

Lecture 09

Model Evaluation 2: Confidence Intervals and Resampling Methods

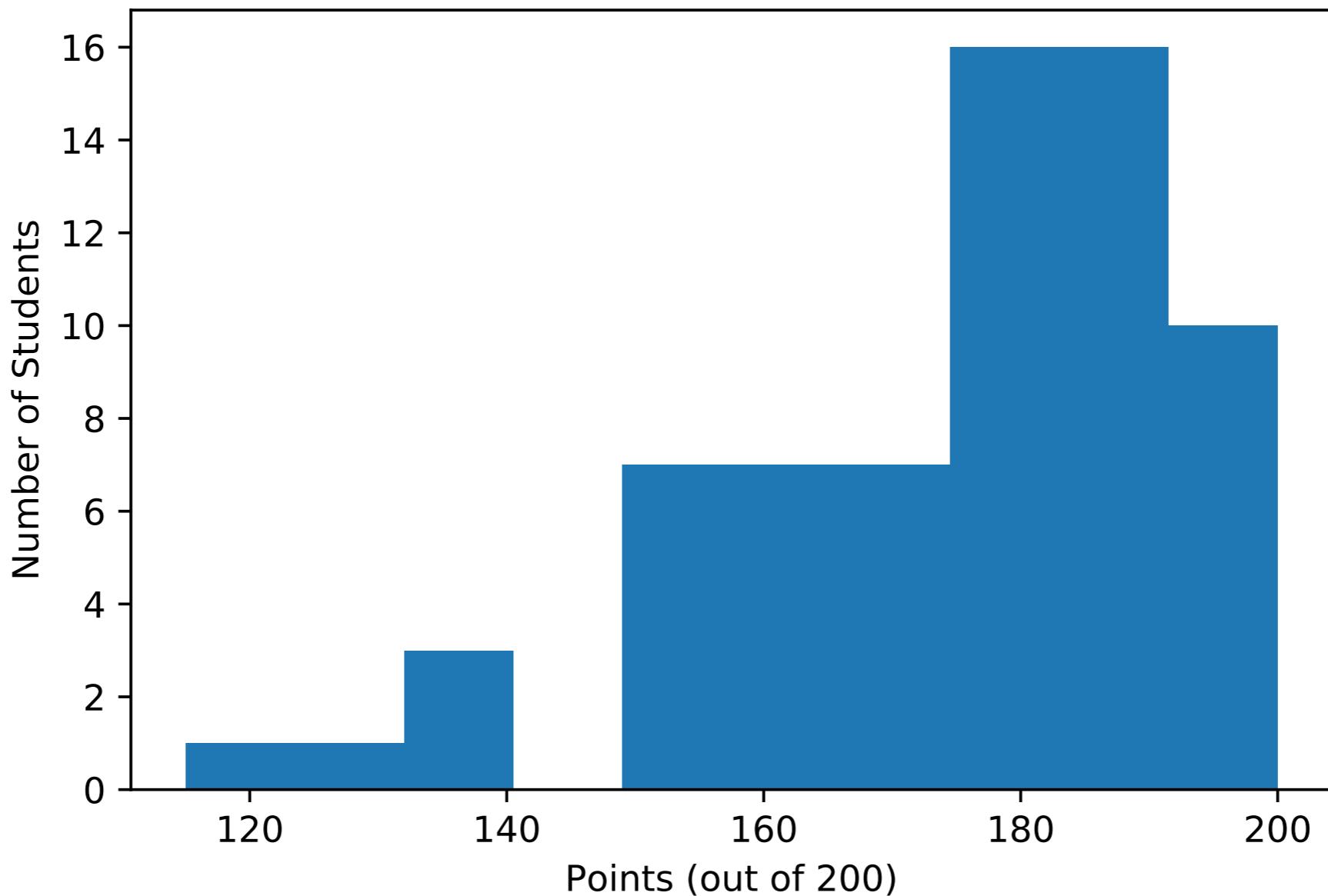
STAT 479: Machine Learning, Fall 2019

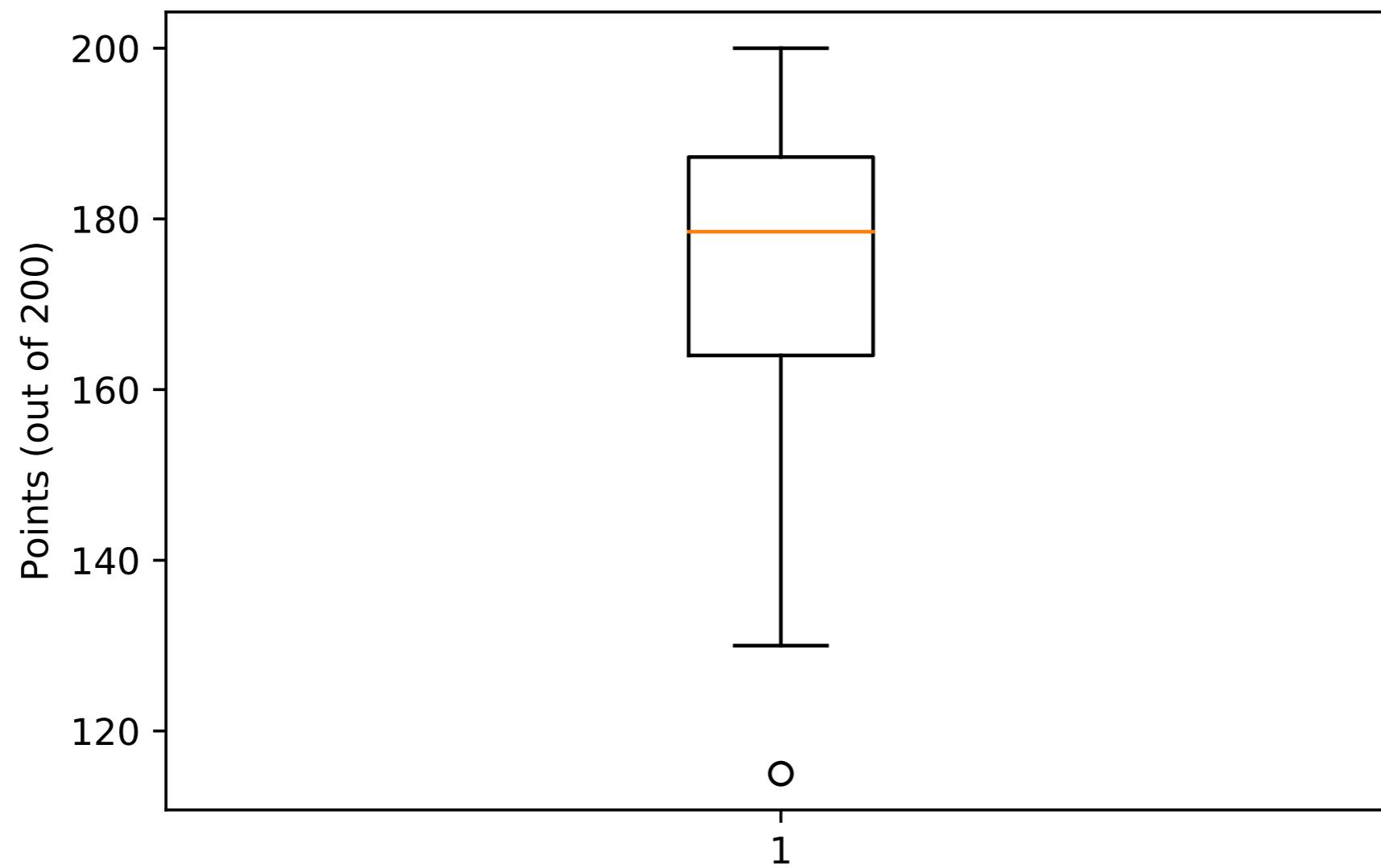
Sebastian Raschka

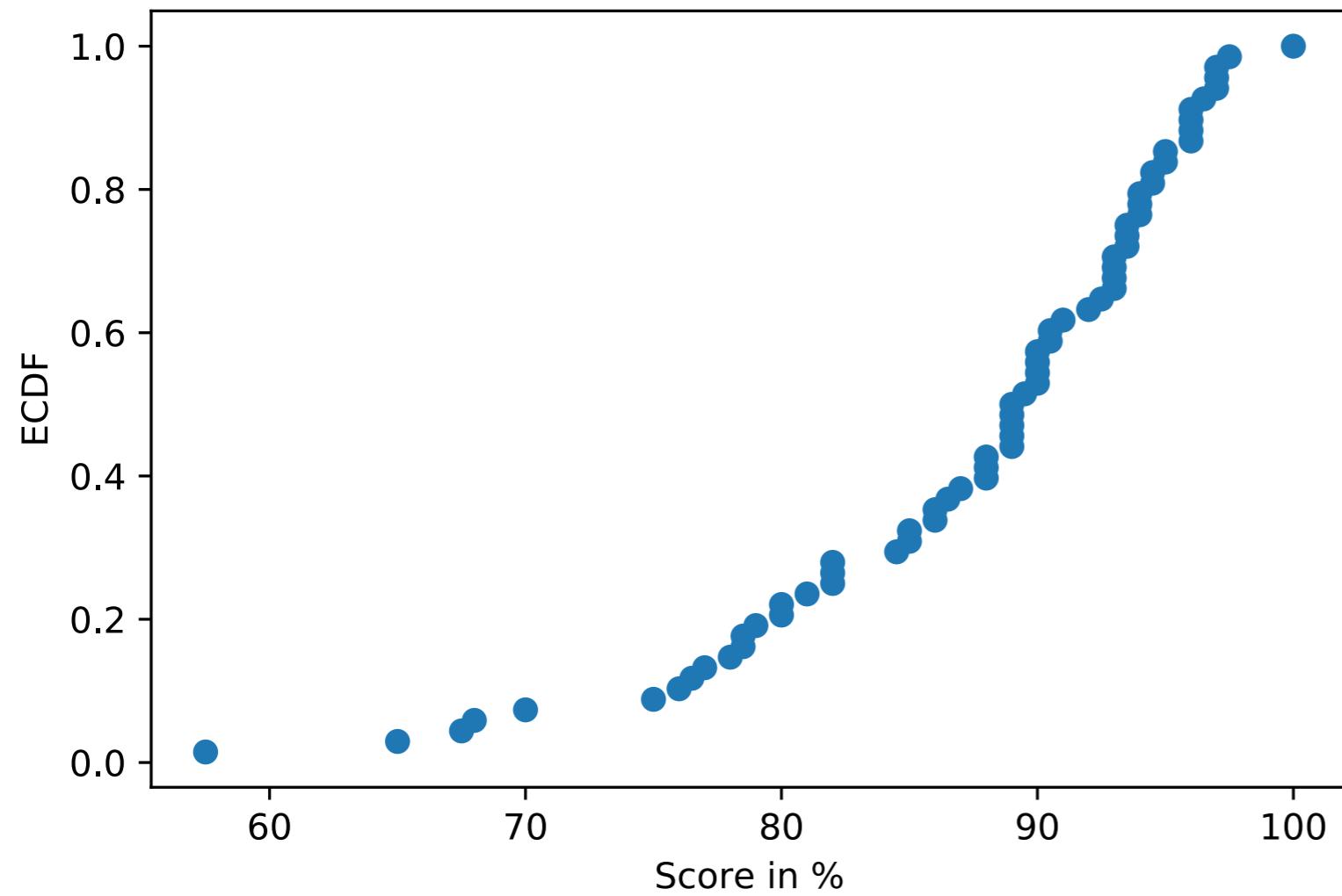
<http://stat.wisc.edu/~sraschka/teaching/stat479-fs2019/>

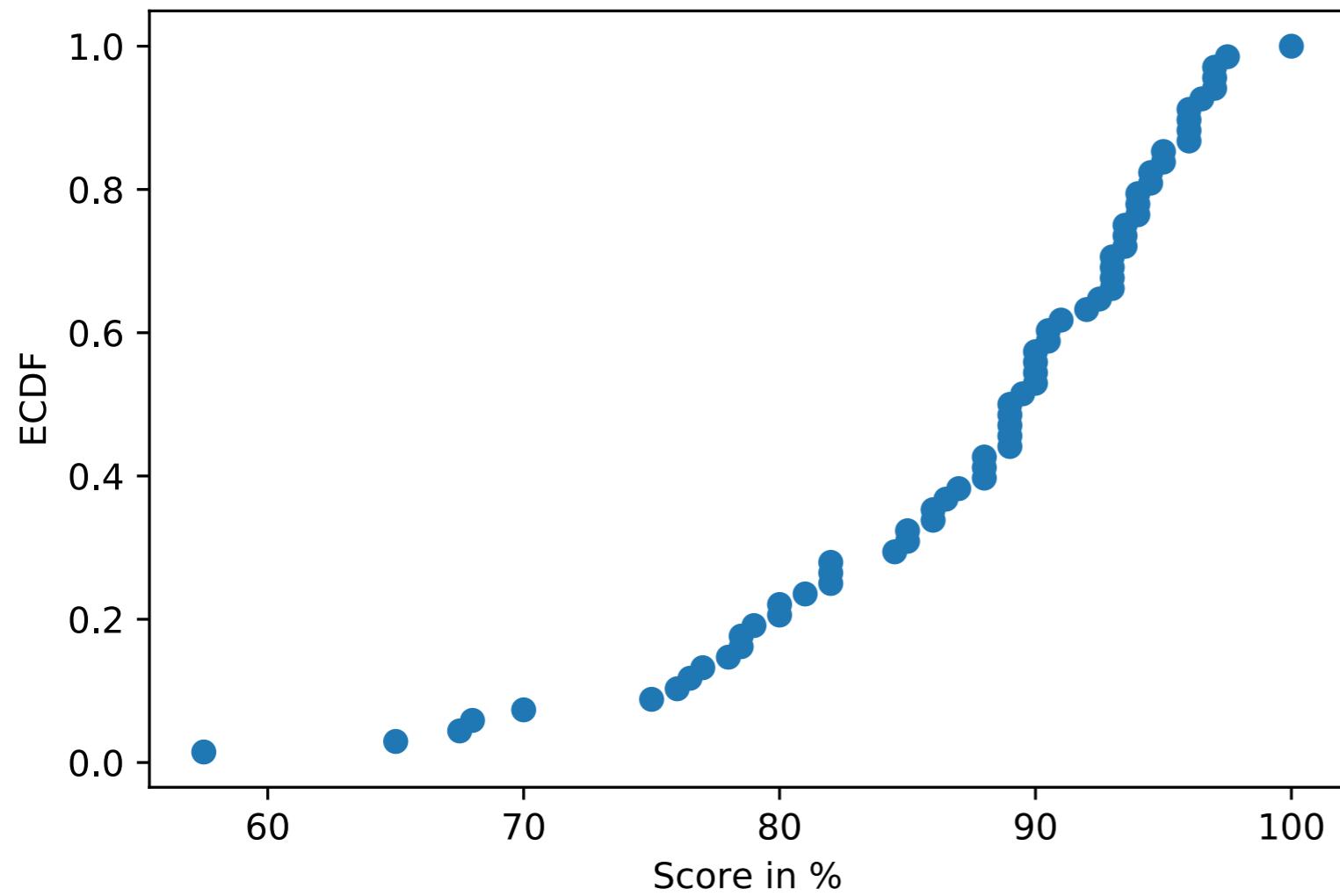
Announcements

Midterm Exam Outcome









A	\geq	93%	:	24
AB	\geq	90%	:	9
B	\geq	85%	:	15
BC	\geq	80%	:	7
C	\geq	70%	:	9
D	\geq	60%	:	3
F	$<$	60%	:	1



Artificial Intelligence (AI)

Lex Fridman

► Resume Episode

✓ SUBSCRIBED



Michio Kaku: Future of Humans, Aliens, Space Travel & Physics: Michio Kaku is a theoretical physicist, futurist, and professor at the City College of New York. He is the author of many fascinating books on the nature of our reality and the future of our civilization. This conversation is part of the Artificial Intelligence podcast. If you would like to get more information about this podcast go to <https://lexfridman.com/ai> or connect with @lexfridman on Twitter, LinkedIn, Facebook,

My Episodes



DeepMind: The Podcast

DeepMind

► Resume Episode

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2. Go to Zero: In March 2016, more than 200 million people watched AlphaGo become first computer program to defeat a professional human player at the game of Go, a milestone in AI research that was considered to be a decade ahead of its time. Since then the team has continued to develop the system and recently unveiled AlphaZero: a program that has taught itself how to play chess, Go, and shogi. Hannah explores the inside story of both with Lead Researcher David Silver and

My Episodes



Talking Machines

Tote Bag Productions

► Play Episode

✓ SUBSCRIBED



20. Children are the Future and Ada Lovelace Day: In episode twenty of season five we talk with Neil about a discussion he had about the impact of ML tools on children talk about the new Diversity Dashboard from the Turing Institute in response to a question about cool things for Ada Lovelace day plus we sit down with Corinna Cortes of Google AI

My Episodes

Model Evaluation 2:

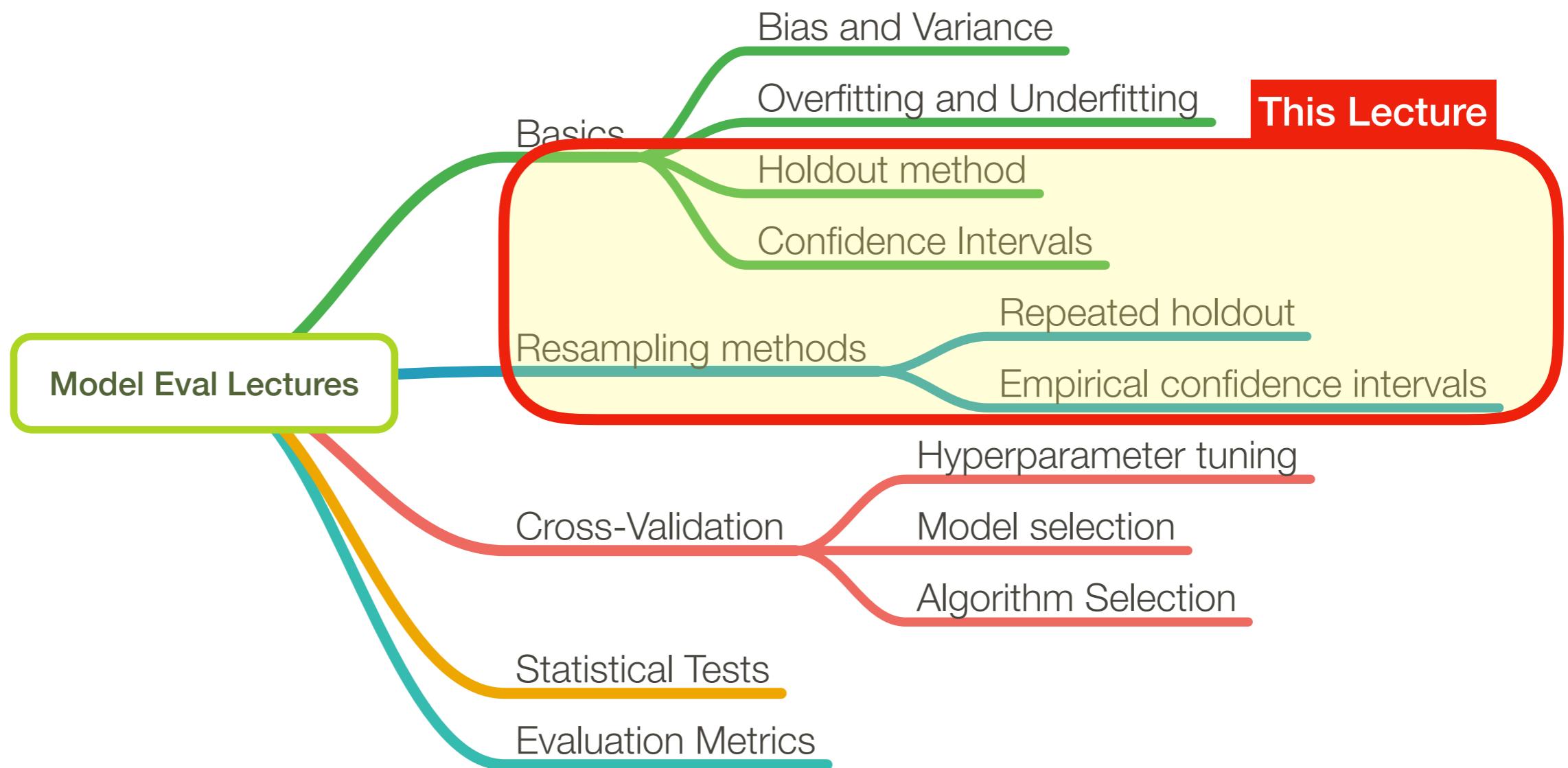
Confidence Intervals

STAT 479: Machine Learning, Fall 2019

Sebastian Raschka

<http://stat.wisc.edu/~sraschka/teaching/stat479-fs2019/>

Overview

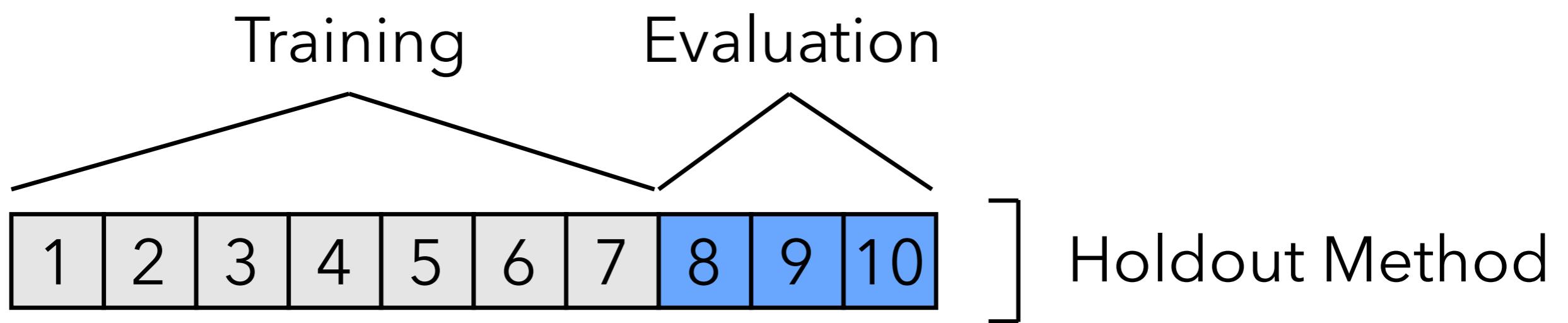


- Concepts first
- Code examples at the end of the lecture

Main points why we evaluate the predictive performance of a model:

1. Want to estimate the generalization performance, the predictive performance of our model on future (unseen) data.
2. Want to increase the predictive performance by tweaking the learning algorithm and selecting the best performing model from a given hypothesis space.
3. Want to identify the ML algorithm that is best-suited for the problem at hand; thus, we want to compare different algorithms, selecting the best-performing one as well as the best performing model from the algorithm's hypothesis space.

- Training set error is an optimistically biased estimator of the generalization error
- Test set error is an unbiased estimator of the generalization error (test sample and hypothesis chosen independently)
- (in practice, the test set error is actually pessimistically biased; why?)



Often using the holdout
method is not a good idea ...

Often using the holdout
method is not a good idea ...

Test set error as generalization error estimator is optimistically
biased (not so bad)

But it does not account for variance in the training data (bad)

Why is pessimistic bias not "so bad"?

Suppose we have the following ranking based on accuracy:

$h_2: 75\% > h_1: 70\% > h_3: 65\%$,

we would still rank them the same way if we add a 10% pessimistic bias:

$h_2: 65\% > h_1: 60\% > h_3: 55\%$.

Do CIFAR-10 Classifiers Generalize to CIFAR-10?

Benjamin Recht
UC Berkeley

Rebecca Roelofs
UC Berkeley

Ludwig Schmidt
MIT

Vaishaal Shankar
UC Berkeley

June 4, 2018

Abstract

Machine learning is currently dominated by largely experimental work focused on improvements in a few key tasks. However, the impressive accuracy numbers of the best performing models are questionable because the same test sets have been used to select these models for multiple years now. To understand the danger of overfitting, we measure the accuracy of CIFAR-10 classifiers by creating a new test set of truly unseen images. Although we ensure that the new test set is as close to the original data distribution as possible, we find a large drop in accuracy (4% to 10%) for a broad range of deep learning models. Yet, more recent models with higher original accuracy show a *smaller* drop and better overall performance, indicating that this drop is likely not due to overfitting based on adaptivity. Instead, we view our results as evidence that current accuracy numbers are brittle and susceptible to even minute natural variations in the data distribution.

Recht, B., Roelofs, R., Schmidt, L., & Shankar, V. (2018). Do CIFAR-10 classifiers generalize to CIFAR-10?. *arXiv preprint arXiv:1806.00451*.

<https://arxiv.org/abs/1806.00451>

The CIFAR-10 dataset

CIFAR -> Canadian Institute For Advanced Research

- 60,000 32x32 color images in 10 classes
- 6,000 images per class
- 50,000 training images and 10,000 test images

airplane



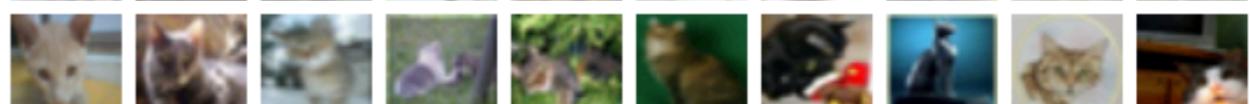
automobile



bird



cat



deer



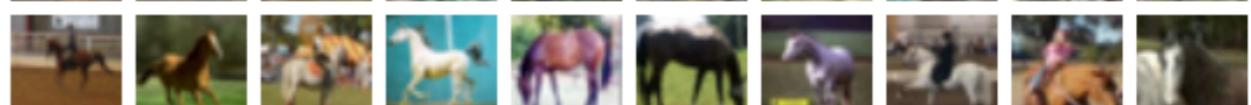
dog



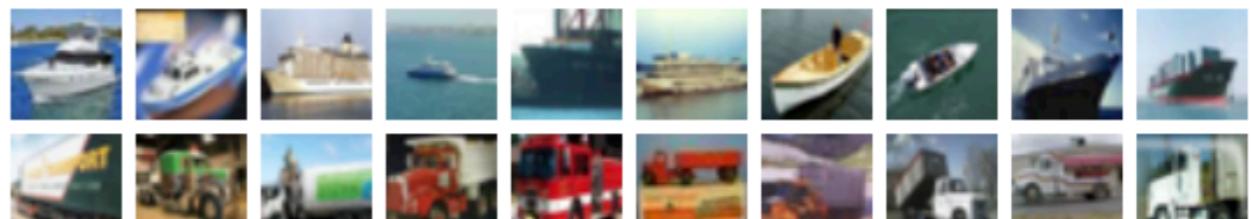
frog



horse



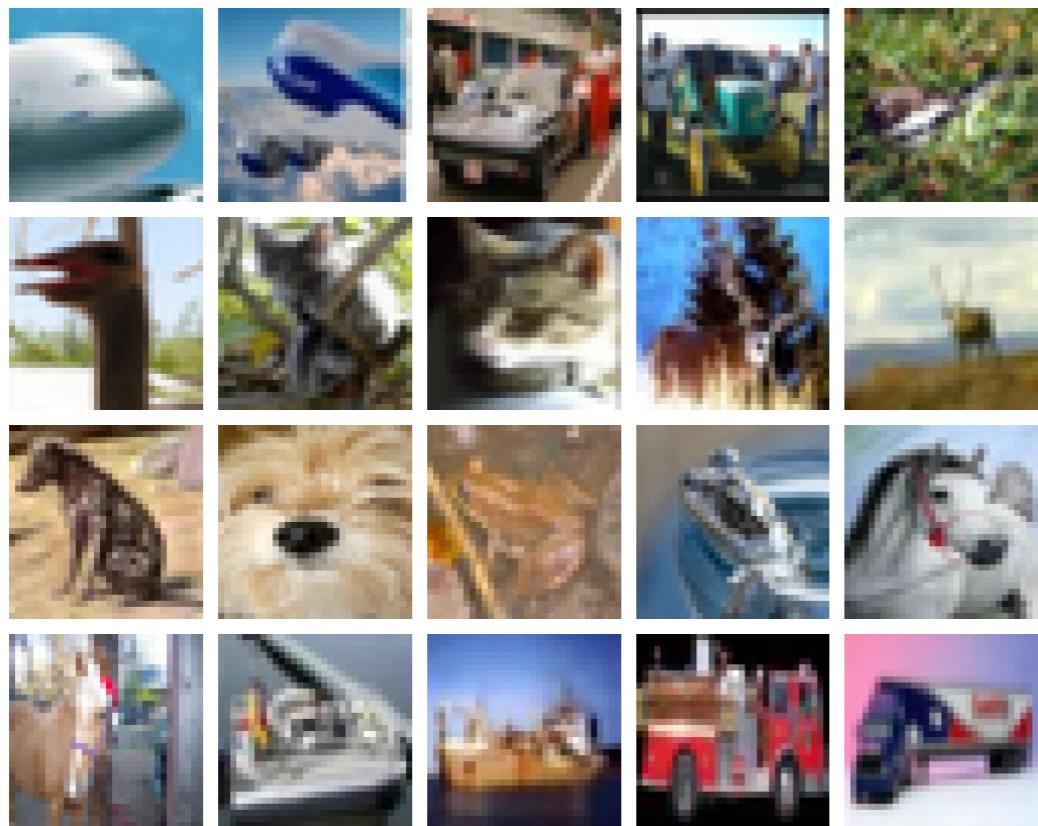
ship



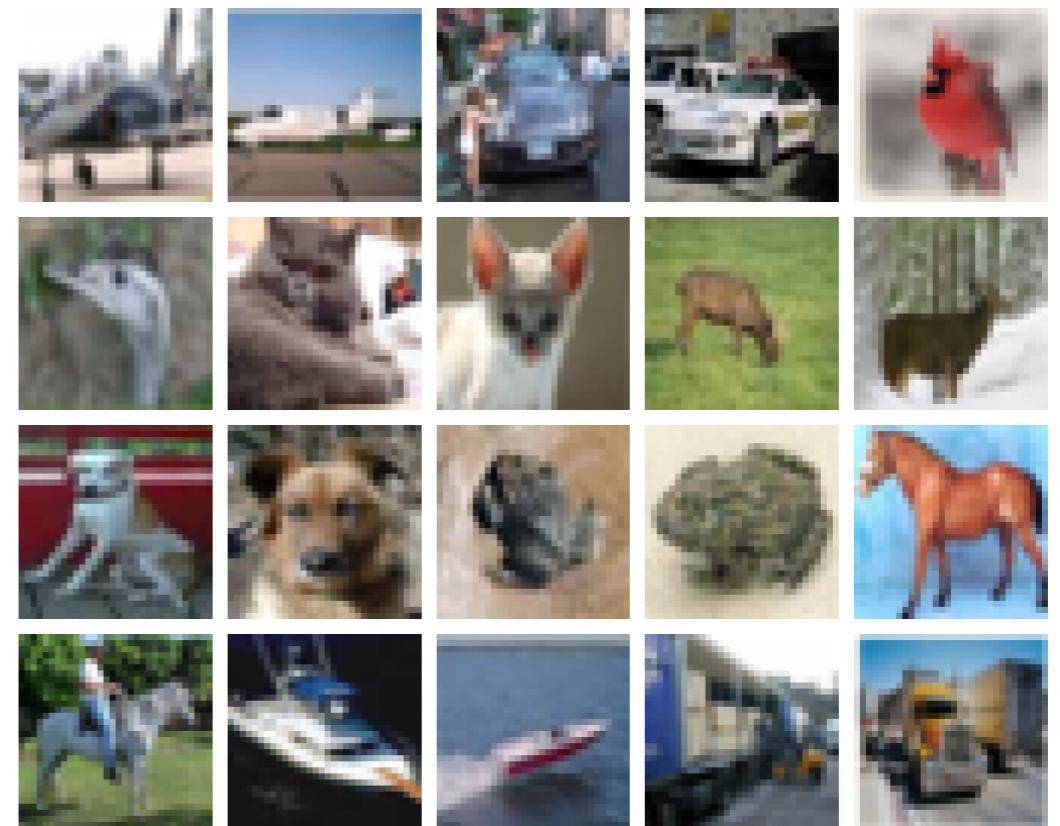
truck



<https://www.cs.toronto.edu/~kriz/cifar.html>

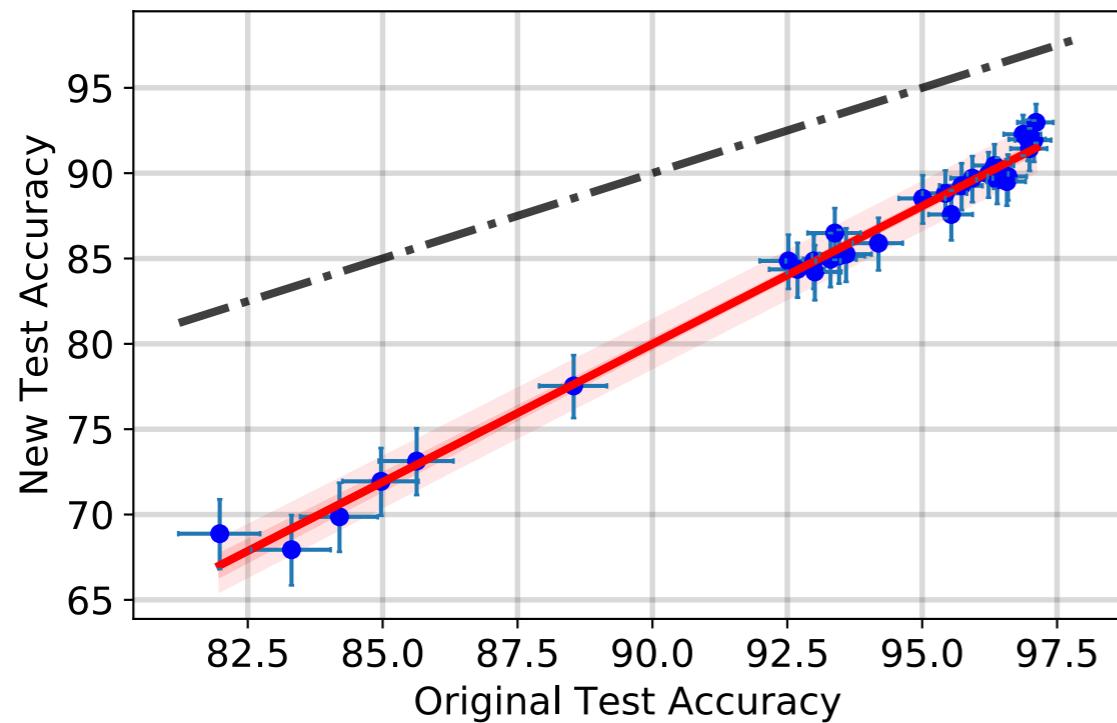


(a) Test Set A



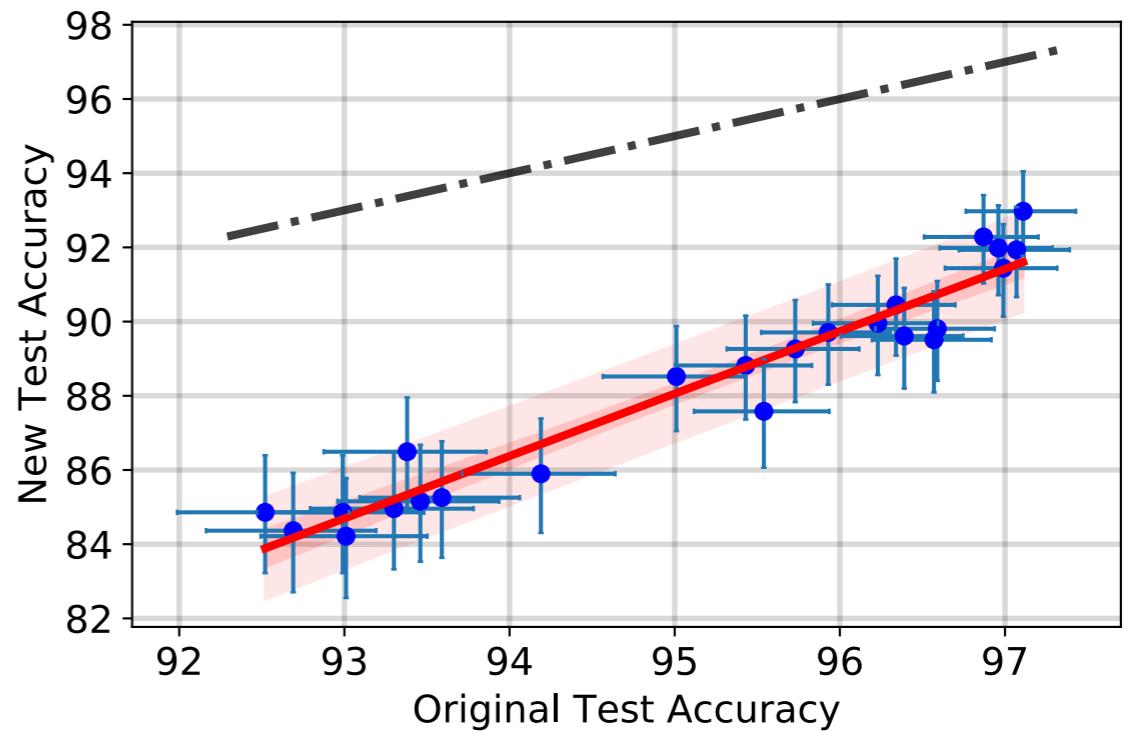
(b) Test Set B

Figure 1: Class-balanced random draws from the new and original test sets.¹



(a) All models

- Model
- · Ideal reproducibility
- Linear Fit
- Linear Fit 95% Prediction Interval
- + Model Confidence Interval



(b) High accuracy models

- Linear Fit 95% Prediction Interval
- + Model Confidence Interval

Figure 2: Model accuracy on new test set vs. model accuracy on original test set.

Recht, B., Roelofs, R., Schmidt, L., & Shankar, V. (2018). Do CIFAR-10 classifiers generalize to CIFAR-10?. *arXiv preprint arXiv:1806.00451*.

Table 1: Model accuracy on the original CIFAR-10 test set and the new test set, with the gap reported as the difference between the two accuracies. Δ Rank is the relative difference in the ranking from the original test set to the new test set. For example, Δ Rank = -2 means a model dropped in the rankings by two positions on the new test set.

	Original Accuracy	New Accuracy	Gap	Δ Rank
shake_shake_64d_cutout [3, 4]	97.1 [96.8, 97.4]	93.0 [91.8, 94.0]	4.1	0
shake_shake_96d [4]	97.1 [96.7, 97.4]	91.9 [90.7, 93.1]	5.1	-2
shake_shake_64d [4]	97.0 [96.6, 97.3]	91.4 [90.1, 92.6]	5.6	-2
wide_resnet_28_10_cutout [3, 22]	97.0 [96.6, 97.3]	92.0 [90.7, 93.1]	5	+1
shake_drop [21]	96.9 [96.5, 97.2]	92.3 [91.0, 93.4]	4.6	+3
shake_shake_32d [4]	96.6 [96.2, 96.9]	89.8 [88.4, 91.1]	6.8	-2
darc [11]	96.6 [96.2, 96.9]	89.5 [88.1, 90.8]	7.1	-4
resnext_29_4x64d [20]	96.4 [96.0, 96.7]	89.6 [88.2, 90.9]	6.8	-2
pyramidnet_basic_110_270 [6]	96.3 [96.0, 96.7]	90.5 [89.1, 91.7]	5.9	+3
resnext_29_8x64d [20]	96.2 [95.8, 96.6]	90.0 [88.6, 91.2]	6.3	+3
wide_resnet_28_10 [22]	95.9 [95.5, 96.3]	89.7 [88.3, 91.0]	6.2	+2
pyramidnet_basic_110_84 [6]	95.7 [95.3, 96.1]	89.3 [87.8, 90.6]	6.5	0
densenet_BC_100_12 [10]	95.5 [95.1, 95.9]	87.6 [86.1, 89.0]	8	-2
neural_architecture_search [23]	95.4 [95.0, 95.8]	88.8 [87.4, 90.2]	6.6	+1
wide_resnet_tf [22]	95.0 [94.6, 95.4]	88.5 [87.0, 89.9]	6.5	+1
resnet_v2_bottleneck_164 [8]	94.2 [93.7, 94.6]	85.9 [84.3, 87.4]	8.3	-1
vgg16_keras [14, 18]	93.6 [93.1, 94.1]	85.3 [83.6, 86.8]	8.3	-1
resnet_basic_110 [7]	93.5 [93.0, 93.9]	85.2 [83.5, 86.7]	8.3	-1
resnet_v2_basic_110 [8]	93.4 [92.9, 93.9]	86.5 [84.9, 88.0]	6.9	+3
resnet_basic_56 [7]	93.3 [92.8, 93.8]	85.0 [83.3, 86.5]	8.3	0
resnet_basic_44 [7]	93.0 [92.5, 93.5]	84.2 [82.6, 85.8]	8.8	-3
vgg_15_BN_64 [14, 18]	93.0 [92.5, 93.5]	84.9 [83.2, 86.4]	8.1	+1
resnet_preact_tf [7]	92.7 [92.2, 93.2]	84.4 [82.7, 85.9]	8.3	0
resnet_basic_32 [7]	92.5 [92.0, 93.0]	84.9 [83.2, 86.4]	7.7	+3
cudacovnet [13]	88.5 [87.9, 89.2]	77.5 [75.7, 79.3]	11	0
random_features_256k_aug [2]	85.6 [84.9, 86.3]	73.1 [71.1, 75.1]	12	0
random_features_32k_aug [2]	85.0 [84.3, 85.7]	71.9 [69.9, 73.9]	13	0
random_features_256k [2]	84.2 [83.5, 84.9]	69.9 [67.8, 71.9]	14	0
random_features_32k [2]	83.3 [82.6, 84.0]	67.9 [65.9, 70.0]	15	-1
alexnet_tf	82.0 [81.2, 82.7]	68.9 [66.8, 70.9]	13	+1

Often using the holdout method is not a good idea ...

- Test set error as generalization error estimator is pessimistically biased (not so bad)
- Does not account for variance in the training data (bad)

Issues with Subsampling (Independence Violation)



The Iris dataset consists of 50 Setosa, 50 Versicolor, and 50 Virginica flowers; the flower species are distributed uniformly:

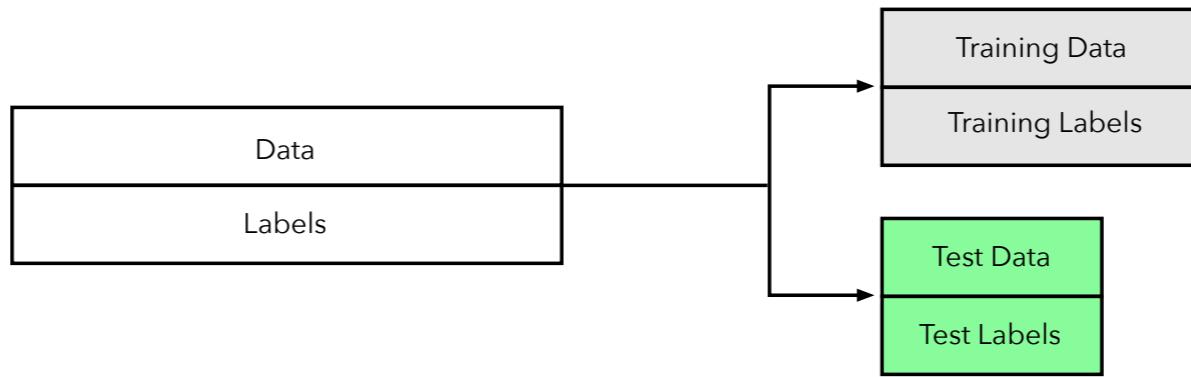
- 33.3% Setosa
- 33.3% Versicolor
- 33.3% Virginia

If our random function assigns 2/3 of the flowers (100) to the training set and 1/3 of the flowers (50) to the test set, it may yield the following:

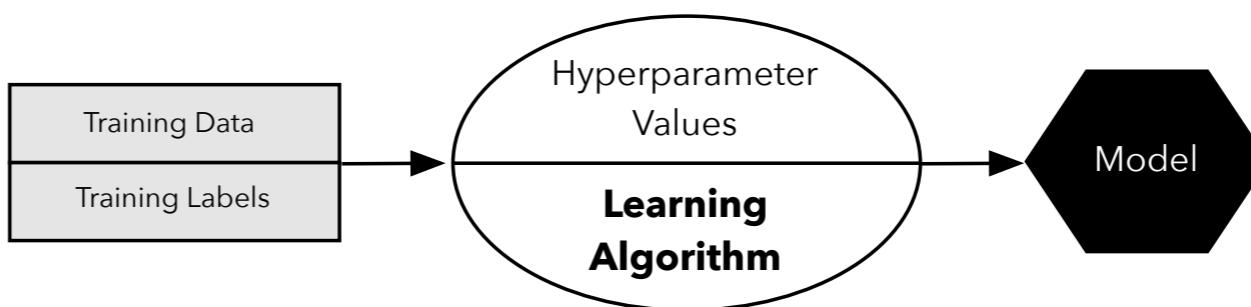
- training set → 38 x Setosa, 28 x Versicolor, 34 x Virginica
- test set → 12 x Setosa, 22 x Versicolor, 16 x Virginica

Holdout evaluation

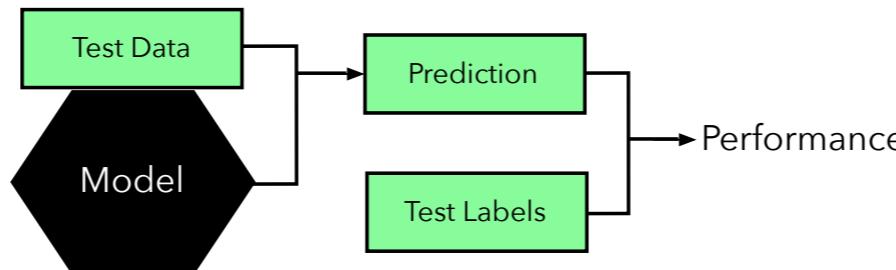
1



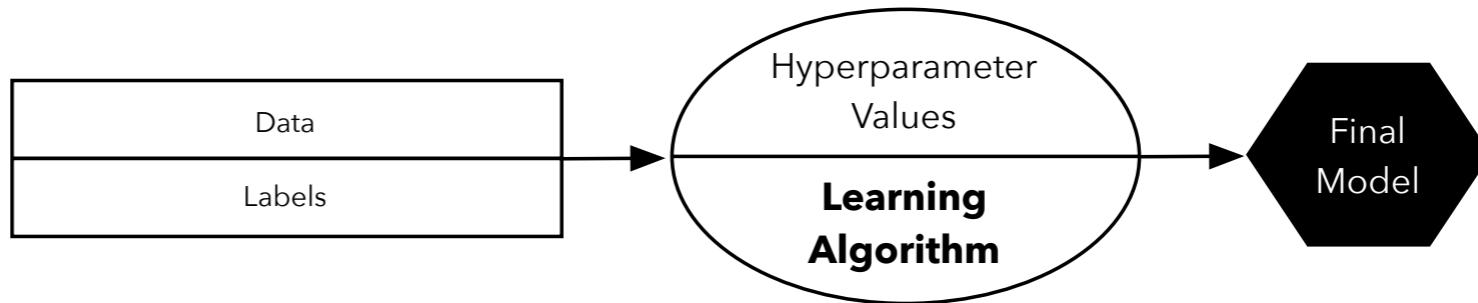
2



3

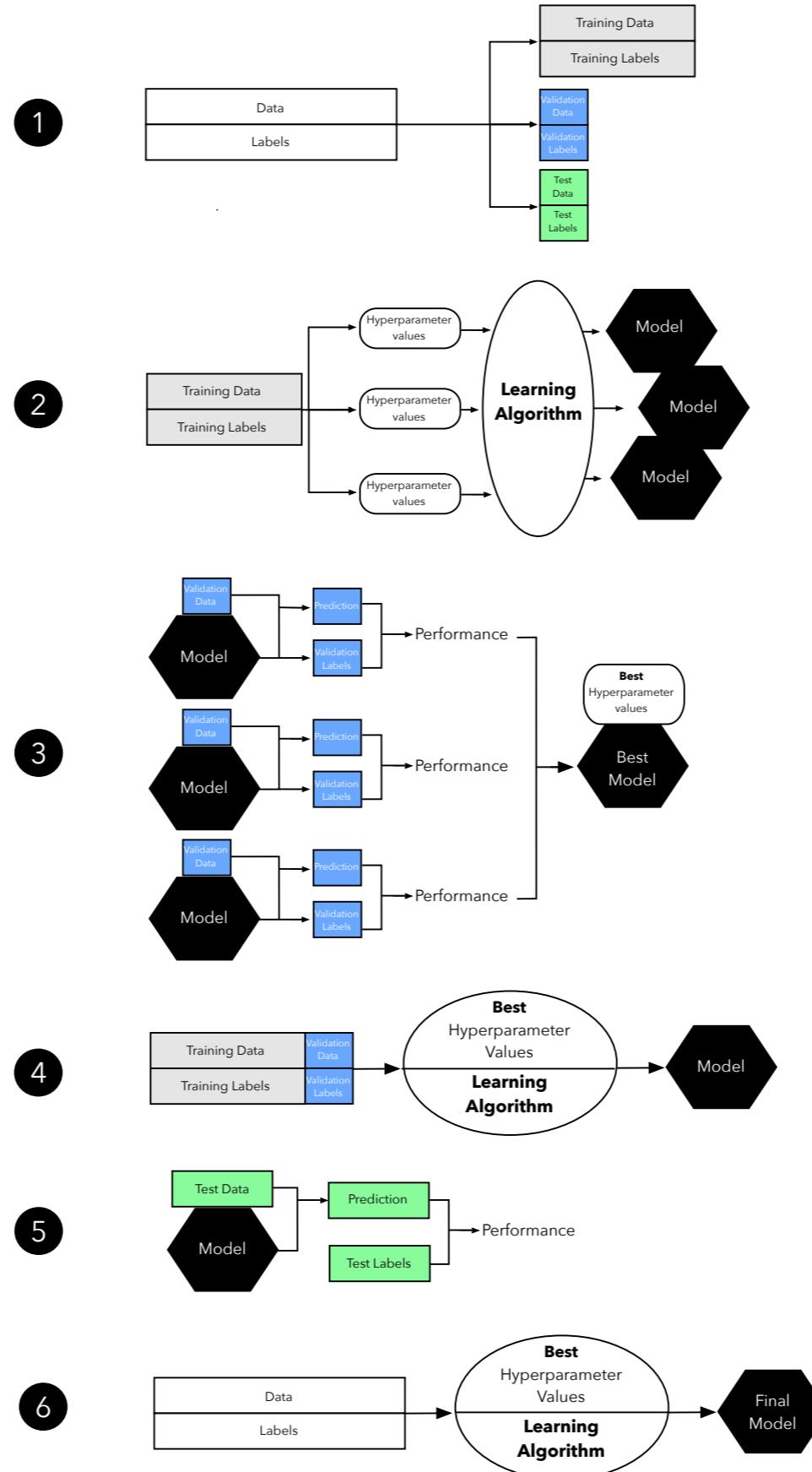


4



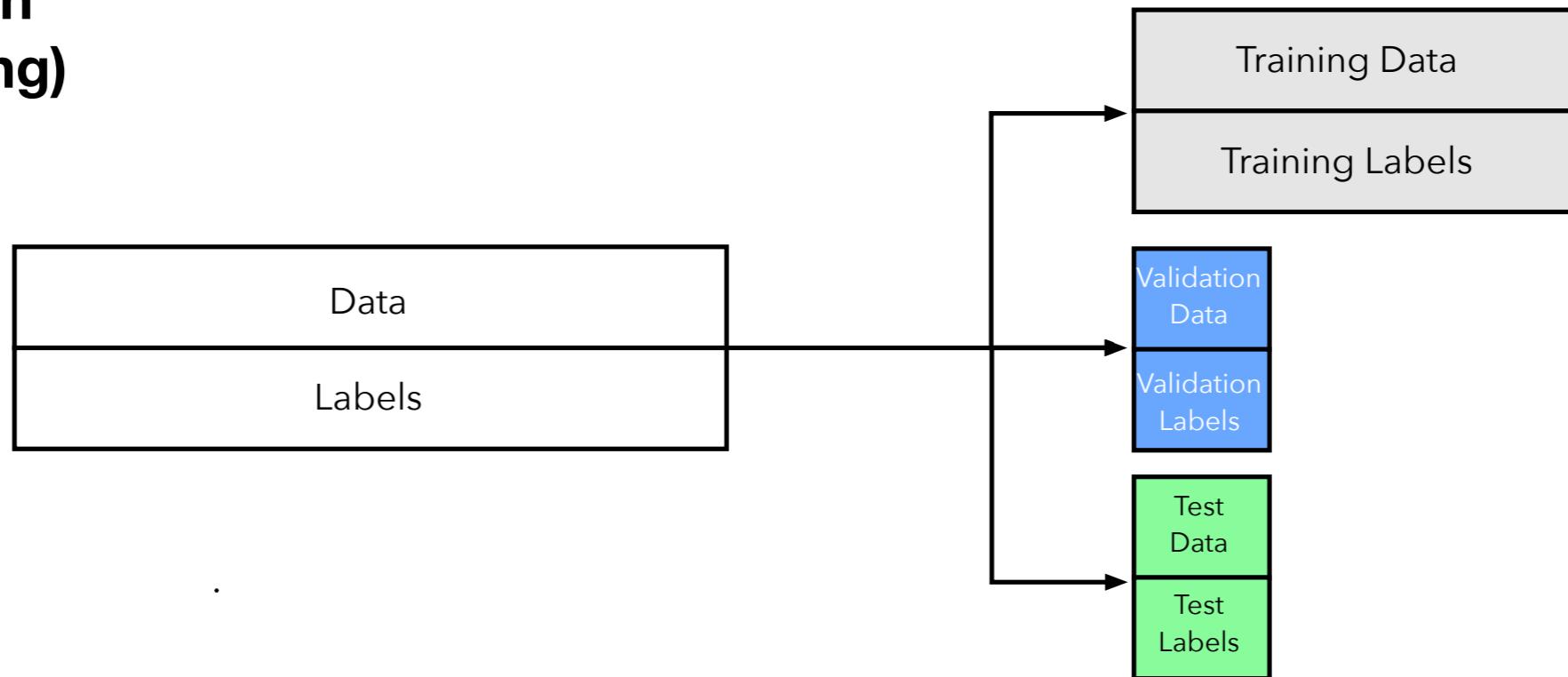
**Can we use the holdout method
for model selection?**

Holdout validation (hyperparam. tuning)

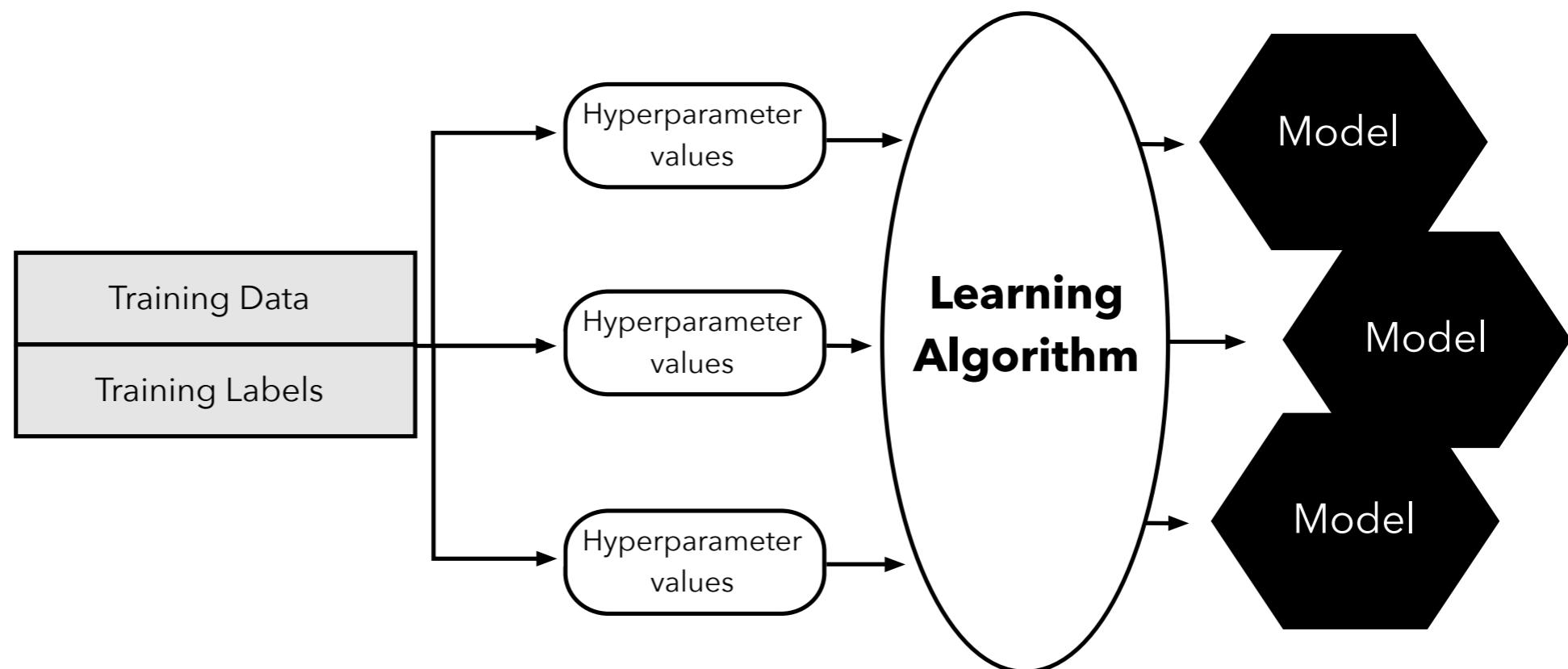


Holdout validation (hyperparam. tuning)

1

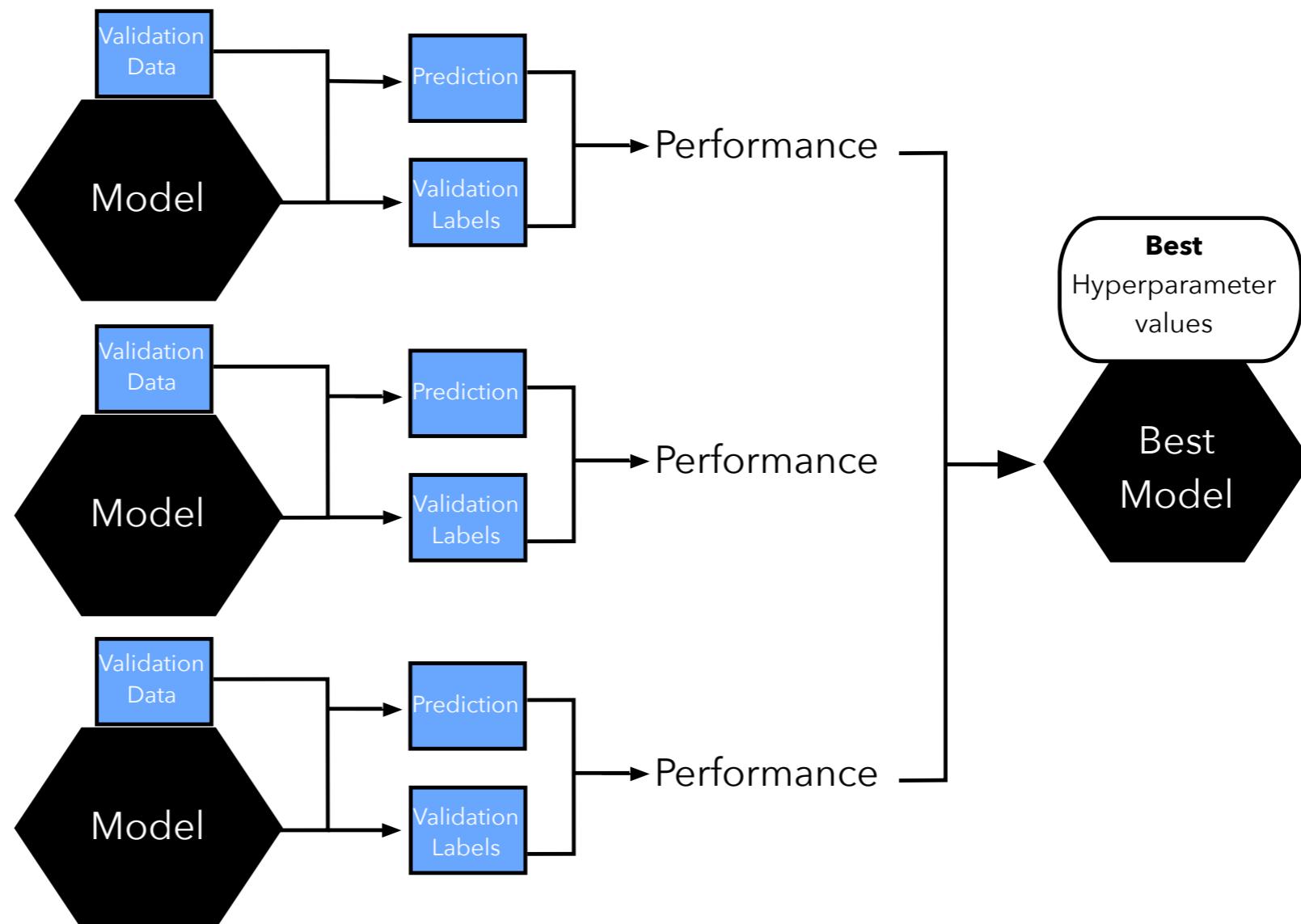


2

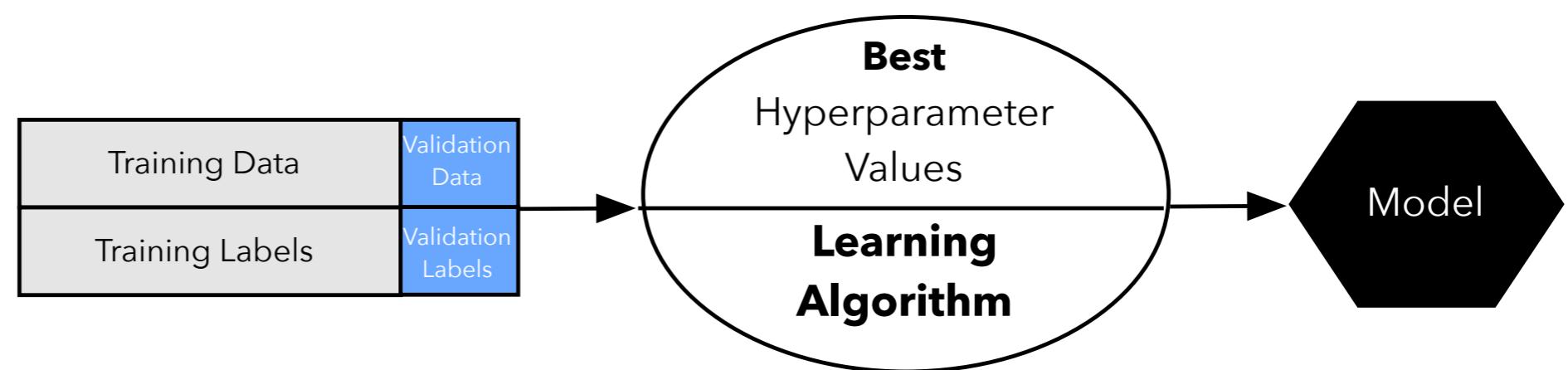


Holdout validation (hyperparam. tuning)

3

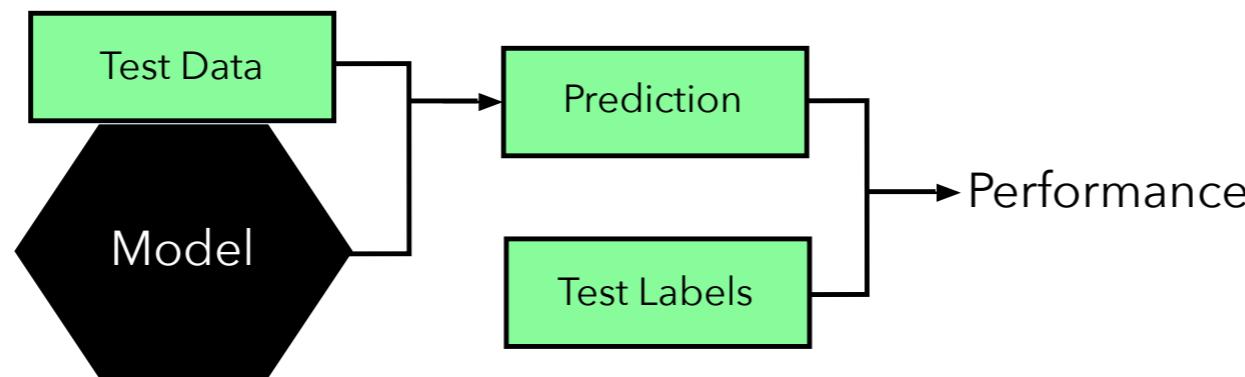


4

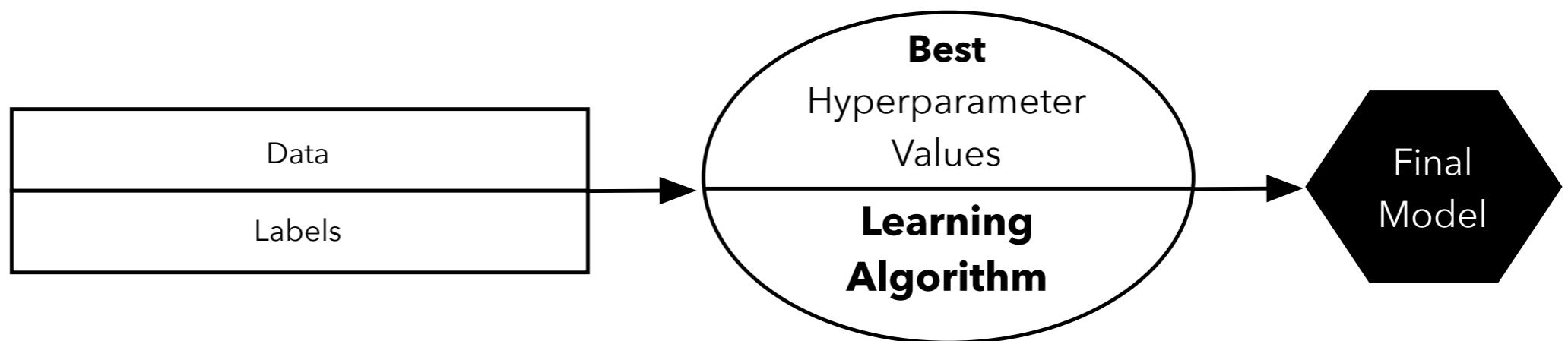


Holdout validation (hyperparam. tuning)

5



6



Cross-Validation is generally better than the holdout method

... but ...

Bengio, Y., & Grandvalet, Y. (2004). No unbiased estimator of the variance of k-fold cross-validation. *Journal of machine learning research*, 5(Sep), 1089-1105.

Bias of Estimators -- Example

Normal Distribution: $\mathcal{N}(\mu, \sigma^2)$

Probability density
function: $f(x^{[i]}; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\frac{(x^{[i]} - \mu)^2}{\sigma^2}\right)$

Is the sample mean an unbiased estimator of the mean of the Gaussian?

$$\hat{\mu} = \frac{1}{n} \sum_i x^{[i]}$$

Bias of Estimators Example

Is the sample mean an unbiased estimator of the mean of the Gaussian?

$$\hat{\mu} = \frac{1}{n} \sum_i x^{[i]}$$

$$\begin{aligned} Bias(\hat{\mu}) &= E[\hat{\mu}] - \mu \\ &= E\left[\frac{1}{n} \sum_i x^{[i]}\right] - \mu \\ &= \frac{1}{n} \sum_i E[x^{[i]}] - \mu \\ &= \frac{1}{n} \sum_i \mu - \mu \\ &= \mu - \mu = 0 \end{aligned}$$

Bias of Estimators Example

Is the sample variance an unbiased estimator of the variance of the Gaussian?

$$\hat{\sigma}^2 = \frac{1}{n} \sum_i (x^{[i]} - \hat{\mu})^2$$

$$\begin{aligned} Bias(\hat{\sigma}^2) &= E[\hat{\sigma}^2] - \sigma^2 \\ &= E\left[\frac{1}{n} \sum_i (x^{[i]} - \hat{\mu})^2\right] - \sigma^2 \\ &= \dots \\ &= \frac{n-1}{n} \sigma^2 - \sigma^2 \end{aligned}$$

Bias of Estimators Example

Is the sample variance an unbiased estimator of the mean of the Gaussian?

$$\begin{aligned}\hat{\sigma}^2 &= \frac{1}{n} \sum_i (x^{[i]} - \hat{\mu})^2 & \text{Bias}(\hat{\sigma}^2) &= E[\hat{\sigma}^2] - \sigma^2 \\ &&&= E\left[\frac{1}{n} \sum_i (x^{[i]} - \hat{\mu})^2\right] - \sigma^2 \\ &&&= \dots \\ &&&= \frac{n-1}{n} \sigma^2 - \sigma^2\end{aligned}$$

The unbiased estimator is actually

$$\hat{\sigma}'^2 = \frac{1}{n-1} \sum_i (x^{[i]} - \hat{\mu})^2$$

k-fold test-fold scores are more similar to each other than repetitions of the experiment with independent data samples

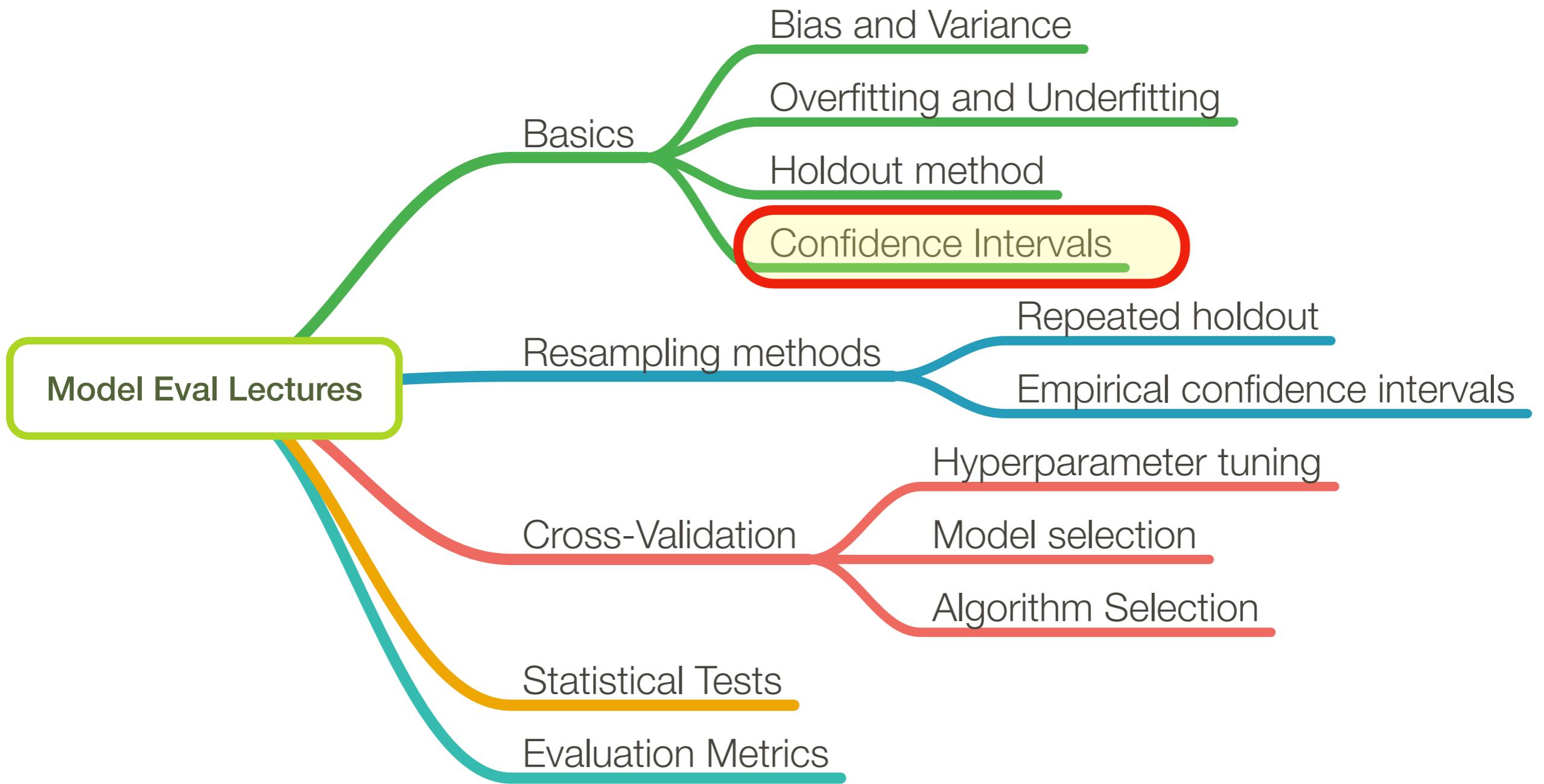
9. Conclusions

It is known that K-fold cross-validation may suffer from high variability, which can be responsible for bad choices in model selection and erratic behavior in the estimated expected prediction error.

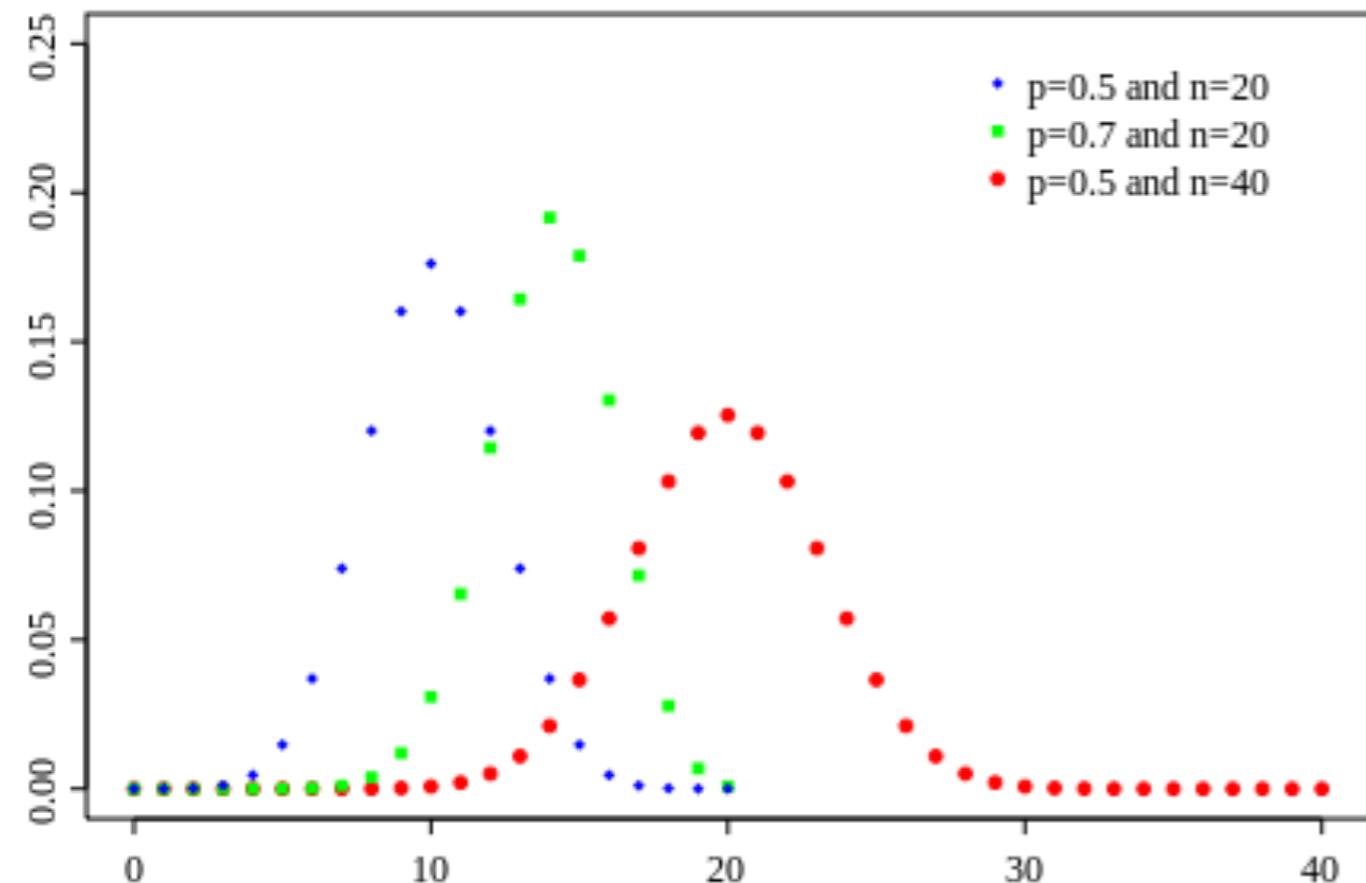
In this paper, we show that estimating the variance of K-fold cross-validation is difficult. Estimating a variance can be done from independent realizations or from dependent realizations whose correlation is known. K-fold cross-validation produces dependent test errors. Our analysis shows that although the correlations are structured in a very simple manner, their values cannot be estimated unbiasedly. Consequently, there is no unbiased estimator of the variance of K-fold cross-validation.

Our experimental section shows that in very simple cases, the bias incurred by ignoring the dependencies between test errors will be of the order of the variance itself. These experiments illustrate thus that the assessment of the significance of observed differences in cross-validation scores should be treated with much caution. The problem being unveiled, the next step of this study consists in building and comparing variance estimators dedicated to the very specific structure of the test error dependencies.

Bengio, Y., & Grandvalet, Y. (2004). No unbiased estimator of the variance of k-fold cross-validation. *Journal of machine learning research*, 5(Sep), 1089-1105.



Binomial distribution



Notation	$B(n, p)$
Parameters	$n \in \mathbf{N}_0$ — number of trials $p \in [0, 1]$ — success probability in each trial
Support	$k \in \{0, \dots, n\}$ — number of successes
pmf	$\binom{n}{k} p^k (1 - p)^{n-k}$
CDF	$I_{1-p}(n - k, 1 + k)$
Mean	np
Median	$\lfloor np \rfloor$ or $\lceil np \rceil$
Mode	$\lfloor (n + 1)p \rfloor$ or $\lceil (n + 1)p \rceil - 1$
Variance	$np(1 - p)$

(Image credit: Screenshot from https://en.wikipedia.org/wiki/Binomial_distribution)

Binomial distribution $Pr(k) = \frac{n!}{k!(n-k)!} p^k (1-p)^{n-k}.$

Coin Flip (Bernoulli Trial)

- coin lands on head ("success")
- probability of success p
- $\frac{k}{n}$, estimator of p
- mean, number of successes
 $\mu_k = np$

0-1 Loss

- example misclassified (0-1 loss)
- true error $ERR_{\mathcal{D}}(h) = \Pr_{x \in \mathcal{D}} [f(x) \neq h(x)]$
- sample (test set) error

$$ERR_S(h) = \frac{1}{n} \sum_{x \in S} \delta(f(x), h(x))$$

Binomial distribution $Pr(k) = \frac{n!}{k!(n-k)!} p^k (1-p)^{n-k}.$

Coin Flip (Bernoulli Trial)

0-1 Loss

- mean, number of successes

$$\mu_k = np$$

- variance $\sigma_k^2 = np(1 - p)$

- standard deviation $\sigma_k = \sqrt{np(1 - p)}$

We are interested in proportions!

$$ERR_S(h) = \frac{1}{n} \sum_{x \in S} \delta(f(x), h(x))$$

$$\sigma_{ERR_S(h)} = \frac{\sigma_k}{n} = \frac{\sqrt{np(1 - p)}}{n} = \sqrt{\frac{p(1 - p)}{n}}$$

$$\sigma_{ERR_S(h)} \approx \sqrt{\frac{ERR_S(h)(1 - ERR_S(h))}{n}}$$

Confidence Intervals

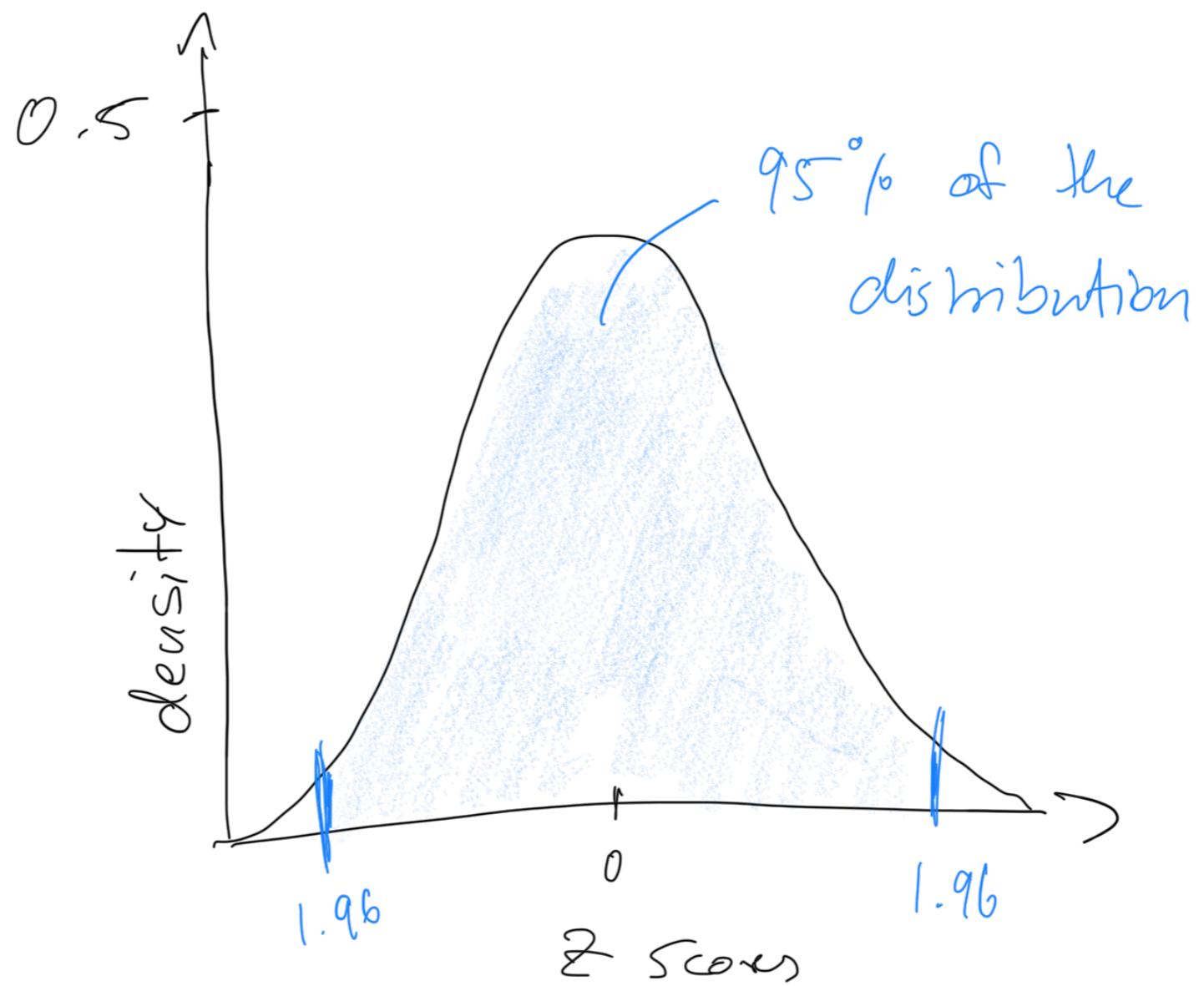
A XX% confidence interval of some parameter p is an interval that is expected to contain p with probability XX%.*

* the more precise definition is "In an infinite long series of trials in which repeated samples of n are taken from the same distribution, the 95% Confidence Interval is calculated using the same method, the proportion of intervals covering the true parameter p is xx%."

Normal Approximation

- Less tedious than confidence interval for Binomial distribution and hence often used in (ML) practice for large n
- Rule of thumb: if n larger than 40, the Binomial distribution can be reasonably approximated by a Normal distribution; and np and $n(1 - p)$ should be greater than 5

$$CI = \text{ERR}_S(h) \pm z \sqrt{\frac{\text{ERR}_S(h)(1 - \text{ERR}_S(h))}{n}}$$



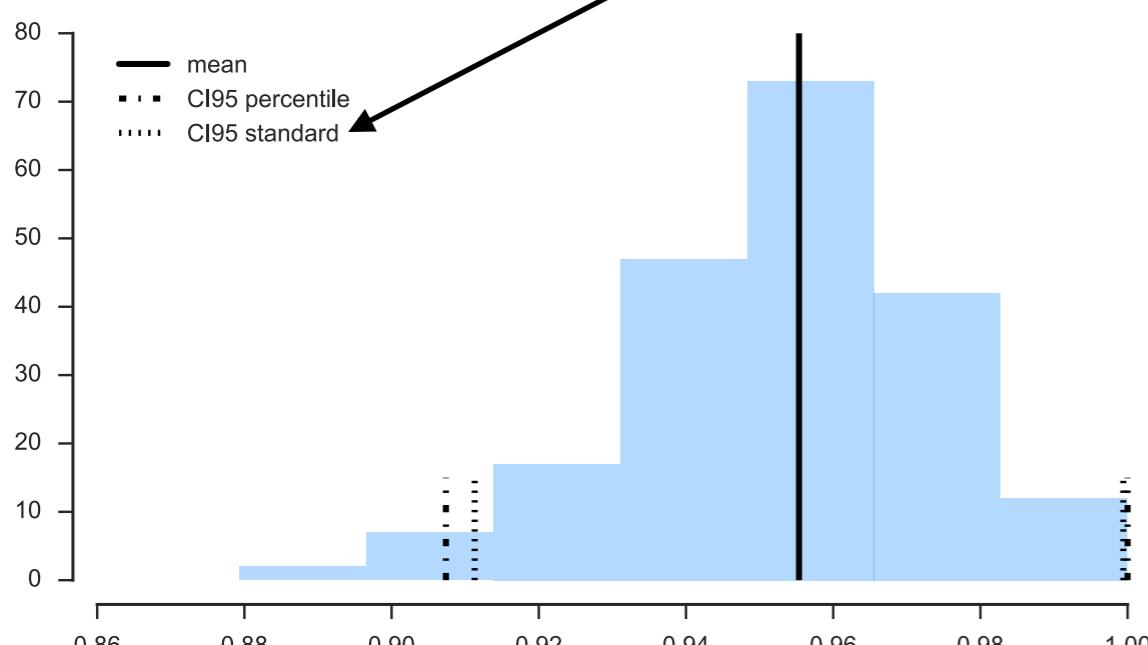
The z constant for different confidence intervals:

- 99%: $z=2.58$
- 95%: $z=1.96$
- 90%: $z=1.64$

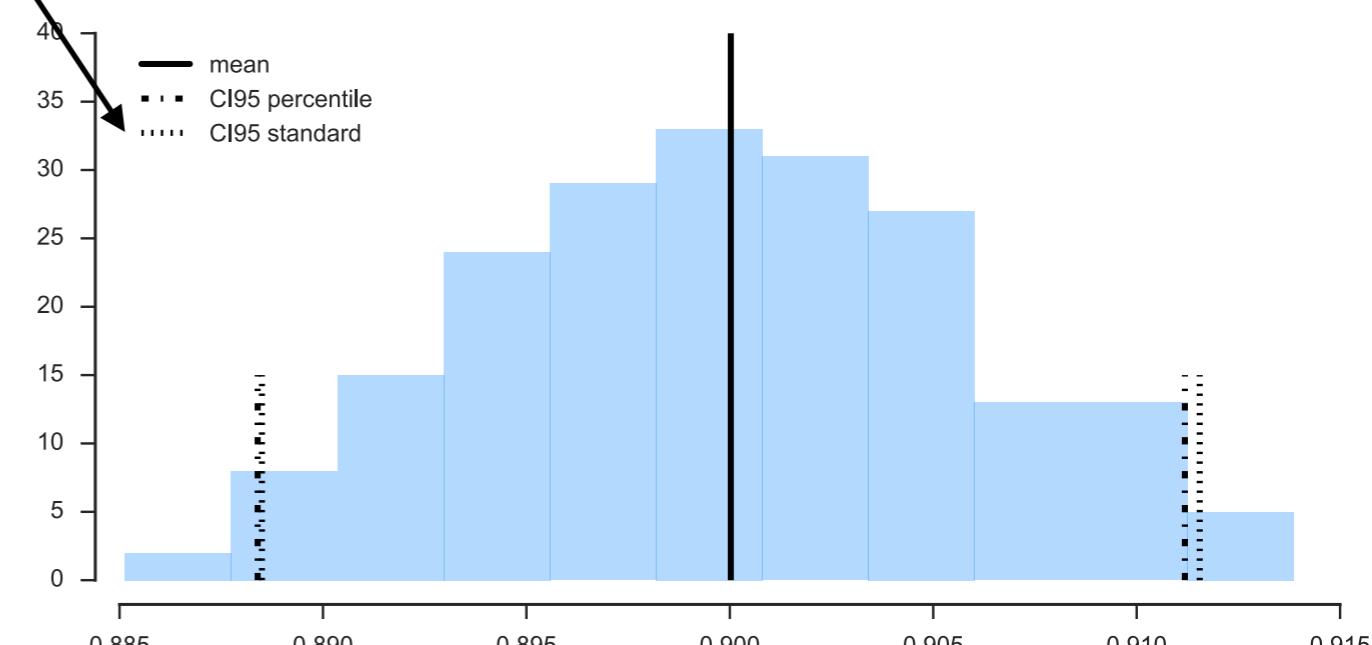
The Bootstrap Method and Empirical Confidence Intervals

normal approximation interval

A



B



In the left subplot, I applied the *Leave-One-Out Bootstrap* technique to evaluate 3-nearest neighbors models on Iris, and the right subplot shows the results of the same model evaluation approach on MNIST, using the same softmax classifier.

Project Proposals

	WengieWang_YuhanXie_HengjialiXu.pdf
	XinranMiao_ZiangyuWang_XinyueWang.pdf
	XueGu_JingHuang_QuihongLi.pdf
	YewonLee_GeorgeLiu_NeilLeonard.pdf
	YuanCao_RunzeYou_JingshanHuang.pdf
	YuhanZhou_YicenLiu_JingyueLou.pdf
	ZiaoyuanZhong_WanjiangWang_ZhilinWang.pdf
	ZihangWang_HaoranLu_ZijinWang.pdf
	zz-AidenSong_BenjaminRoss...rentNicolet_ZamielSchwarz.pdf
	zz-ChenhaoFang_XizhiDeng_YixianWang.pdf
	zz-DevinKestell_JungwonWoo_LareinaLiu.pdf
	zz-EmilyXu_YanxiZhou_ChuckWhite.pdf
	zz-FeliceHao_YifanMo_SiruiYi.pdf
	zz-HanyuCai_DavidFei_ElaineHuang.pdf
	zz-JiaweiHuang_ZijunFeng_ZhipanZhang.pdf
	zz-JuntingWang_XiHe_XinyiYu.pdf
	zz-KyleWang_FeiyuYue_Tz-RueiLiu.pdf
	zz-MaozeWang_ShixuanSong_XuchenXue_TianchangLi.pdf
	zz-MengqiLi_YanyiJiang_JihanChang.pdf
	zz-RuiHuang_BoPeng_HaoyueShi.pdf
	zz-ShaunCampbell_BaileyRusso_RuichaoMa.pdf
	zz-TongLi_RunxinGao_KennyJin.pdf

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Uncovering the Truth of Love: A Modern Approach

1. Introduction

Throughout the long history of human beings, love has been a super popular, exciting, and long-lasting topic in daily life. Love is said to be a kind of magic or miracle. Statistically, it actually is if you consider it in this way: given a person, try to find another one who he or she can call as his or her "soul mate" from more than 7.7 billion people living on Earth (excluding other creatures and potential aliens to reduce the "heavy" computing followed) [1]. The probability of finding such a unique match could be as low as $1.2987013e-10$ (if we consider this as it follows a Binomial Distribution). Love is also a mystery as it cannot be simply defined or explained. People have been trying to find what is the thing that connects two people with a variety of different "features" together closely. There are at least thousands of poems or books talking about what love is by Literature people [2]. Neuroscience or Psychology people may define love as a property of a complex mixture of neuropeptides and neurotransmitters [3]. As Statistic, Mathematics, or Computer Science(s) people, even though we are always considered as indifferent to romance, we still find models (in mathematics instead of those in real-life) to be sexy enough to help with defining love.

2. Motivation

According to a study from The Washington Post, approximately 51 percent of Americans between the ages of 18 and 34 said that they do not have a steady romantic partner. In fact, this 2018 figure has increased significantly from 33 percent in 2004 [4]. However, it's not just the United States that is experiencing this high single proportion. Recently, the United Nations gathered data for roughly 100 countries, showing how marriage rates changed from 1970 to 2005. Marriage rates indeed "had fallen in four-fifths of the countries" [5]. Ford Torney, a 26-year-old man in Baltimore, USA, really wants a steady partner but he just cannot find the right connection despite wandering through numerous date apps. He does not know how to find a partner that matches him the best and he needs to keep reminding himself that most people are not married within the country, and he is only an outlier within his own social group [4].



Figure 1. Speed dating [6]

Many people are experiencing the same thing as Torney and have been struggling to find the person that best matches his or her interest. Therefore, our group is interested in finding out how well two people are matched using machine learning tools learned in class. Given one individual's features including gender, position, country, income, and etc, our group aims to find out whether another individual is a perfect match for him/her. By applying the machine learning algorithms including decision trees and random forests, we would like to help people to overcome the partner barrier by providing everyone the best choice.

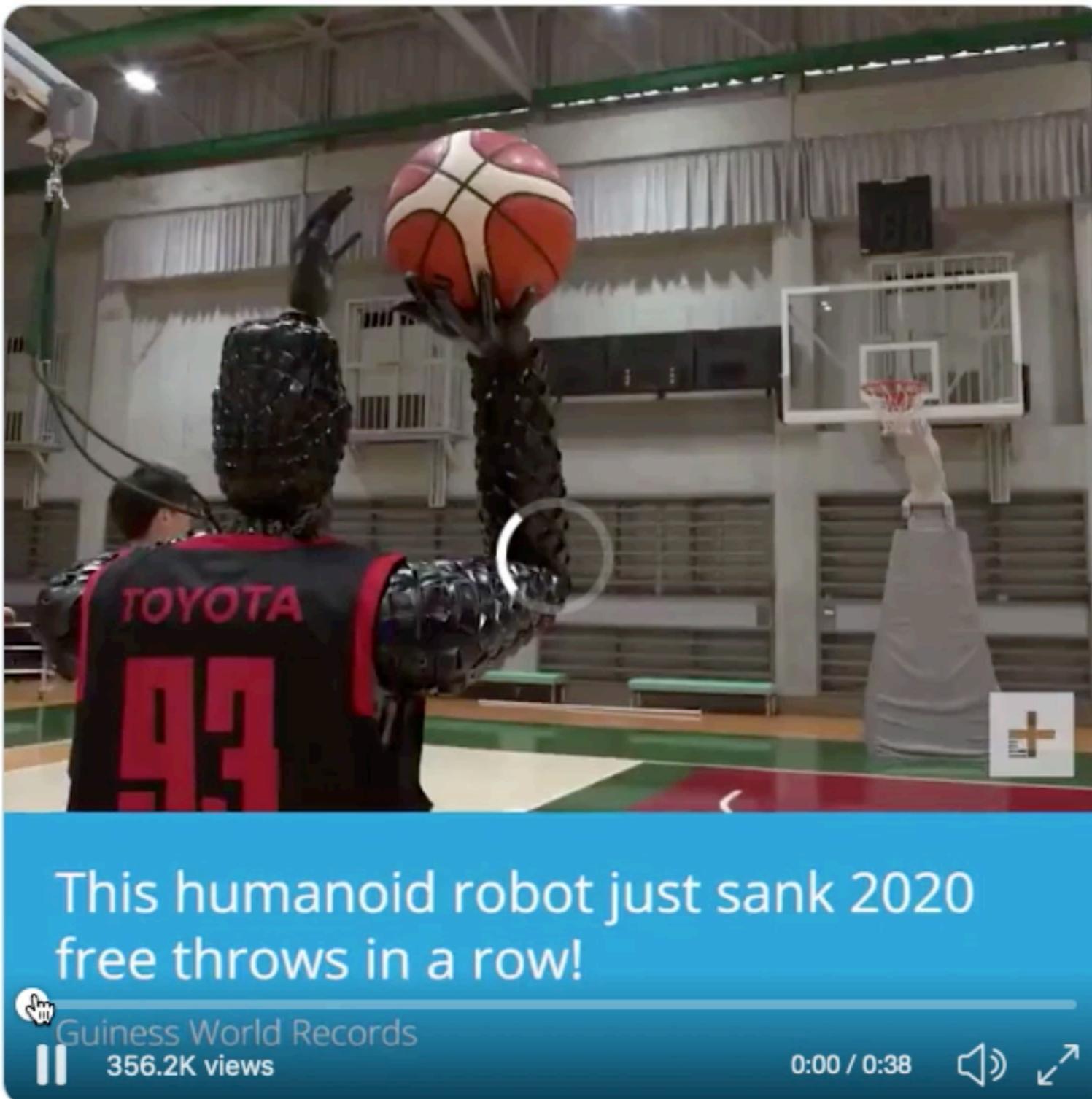
In addition, if there are some features that appeal to people the most, we would like to explore them more and illustrate how these features can increase the probability of an individual being successfully matched. These will be regarded as valuable resources for people struggling to find a romantic partner—to become someone that attracts others the most.

3. Evaluation

We hope to train models that can predict whether two people would like to see their date again after a fast "first date", which serves as a pre-survey. In other words, given two people's information with their first-date's feedback, our final model is expected to tell whether they will have a second date (return 1) or not (return 0) with high level of accuracy.



This humanoid robot just sank 2,020 free throws in a row.



5:00 AM · Oct 29, 2019 · Twitter Media Studio

<https://twitter.com/DigitalTrends/status/1189119686685933569?s=20>



Sebastian Raschka @rasbt · Oct 25

GitHub does support Jupyter Notebooks for viewing, it's just super unreliable (sometimes requires 3-5 presses on the reload button; sometimes it doesn't work at all but will work 10 min later).



1

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Nat Friedman @natfriedman · Oct 25

We're going to fix it

3

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15

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Nat Friedman @natfriedman · 44m

Band-aid implemented. Should be a bit better now. Large-scale improvements coming.

2

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6

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 rasbt add missing example to 1.4

2c54d1c yesterday

1 contributor

1371 lines (1370 sloc) | 47.7 KB

 [Raw](#) [Blame](#) [History](#)

Homework 2 (78 Pts)

STAT 479: Machine Learning (Fall 2019)

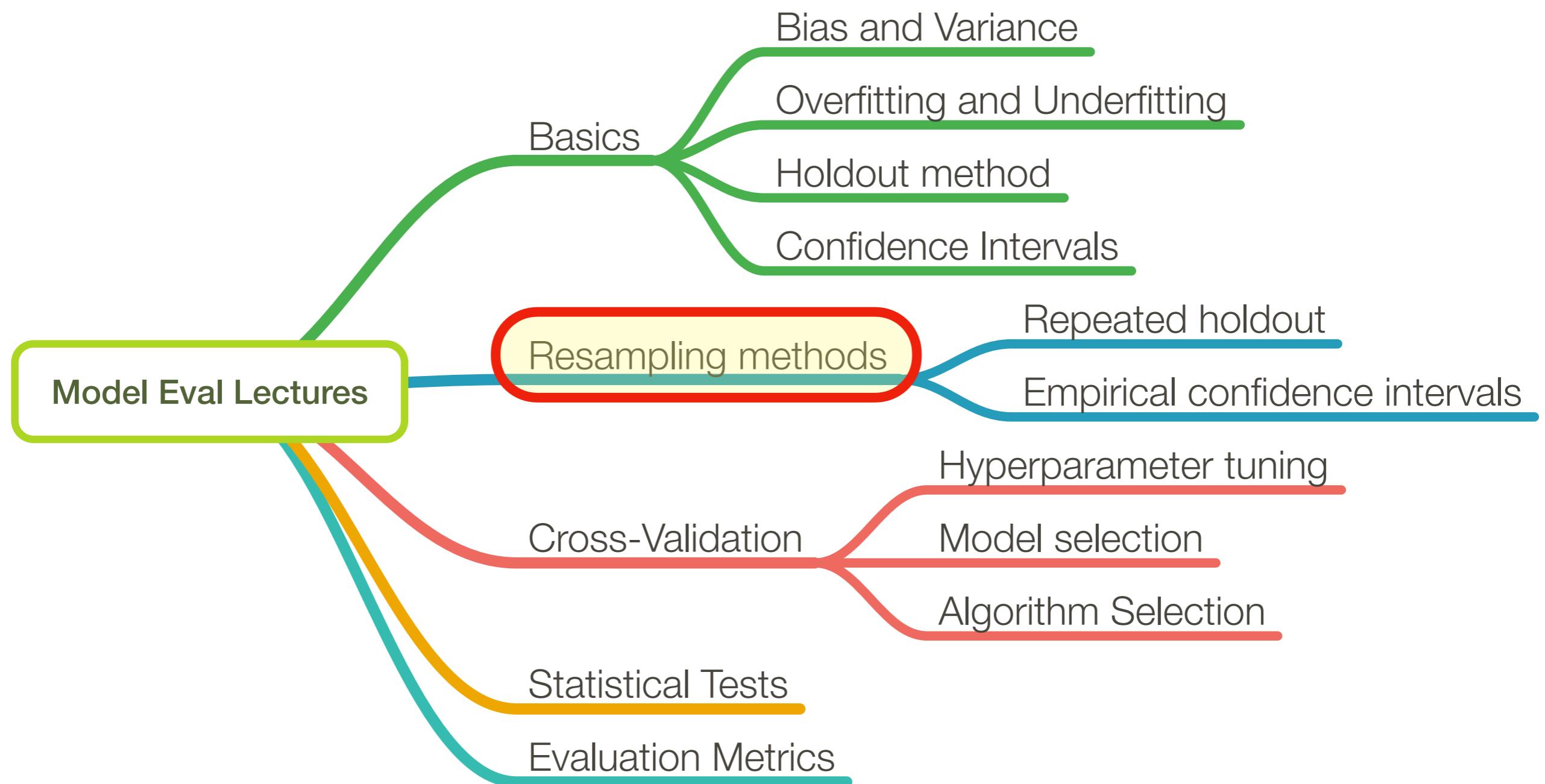
Instructor: Sebastian Raschka (sraschka@wisc.edu)

Course website: <http://pages.stat.wisc.edu/~sraschka/teaching/stat479-fs2019/>

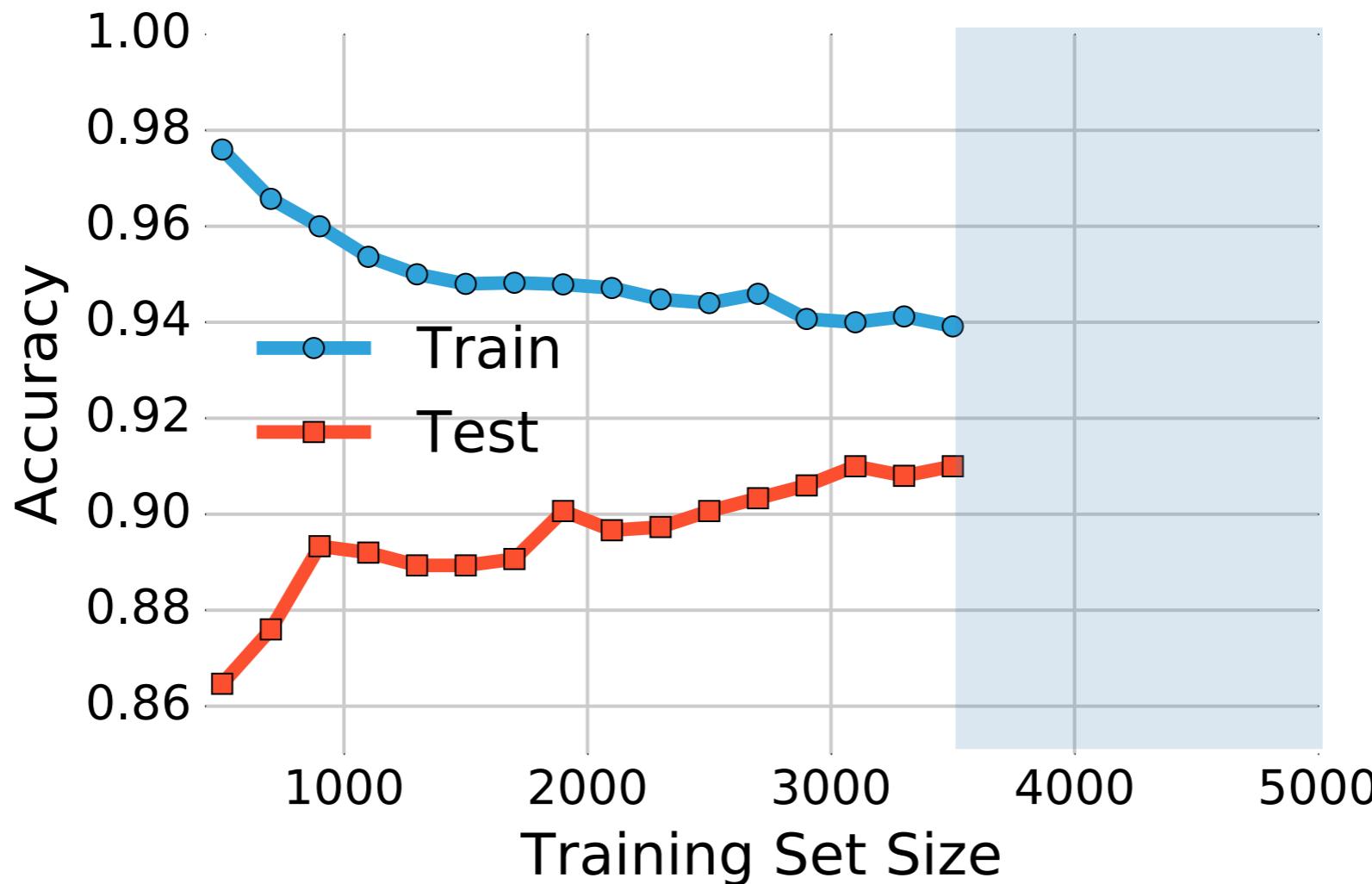
Due: Nov 05, (before 11:59 pm).

1) Implementing a "CART" Decision Tree from Scratch

In this first part of the homework, you are going to implement the CART decision tree algorithm we discussed in class. This decision tree algorithm will construct a binary decision tree based on maximizing Information Gain using the Gini Impurity measure on continuous features.

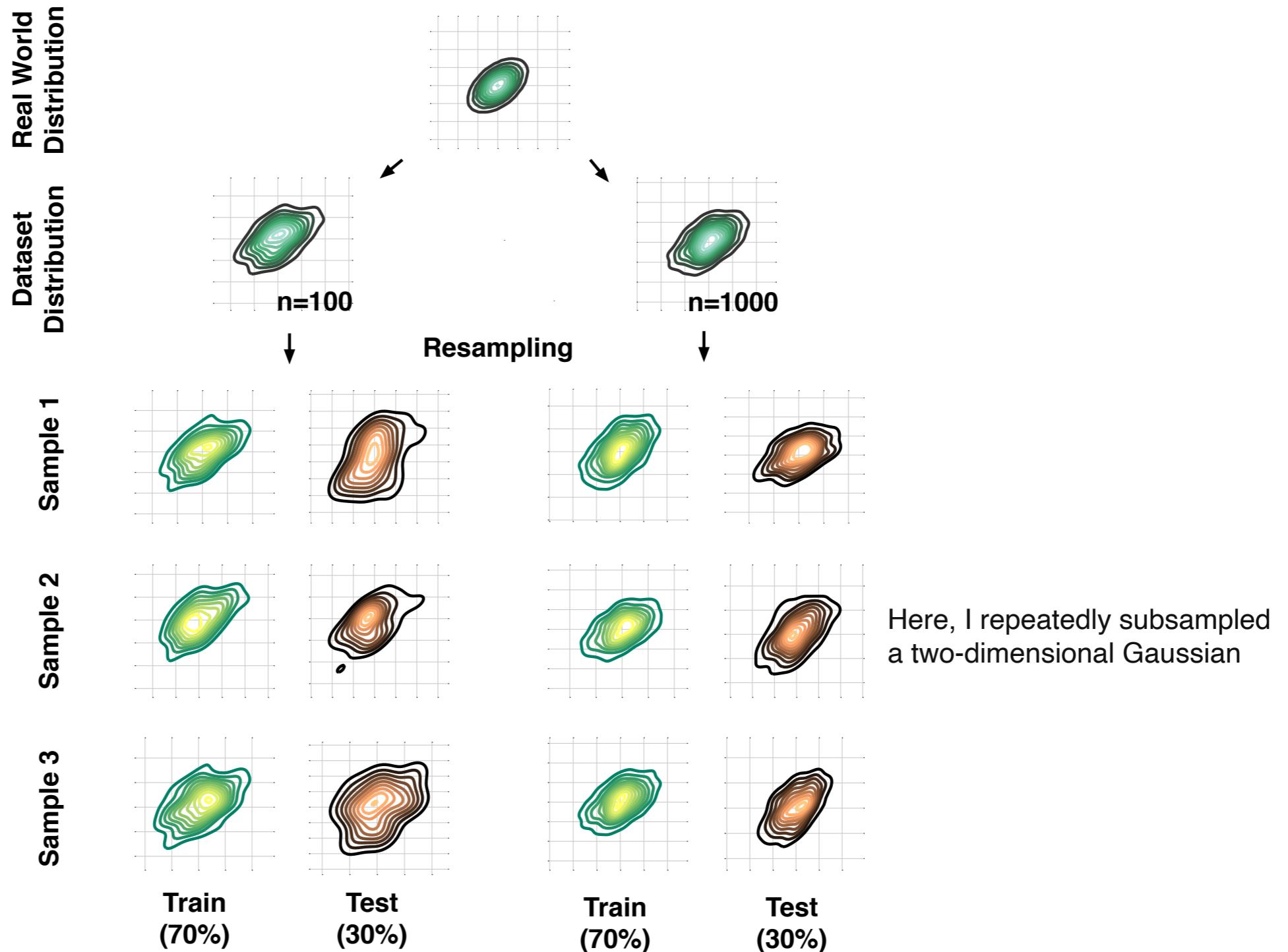


Proportionally large test sets increase the pessimistic bias if a model has not reached its full capacity, yet.



- To produce the plot above, I took 500 random samples of each of the ten classes from MNIST
- The sample was then randomly divided into a 3500-example training subset and a test set (1500 examples) via stratification.
- Even smaller subsets of the 3500-sample training set were produced via randomized, stratified splits, and I used these subsets to fit softmax classifiers and used the same 1500-sample test set to evaluate their performances; samples may overlap between these training subsets.

Decreasing the size of the test set brings up another problem:
It may result in a substantial variance increase of our model's
performance estimate.



The reason is that it depends on which instances end up in training set, and which particular instances end up in test set.
Keeping in mind that each time we resample our data, we alter the statistics of the distribution of the sample.

Repeated Holdout: Estimate Model Stability

(also called Monte Carlo Cross-Validation)

Average performance over k repetitions

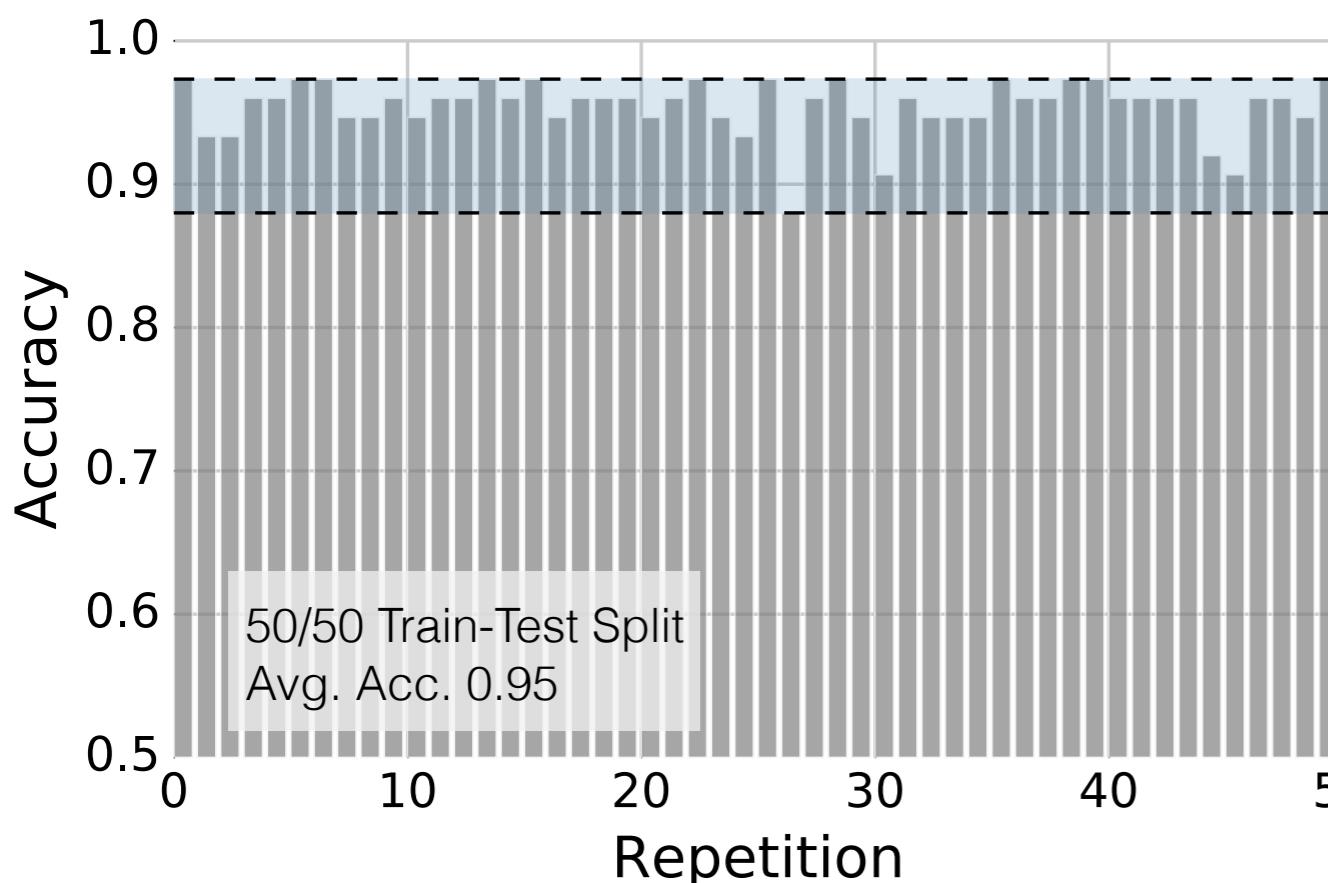
$$\mathbf{ACC}_{avg} = \frac{1}{k} \sum_{j=1}^k ACC_j,$$

where ACC_j is the accuracy estimate of the j th test set of size m ,

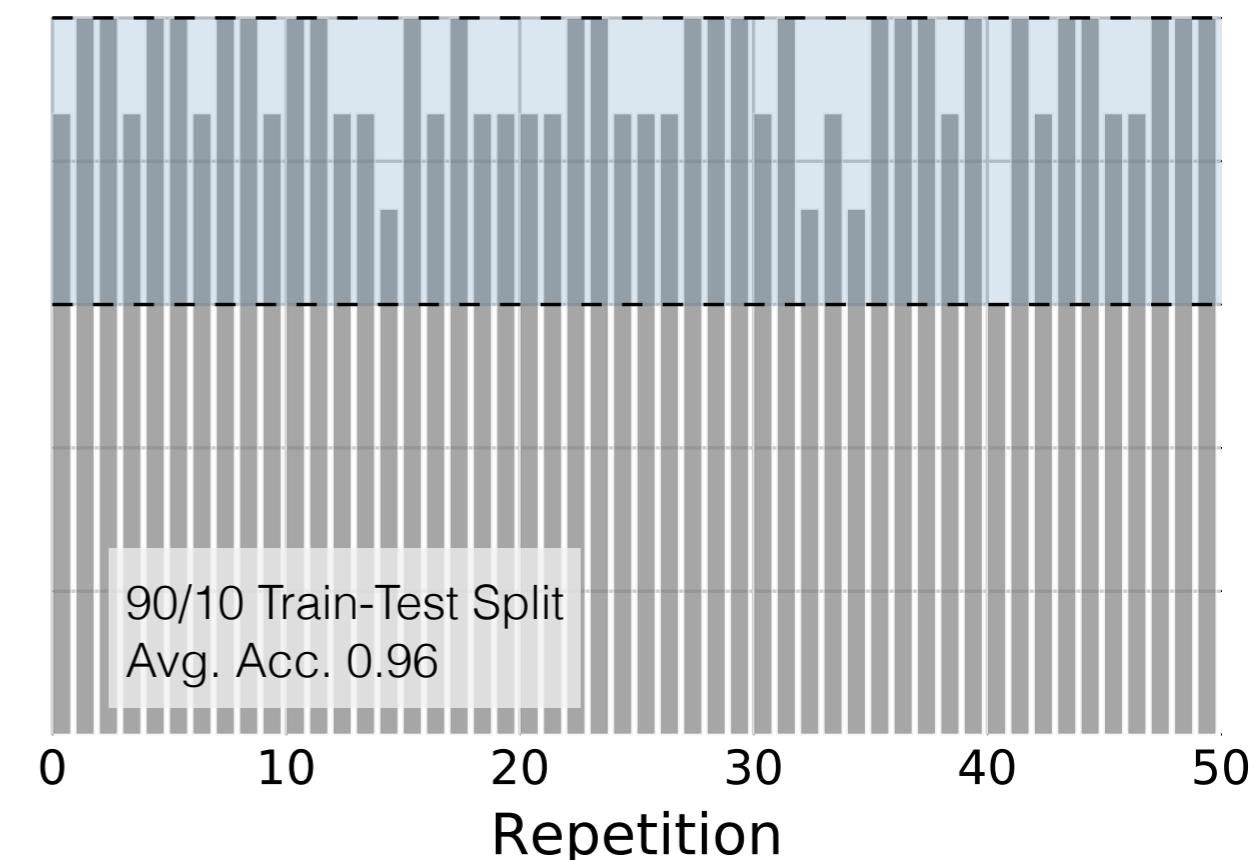
$$ACC_j = 1 - \frac{1}{n} \sum_{i=1}^n L\left(h(x^{[i]}), f(x^{[i]})\right).$$

Repeated Holdout: Estimate Model Stability

How repeated holdout validation may look like for different training-test split using the Iris dataset to fit to 3-nearest neighbors classifiers:



Left: I performed 50 stratified training/test splits with 75 samples in the test and training set each; a K-nearest neighbors model was fit to the training set and evaluated on the test set in each repetition.



Right: Here, I repeatedly performed 90/10 splits, though, so that the test set consisted of only 15 samples.

The Bootstrap Method and Empirical Confidence Intervals

Circa 1900, to pull (oneself) up by (one's) bootstraps was used figuratively of an impossible task (Among the “practical questions” at the end of chapter one of Steele’s “Popular Physics” schoolbook (1888) is, “30. Why can not a man lift himself by pulling up on his boot-straps?”). By 1916 its meaning expanded to include “better oneself by rigorous, unaided effort.” The meaning “fixed sequence of instructions to load the operating system of a computer” (1953) is from the notion of the first-loaded program pulling itself, and the rest, up by the bootstrap.

(Source: [Online Etymology Dictionary](#))

The Bootstrap Method and Empirical Confidence Intervals

- The bootstrap method is a resampling technique for estimating a sampling distribution
- Here, we are particularly interested in estimating the uncertainty of our performance estimate
- The bootstrap method was introduced by Bradley Efron in 1979 [1]
- About 15 years later, Bradley Efron and Robert Tibshirani even devoted a whole book to the bootstrap, “An Introduction to the Bootstrap” [2]
- In brief, the idea of the bootstrap method is to generate *new* data from a population by repeated sampling from the original dataset *with replacement* – in contrast, the repeated holdout method can be understood as sampling *without* replacement.

[1] Efron, Bradley. 1979. “Bootstrap Methods: Another Look at the Jackknife.” *The Annals of Statistics* 7 (1). Institute of Mathematical Statistics: 1–26. doi:10.1214/aos/1176344552.

[2] Efron, Bradley, and Robert Tibshirani. 1994. *An Introduction to the Bootstrap*. Chapman & Hall.

The Bootstrap Method and Empirical Confidence Intervals

Using the bootstrap, we can estimate sample statistics and compute the standard error of the mean and confidence intervals as if we have drawn a number of samples from an infinite population. In a nutshell, the bootstrap procedure can be described as follows:

1. Draw a sample with replacement
2. Compute the sample statistic
3. Repeat step 1-2 n times
4. Compute the standard deviation (standard error of the mean of the statistic)
5. Compute the confidence interval

The Bootstrap Method and Empirical Confidence Intervals For Evaluating Classifier Performance

1. We are given a dataset of size n .
2. For b bootstrap rounds:
 1. We draw one single instance from this dataset and assign it to our j th bootstrap sample. We repeat this step until our bootstrap sample has size n (the size of the original dataset). Each time, we draw samples from the same original dataset so that certain samples may appear more than once in our bootstrap sample and some not at all.
3. We fit a model to each of the b bootstrap samples and compute the resubstitution accuracy.
4. We compute the model accuracy as the average over the b accuracy estimates

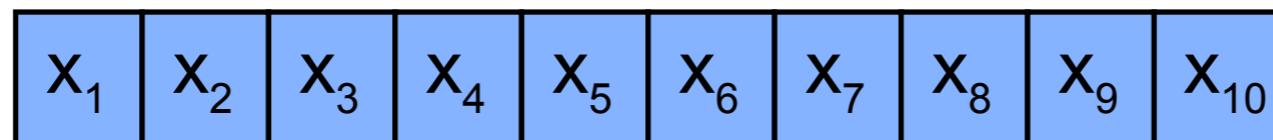
$$\mathbf{ACC}_{boot} = \frac{1}{b} \sum_{j=1}^b \frac{1}{n} \sum_{i=1}^n \left(1 - L(h(x^{[i]}), f(x^{[i]})) \right).$$

The Bootstrap Method and Empirical Confidence Intervals

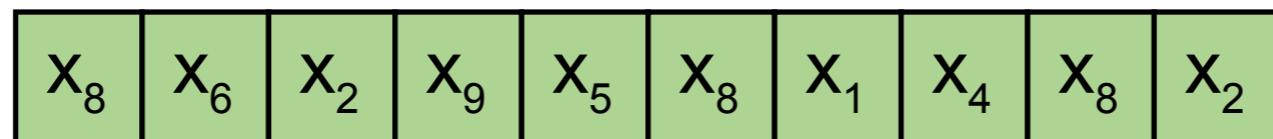
- As we discussed previously, the resubstitution accuracy usually leads to an extremely optimistic bias, since a model can be overly sensible to noise in a dataset.
- Originally, the bootstrap method aims to determine the statistical properties of an estimator when the underlying distribution was unknown and additional samples are not available.
- So, in order to exploit this method for the evaluation of predictive models, such as hypotheses for classification and regression, we may prefer a slightly different approach to bootstrapping using the so-called *Leave-One-Out Bootstrap* (LOOB) technique.
- Here, we use *out-of-bag* samples as test sets for evaluation instead of evaluating the model on the training data. Out-of-bag samples are the unique sets of instances that are not used for model fitting

Bootstrap Sampling

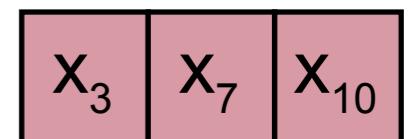
Original Dataset



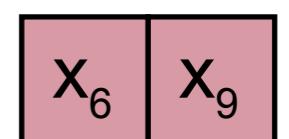
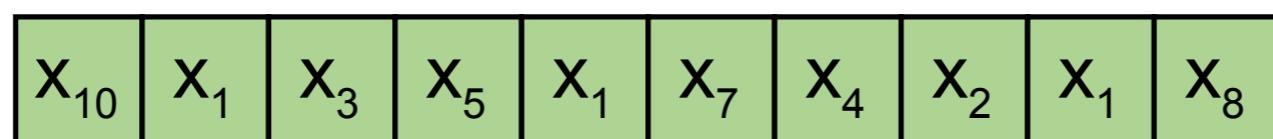
Bootstrap 1



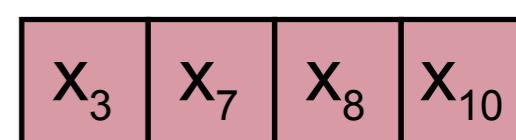
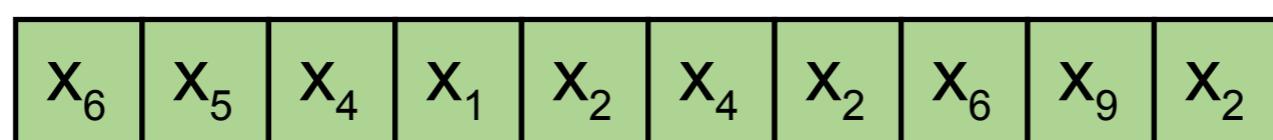
Out-of-bag samples



Bootstrap 2



Bootstrap 3



Training Sets

The Bootstrap Method and Empirical Confidence Intervals

We can compute the 95% confidence interval of the bootstrap estimate as

$$\mathbf{ACC}_{boot} = \frac{1}{b} \sum_{i=1}^b \mathbf{ACC}_i$$

and use it to compute the standard error

$$\mathbf{SE}_{boot} = \sqrt{\frac{1}{b-1} \sum_{i=1}^b (\mathbf{ACC}_i - \mathbf{ACC}_{boot})^2}.$$

Finally, we can then compute the confidence interval around the mean estimate as

$$\mathbf{ACC}_{boot} \pm t \times \mathbf{SE}_{boot}.$$

For instance, given a sample with $n=100$, we find that $t_{95} = 1.984$

(In practice, at least 200 bootstrap rounds are recommended)

The Bootstrap Method and Empirical Confidence Intervals

And if our samples do *not* follow a normal distribution? A more robust, yet computationally straight-forward approach is the **percentile method** as described by B. Efron (Efron, 1981). Here, we pick our lower and upper confidence bounds as follows:

$$\mathbf{ACC}_{lower} = \alpha_1^{th} \text{ percentile of the } \mathbf{ACC}_{boot} \text{ distribution}$$

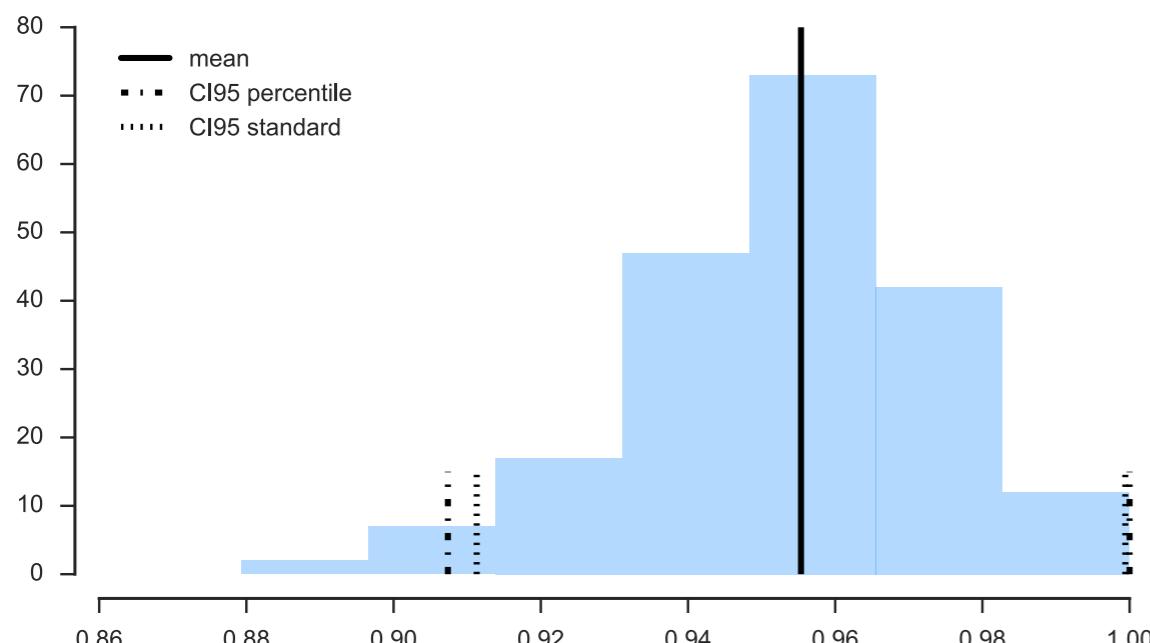
$$\mathbf{ACC}_{upper} = \alpha_2^{th} \text{ percentile of the } \mathbf{ACC}_{boot} \text{ distribution}$$

where $\alpha_1 = \alpha$ and $\alpha_2 = 1 - \alpha$ and α is our degree of confidence to compute the $100 \times (1 - 2 \times \alpha)$ confidence interval.

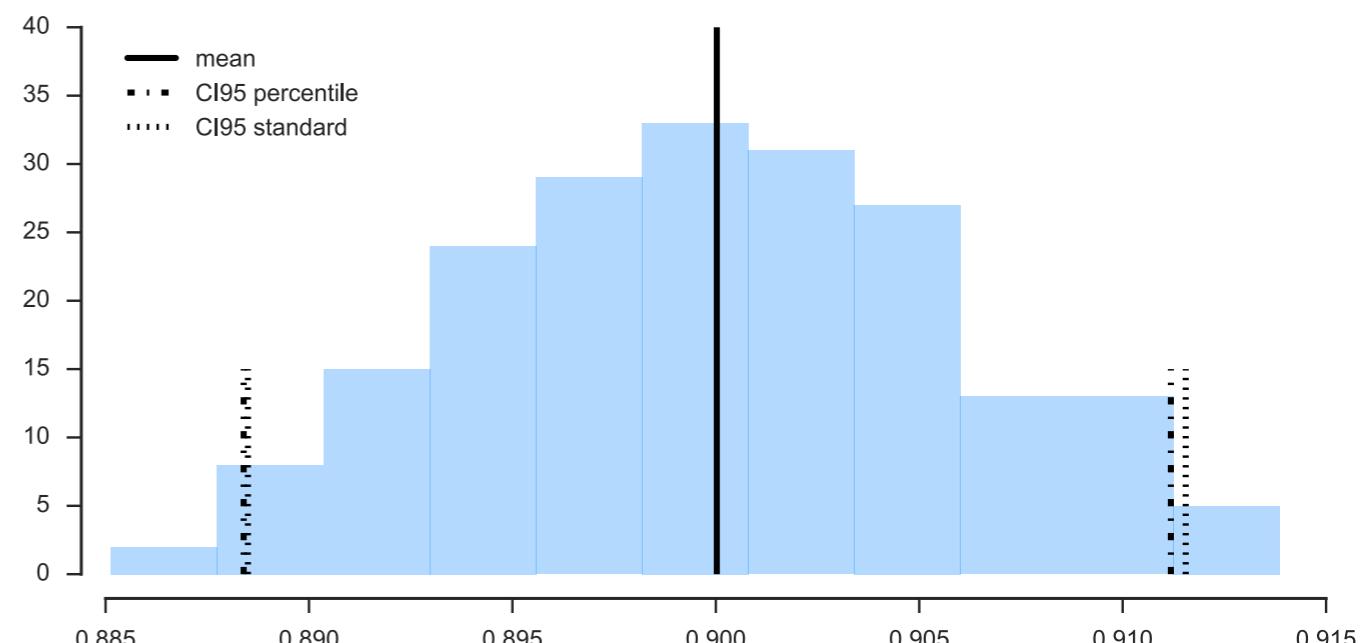
For instance, to compute a 95% confidence interval, we pick $\alpha = 0.025$ to obtain the 2.5th and 97.5th percentiles of the b bootstrap samples distribution as our upper and lower confidence bounds.

The Bootstrap Method and Empirical Confidence Intervals

A



B



In the left subplot, I applied the *Leave-One-Out Bootstrap* technique to evaluate 3-nearest neighbors models on Iris, and the right subplot shows the results of the same model evaluation approach on MNIST, using the same softmax algorithm as mentioned earlier.

The 0.632 Bootstrap Method

- In 1983, Bradley Efron described the *.632 Estimate*, a further improvement to address the pessimistic bias of the bootstrap [1].
- The pessimistic bias in the “classic” bootstrap method can be attributed to the fact that the bootstrap samples only contain approximately 63.2% of the unique samples from the original dataset.

[1] Efron, Bradley. 1983. “Estimating the Error Rate of a Prediction Rule: Improvement on Cross-Validation.” *Journal of the American Statistical Association* 78 (382): 316. doi:10.2307/2288636.

Bootstrap Sampling

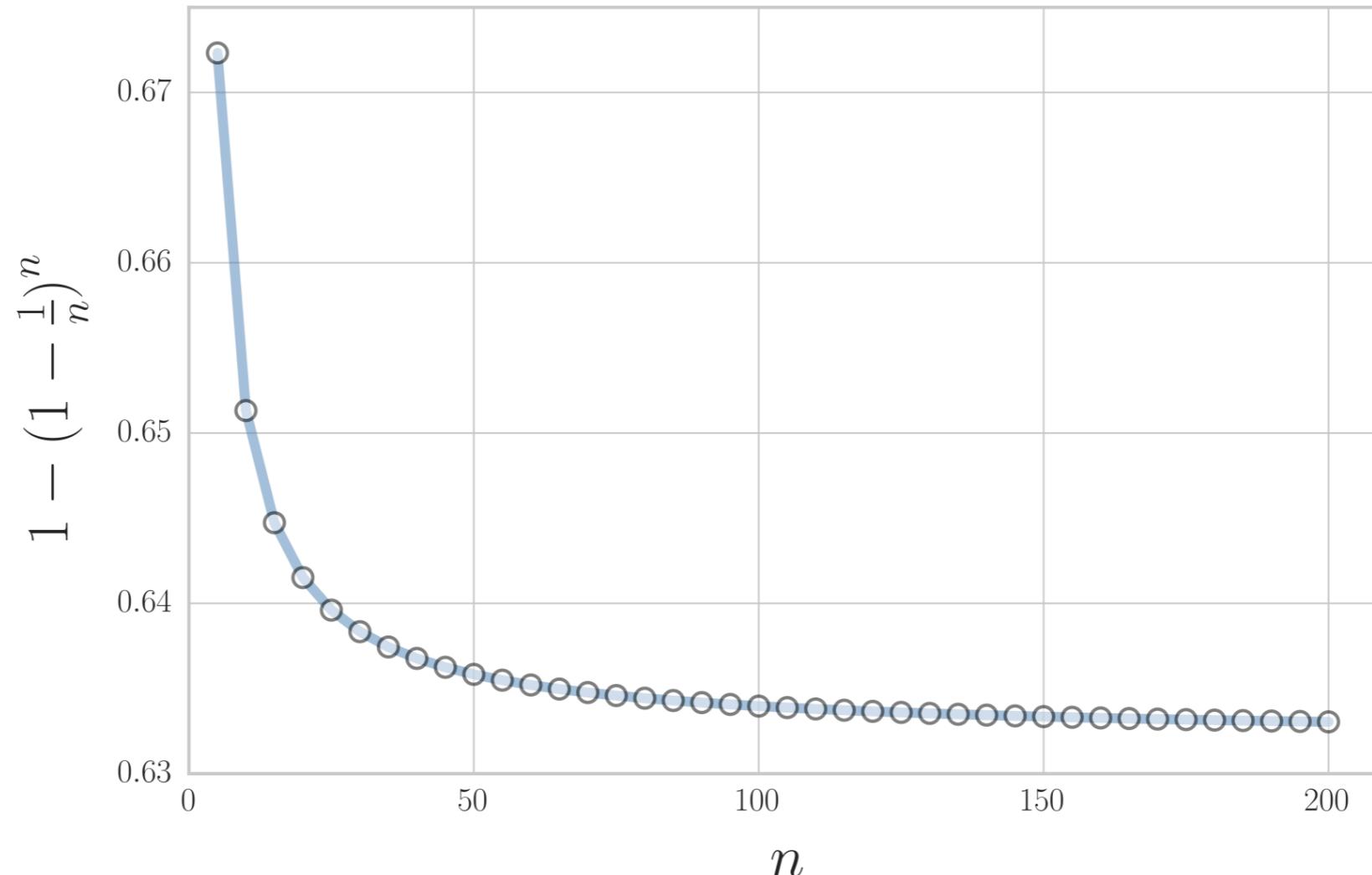
$$P(\text{not chosen}) = \left(1 - \frac{1}{n}\right)^n,$$

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

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

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

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



The .632 Bootstrap Method

The *.632 Estimate*, is computed via the following equation:

$$\mathbf{ACC}_{boot} = \frac{1}{b} \sum_{i=1}^b (0.632 \cdot \mathbf{ACC}_{h,i} + 0.368 \cdot \mathbf{ACC}_{r,i}),$$

where

$\mathbf{ACC}_{r,i}$ is the resubstitution accuracy

$\mathbf{ACC}_{h,i}$ is the accuracy on the out-of-bag sample.

[1] Efron, Bradley. 1983. “Estimating the Error Rate of a Prediction Rule: Improvement on Cross-Validation.” *Journal of the American Statistical Association* 78 (382): 316. doi:10.2307/2288636.

The .632+ Bootstrap Method

Now, while the *.632 Bootstrap* attempts to address the pessimistic bias of the estimate, an optimistic bias may occur with models that tend to overfit so that Bradley Efron and Robert Tibshirani proposed the *The .632+ Bootstrap Method* [1].

Instead of using a fixed “weight” $\omega = 0.632$ in

$$ACC_{\text{boot}} = \frac{1}{b} \sum_{i=1}^b (\omega \cdot ACC_{h,i} + (1 - \omega) \cdot ACC_{r,i}),$$

we compute the weight as

$$\omega = \frac{0.632}{1 - 0.368 \times R},$$

where R is the *relative overfitting rate*

$$R = \frac{(-1) \times (ACC_{h,i} - ACC_{r,i})}{\gamma - (1 - ACC_{h,i})}.$$

[1] Efron, Bradley, and Robert Tibshirani. 1997. “Improvements on Cross-Validation: The .632+ Bootstrap Method.” *Journal of the American Statistical Association* 92 (438): 548. doi:10.2307/2965703.

The .632+ Bootstrap Method

R is the *relative overfitting rate*

$$R = \frac{(-1) \times (\mathbf{ACC}_{h,i} - \mathbf{ACC}_{r,i})}{\gamma - (1 - \mathbf{ACC}_{h,i})}.$$

Now, we need to determine the *no-information rate* γ in order to compute R .

For instance, we can compute γ by fitting a model to a dataset that contains all possible combinations between the examples and target class labels:

$$\gamma = \frac{1}{n^2} \sum_{i=1}^n \sum_{i'=1}^n (1 - L(h(x^{[i]}), f(x^{[i']}))) .$$

[1] Efron, Bradley, and Robert Tibshirani. 1997. "Improvements on Cross-Validation: The .632+ Bootstrap Method." *Journal of the American Statistical Association* 92 (438): 548. doi:10.2307/2965703.

Code Examples

[https://github.com/rasbt/stat479-machine-learning-fs19/
blob/master/09_eval2-ci/code/09-eval2-ci_code.ipynb](https://github.com/rasbt/stat479-machine-learning-fs19/blob/master/09_eval2-ci/code/09-eval2-ci_code.ipynb)

Reading Assignment

L09 Lecture Notes:

[https://github.com/rasbt/stat479-machine-learning-fs19/blob/
master/09_eval2-ci/09-eval2-ci_notes.pdf](https://github.com/rasbt/stat479-machine-learning-fs19/blob/master/09_eval2-ci/09-eval2-ci_notes.pdf)

Overview

