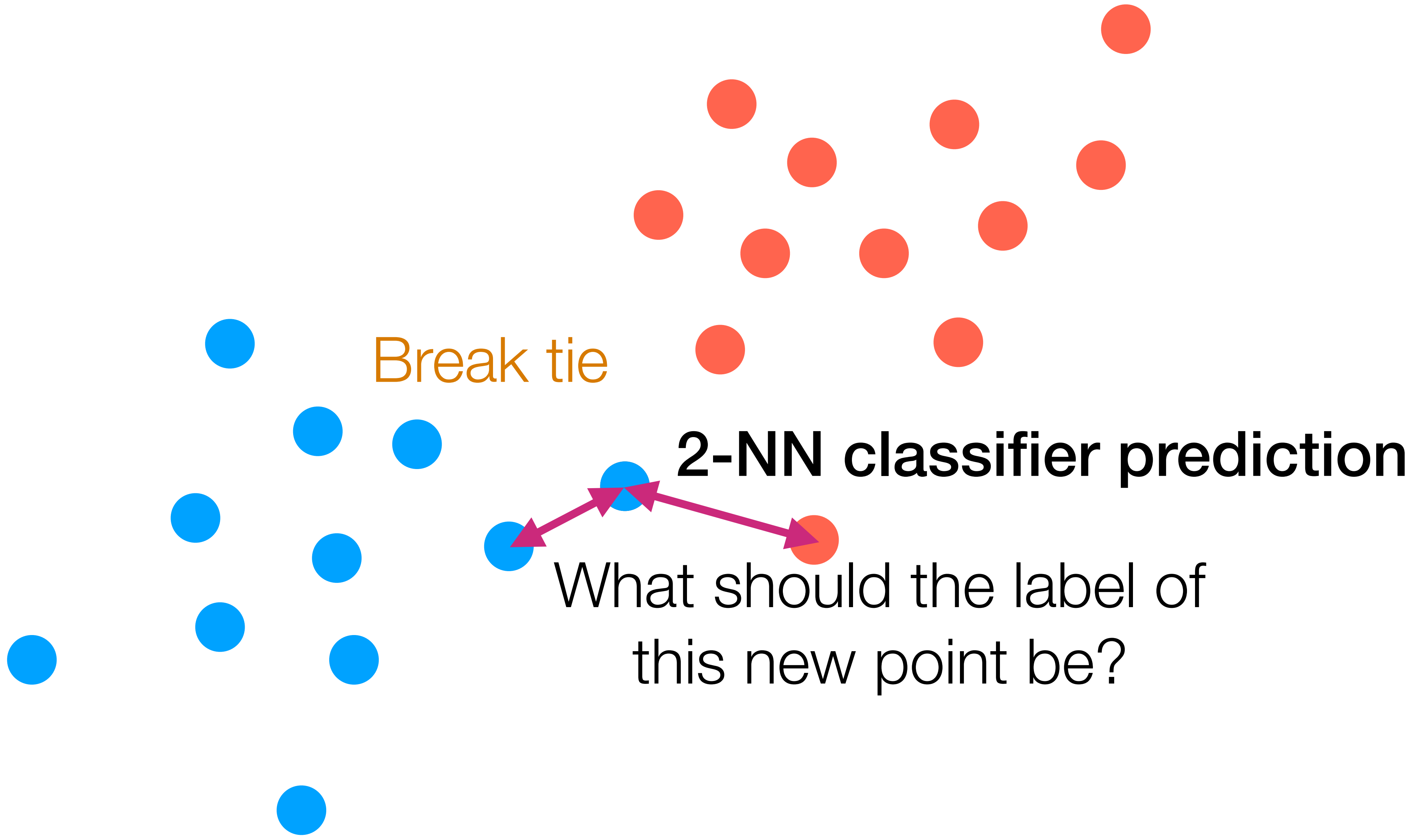


What should the label of
this new point be?

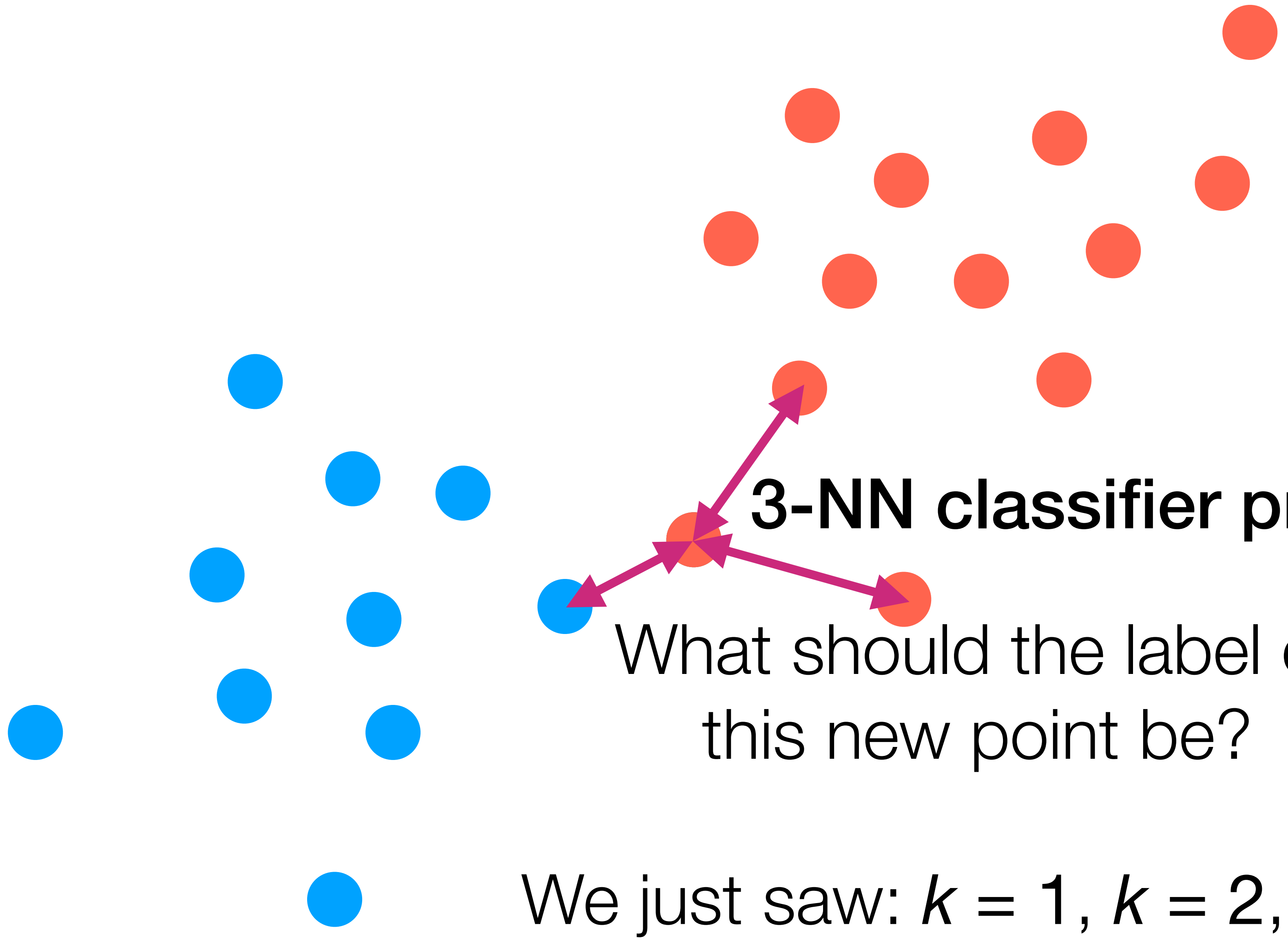
Example: *k*-NN Classification


1-NN classifier prediction
What should the label of this new point be?

Example: *k*-NN Classification


Break tie
2-NN classifier prediction
What should the label of this new point be?

Example: *k*-NN Classification



3-NN classifier prediction

What should the label of
this new point be?

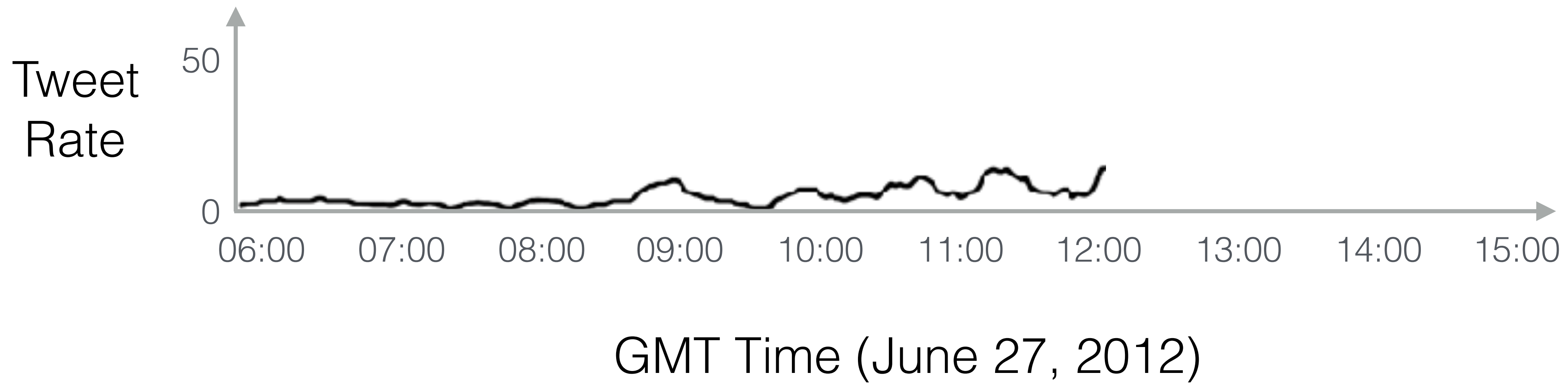
We just saw: k = 1, k = 2, k = 3

What happens if $k = n$?

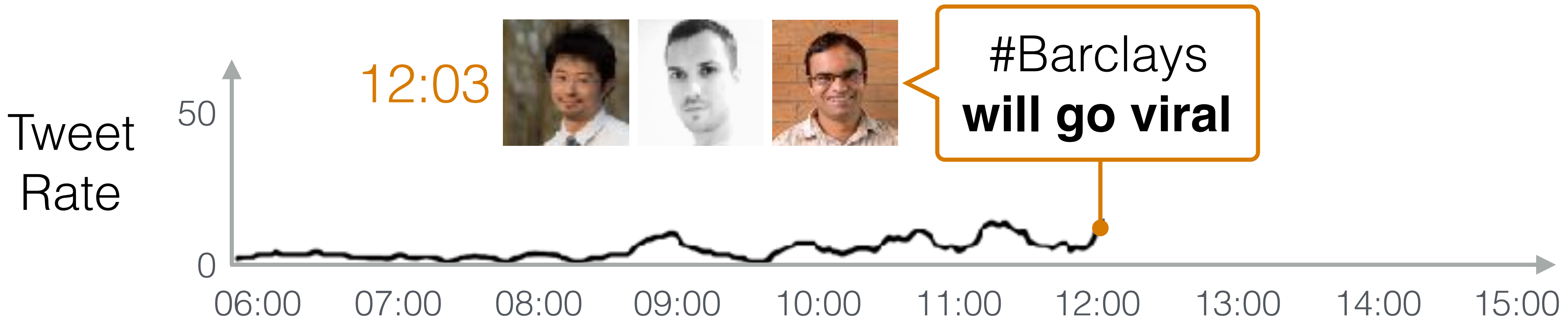
Generalization of *k*-NN classification: weighted majority voting

BARCLAYS

News Activity for #Barclays

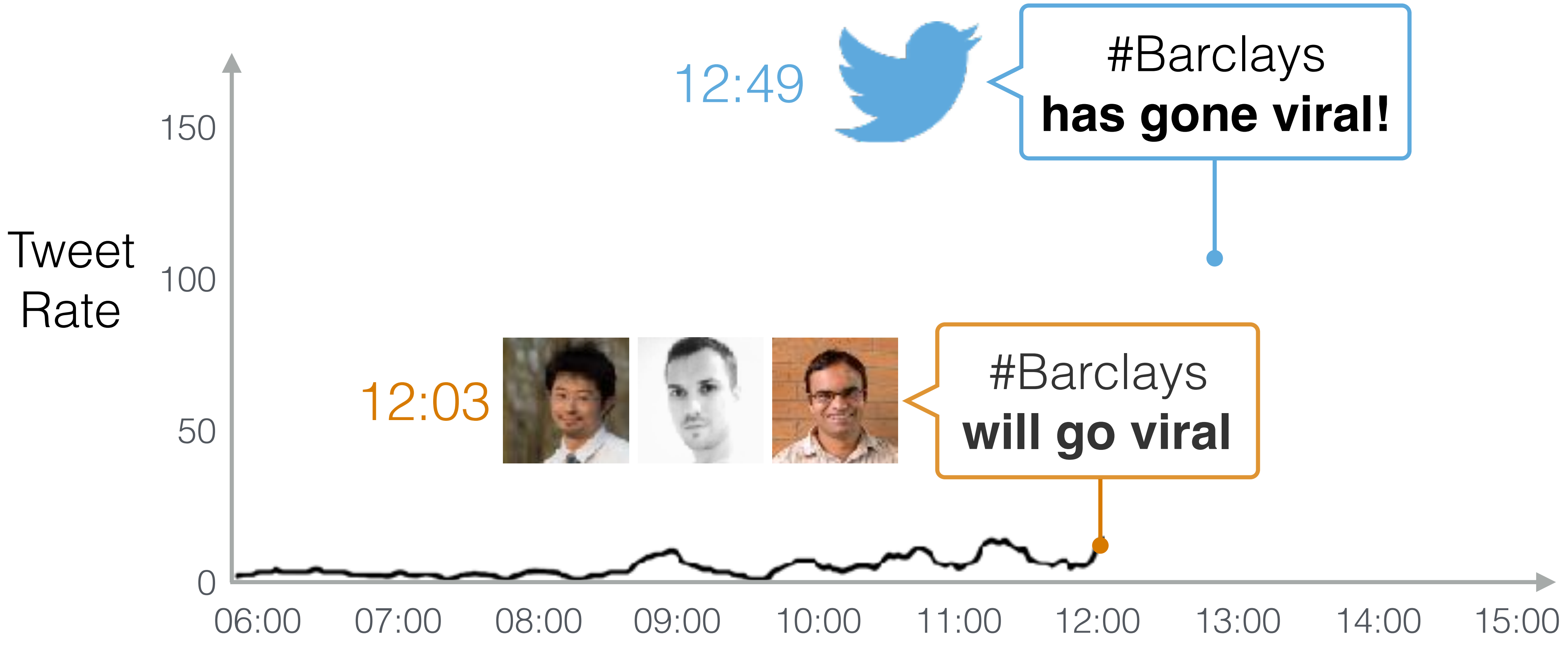


News Activity for #Barclays



GMT Time (June 27, 2012)

News Activity for #Barclays

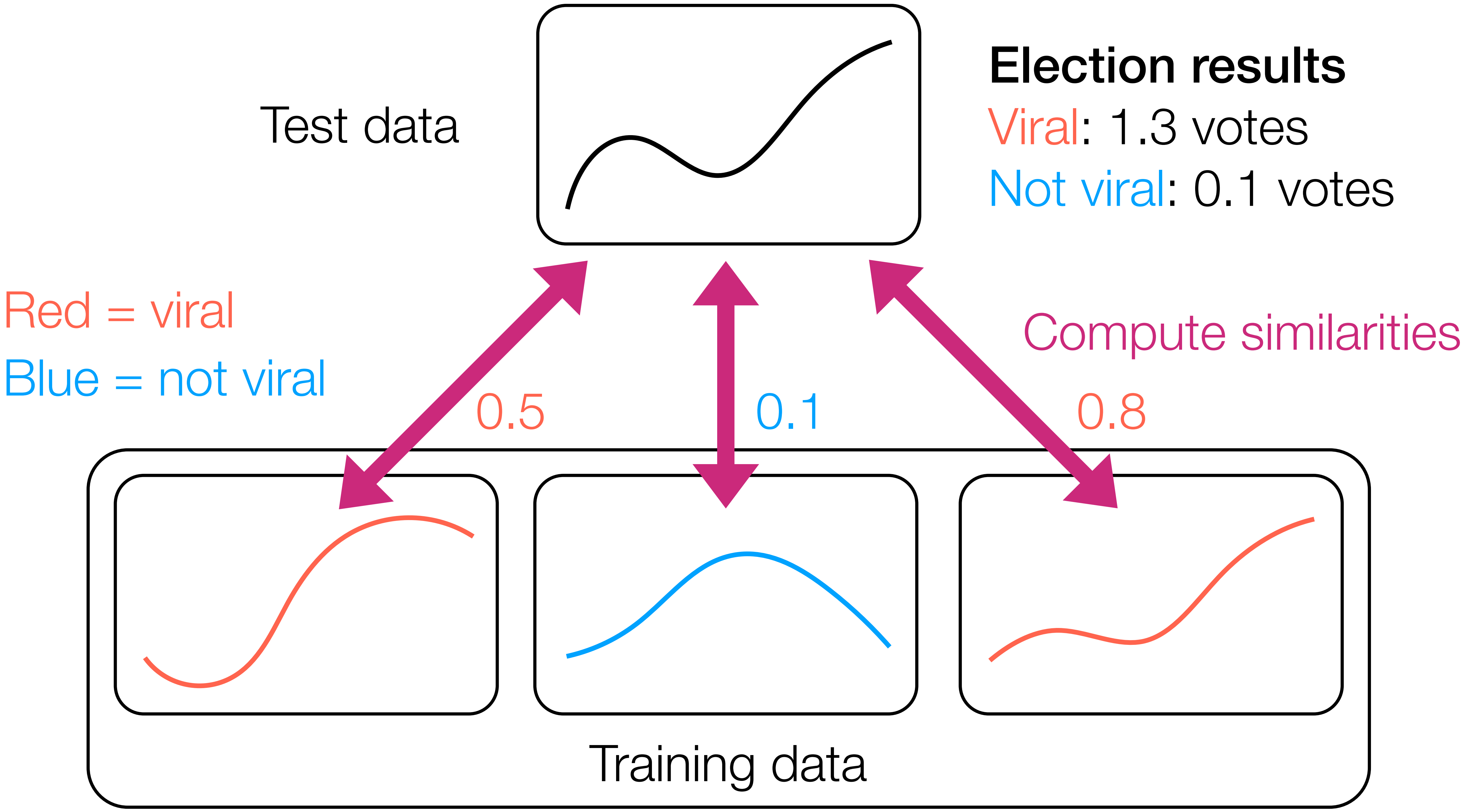


GMT Time (June 27, 2012)

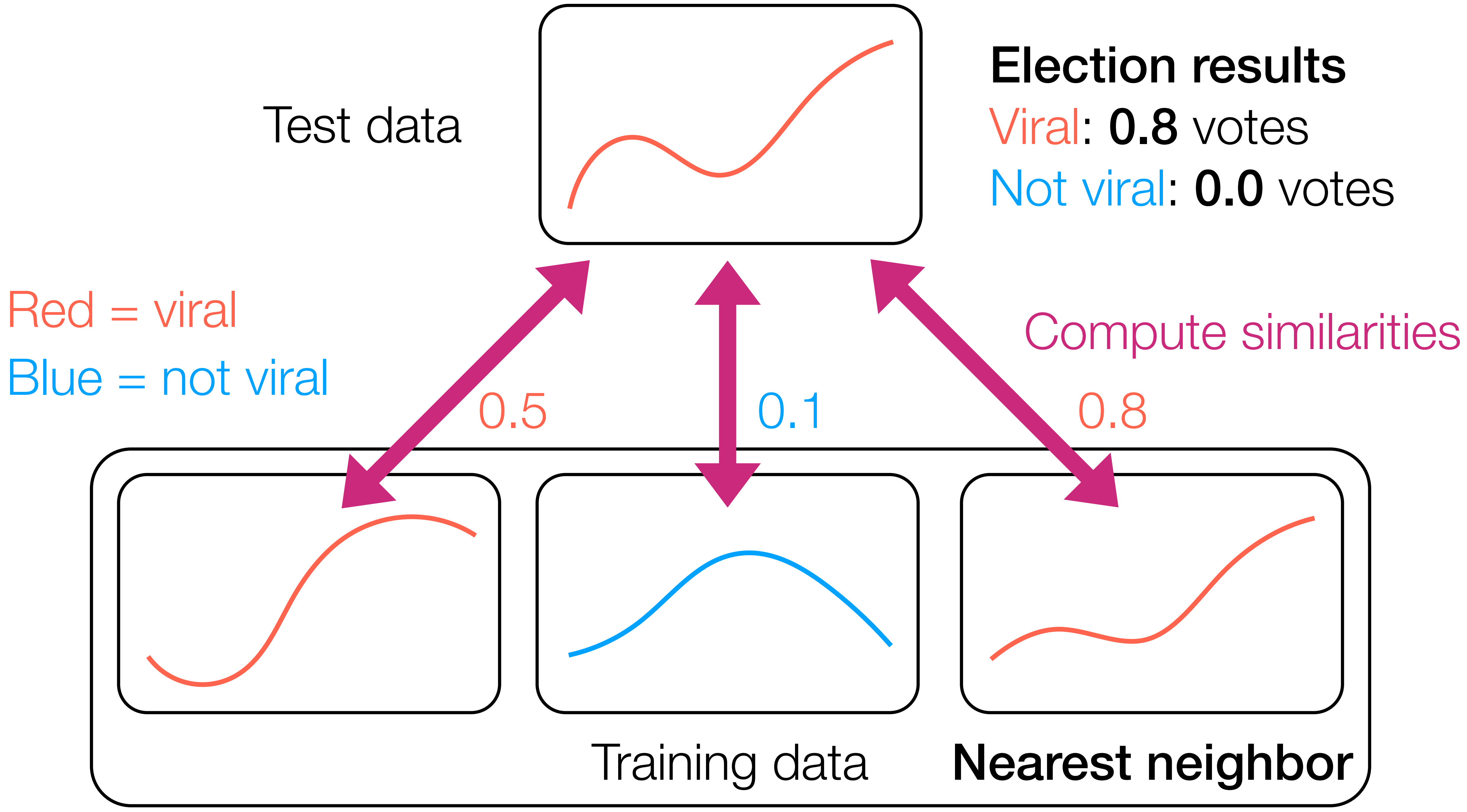
How we did this: **weighted majority voting**

Chen, Nikolov, and Shah. A Latent Source Model for Nonparametric Time Series Classification. NIPS 2013.

Weighted Majority Voting



Nearest Neighbor Classification



NN Classification Variants

not the same *k* as in *k*-means

- ***k*-NN classification:** consider *k* most similar training data to test data point
    - **Weighted:** when tallying up votes, use the similarities that we computed
    - **Unweighted:** when tallying up votes, have each of the *k* nearest neighbors have an equal vote of 1
      (terminology: "*k*-NN classification" by default is unweighted)

- **Fixed-radius near neighbor classification:** consider all training data at least some similarity threshold close to test data point (i.e., use all training data distance ≤ *h* away)
    - Once again, can use weighted or unweighted votes

How do we choose *k*?

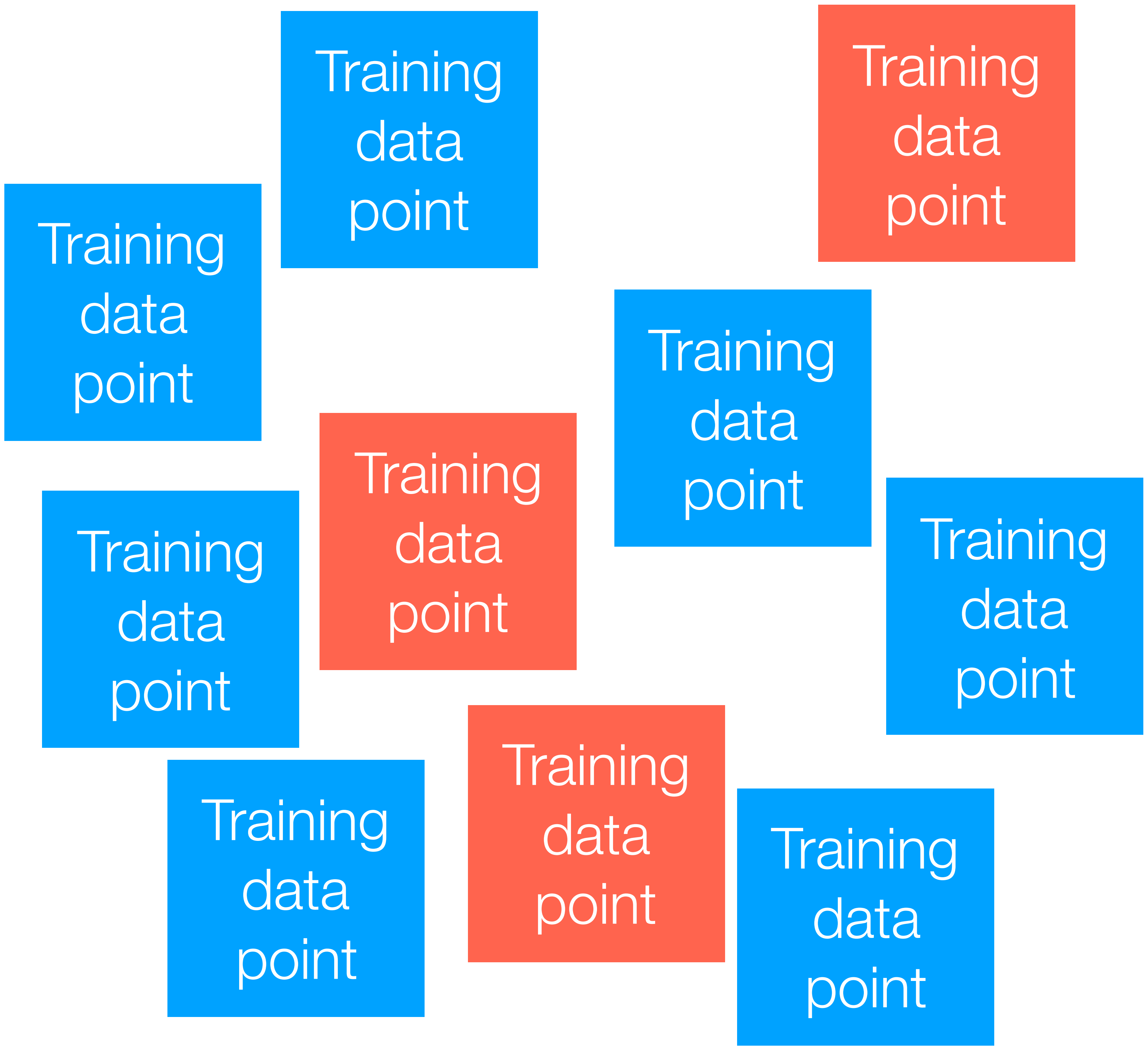
What I'll describe next can be used to select hyperparameter(s) for any prediction method

First: How do we assess how good a prediction method is?

Hyperparameters vs. Parameters

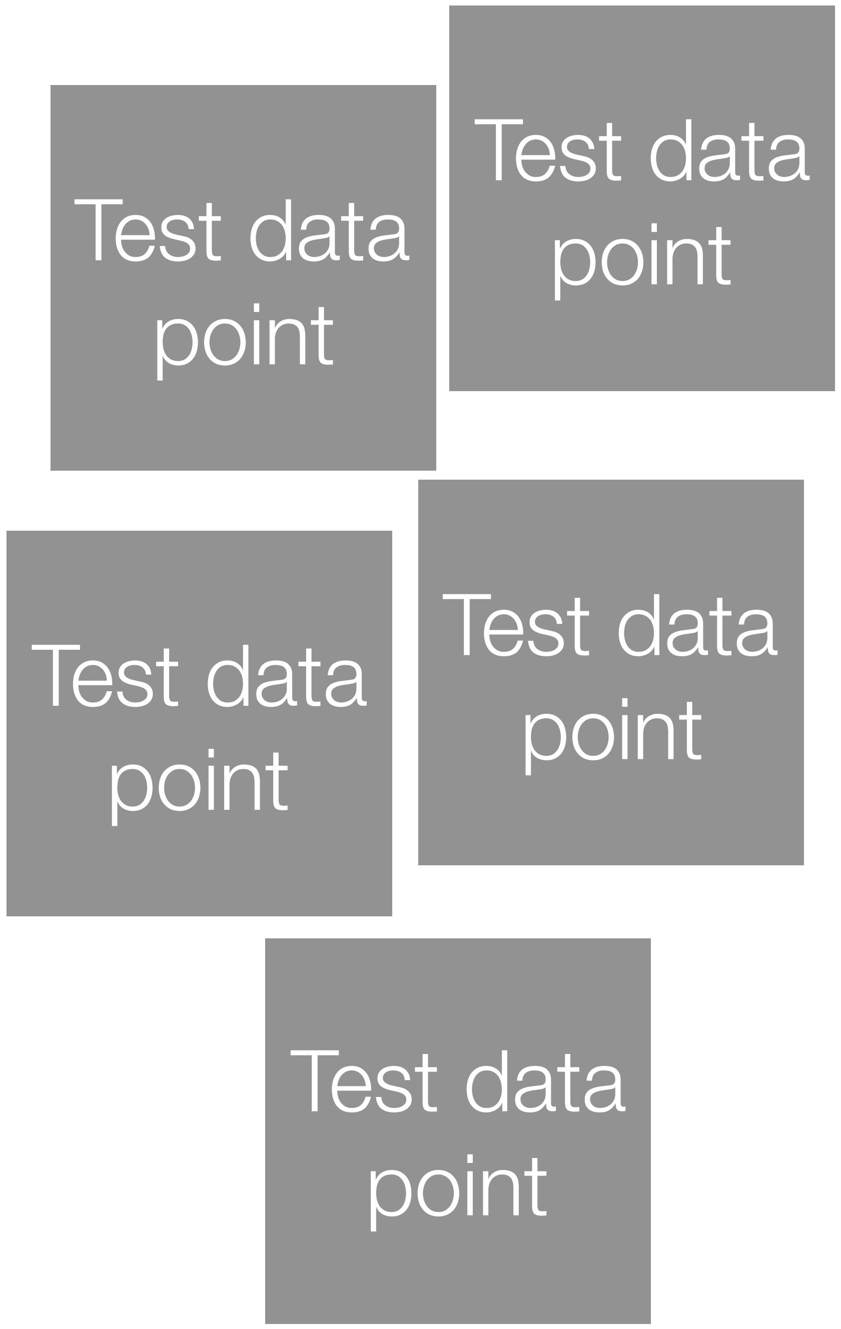
- We fit a model’s parameter to training data (terminology: we “learn” the parameters)
- We pick values of hyperparameters and they do *not* get fit to training data
- Example: Gaussian mixture model
    - Hyperparameter: number of clusters *k*
    - Parameters: cluster probabilities, means, covariances
- Example: *k*-NN classification
    - Hyperparameter: number of nearest neighbors *k*
    - Parameters: N/A

Training data



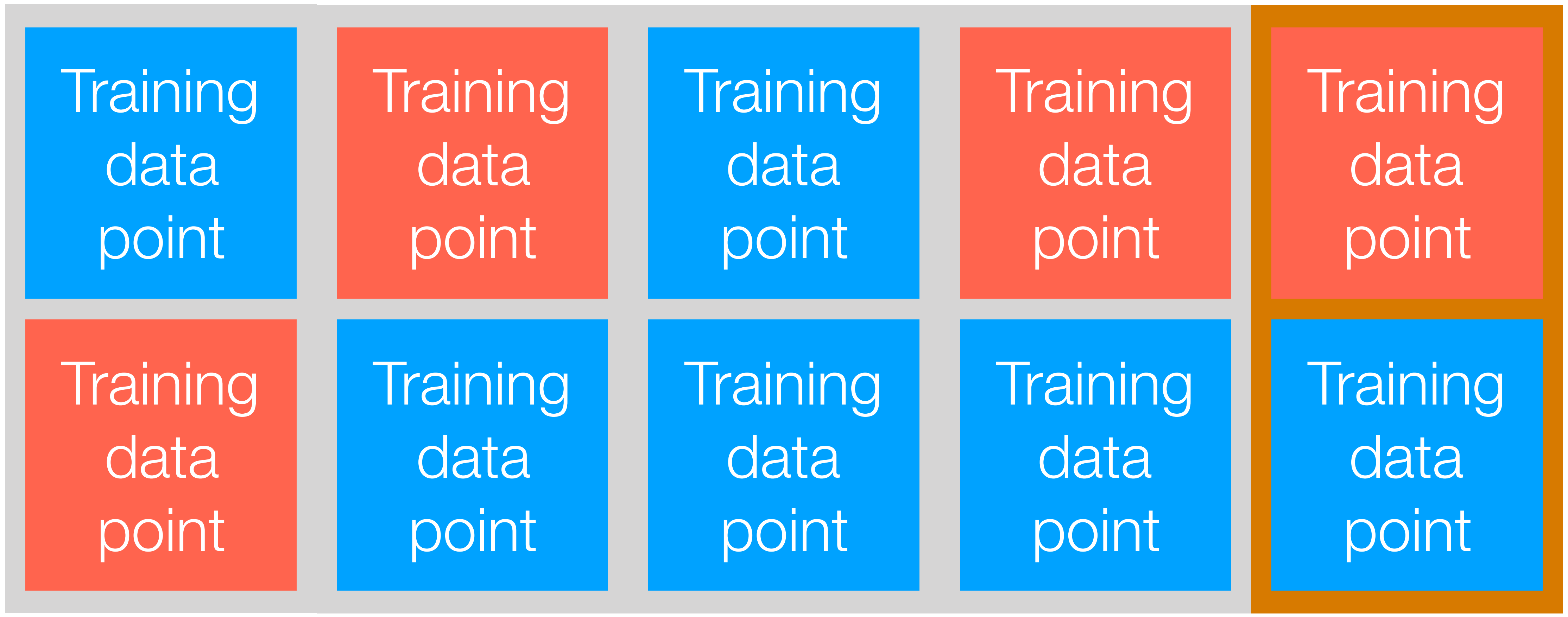
Example: Each data point is an email and we know whether it is spam/ham

Want to classify these points correctly



Example: future emails to classify as spam/ham

Predicted labels

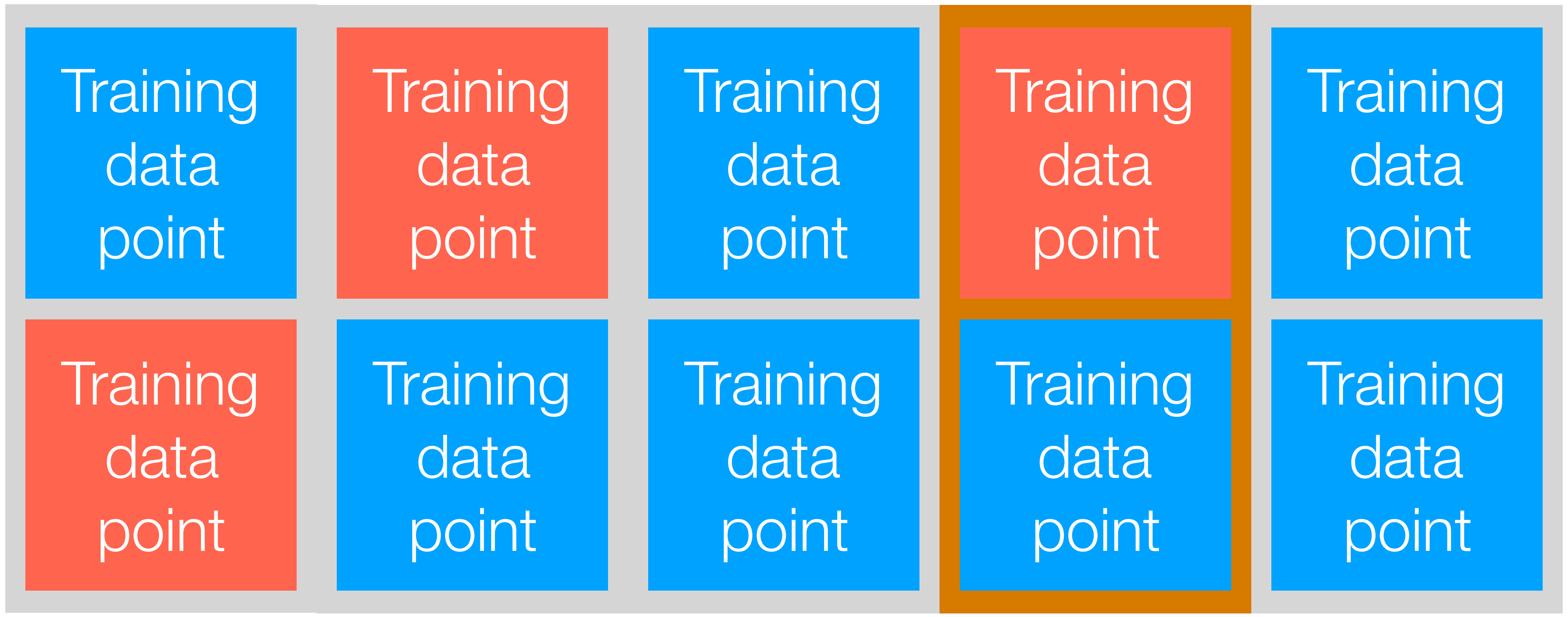


Train method on data in gray

Predict on data in orange

Compute prediction error

50%

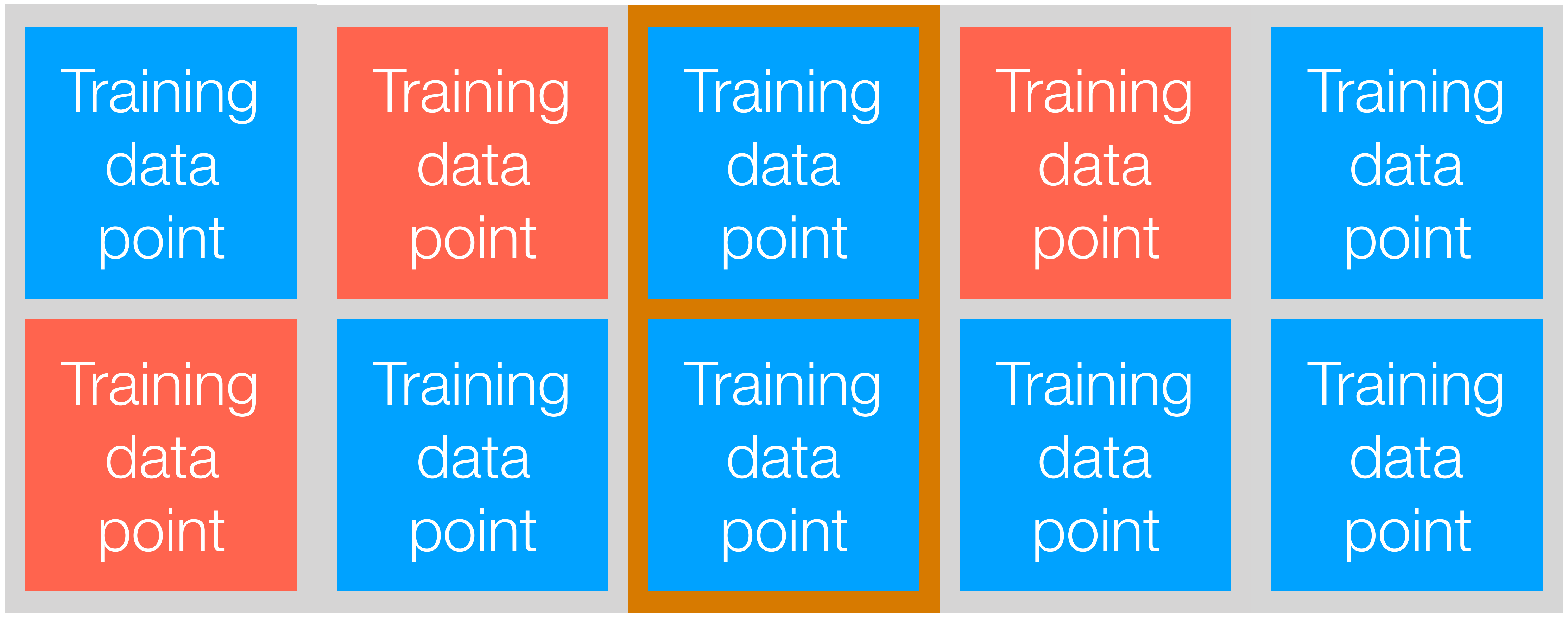


Train method on data in gray

Predict on data in orange

Compute prediction error

0% 50%

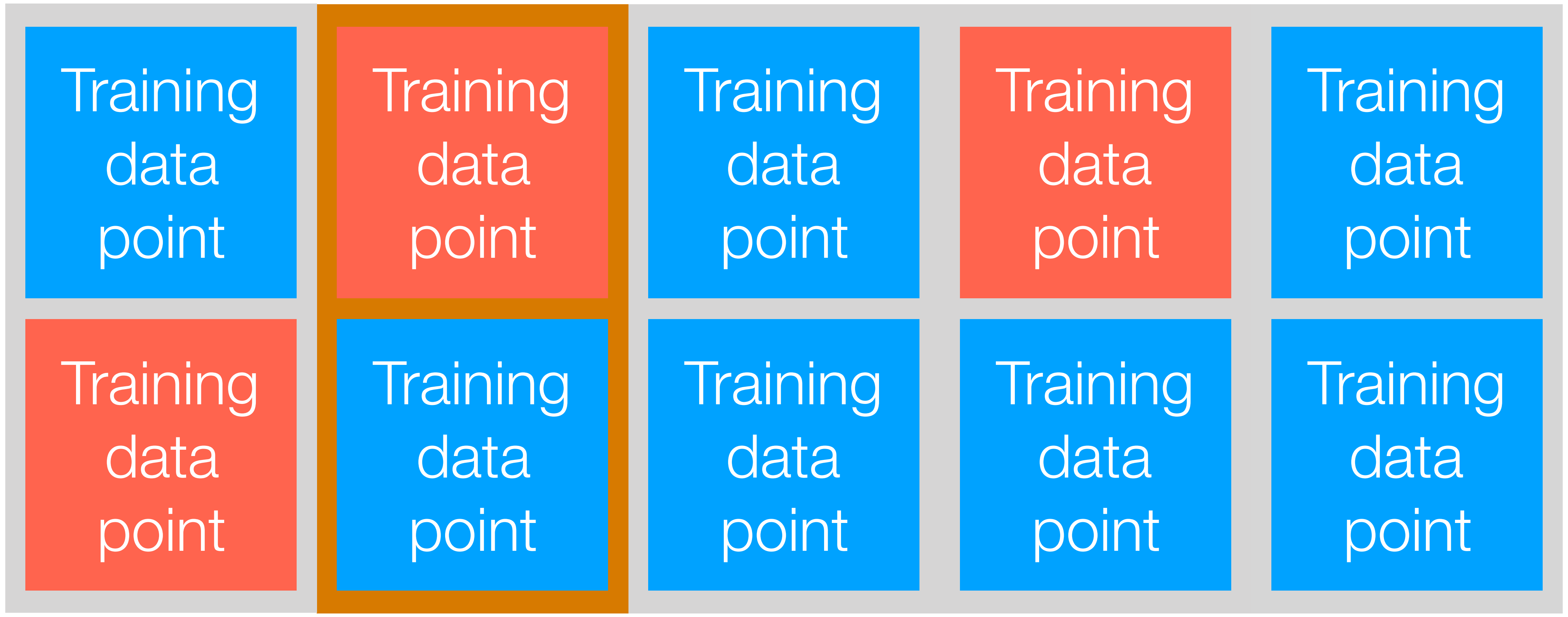


Train method on data in gray

Predict on data in orange

Compute prediction error

50%   0%   50%



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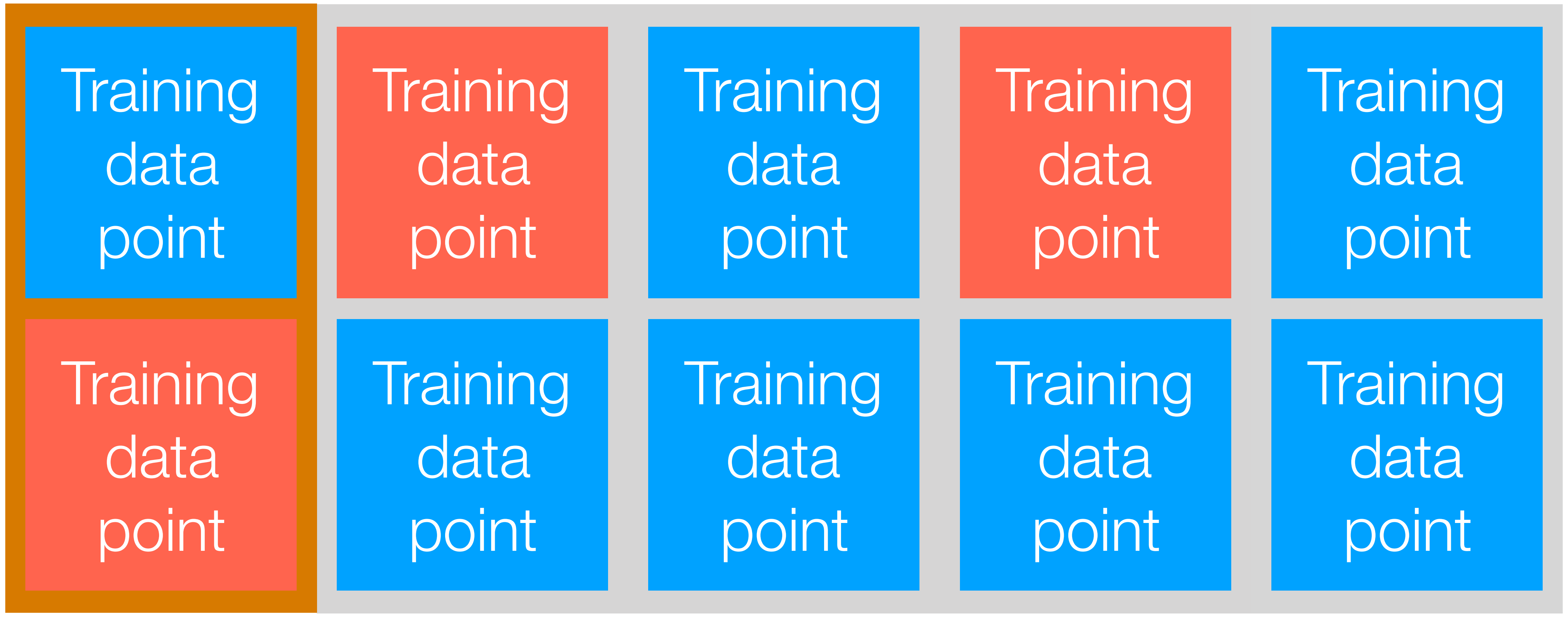
Compute prediction error

0%   50%   0%   50%



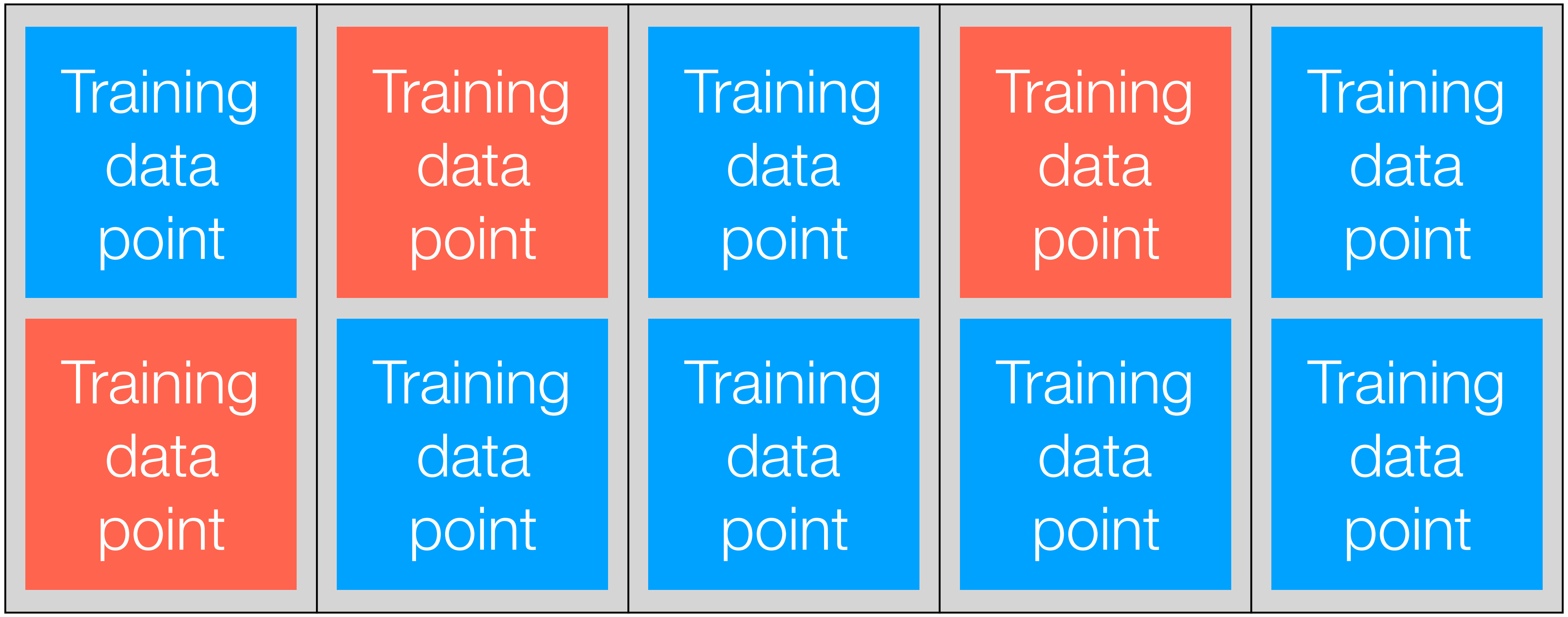
Train method on data in gray

Predict on data in orange

Compute prediction error

0% 0% 50% 0% 50%

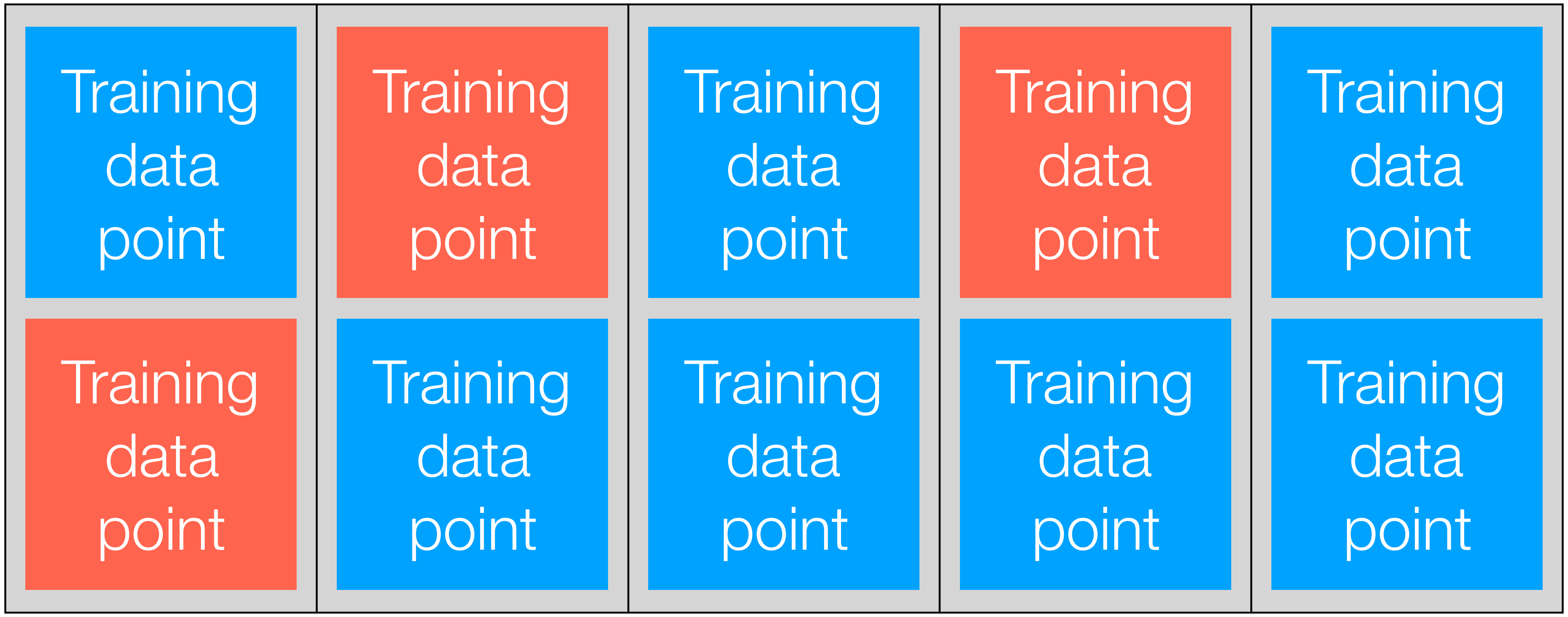
Average error: (0+0+50+0+50)/5 = 20%



1. Shuffle data and put them into “folds” (5 folds in this example)
2. For each fold (which consists of its own train/validation sets):
   (a) Predict on fold’s training data, test on fold’s validation data
   (b) Compute prediction error
3. Compute average prediction error across the folds

not the same *k* as in *k*-means or *k*-NN classification

k-fold Cross Validation



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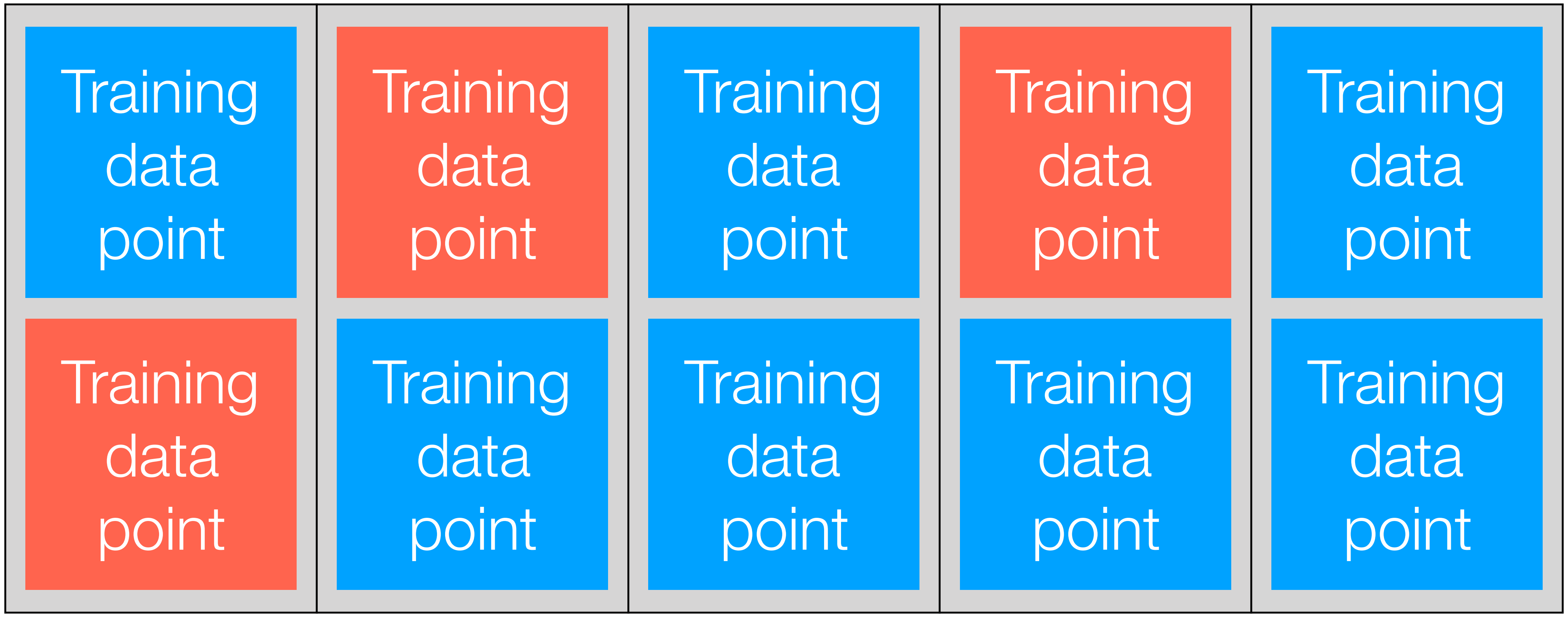


1. Shuffle data and put them into "folds" (*k*=5 folds in this example)
2. For each fold (which consists of its own train/validation sets):
   (a) Predict on fold's training data, test on fold's validation data
   (b) Compute **some sort of prediction score**
3. Compute **average prediction score** across the folds
   "cross validation score"

Choosing *k* in *k*-NN Classification

Note: *k*-NN classifier has a single parameter *k*

For each *k* = 1, 2, 3, …, the maximum *k* you are willing to try:

  Compute 5-fold cross validation score using *k*-NN classifier as prediction method

Use whichever *k* has the best cross validation score

Automatic Hyperparameter Selection

Suppose the prediction algorithm you're using has hyperparameters θ

For each hyperparameter setting θ you are willing to try:

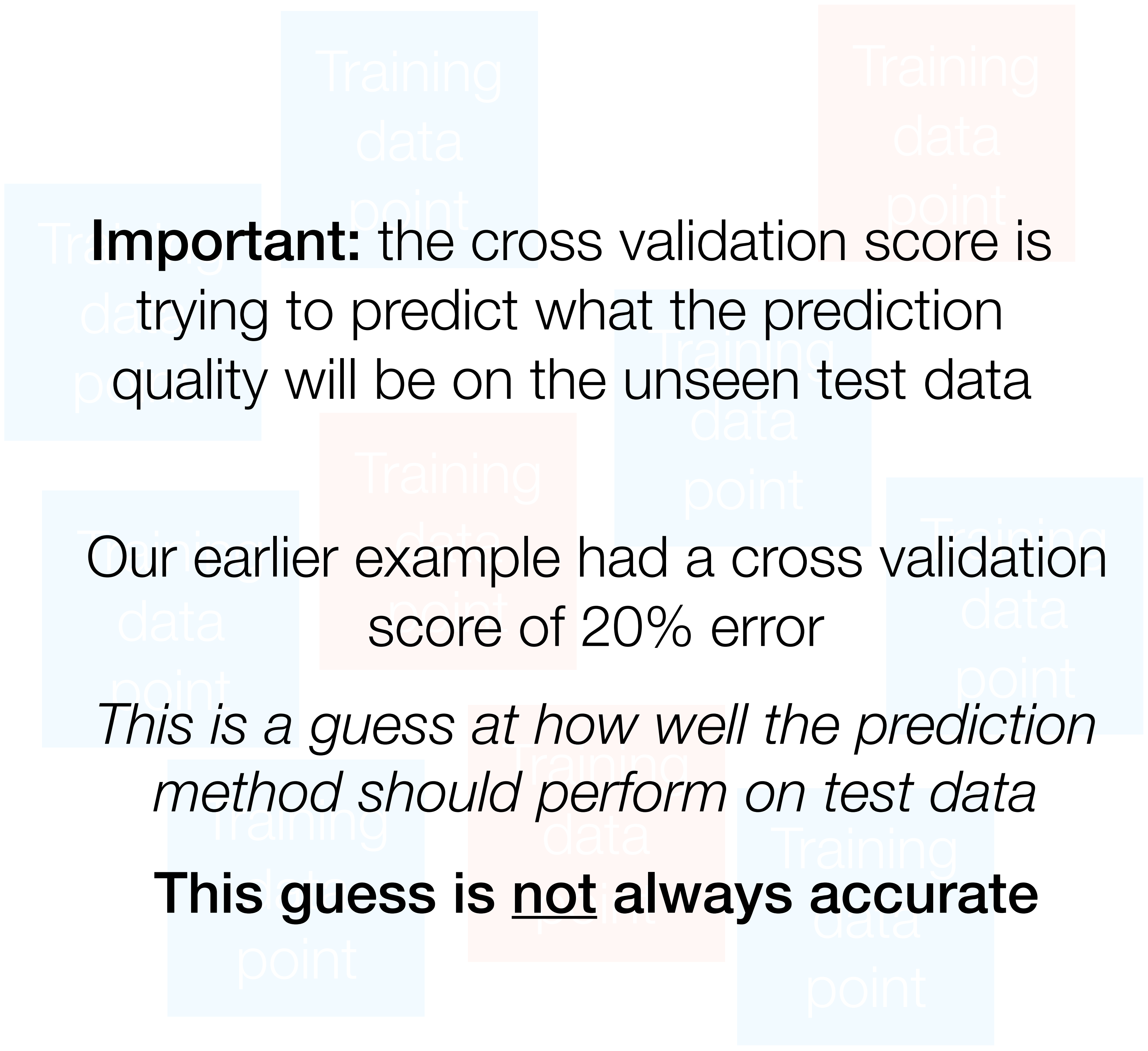
> Compute 5-fold cross validation score using your algorithm with hyperparameters θ

Use whichever θ has the best cross validation score

Why 5?

People have found using 10 folds or 5 folds to work well in practice but it's just empirical — there's no deep reason

Training data



Important: the cross validation score is trying to predict what the prediction quality will be on the unseen test data

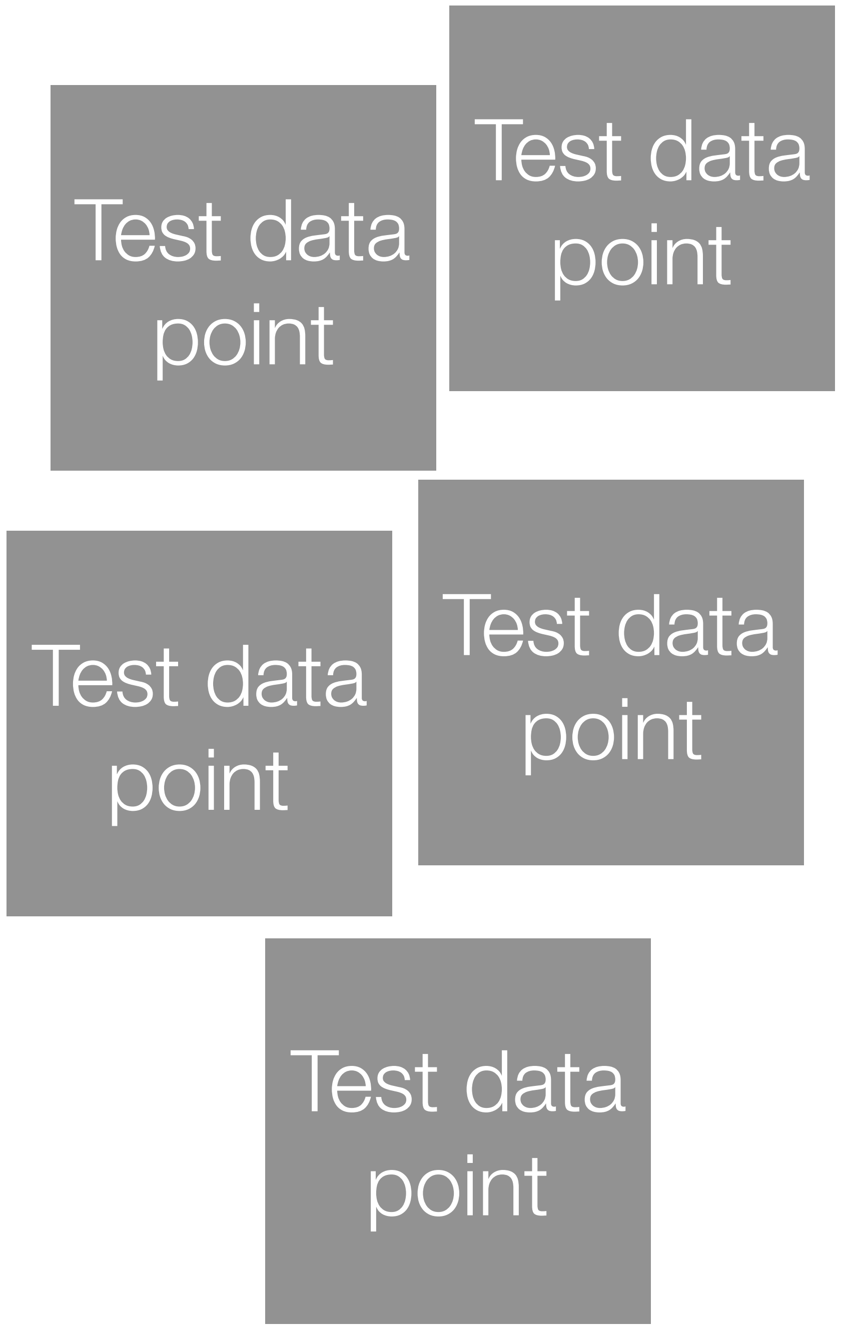
Our earlier example had a cross validation score of 20% error

This is a guess at how well the prediction method should perform on test data

This guess is <u>not</u> always accurate

Example: Each data point is an email and we know whether it is spam/ham

Want to classify these points correctly



Example: future emails to classify as spam/ham

Different Ways to Measure Accuracy

Simplest way:

- **Raw error rate:** fraction of predicted labels that are wrong (this was in our cross validation example earlier)

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

- **Precision:** among data points predicted to be “positive”, what fraction of these predictions is correct?
- **Recall:** among data points that are actually “positive”, what fraction of these points is predicted correctly as “positive”? (also called **true positive rate**)
- **F1 score:** $$\frac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

Naive Bayes

(a generative model)

Many other ways to specify a naive Bayes model (features need not be binary)

Email spam classification example

Each email represented by feature vector saying whether a word is present or not (for pre-specified dictionary of words)

```
1. Flip coin with unknown probability $s$:
   If heads: new email is spam
   If tails: new email is ham
2. If new email is spam:
     For each word $w$ in vocabulary:
       Flip coin with probability $p_w$ for whether word w appears
   If new email is ham:
     For each word $w$ in vocabulary:
       Flip coin with probability $q_w$ for whether word w appears
```

Whether one word appears has no effect on whether another word appears! (why model is called "naive")

How many parameters are there in this example?