Lecture 11 pre-video

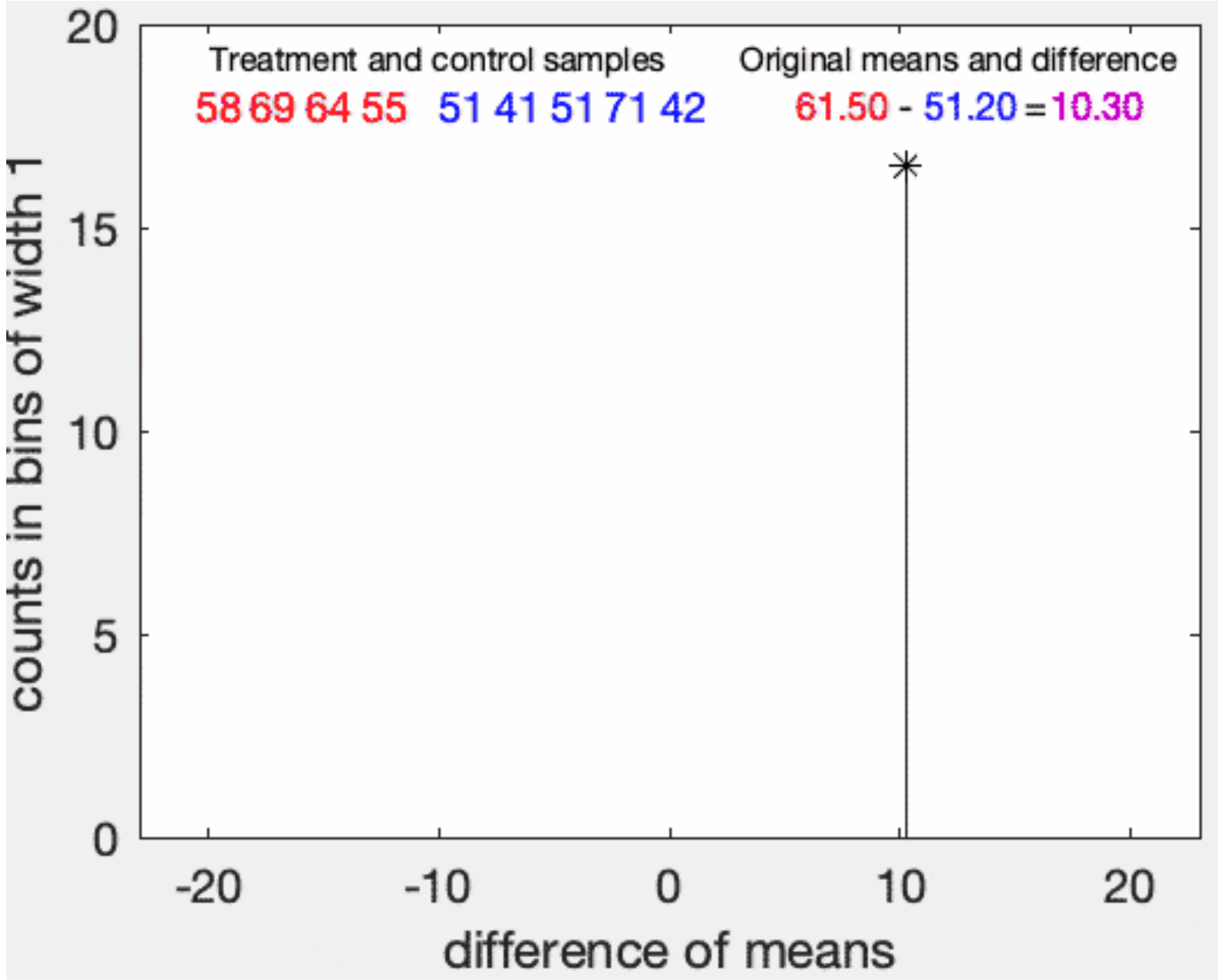
Resampling methods

Resampling

- Why do it?
  - More accurate estimation of population from sample measurements
  - Make better use of limited sample size
  - A static technique: don’t need more experiments
- Why not?
  - Could get better results by doing experiments and actively choosing new samples
  - Computationally intensive

Resampling techniques

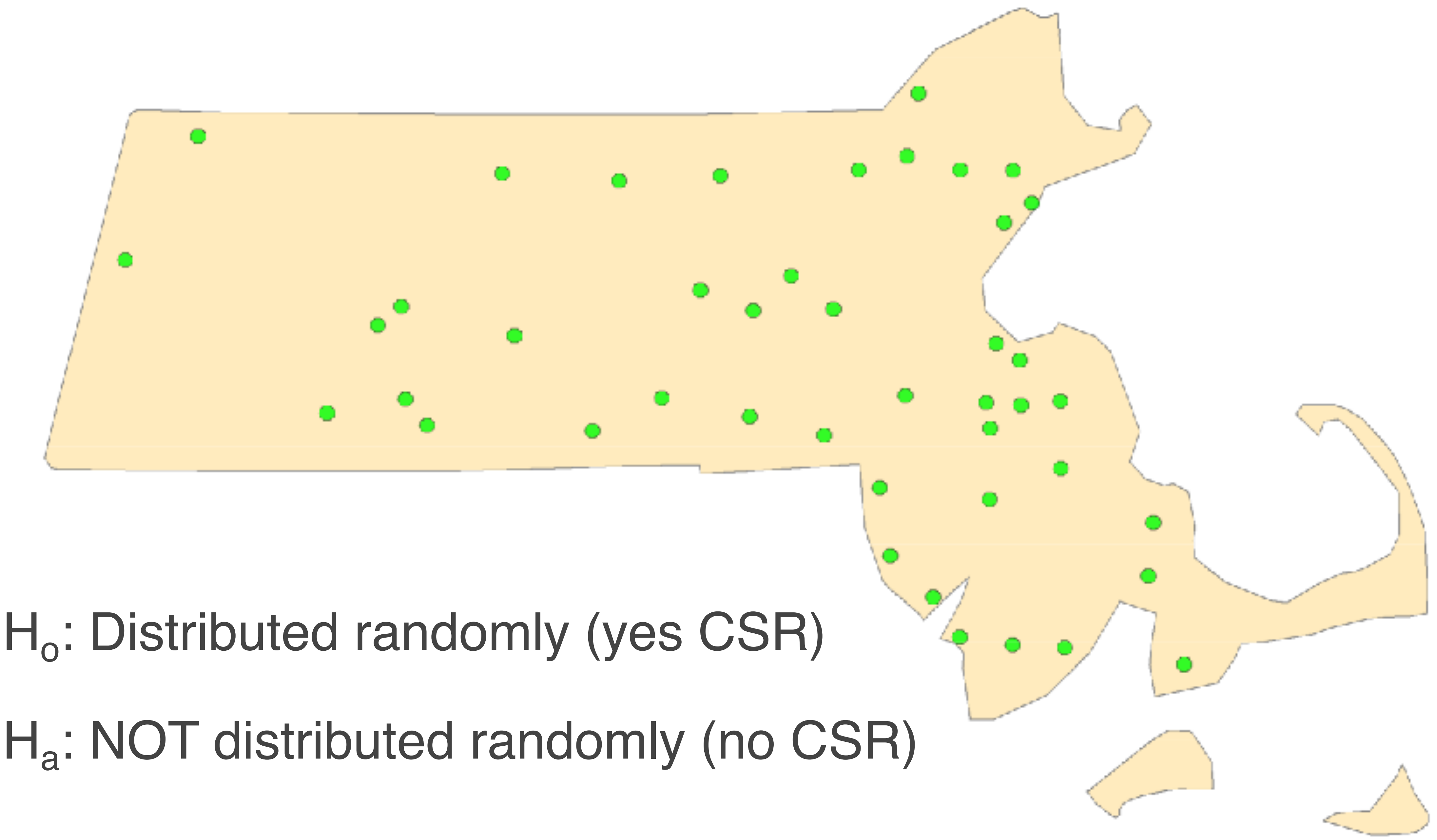
Permutation tests, e.g. Fisher's exact test



Resampling techniques

Monte Carlo simulation

Is this distribution of Walmarts in MA the result of CSR?



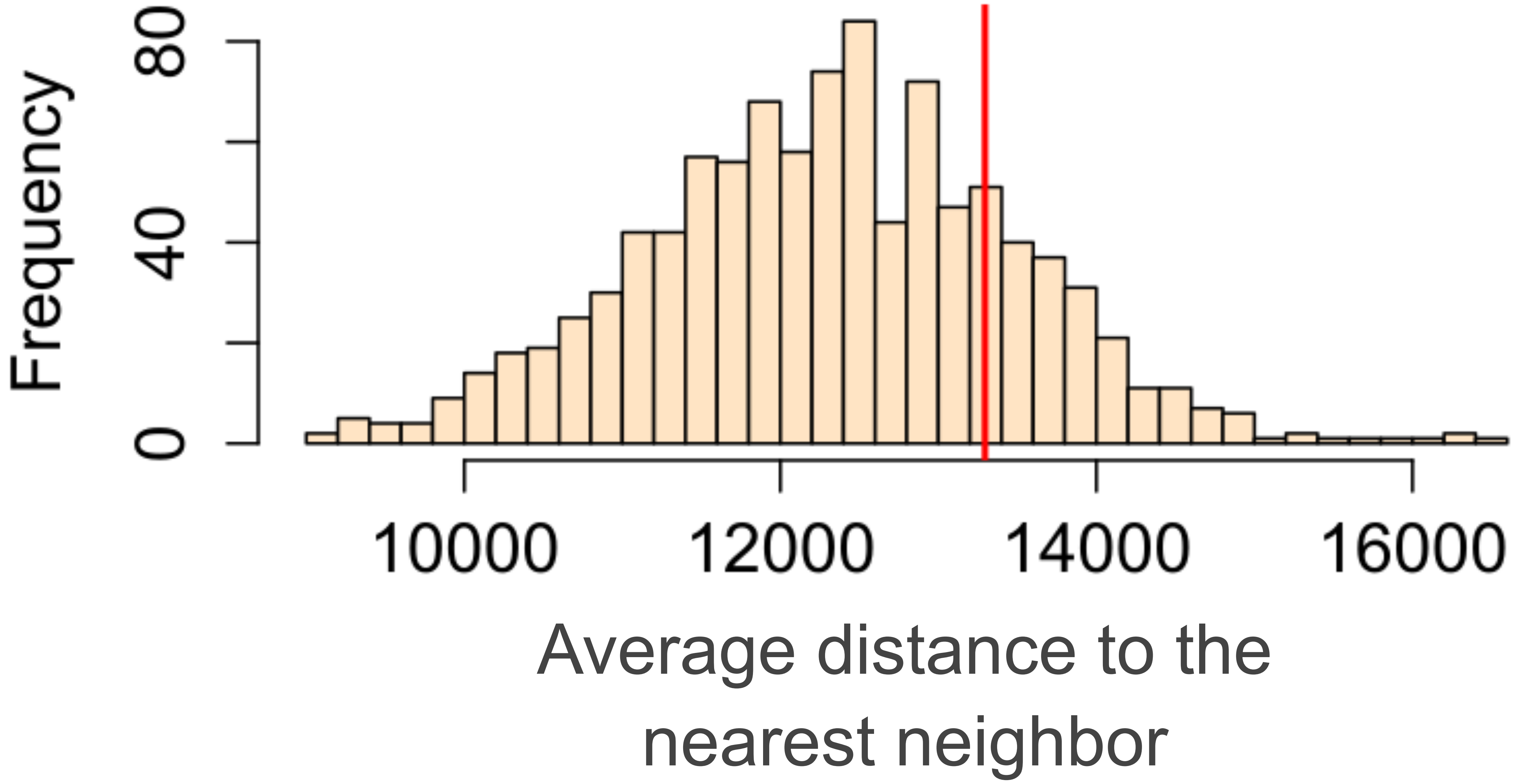
H_o: Distributed randomly (yes CSR)

H_a: NOT distributed randomly (no CSR)

p = # more extreme / # simulations

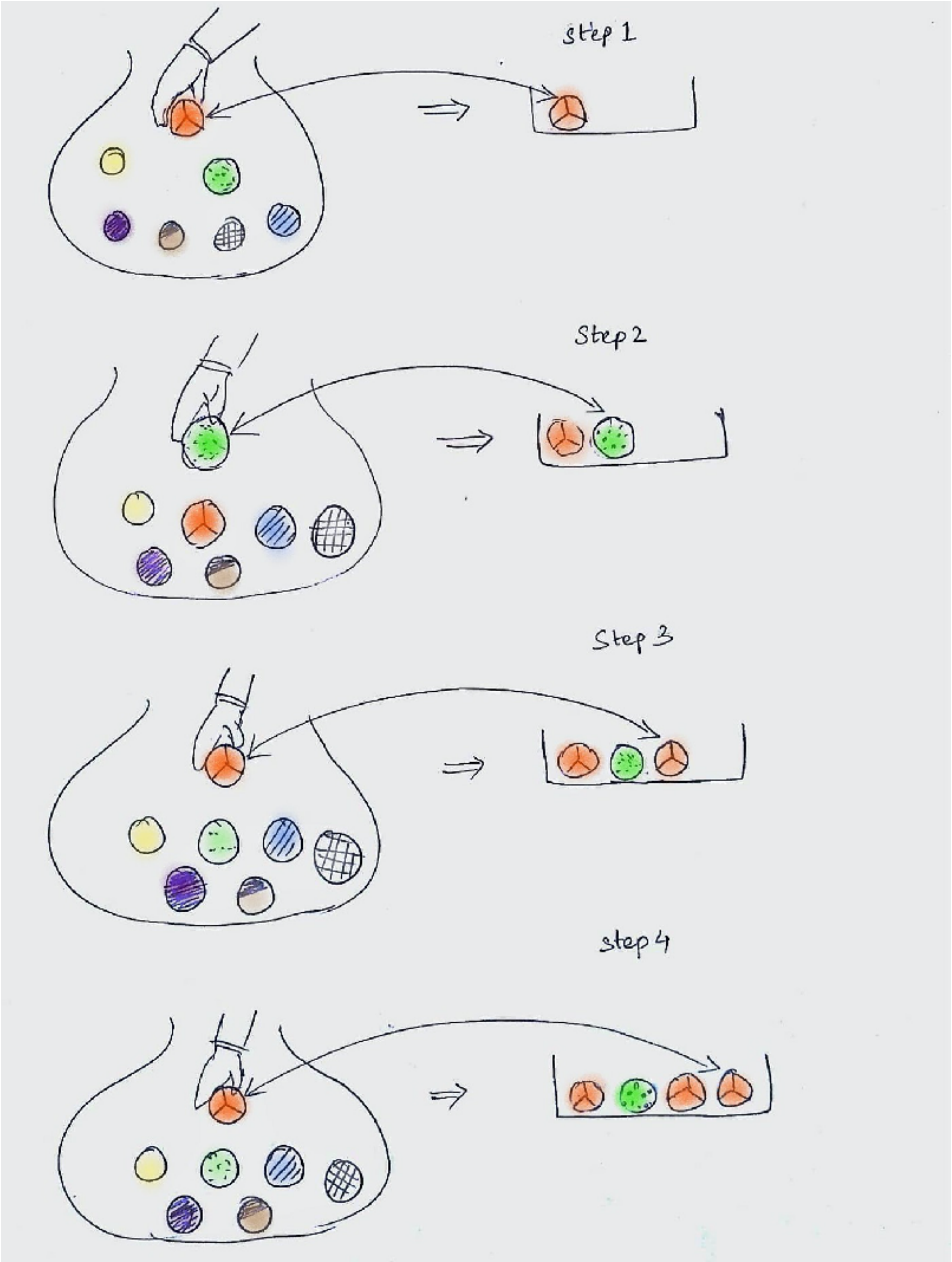
p = (319 + 1) / (1000 + 1)

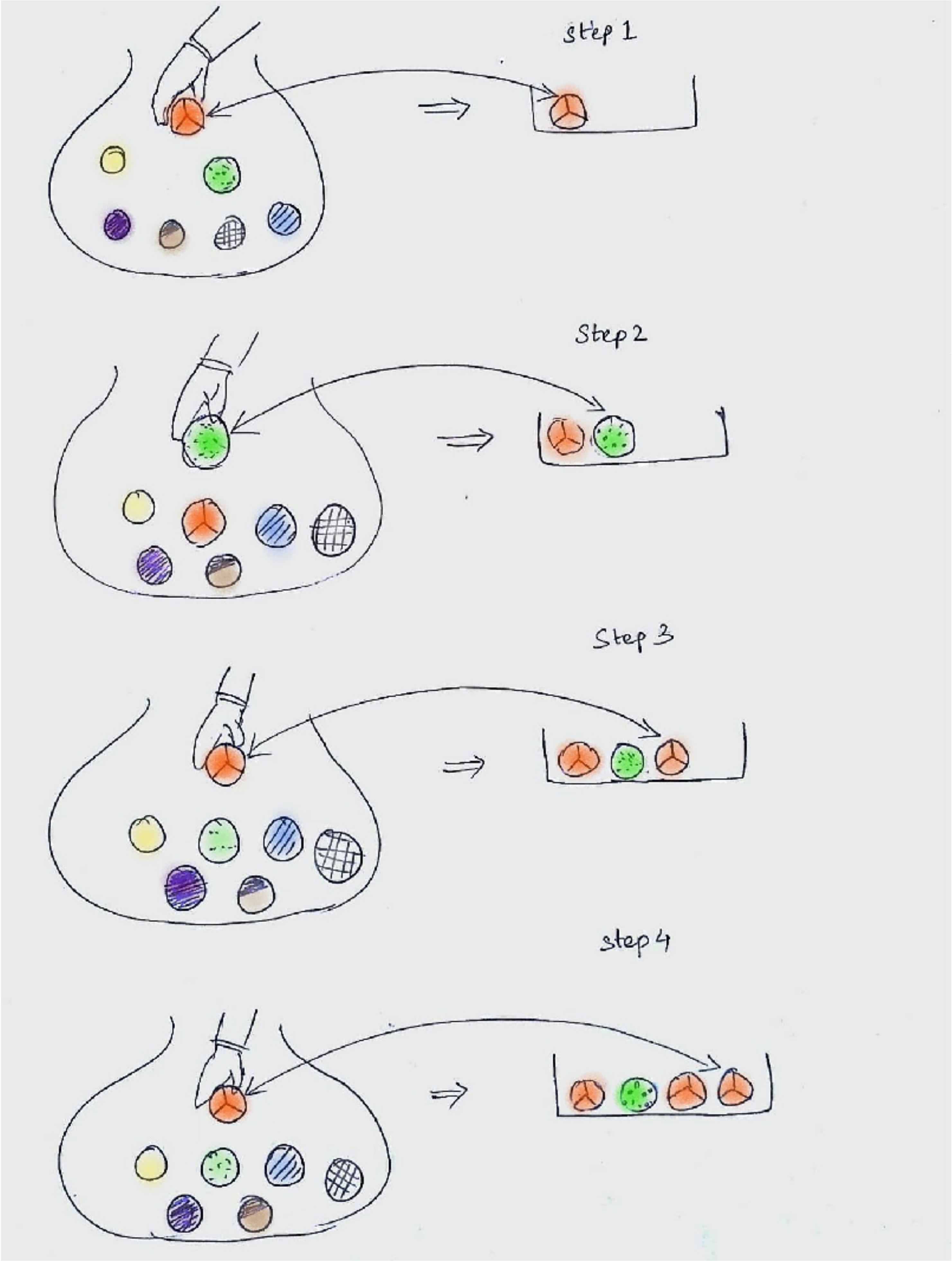
p = 0.32



Resampling techniques

Bootstrap aka
resample with replacement

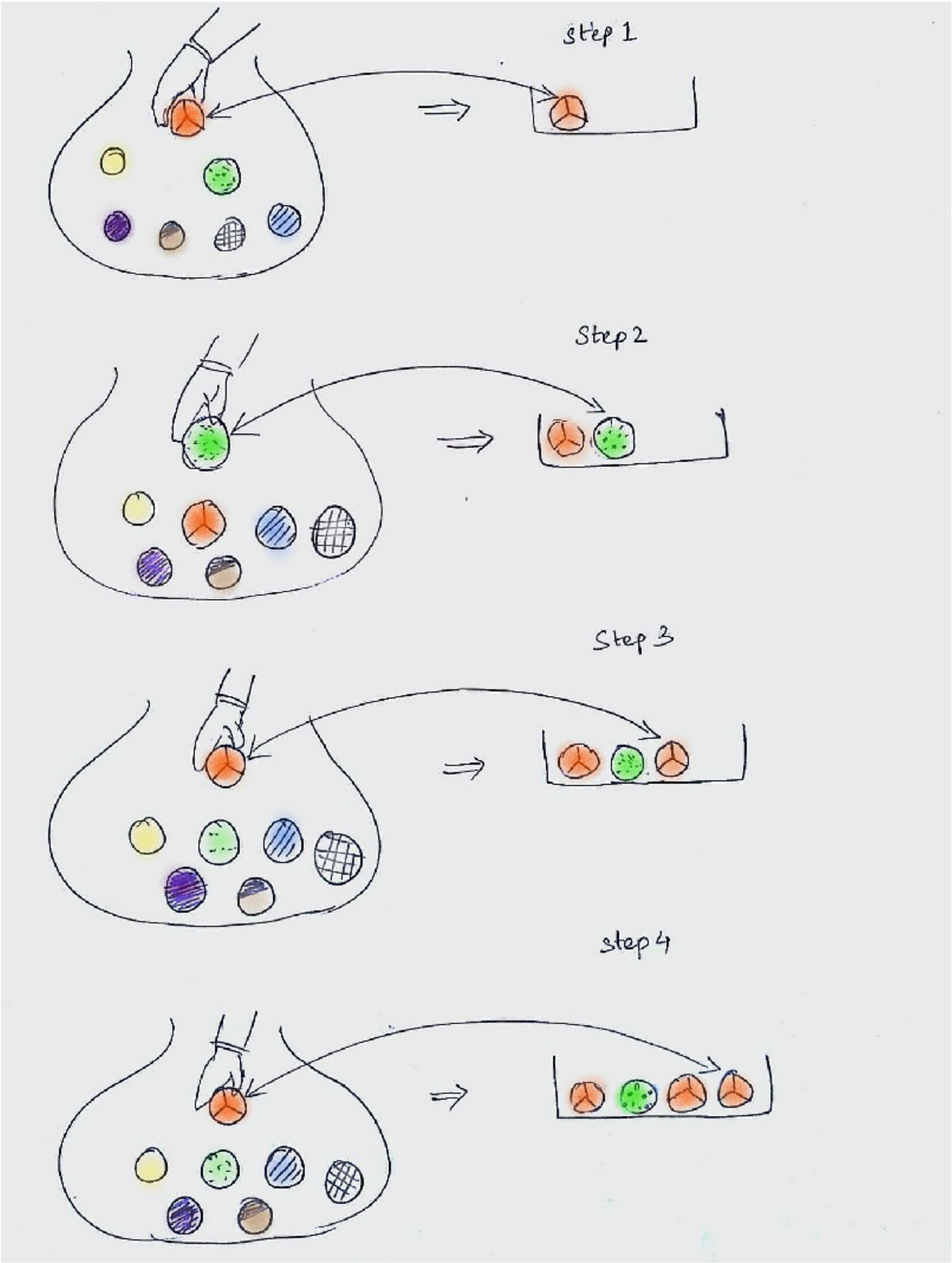




Bootstrap Sampling

$$P(\textbf{not chosen}) = \left(1 - \frac{1}{n}\right)^n,$$

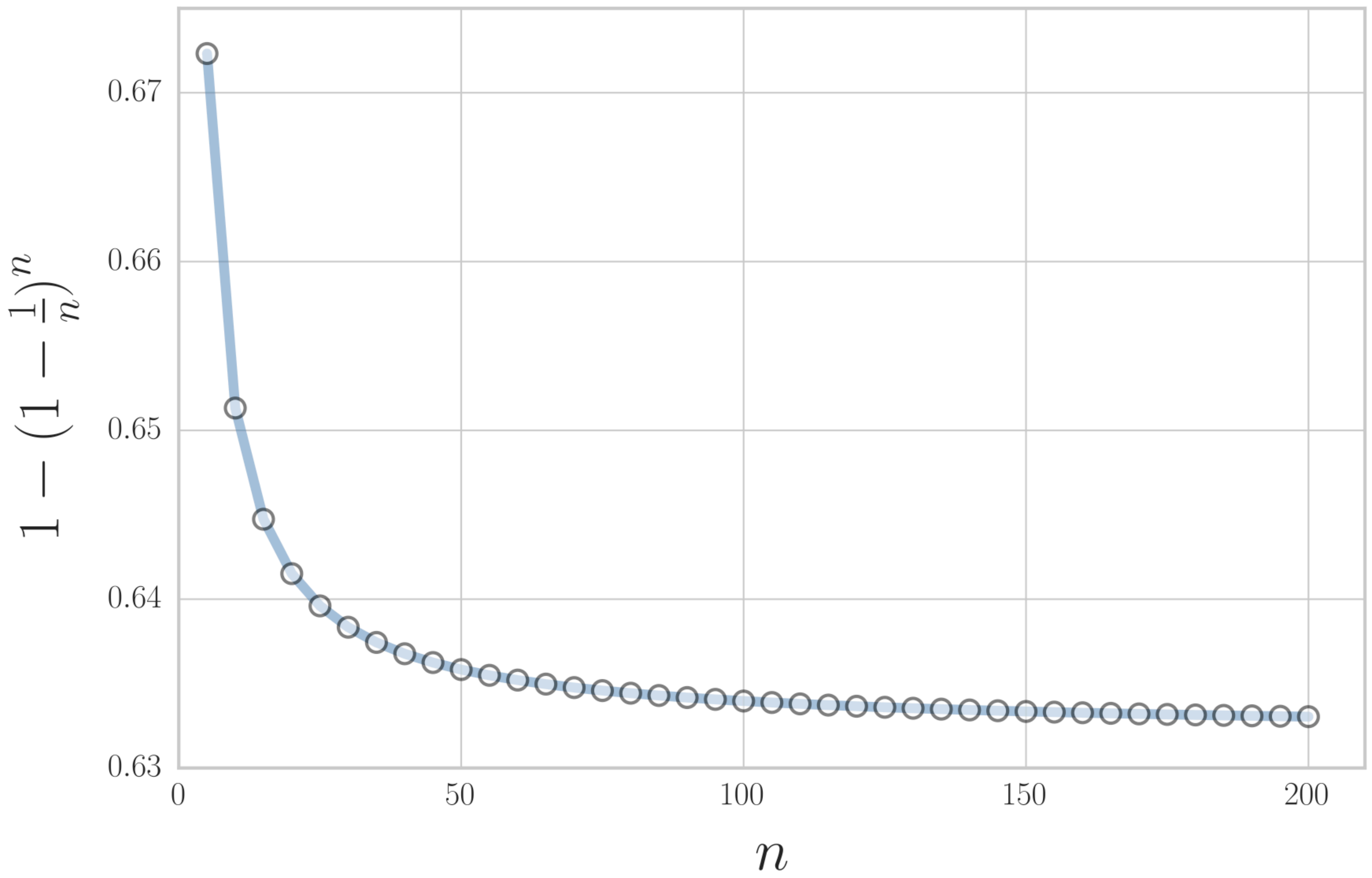
$$\frac{1}{e} \approx 0.368, \quad n \to \infty .$$



$$P(\textbf{not chosen}) = \left(1 - \frac{1}{n}\right)^n,$$

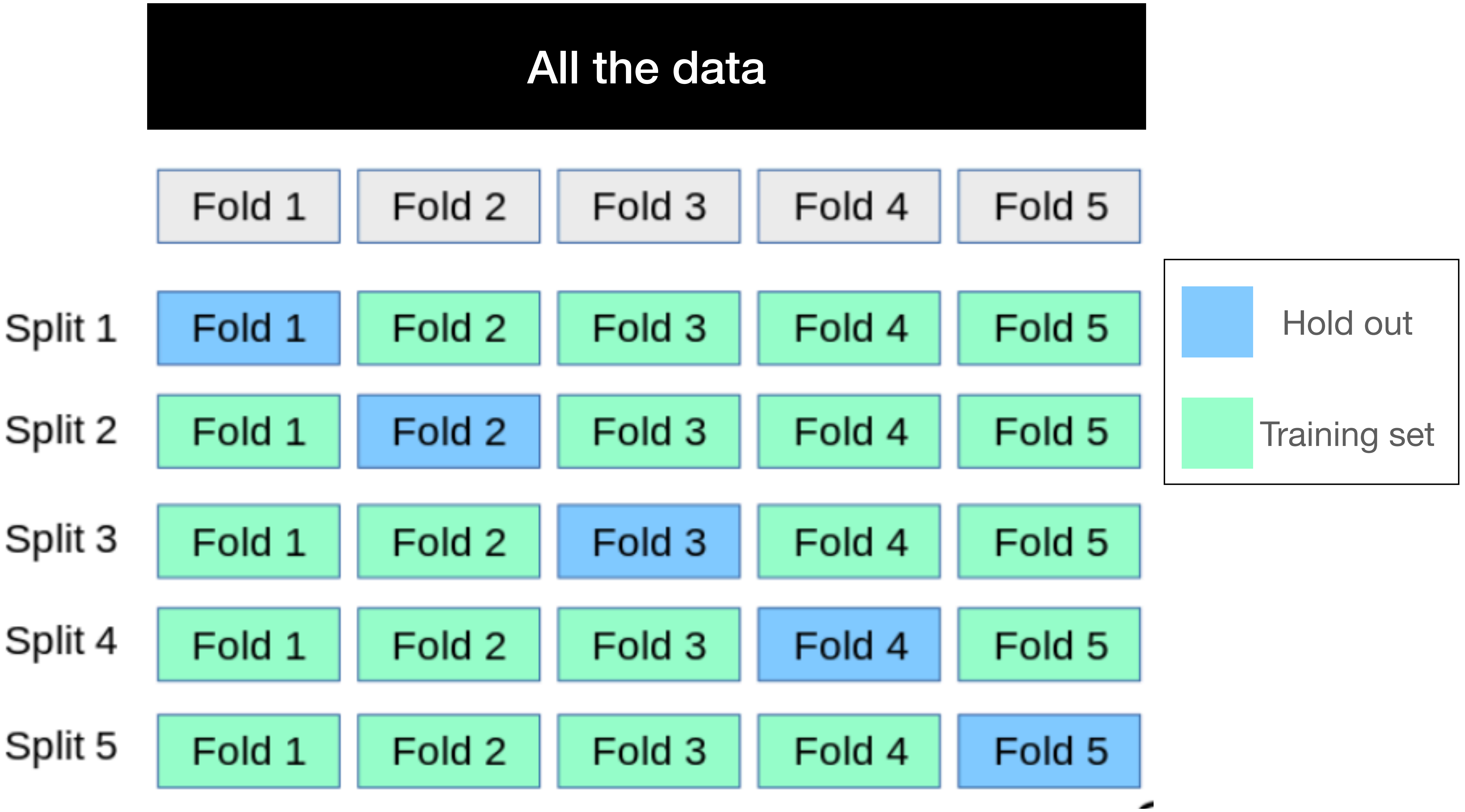
$$\frac{1}{e} \approx 0.368, \quad n \to \infty.$$

$$P(\textbf{chosen}) = 1 - \left(1 - \frac{1}{n}\right)^n \approx 0.632$$



Resampling techniques

Cross validation



Use the mean of the hold out set performances to estimate either test or validation error

Resampling techniques

- Permutation tests, e.g. Fisher’s test, Monte Carlo simulation
  - Estimate if model #1 is really better than model #2 or if its just by chance
- Bootstrap sampling, Cross validation:
  - Reuse limited data to get a better estimate of a metric

Cross validation

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Slides in this presentation are from material kindly provided by Shannon Ellis and Sebastian Rashka

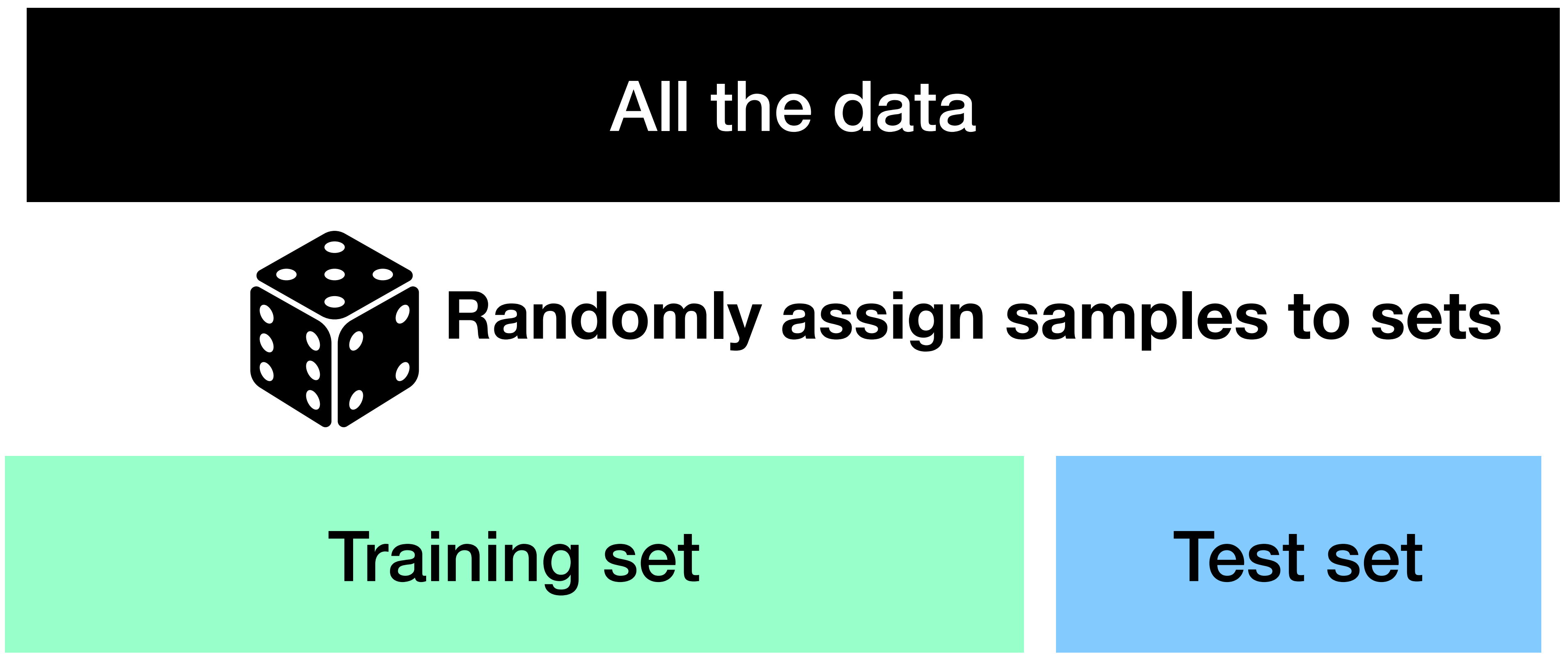
Drowning in data?

Image borrowed from
https://medium.com/@tmaoconnor/marketing-is-drowning-in-data-yet-its-starving-for-answers-f15ee890a732

Limited data?

Evaluating generalization via train - test

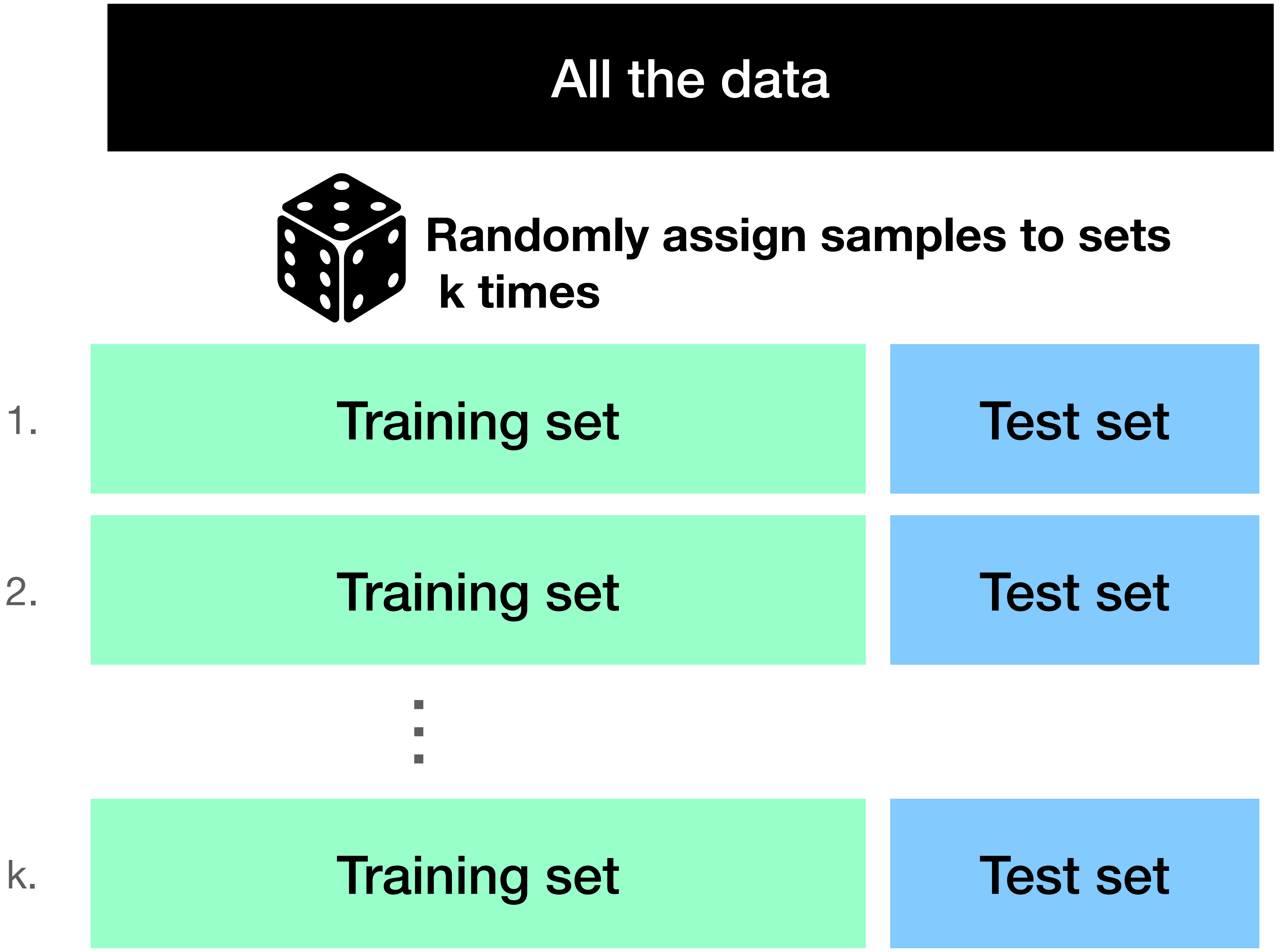
Huge data technique



$$\epsilon_{\text{testing}} = \epsilon_{\text{training}} + \epsilon_{\text{generalization}}$$

Evaluating generalization via k shuffle splits

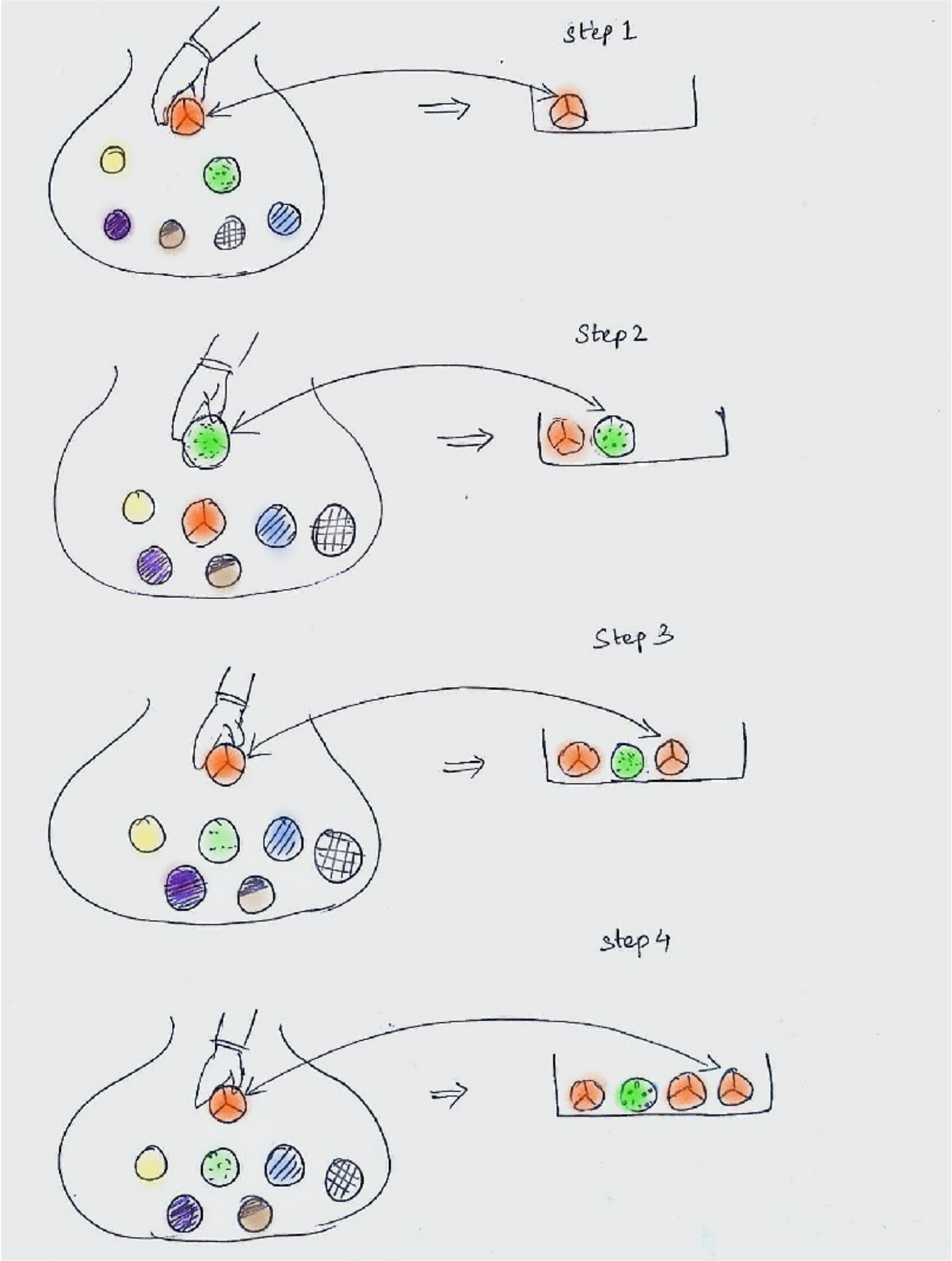
Limited data technique



Use the mean of the k test set performances

$$\bar{\epsilon}_{\text{testing}} = \epsilon_{\text{training}} + \epsilon_{\text{generalization}}$$

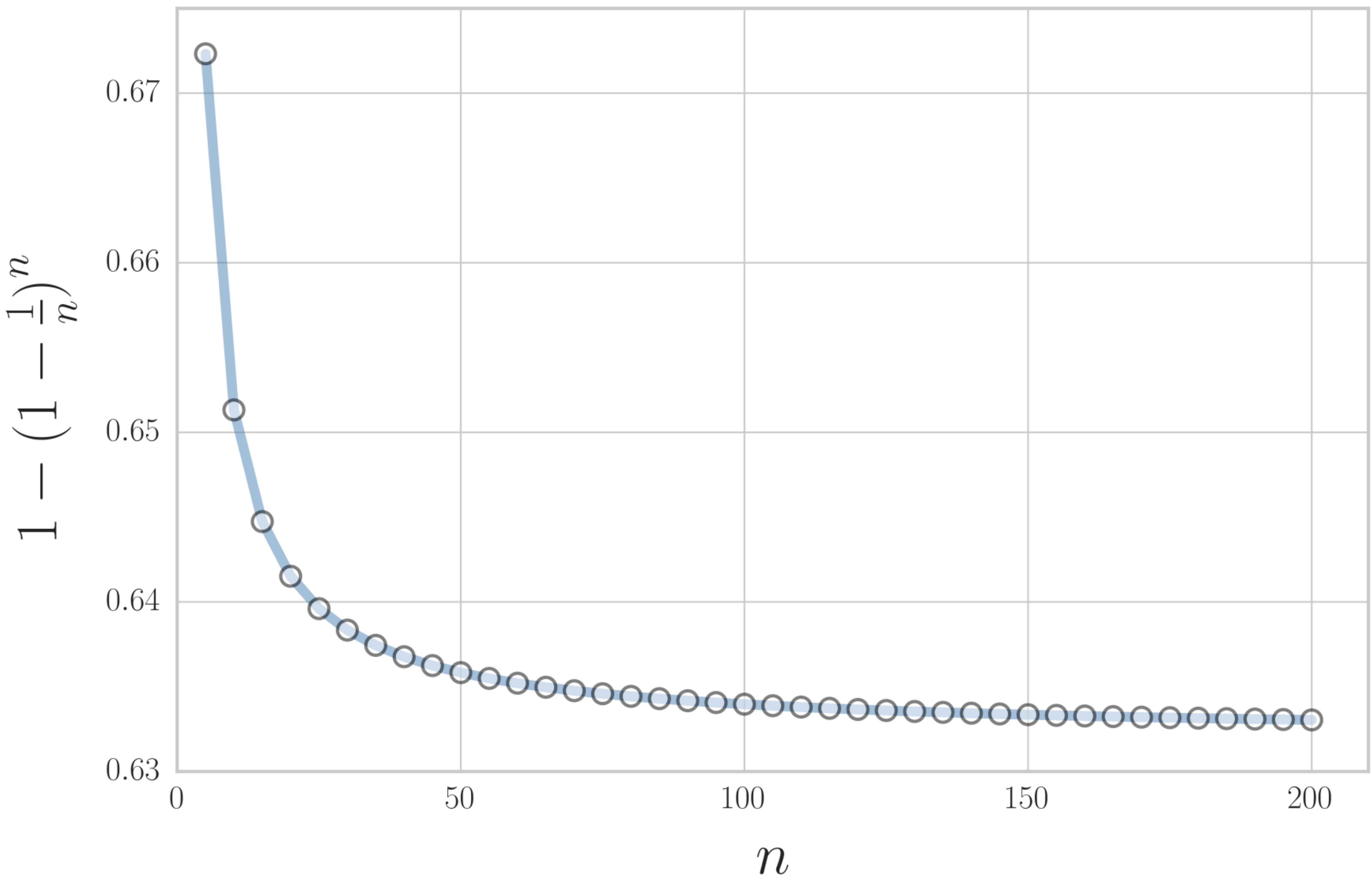
$$\bar{\epsilon}_{\text{testing}} = 1/n \sum_{i\in[0,n]} \epsilon_{\text{test}_i}$$



$$P(\textbf{not chosen}) = \left(1 - \frac{1}{n}\right)^n,$$

$$\frac{1}{e} \approx 0.368, \quad n \to \infty\,.$$

$$P(\textbf{chosen}) = 1 - \left(1 - \frac{1}{n}\right)^n \approx 0.632$$



Evaluating generalization via bootstrap sampling

Limited data technique

All the data

Build k bootstrap samples

1. Training set | Out of bag set
2. Training set | Out of bag set

⋮

k. Training set | Out of bag set

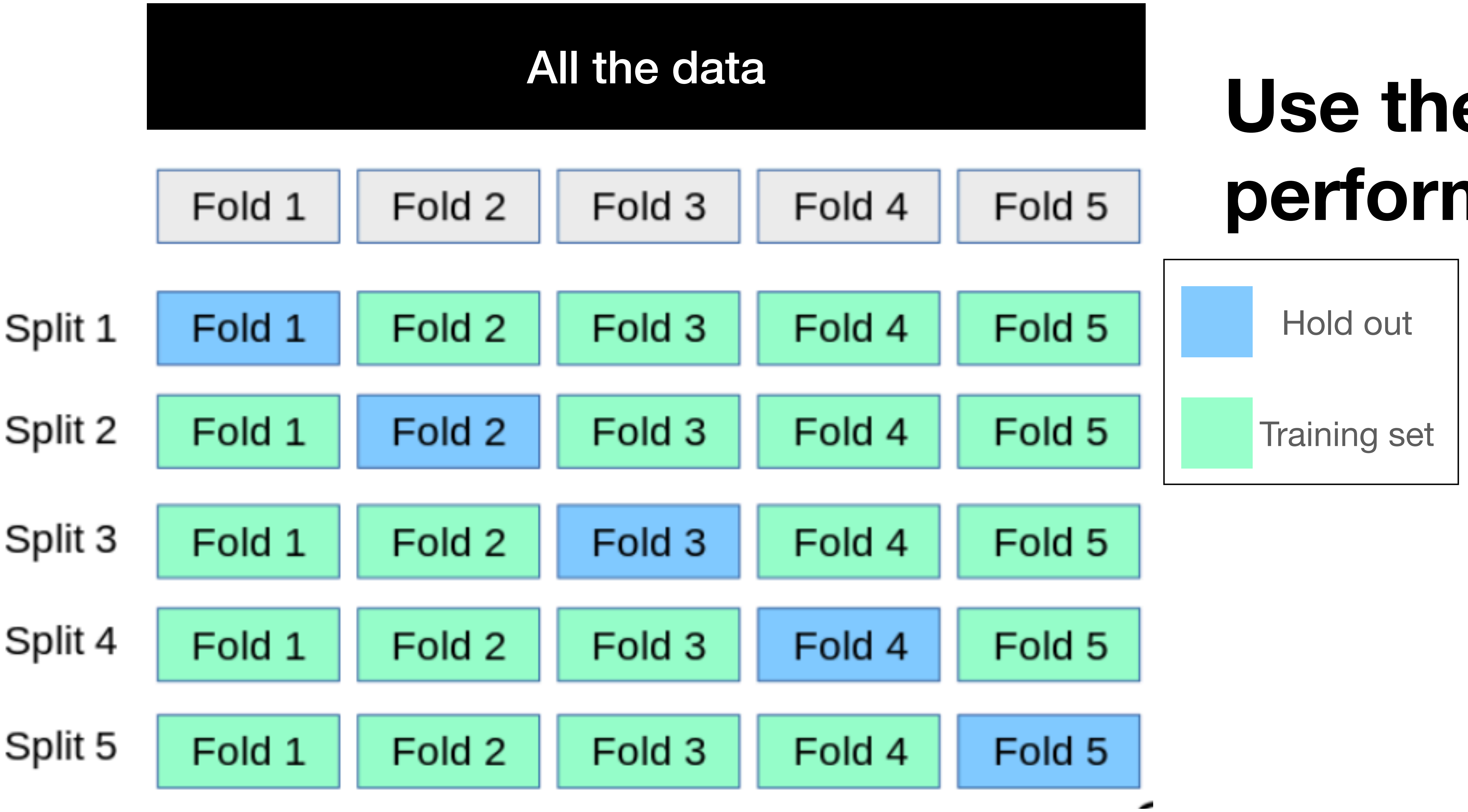
Use the mean of the k test set performances

$$\bar{\epsilon}_{.632+} = 1/n \sum_{i\in[0,n]} \left(\omega * \epsilon_{\text{OOB}_i} + (1-\omega) * \epsilon_{\text{training}_i}\right)$$

$\omega = \dfrac{.632}{(1-.368)R}$, $R = -\dfrac{\epsilon_{\text{OOB}_i} - \epsilon_{\text{training}_i}}{\gamma - (1-\epsilon_{\text{OOB}_i})}$, where γ is a constant calulated on the dataset

Evaluating generalization via k-folds cross-validation

Limited data technique

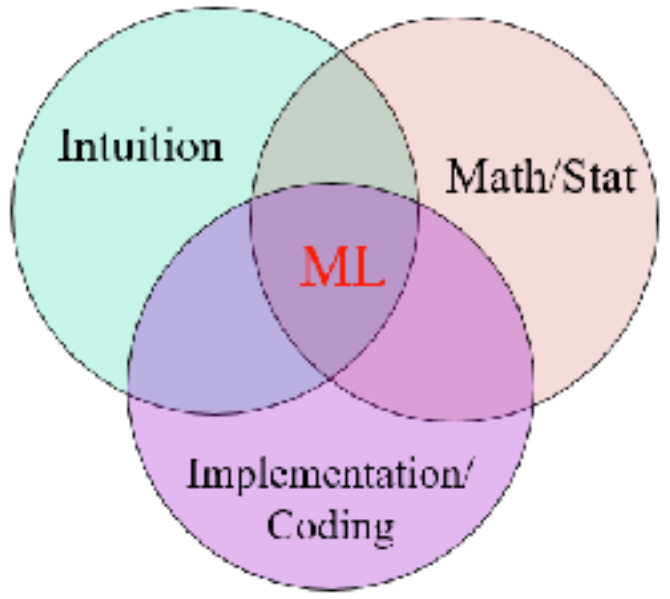


Use the mean of the k hold out set performances

$$\bar{\epsilon}_{\text{testing}} = \epsilon_{\text{training}} + \epsilon_{\text{generalization}}$$

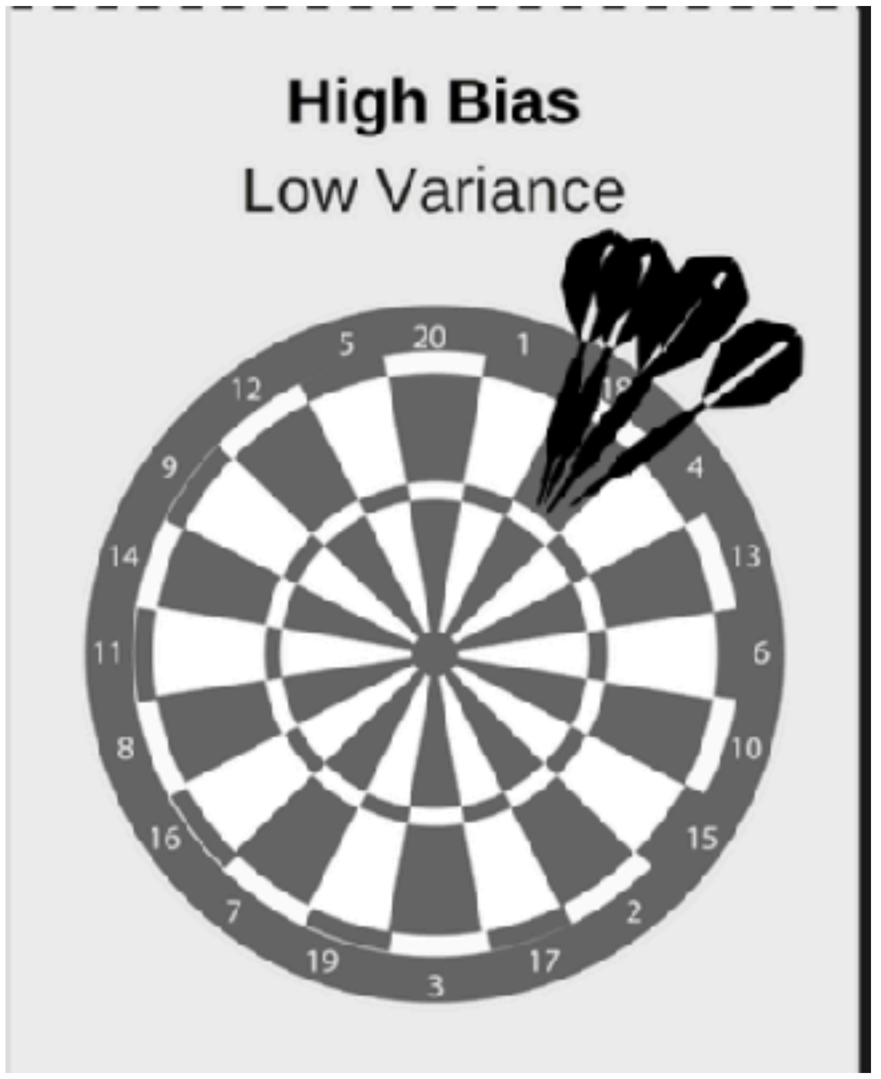
$$\bar{\epsilon}_{\text{testing}} = 1/n \sum_{i \in [0,n]} \epsilon_{\text{hold out}_i}$$

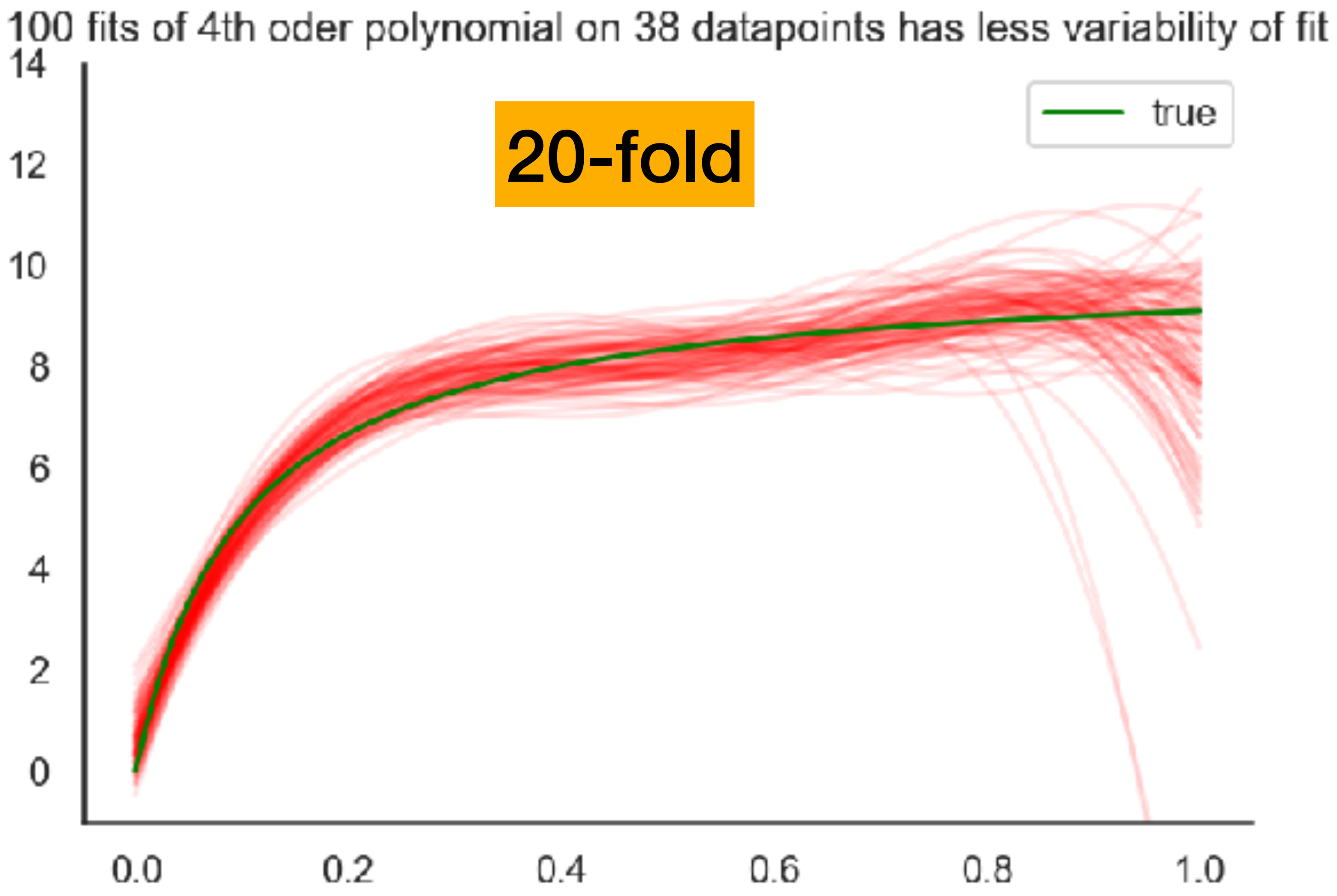
When k = # samples, this is Leave One Out Cross Validation



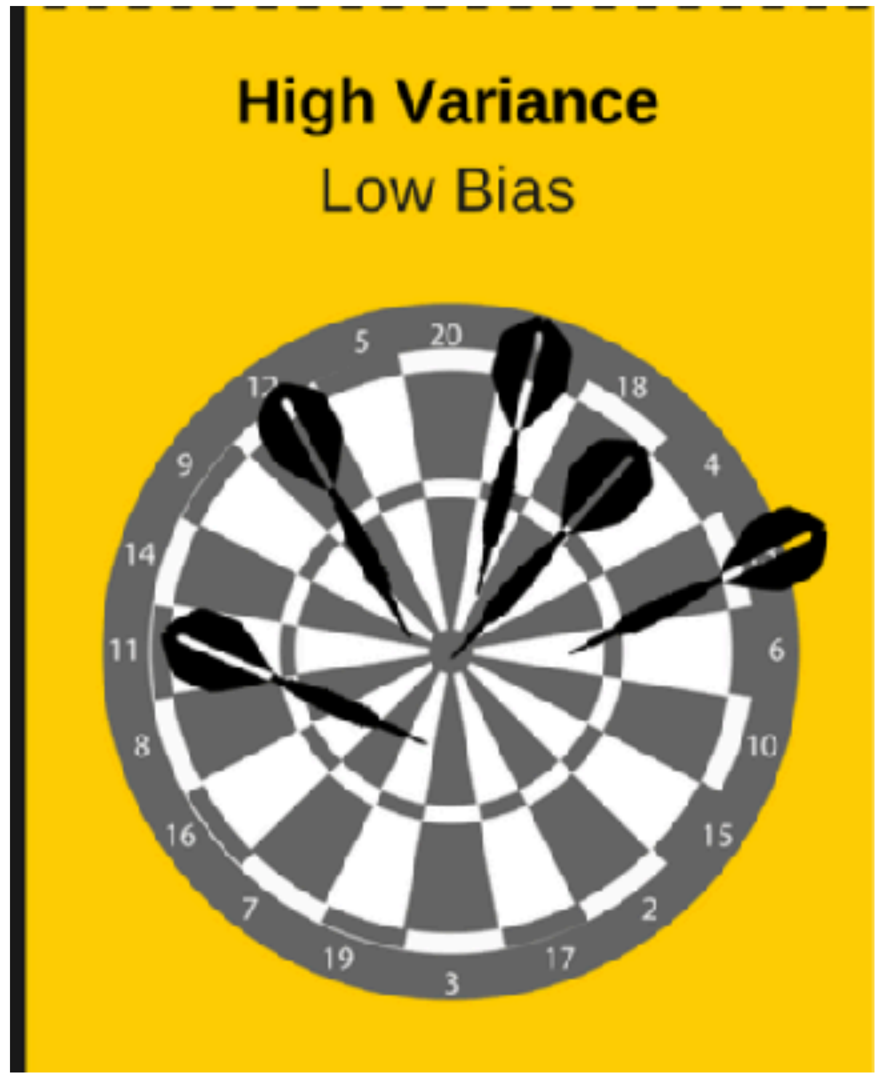
Bias-variance tradeoff in cross validation

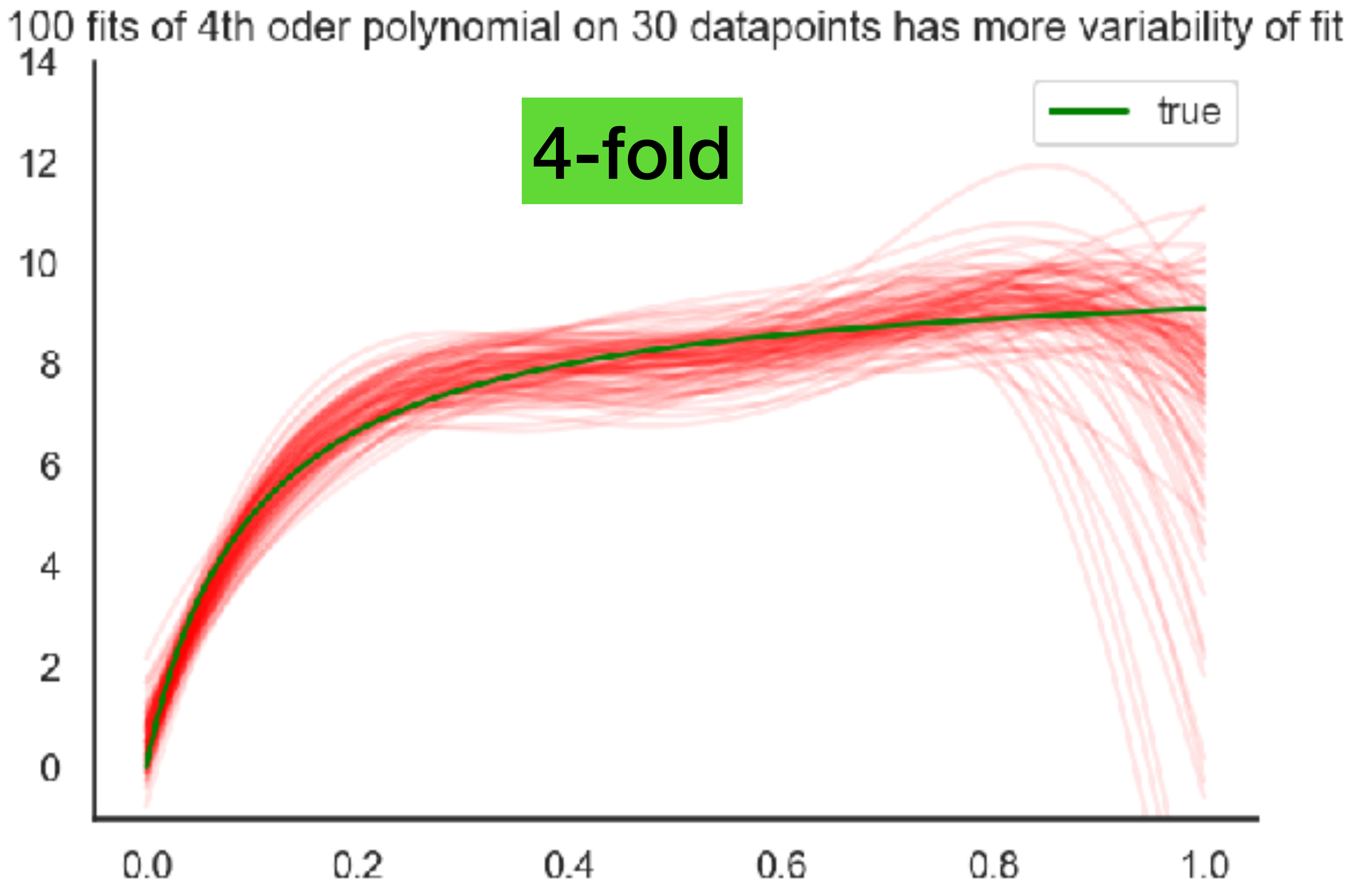
In terms of sample size effects on fit





Larger training set size
(K-folds as k gets large -> LOOCV)
more uniformity of fit





Smaller training set size
(K-folds as k gets small)
more variety of fit

Bias-variance tradeoff in cross validation

In terms of error estimate its the opposite, ⬆️ fit variability == ⬇️ estimate var