Experimentation

Jaime Arguello
INLS 613: Text Data Mining
jarguell@email.unc.edu

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Outline

Parameter Tuning

Cross-Validation

Significance tests

Evaluation

- The goal of evaluation is to determine a model's performance on previously unseen data
  - Parameter-tuning
  - Comparing between alternative approaches
  - Feature-ablation studies

Parameter Tuning

motivation

- Supervised machine learning algorithms have lots of moving parts
- We can think of these parameters as “knobs” that need to be tweaked or tuned
- The goal is to set these parameter values such that we maximize performance
- We need to do this for both systems, not just the one we want to win!
- Can you think of some example parameters?

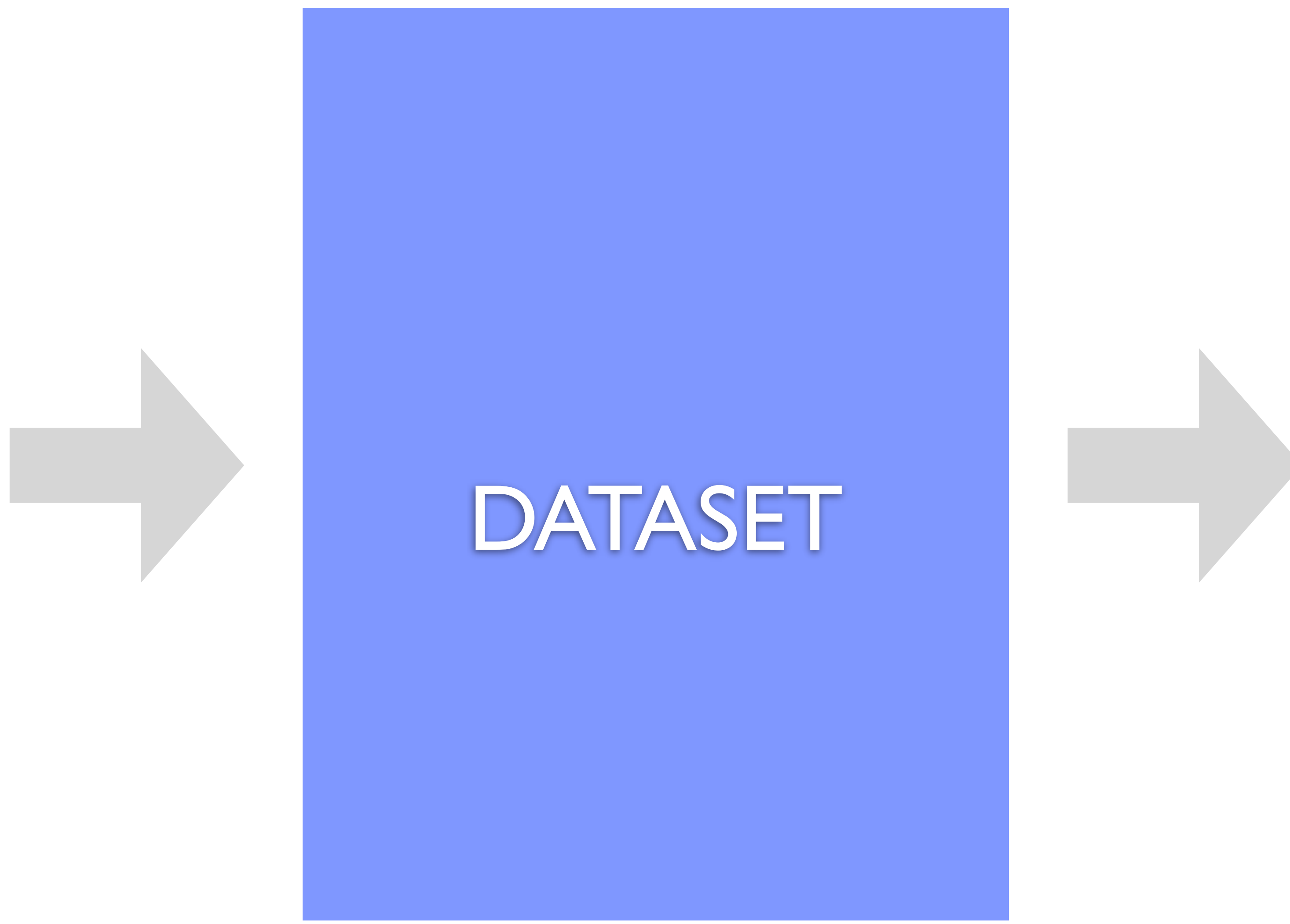
Parameter Tuning

- K-nearest Neighbor
  - Compute the similarity between a previously unseen instance and all the instances in the training set
  - Assign the majority class associated with its K nearest neighbors
- Parameter K determines the number of training set instances that are used in the voting
- Goals:
  - How do we set K?
  - What is the expected performance of the system with a good value of K?

Parameter Tuning

- How should we determine the value of K?
- Option -1: roll the dice, close your eyes, and hope for the best
- Option 0: take a conservative guess (e.g., K = 5)?
- Option 1: try out a range of values (e.g., K = 1, 5, 10, 20, 50, 100) and set it to the value that maximizes performance based on a sensible metric?

Parameter Tuning



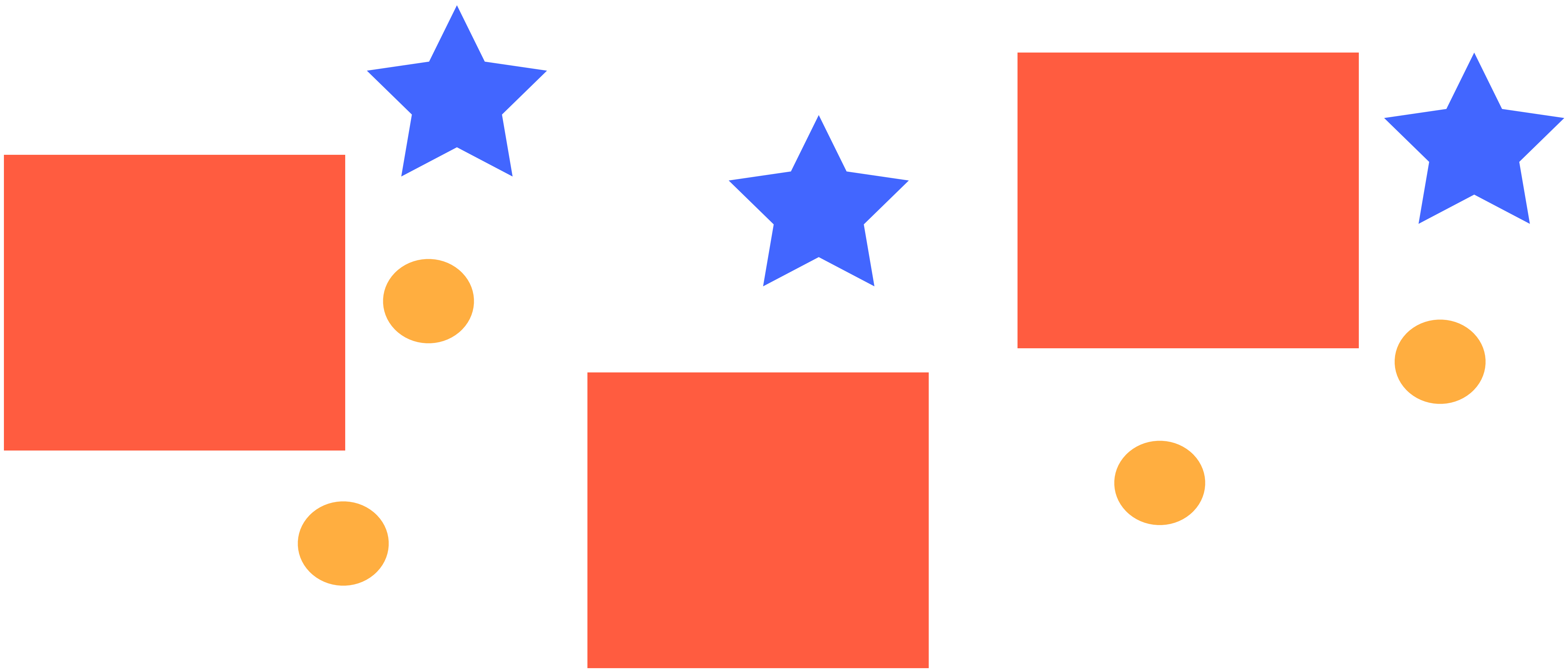
K =	F-measure =
1	0.25
2	0.27
3	0.29
4	0.35
5	0.45
6	0.50
7	**0.55**
8	0.47
9	0.35
10	0.20

Why is this a bad idea?

Parameter Tuning

toy example

- Objective: distinguish between stars, squares, and circles



- Parameters: the relative importance between (1) size, (2) color, and (3) number of sides

Parameter Tuning

- The goal is to set parameter values such that we maximize performance
- What is the performance that we are really interested in?
- We care about performance on <u>previously unseen</u> data
- We care about <u>generalization</u> performance!
- Our training set may contain regularities that are not meaningful
- We care about those regularities that are meaningful for the overall population!

Parameter Tuning

- Option 2:

1. divide the data set into two sets
    - training set: a set used to find the best parameter values (e.g., 80%)
    - test set: a held-out set used to evaluate model performance (e.g., 20%)
2. train: find the parameter value that maximize performance on the training set
3. test: evaluate the model (with the best training-set parameter value) on the test set

Parameter Tuning

Parameter Tuning

- Split the data into two sets.
- Find the parameter value that maximizes performance on the training set.
- Evaluate the system with that parameter value on the test set.

TRAINING SET (80%)

K = 5

TEST SET (20%)

F = 0.50

Parameter Tuning

- Split the data into two sets.
- Find the parameter value that maximizes performance on the training set.
- Evaluate the system with that parameter value on the test set.

TRAINING SET (80%)

K = 5

TEST SET (20%)

F = 0.50

Advantages and Disadvantages?

Single Train/Test Split

- Advantage
  - the data used to find the optimal parameter value is not the same data used to test!
  - we are testing generalization performance.
- Disadvantage
  - we are putting all our eggs in one basket!
  - out of pure coincidence, the training set may have regularities that don't generalize to the test set

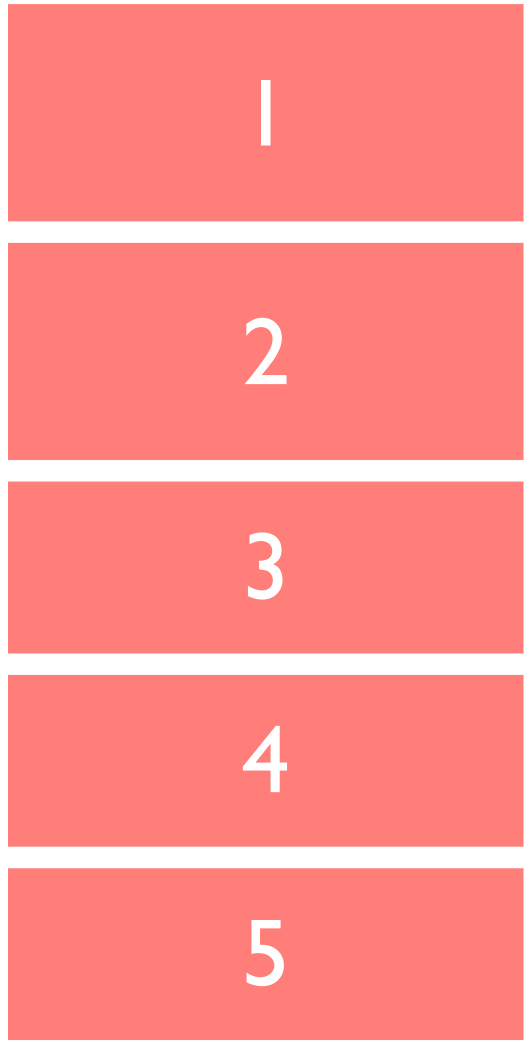
Parameter Tuning

- Option 3: cross-validation
  1. divide the data into N sets of instances
  2. use the union of N-1 sets to find the best parameter values
  3. measure performance (using the best parameters) on the held-out set
  4. do steps 2-3 N times
  5. average performance across the N held-out sets
- This is called N-fold cross-validation (usually, N=10)

Cross-Validation

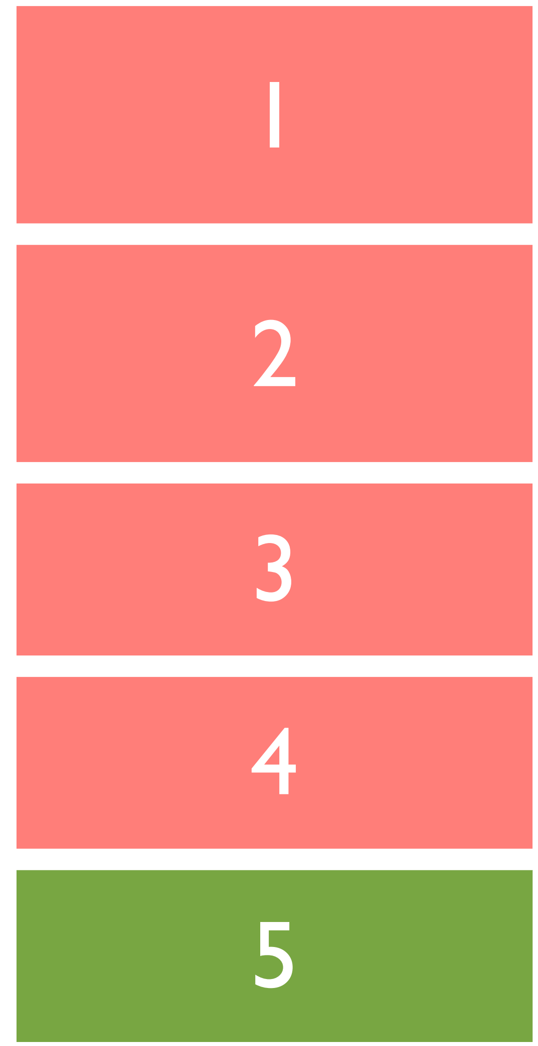
Cross-Validation

- Split the data into $N = 5$ folds



Cross-Validation

- For each fold, find the parameter value that maximizes performance on the union of N - 1 folds and test (using this parameter value) on the held-out fold.

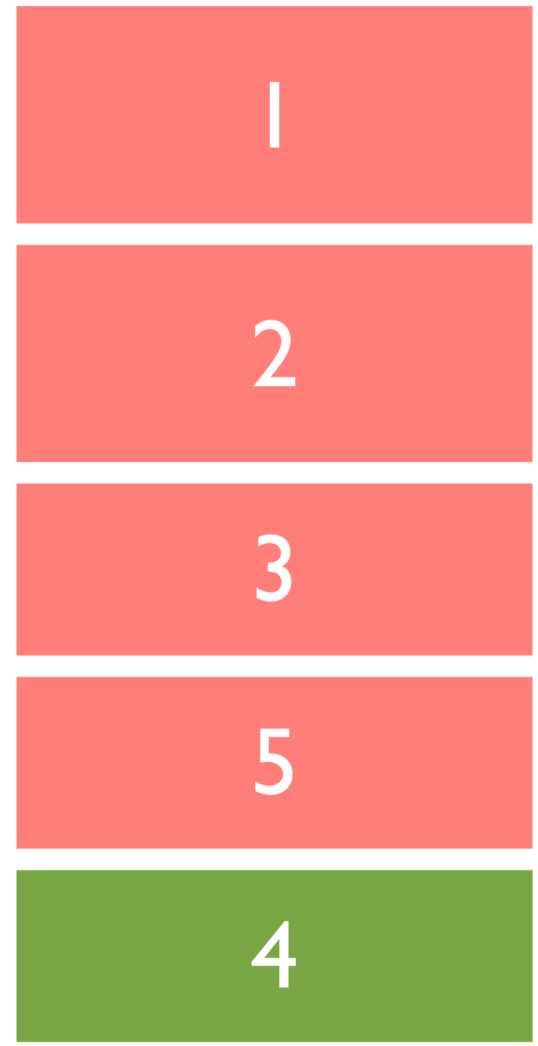


K = 5

F = 0.50

Cross-Validation

- For each fold, find the parameter value that maximizes performance on the union of N - 1 folds and test (using this parameter value) on the held-out fold.

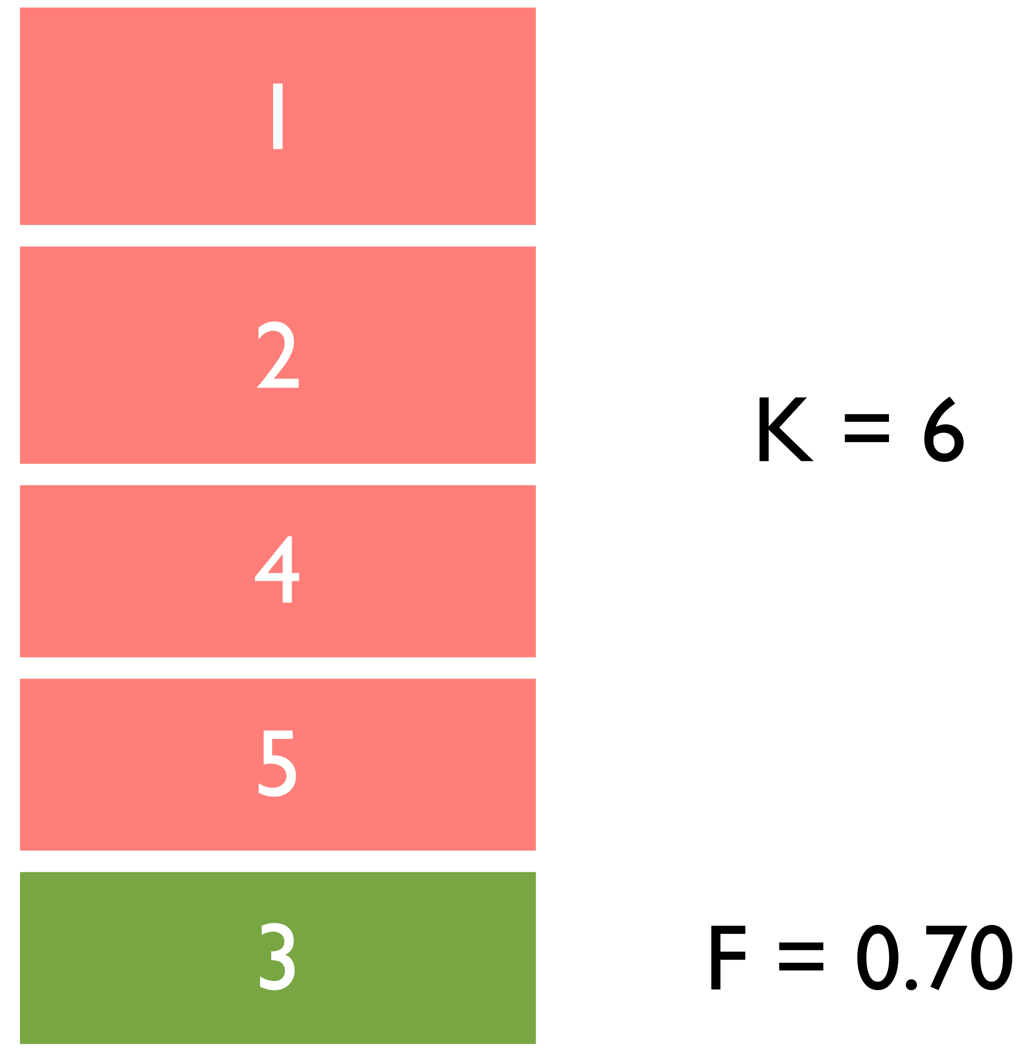


K = 6

F = 0.60

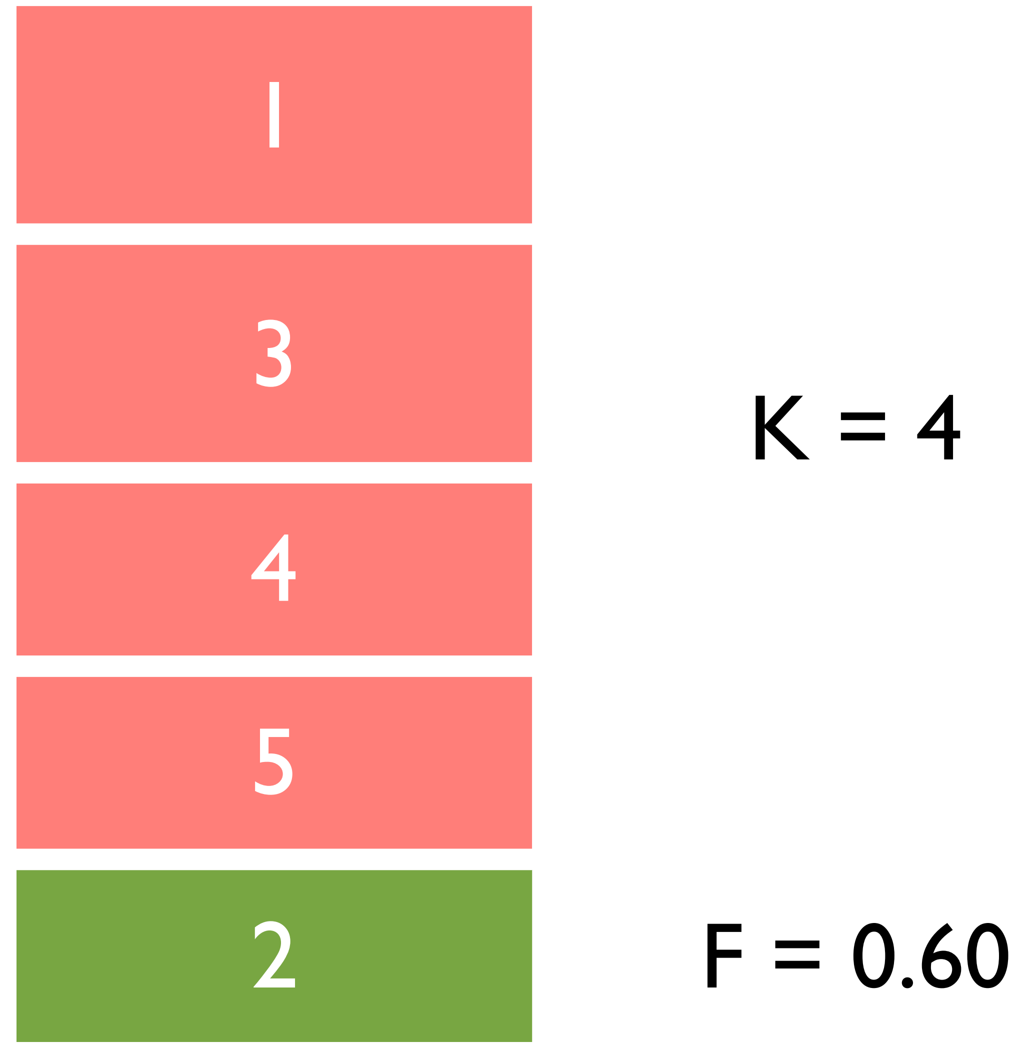
Cross-Validation

- For each fold, find the parameter value that maximizes performance on the union of N - 1 folds and test (using this parameter value) on the held-out fold.



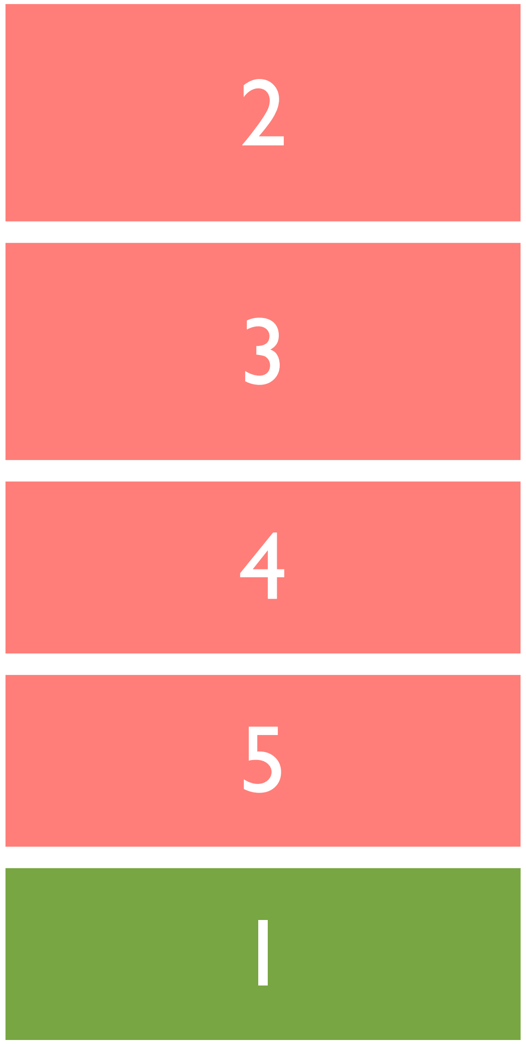
Cross-Validation

- For each fold, find the parameter value that maximizes performance on the union of N - 1 folds and test (using this parameter value) on the held-out fold.



Cross-Validation

- For each fold, find the parameter value that maximizes performance on the union of N - 1 folds and test (using this parameter value) on the held-out fold.



K = 5

F = 0.50

Cross-Validation

- Average the performance across held-out folds

1	F = 0.50
2	F = 0.60
3	F = 0.70
4	F = 0.60
5	F = 0.50
Average	**F = 0.58**

Cross-Validation

- Average the performance across held-out folds

1	F = 0.50
2	F = 0.60
3	F = 0.70
4	F = 0.60
5	F = 0.50
Average	**F = 0.58**

Advantages and Disadvantages?

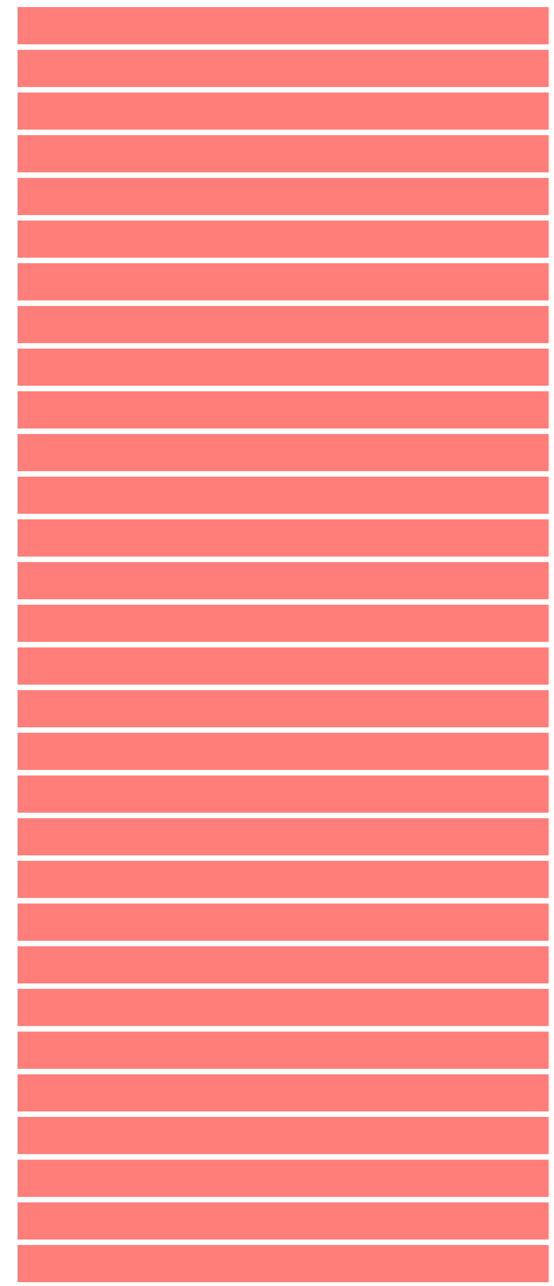
N-Fold Cross-Validation

- Advantage
  - multiple rounds of generalization performance.
- Disadvantage
  - ultimately, we'll tune parameters on the whole dataset and send our system into the world.
  - a model trained on 100% of the data should perform better than one trained on 80%.
  - thus, we may be underestimating the model's performance!

Leave-One-Out Cross-Validation

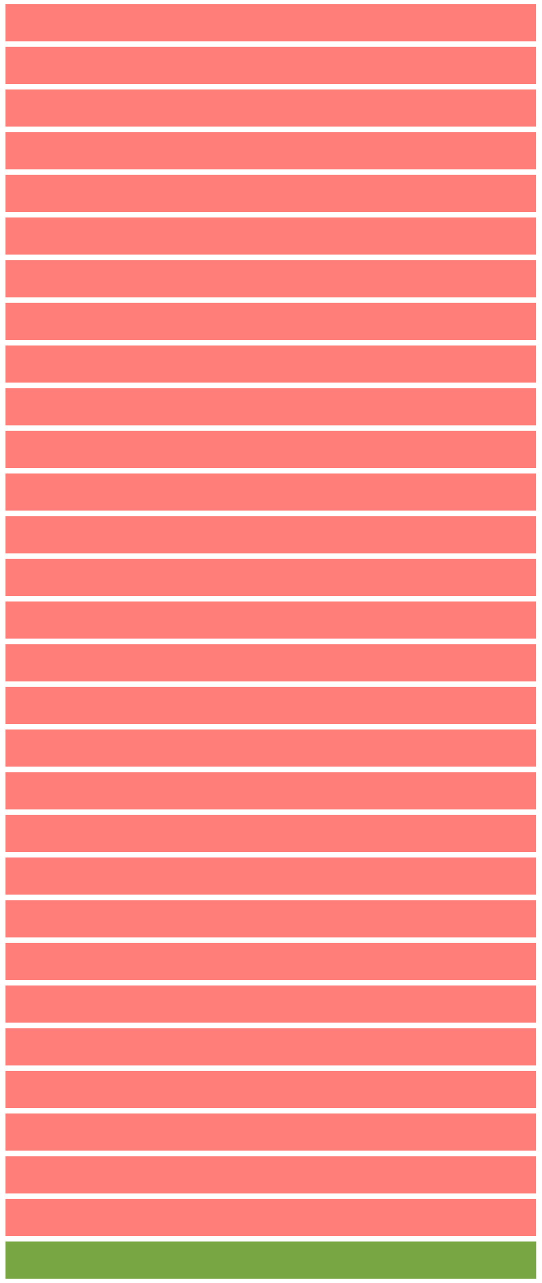
Leave-One-Out Cross-Validation

- Split the data into N folds of 1 instance each



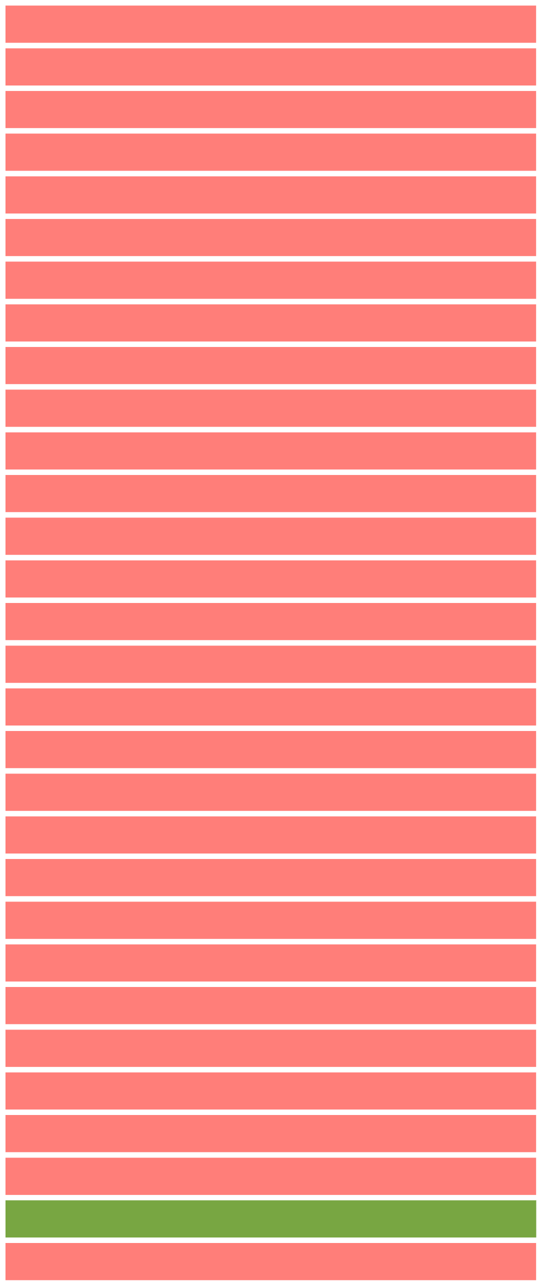
Leave-One-Out Cross-Validation

- For each instance, find the parameter value that maximize performance on for the other instances and and test (using this parameter value) on the held-out instance.



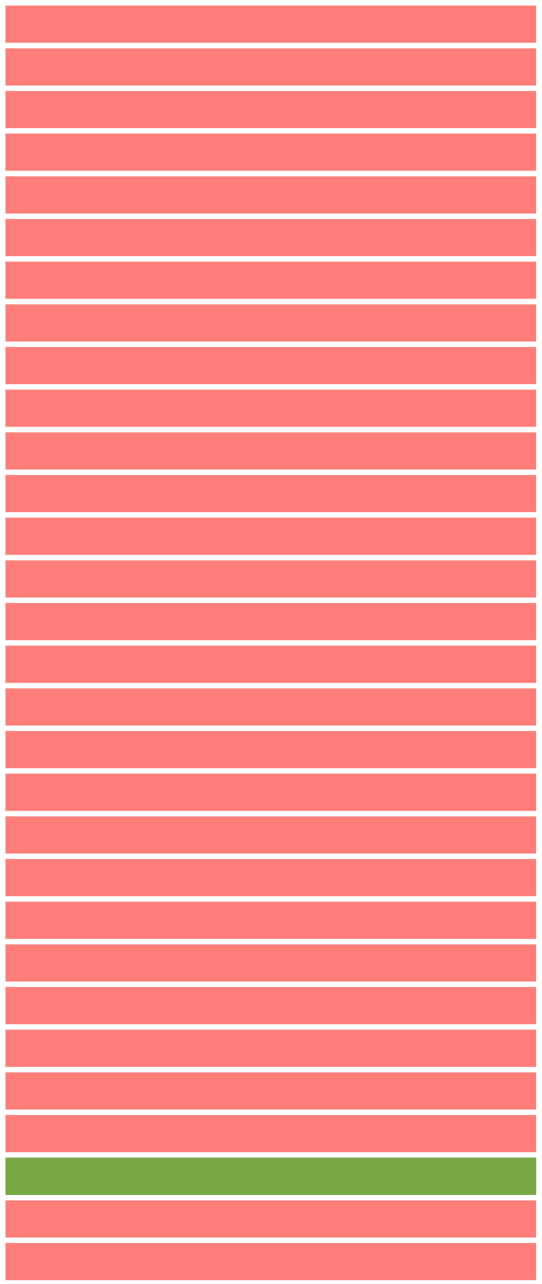
Leave-One-Out Cross-Validation

- For each instance, find the parameter value that maximize performance on for the other instances and and test (using this parameter value) on the held-out instance.



Leave-One-Out Cross-Validation

- For each instance, find the parameter value that maximize performance on for the other instances and and test (using this parameter value) on the held-out instance.
- And so on ...
- Finally, average the performance for each held-out instance



Leave-One-Out Cross-Validation

- For each instance, find the parameter value that maximize performance on for the other instances and and test (using this parameter value) on the held-out instance.
- And so on ...
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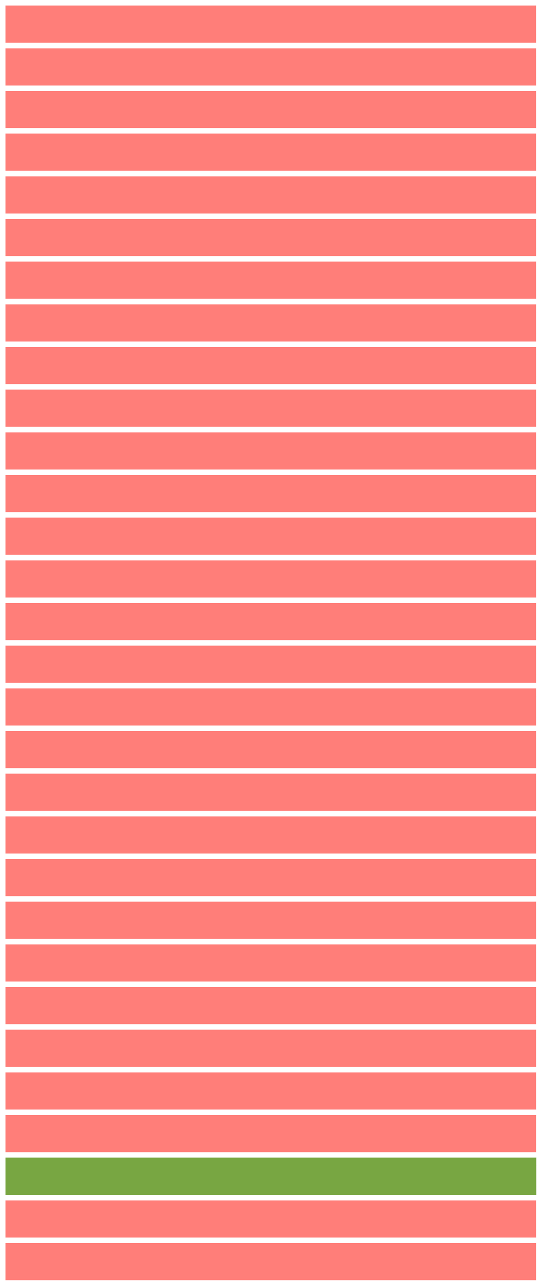


Advantages and Disadvantages?

Leave-One-Out Cross-Validation

- Advantages
  - multiple rounds of generalization performance.
  - each training fold is as similar as possible to the one we will ultimately use to tune parameters before sending the system out into the world.
- Disadvantage
  - our estimate of generalization performance may still be artificially high
  - why?

Leave-One-Out Cross-Validation

- Advantages
  - multiple rounds of generalization performance.
  - each training fold is as similar as possible to the one we will ultimately use to tune parameters before sending the system out into the world.
- Disadvantage
  - our estimate of generalization performance may still be artificially high
  - we are likely to try lots of different things and pick the one with the best "generalization" performance
  - still indirectly over-training to the dataset (sigh...)

Outline

Parameter Tuning

Cross-Validation

Significance tests

Comparing Systems

- Train and test both systems using 10-fold cross validation
- Use the same folds for both systems
- Compare the difference in average performance across held-out folds

Fold	System A	System B
1	0.20	0.50
2	0.30	0.30
3	0.10	0.10
4	0.40	0.40
5	1.00	1.00
6	0.80	0.90
7	0.30	0.10
8	0.10	0.20
9	0.00	0.50
10	0.90	0.80
Average	0.41	0.48
	Difference	0.07

Significance Tests
motivation

- Why would it be risky to conclude that System B is better System A?
- Put differently, what is it that we're trying to achieve?

Significance Tests

motivation

- In theory: that the average performance of System B is greater than the average performance of System A for all possible test sets.
- However, we don't have all test sets. We have a sample
- And, this sample may favor one system vs. the other!

Significance Tests
definition

- A significance test is a statistical tool that allows us to determine whether a difference in performance reflects a true pattern or just random chance

Significance Tests
ingredients

- Test statistic: a measure used to judge the two systems (e.g., the difference between their average F-measure)
- Null hypothesis: no “true” difference between the two systems
- P-value: take the value of the observed test statistic and compute the probability of observing a value that large (or larger) under the null hypothesis

Significance Tests
ingredients

- If the p-value is large, we cannot reject the null hypothesis
- That is, we cannot claim that one system is better than the other
- If the p-value is small (p<0.05), we can reject the null hypothesis
- That is, the observed test-statistic is not due to random chance

Fisher's Randomization Test

procedure

- **Inputs:** counter = 0, N = 100,000
- Repeat N times:

  Step 1: for each fold, flip a coin and if it lands 'heads', flip the result between System A and B

  Step 2: see whether the test statistic is equal to or greater than the one observed and, if so, increment counter

- **Output:** counter / N

Fisher's Randomization Test

Fold	System A	System B
1	0.20	0.50
2	0.30	0.30
3	0.10	0.10
4	0.40	0.40
5	1.00	1.00
6	0.80	0.90
7	0.30	0.10
8	0.10	0.20
9	0.00	0.50
10	0.90	0.80
Average	0.41	0.48
	Difference	0.07

Fisher's Randomization Test

Fold	System A	System B
1	**0.50**	**0.20**
2	0.30	0.30
3	0.10	0.10
4	0.40	0.40
5	1.00	1.00
6	**0.90**	**0.80**
7	0.30	0.10
8	0.10	0.20
9	**0.50**	**0.00**
10	0.90	0.80
Average	0.5	0.39
	Difference	-0.11

at least 0.07?

iteration = 1 counter = 0

Fisher's Randomization Test

Fold	System A	System B
1	0.20	0.50
2	0.30	0.30
3	**0.10**	**0.10**
4	0.40	0.40
5	**1.00**	**1.00**
6	0.80	0.90
7	**0.10**	**0.30**
8	**0.20**	**0.10**
9	0.00	0.50
10	**0.08**	**0.90**
Average	0.318	0.5
	Difference	0.182

at least 0.07?

iteration = 2   counter = 1

Fisher's Randomization Test

Fold	System A	System B
1	**0.50**	**0.20**
2	0.30	0.30
3	**0.10**	**0.10**
4	**0.40**	**0.40**
5	1.00	1.00
6	**0.90**	**0.80**
7	0.30	0.10
8	0.10	0.20
9	**0.50**	**0.00**
10	0.90	0.80
Average	0.5	0.39
	Difference	-0.11

at least 0.07?

iteration = 100,000 counter = 25,678

Fisher’s Randomization Test

procedure

- **Inputs:** counter = 0, N = 100,000
- Repeat N times:

  Step 1: for each query, flip a coin and if it lands ‘heads’, flip the result between System A and B

  Step 2: see whether the test statistic is equal to or greater than the one observed and, if so, increment counter

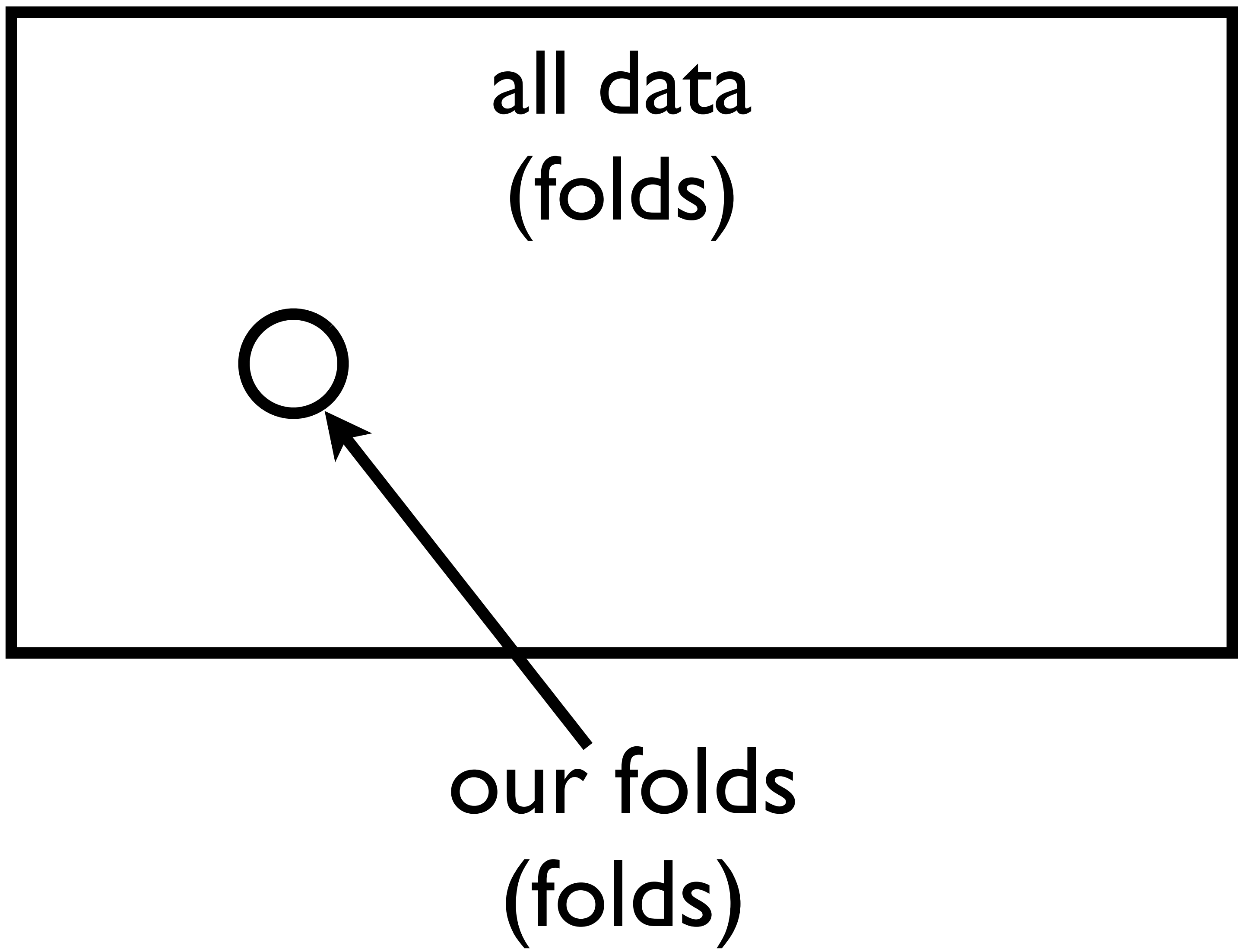
- **Output:** counter / N = (25,678/100,00) = 0.25678

Fisher's Randomization Test

- Under the null hypothesis, the probability of observing a value of the test statistic of 0.07 or greater is about 0.26.
- Because $p > 0.05$, we cannot confidently say that the value of the test statistic is <u>not</u> due to random chance.
- A difference between the average F-measure values of 0.07 is not significant

Bootstrap-Shift Test
motivation

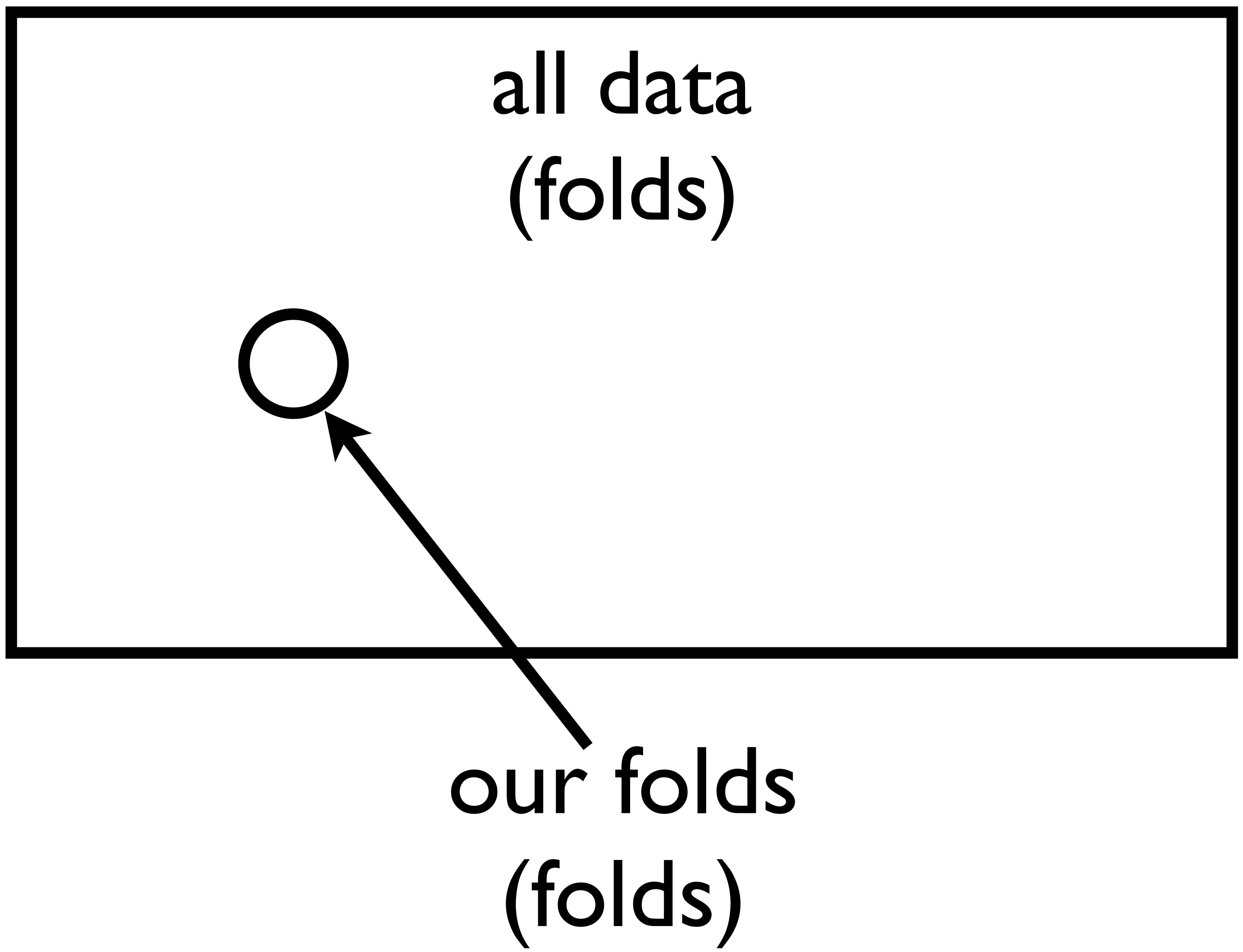
- Our sample is a representative sample of all data



Bootstrap-Shift Test

motivation

- If we sample (with replacement) from our sample, we can generate a new representative sample of all data



Bootstrap-Shift Test

procedure

- **Inputs:** Array T = {}, N = 100,000
- Repeat N times:

  Step 1: sample 10 folds (with replacement) from our set of 10 folds (called a subsample)

  Step 2: compute test statistic associated with new sample and add to T
- **Step 3:** compute <u>average</u> of numbers in T
- **Step 4:** reduce every number in T by <u>average</u>
- **Output:** % of numbers in T greater than or equal to the observed test statistic

Bootstrap-Shift Test

Fold	System A	System B
1	0.20	0.50
2	0.30	0.30
3	0.10	0.10
4	0.40	0.40
5	1.00	1.00
6	0.80	0.90
7	0.30	0.10
8	0.10	0.20
9	0.00	0.50
10	0.90	0.80
Average	0.41	0.48
	Difference	0.07

Bootstrap-Shift Test

Fold	System A	System B	**sample**
1	0.20	0.50	**0**
2	0.30	0.30	**1**
3	0.10	0.10	**2**
4	0.40	0.40	**2**
5	1.00	1.00	**0**
6	0.80	0.90	**1**
7	0.30	0.10	**1**
8	0.10	0.20	**1**
9	0.00	0.50	**2**
10	0.90	0.80	**0**

iteration = 1

Bootstrap-Shift Test

Fold	System A	System B
2	0.30	0.30
3	0.10	0.10
3	0.10	0.10
4	0.40	0.40
4	0.40	0.40
6	0.80	0.90
7	0.30	0.10
8	0.10	0.20
9	0.00	0.50
9	0.00	0.50
Average	0.25	0.35
	Difference	**0.1**

T = {**0.10**}

iteration = 1

Bootstrap-Shift Test

Fold	System A	System B	**sample**
1	0.20	0.50	**0**
2	0.30	0.30	**0**
3	0.10	0.10	**3**
4	0.40	0.40	**2**
5	1.00	1.00	**0**
6	0.80	0.90	**1**
7	0.30	0.10	**1**
8	0.10	0.20	**1**
9	0.00	0.50	**1**
10	0.90	0.80	**1**

T = {**0.10**}

iteration = 2

Bootstrap-Shift Test

Fold	System A	System B
3	0.10	0.10
3	0.10	0.10
3	0.10	0.10
4	0.40	0.40
4	0.40	0.40
6	0.80	0.90
7	0.30	0.10
8	0.10	0.20
9	0.00	0.50
10	0.90	0.80
Average	0.32	0.36
	Difference	**0.04**

T = {**0.10**, **0.04**}

iteration = 2

Bootstrap-Shift Test

Fold	System A	System B
1	0.20	0.50
1	0.20	0.50
4	0.40	0.40
4	0.40	0.40
4	0.40	0.40
6	0.80	0.90
7	0.30	0.10
8	0.10	0.20
8	0.10	0.20
10	0.90	0.80
Average	0.38	0.44
	Difference	**0.06**

T = {**0.10**,
0.04,
……,
0.06}

iteration = 100,000

Bootstrap-Shift Test
procedure

- **Inputs:** Array T = {}, N = 100,000
- Repeat N times:

  Step 1: sample 10 folds (with replacement) from our set of 10 folds (called a subsample)

  Step 2: compute test statistic associated with new sample and add to T
- **Step 3:** compute average of numbers in T
- **Step 4:** reduce every number in T by average
- **Output:** % of numbers in T' greater than or equal to the observed test statistic

Bootstrap-Shift Test

procedure

- For the purpose of this example, let's assume N = 10.

T = {**0.10**, **0.04**, **0.21**, **0.20**, **0.13**, **0.09**, **0.22**, **0.07**, **0.03**, **0.11**}

Step 3

Average = **0.12**

Step 4

T'= {**-0.02**, **-0.08**, **0.09**, **0.08**, **0.01**, **-0.03**, **0.10**, **-0.05**, **-0.09**, **-0.01**}

Bootstrap-Shift Test

procedure

- **Inputs:** Array T = {}, N = 100,000
- Repeat N times:

  Step 1: sample 10 folds (with replacement) from our set of 10 folds (called a subsample)

  Step 2: compute test statistic associated with new sample and add to T

- **Step 3:** compute <u>average</u> of numbers in T
- **Step 4:** reduce every number in T by <u>average</u>
- **Output:** % of numbers in T' greater than or equal to the observed test statistic

Bootstrap-Shift Test

procedure

- **Output:** (3/10) = **0.30**

T = {**0.10**, **0.04**, **0.21**, **0.20**, **0.13**, **0.09**, **0.22**, **0.07**, **0.03**, **0.11**}

Step 3

Average = **0.12**

Step 4

T'= {**-0.02**, **-0.08**, **0.09**, **0.08**, **0.01**, **-0.03**, **0.10**, **-0.05**, -**0.09**, **-0.01**}

Significance Tests

summary

- Significance tests help us determine whether the outcome of an experiment signals a "true" trend
- The null hypothesis is that the observed outcome is due to random chance (sample bias, error, etc.)
- There are many types of tests
- Parametric tests: assume a particular distribution for the test statistic under the null hypothesis
- Non-parametric tests: make no assumptions about the test statistic distribution under the null hypothesis
- The randomization and bootstrap-shift tests make no assumptions, are robust, and easy to understand