Lecture 11

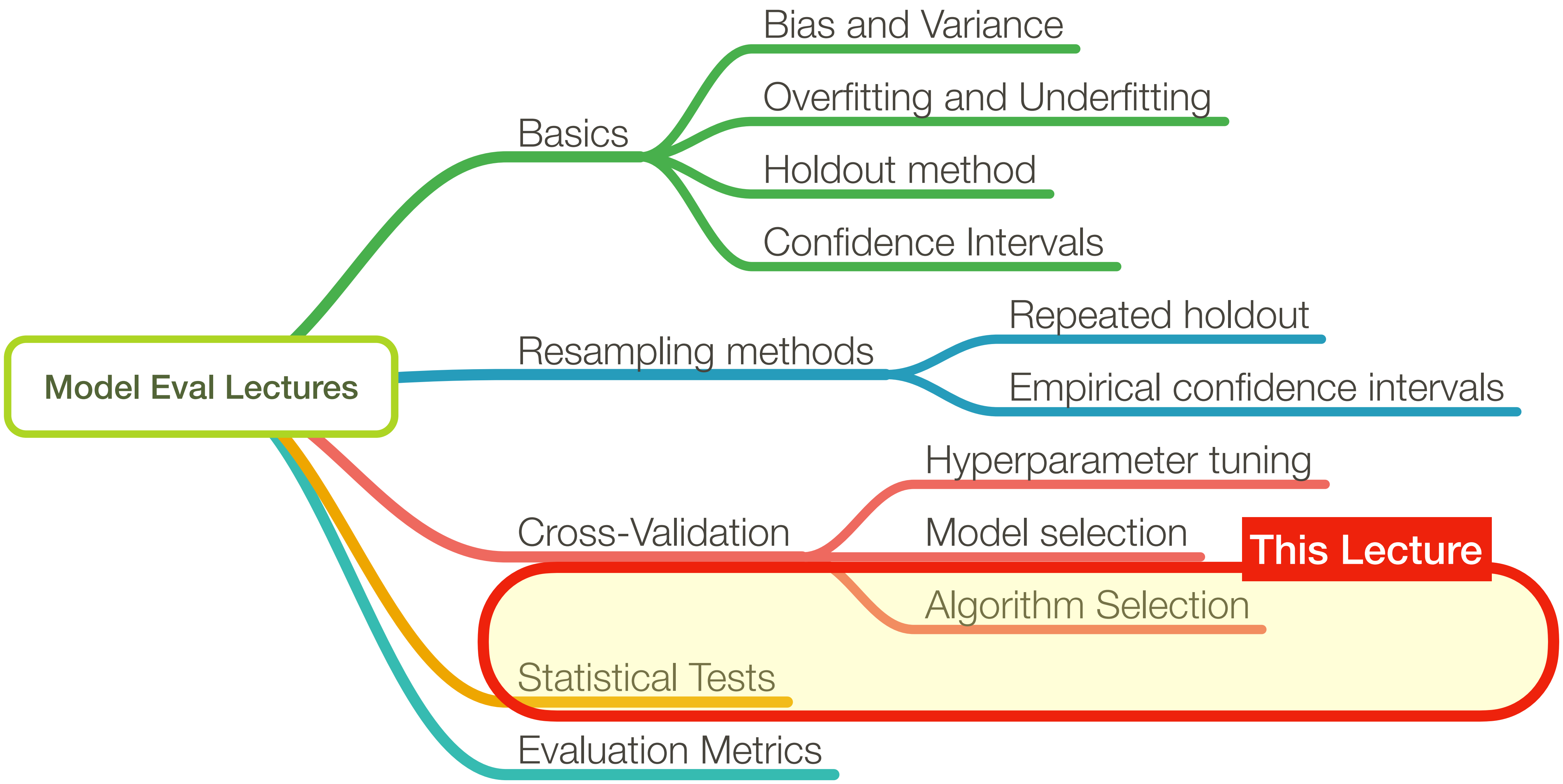
Model Evaluation 4:
Algorithm Comparisons

STAT 479: Machine Learning, Fall 2018

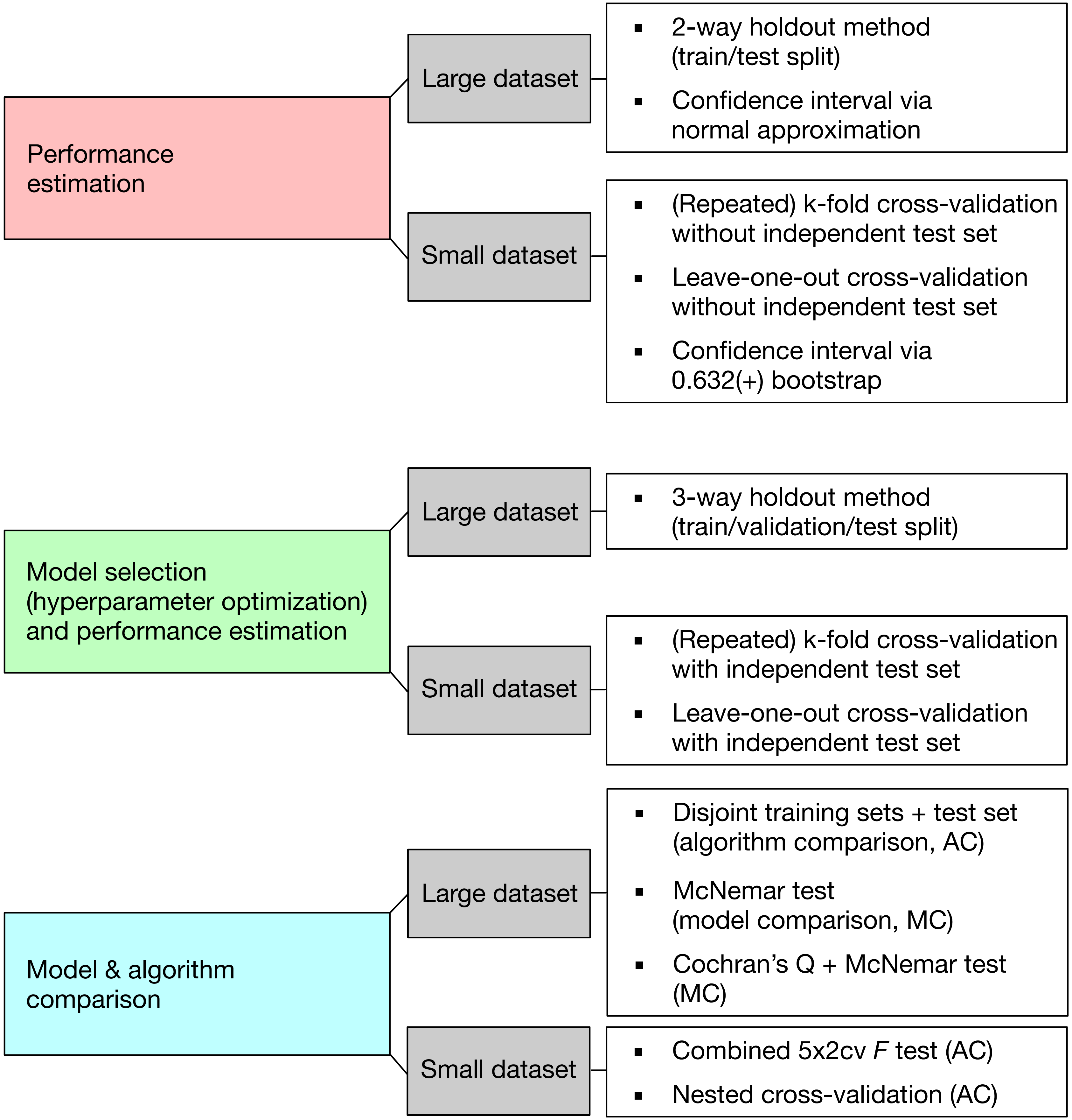
Sebastian Raschka

http://stat.wisc.edu/~sraschka/teaching/stat479-fs2018/

Overview


Model Eval Lectures
Basics
Bias and Variance
Overfitting and Underfitting
Holdout method
Confidence Intervals
Resampling methods
Repeated holdout
Empirical confidence intervals
Cross-Validation
Hyperparameter tuning
Model selection
This Lecture
Algorithm Selection
Statistical Tests
Evaluation Metrics

Overview, (my) "recommendations"



Performance estimation

Large dataset

- 2-way holdout method (train/test split)
- Confidence interval via normal approximation

Small dataset

- (Repeated) k-fold cross-validation without independent test set
- Leave-one-out cross-validation without independent test set
- Confidence interval via 0.632(+) bootstrap

Model selection (hyperparameter optimization) and performance estimation

Large dataset

- 3-way holdout method (train/validation/test split)

Small dataset

- (Repeated) k-fold cross-validation with independent test set
- Leave-one-out cross-validation with independent test set

Model & algorithm comparison

Large dataset

- Disjoint training sets + test set (algorithm comparison, AC)
- McNemar test (model comparison, MC)
- Cochran’s Q + McNemar test (MC)

Small dataset

- Combined 5x2cv *F* test (AC)
- Nested cross-validation (AC)

Comparing two machine learning classifiers -- McNemar's Test

McNemar's test, introduced by Quinn McNemar in 1947 [1], is a non-parametric statistical test for paired comparisons that can be applied to compare the performance of two machine learning classifiers:

Task	Gaussian data	…	Paired nominal data
Compare a group to a reference value			Binomial test
Compare a pair of groups			McNemar's test
Compare two unpaired groups			χ^2 test, Fisher's exact test

[1] McNemar, Quinn. "Note on the sampling error of the difference between correlated proportions or percentages." *Psychometrika* 12.2 (1947): 153-157.

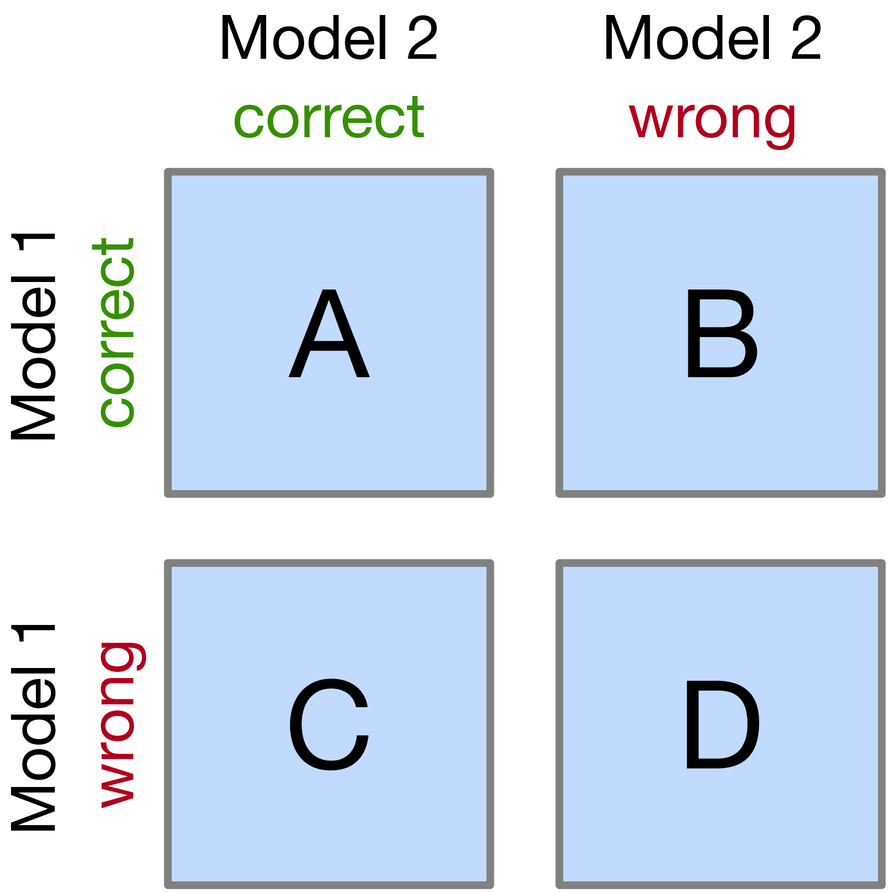
Comparing two machine learning classifiers -- McNemar's Test

- Also referred to as "within-subjects chi-squared test"
- Applied to paired nominal data based on *a version of a* 2x2 confusion matrix
- Compares the predictions of two models to each other rather than listing false positive, true positive, false negative, and true negative counts of a single model
- The layout of the 2x2 confusion matrix suitable for McNemar's test is shown in the following figure:

	Model 2 correct	Model 2 wrong
Model 1 correct	A	B
Model 1 wrong	C	D

Comparing two machine learning classifiers -- McNemar's Test

- Given such a 2x2 confusion matrix as shown in the previous figure, we can compute the accuracy of a *Model 1* via *(A+B) / (A+B+C+D)*
- Similarly, we can compute the accuracy of Model 2 as *(A+B) / N*
- Cells B and C (the off-diagonal entries) tell us how the models differ



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Comparing two machine learning classifiers -- McNemar's Test

- Let's take a look at the following example:

A

	Model 2 correct	Model 2 wrong
Model 1 correct	9959	11
Model 1 wrong	1	29

B

	Model 2 correct	Model 2 wrong
Model 1 correct	9945	25
Model 1 wrong	15	15

- What is the prediction accuracy of models 1 and 2?

Comparing two machine learning classifiers -- McNemar's Test

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- Model 1 accuracy subpanel A: ?? %
- Model 1 accuracy subpanel B: ?? %
- Model 2 accuracy subpanel A: ?? %
- Model 2 accuracy subpanel B: ?? %

Comparing two machine learning classifiers -- McNemar's Test

In both subpanel A and B, the accuracy of *Model 1* and *Model 2* are 99.6% and 99.7%, respectively.

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<u>In subpanel A:</u>

- *Model 1* got 11 predictions right that *Model 1* got wrong
- *Model 2* got 1 prediction right that *Model 2* got wrong
- Based on this 11:1 ratio (based on our intuition), *Model 2* performs substantially better than *Model 1?*

<u>In subpanel B:</u>

- The *Model 1*:*Model 2* ratio is 25:15
- This is less conclusive about which model is the better one to choose.

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In McNemar's Test, we formulate the

- null hypothesis: the probabilities *p(B*) and *p(C)* are the same
- alternative hypothesis: the performances of the two models are not equal

Comparing two machine learning classifiers -- McNemar's Test

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The McNemar test statistic ("chi-squared") can be computed as follows:

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- Set a significance threshold, for example, $\alpha = 0.05$
- Compute the p-value -- assuming that the null hypothesis is true, the p-value is the probability of observing the given empirical (or a larger) chi-squared value (chi^2 distribution with 1 degree of freedom, and relatively large numbers in cells B and C, say > 25)
- If the p-value is lower than our chosen significance level, we can reject the null hypothesis that the two model's performances are equal

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- If we did this for scenario B in the previous figure (chi^2=2.5), we would obtain a p-value of 0.1138, which is larger than our significance threshold, and thus, we cannot reject the null hypothesis.

- If we computed the p-value for scenario A (chi^2=8.3), we would obtain a p-value of 0.0039, which is below the set significance threshold (alpha=0.05) and leads to the rejection of the null hypothesis; we can conclude that the models' performances are different (for instance, Model 1 performs better than Model 2).

Comparing two machine learning classifiers -- McNemar's Test

Continuity Correction

Approximately 1 year after Quinn McNemar published the McNemar Test (McNemar 1947), Allen L. Edwards [1] proposed a continuity corrected version, which is the more commonly used variant today:

$$\chi^2 = \frac{\left(|B - C| - 1 \right)^2}{B + C}.$$

"This correction will have the obvious result of reducing the absolute value of the difference, [B - C], by unity." [1]

[1] Edwards, Allen L. "Note on the “correction for continuity” in testing the significance of the difference between correlated proportions." *Psychometrika* 13.3 (1948): 185-187.

Comparing two machine learning classifiers -- McNemar's Test

Exact p-values via the Binomial test

- McNemar's test approximates the p-values reasonably well if the values in cells B and C are larger than 50
- But it makes sense to use a computationally more expensive binomial test to compute the exact p-values (esp. if B and C are relatively small) -- since the chi-squared value from McNemar's test may not be well-approximated by the chi-squared distribution

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The exact p-value can be computed as follows:

$$p = 2 \sum_{i=B}^{n} \binom{n}{i} 0.5^{i}(1-0.5)^{n-i},$$

where n=b+c, and the factor 2 is used to compute the two-sided p-value.

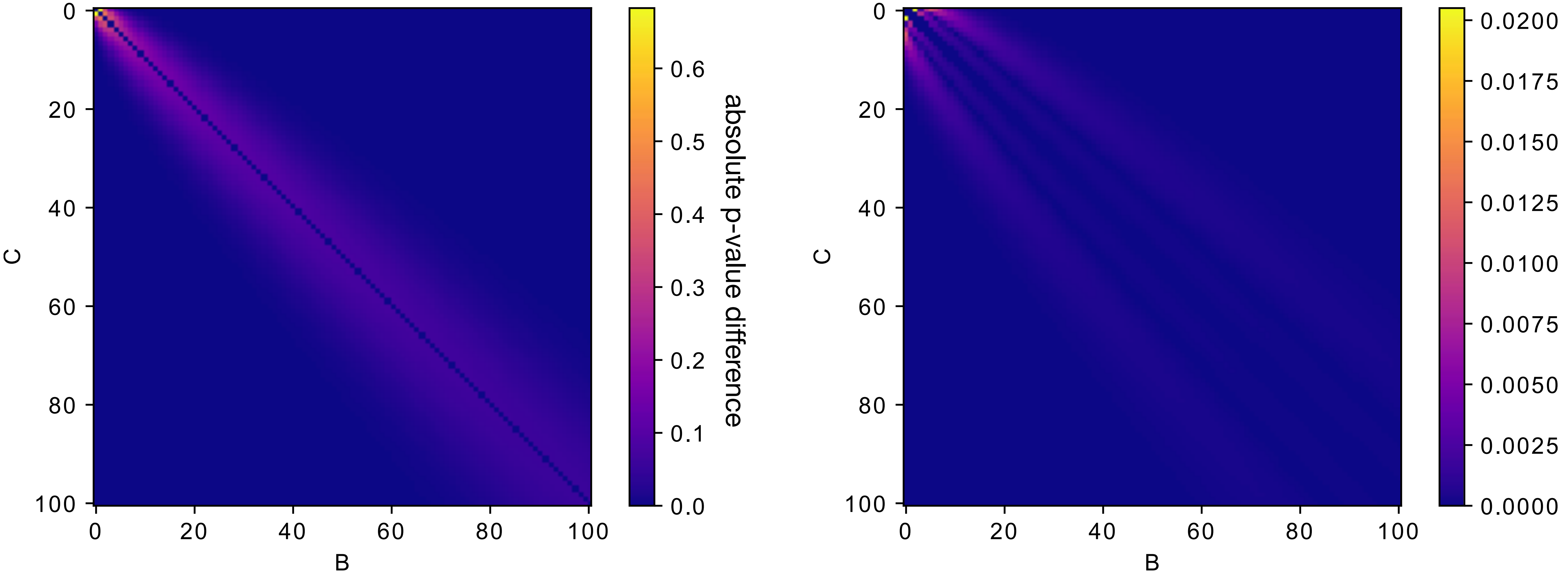
Comparing two machine learning classifiers -- McNemar's Test

Exact p-values via the Binomial test

- The following heat map illustrates the differences between the McNemar approximation of the chi-squared value (with and without Edward's continuity correction) to the exact p-values computed via the binomial test:

Uncorrected vs. exact

Corrected vs. exact



(As we can see in this heat map, the p-values from the continuity-corrected version of McNemar's test are almost identical to the p-values from a binomial test if both B and C are larger than 50.)

Multiple Hypothesis Testing Issue

1. Conduct an omnibus test under the null hypothesis that there is no difference between the classification accuracies

2. If the omnibus test led to the rejection of the null hypothesis, conduct pairwise post hoc tests, with adjustments for multiple comparisons, to determine where the differences between the model performances occurred

Multiple Hypothesis Testing Issue

1. Conduct an omnibus test under the null hypothesis that there is no difference between the classification accuracies (Cochran's Q test would be a good choice, which is a generalized version of McNemar's test for three or more models)

2. If the omnibus test led to the rejection of the null hypothesis, conduct pairwise post hoc tests, with adjustments for multiple comparisons, to determine where the differences between the model performances occurred (McNemar's Test would be a candidate here)

Cochran's Q Test

- Cochran's Q test is analogous to ANOVA for binary outcomes
- The test statistic is approximately (similar to McNemar's test) distributed as chi-squared with L–1 degrees of freedom, where L is the number of models we evaluate (since L=2 for McNemar's test, McNemars test statistic approximates a chi-squared distribution with one degree of freedom)

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- Cochran's Q test is analogous to ANOVA for binary outcomes
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More formally, Cochran's Q test tests the hypothesis that there is no difference between the classification accuracies

$$p_i : H_0 = p_1 = p_2 = \cdots = p_L \,.$$

Cochran's Q Test

Let $\{C_1, \ldots, C_L\}$

be a set of classifiers who have all been tested on the same dataset. If the L classifiers don't perform differently, then the following Q statistic is distributed approximately as "chi-squared" with *L-1* degrees of freedom

$$Q_C = (L-1)\frac{L\sum_{i=1}^{L} G_i^2 - T^2}{LT - \sum_{j=1}^{N_{ts}} (L_j)^2}.$$

G_i is the number of objects out of N_{ts} correctly classified by $C_i = 1, \ldots L$

L_j is the number of classifiers out of *L* that correctly classified object $\mathbf{z}_j \in \mathbf{Z}_{ts}$

where $\mathbf{Z}_{ts} = \{\mathbf{z}_1, \ldots \mathbf{z}_{N_{ts}}\}$

is the test dataset on which the classifiers are tested on;
and *T* is the total number of correct number of votes among the *L* classifiers

$$T = \sum_{i=1}^{L} G_i = \sum_{j=1}^{N_{ts}} L_j.$$

McNemar's Test with Bonferroni Correction to counteract the problem of multiple comparisons

Unfortunately, the problem of multiple comparisons receives little attention in literature. However, Peter H. Westfall, James F. Troendl, and Gene Pennello wrote a nice article on how to approach such situations where we want to compare multiple models to each other if you are interested:

- Westfall, Peter H., James F. Troendle, and Gene Pennello. "Multiple mcnemar tests." *Biometrics* 66.4 (2010): 1185-1191.

McNemar's Test with Bonferroni Correction to counteract the problem of multiple comparisons

Perneger, Thomas V. "What’s wrong with Bonferroni adjustments." *BMJ: British Medical Journal* 316.7139 (1998): 1236:

> "Type I errors [False Positives] cannot decrease (the whole point of Bonferroni adjustments) without inflating type II errors (the probability of accepting the null hypothesis when the alternative is true) (Rothman, 1990). And type II errors [False Negatives] are no less false than type I errors."

Eventually, once more it comes down to the "no free lunch" -- in this context, let us refer of it as the "no free lunch theorem of statistical tests."

> "The answer is that such adjustments are correct in the original framework of statistical test theory, proposed by Neyman and Pearson in the 1920s (Neyman, 1928). This theory was intended to aid decisions in repetitive situations."

Dietterich, T. G. (1998). Approximate statistical tests for comparing supervised classification learning algorithms. *Neural computation*, *10*(7), 1895-1923:

Summary:

1. McNemar's test
    - low false positive rate
    - fast, only needs to be executed once

2. Difference in proportions, by Snedecor and Cochran
    - high false positive rate (here, incorrectly detect difference when there is none)
    - cheap to compute though

3. Resampled paired t-test
    - high false positive rate
    - computationally very expensive

4. k-fold cross-validated t-test
    - somewhat elated false positive rate

5. 5x2cv paired t-test
    - low false positive rate (similar to McNemarr)
    - slightly more powerful than McNemar; recommended if computational efficiency (runtime) is not an issue (10 times more computations than McNemar)

K-fold cross-validation with paired t test

$$t = \frac{\Delta ACC_{avg}\sqrt{k}}{\sqrt{\sum_{i=1}^{k} (\Delta ACC_i - \Delta ACC_{avg})^2/(k-1)}}$$

$$\Delta ACC_{avg} = \frac{1}{k}\sum_{i=1}^{k} \Delta ACC_i |$$

$$\Delta ACC_i = ACC_i^A - ACC_i^B$$

H_0: equal accuracies

Dietterich, T. G. (1998). Approximate statistical tests for comparing supervised classification learning algorithms. *Neural computation*, *10*(7), 1895-1923:

5x2 CV Cross-Validation + paired t test

Dietterich, T. G. (1998). Approximate statistical tests for comparing supervised classification learning algorithms. *Neural computation*, *10*(7), 1895-1923:

Argument: independent training sets for 2-fold

Now we get 2 differences, since we use 2-fold cross-validation:

$$\Delta ACC_i^{(1)} = ACC_i^{A(1)} - ACC_i^{B(1)}$$

$$\Delta ACC_i^{(2)} = ACC_i^{A(2)} - ACC_i^{B(2)}$$

$$\Delta ACC_{avg,i} = (\Delta ACC_i^{(1)} + \Delta ACC_i^{(2)})/2$$

est. variance: $s_i^2 = (ACC^{(1)} - \Delta ACC_{avg,i})^2 + (ACC^{(2)} - \Delta ACC_{avg,i})^2$

$$t = \frac{\Delta ACC_1^{(1)}}{\sqrt{(1/5)\sum_{i=1}^{5} s_i^2}}$$

(note that the subscript 1 in denominator is not a typo, it only refers to the first run)

F Test for classifiers

Looney, S. W. (1988). A statistical technique for comparing the accuracies of several classifiers. *Pattern Recognition Letters*, *8*(1), 5-9.

Assume 1 test set and L independent classifiers with accuracies $ACC_1, \dots ACC_L$

$$SSC = N_{ts} \sum_{i=1}^{L} ACC_i^2 - N_{ts} \cdot L \cdot ACC_{avg}^2$$

$$SST = N_{ts} \cdot L \cdot ACC_{avg}(1 - ACC_{avg})$$

$$SSO = \frac{1}{L} \sum_{j=1}^{N_t s} (L_j)^2 - N_{ts} \cdot L \cdot ACC_{avg}^2$$

$$SSCOMB = SST - SSC - SSO$$

(where L_j is the number of classifiers that correctly classified the *j*th example)

$$MSC = \frac{SSC}{L-1} \qquad MSCOMB = \frac{SSCOMB}{(L-1)(N_{ts}-1)} \qquad F = \frac{MSC}{MSCOMB}$$

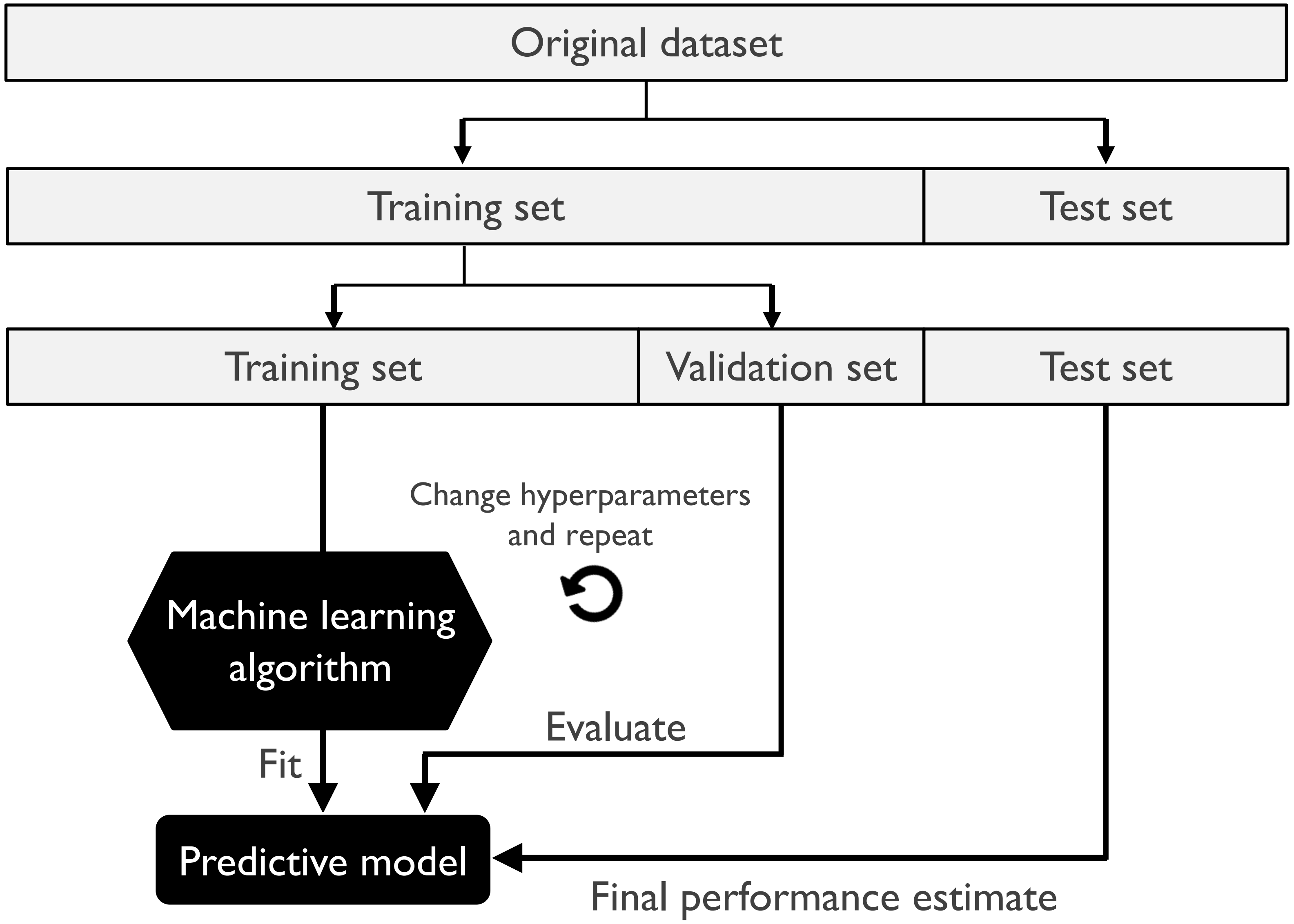
Combined 5 × 2 cv F Test for Comparing Supervised Classification Learning Algorithms

Alpaydm, Ethem. "Combined 5× 2 cv F test for comparing supervised classification learning algorithms." *Neural computation* 11.8 (1999): 1885-1892.

More robust than Dietterich 1998's 5x2 CV + t test

Back to "Computational/Empirical" Methods

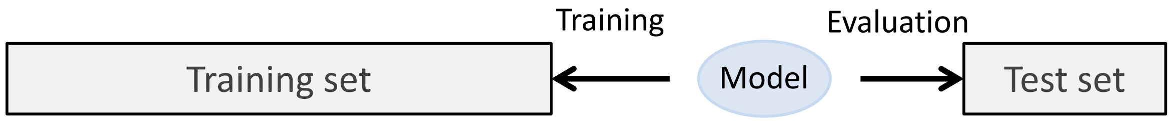
Recap: Model Selection with 3-way Holdout



Recap: Model Selection with k-fold Cross.-Val.

1)

good or bad ?



Training set

Training

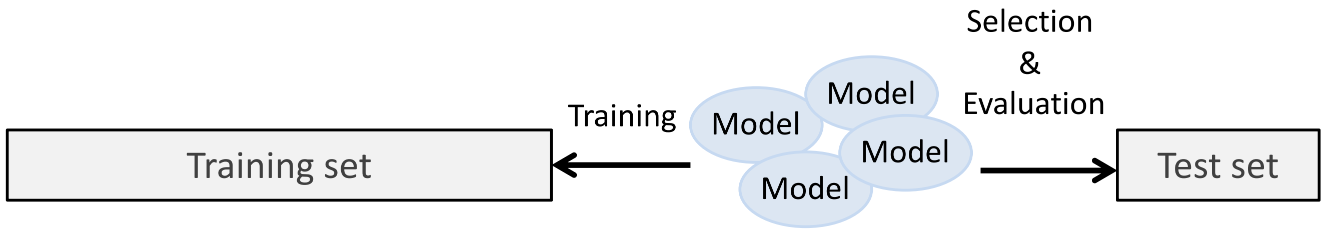
Model

Evaluation

Test set

2)

good or bad ?



Training set

Training

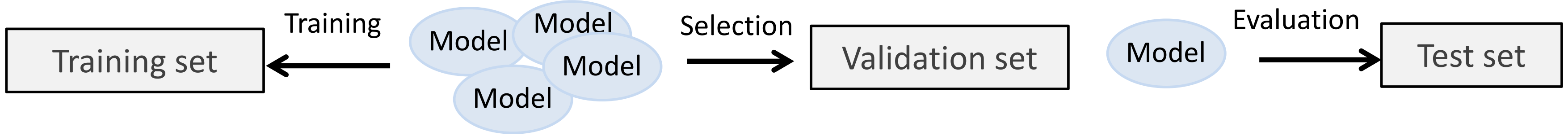
Model Model Model Model

Selection & Evaluation

Test set

3)

good or bad ?



Training set

Training

Model Model Model Model

Selection

Validation set

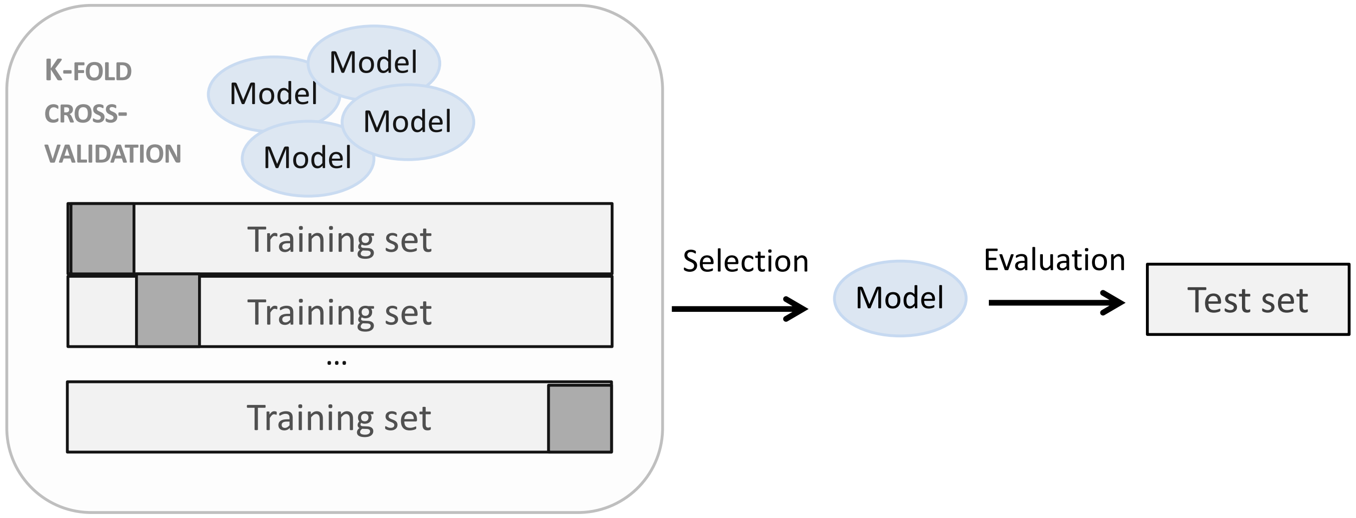
Model

Evaluation

Test set

4)

good or bad ?



K-FOLD CROSS-VALIDATION

Model Model Model Model

Training set

Training set

...

Training set

Selection

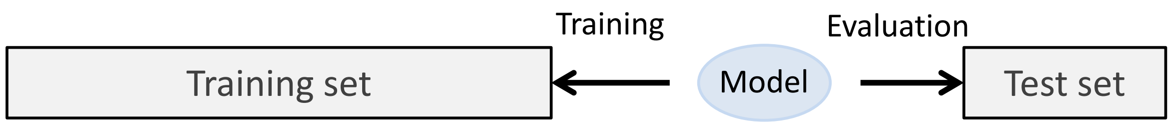
Model

Evaluation

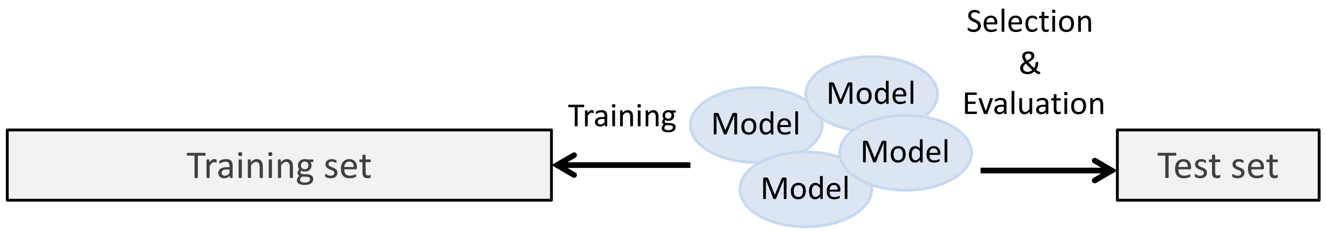
Test set

Recap: Model Selection with k-fold Cross.-Val.

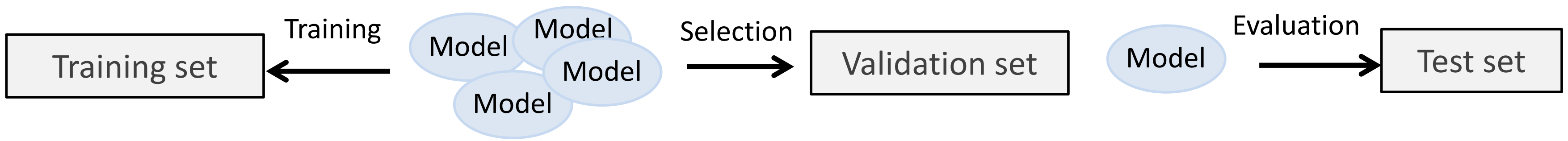
1) ✓



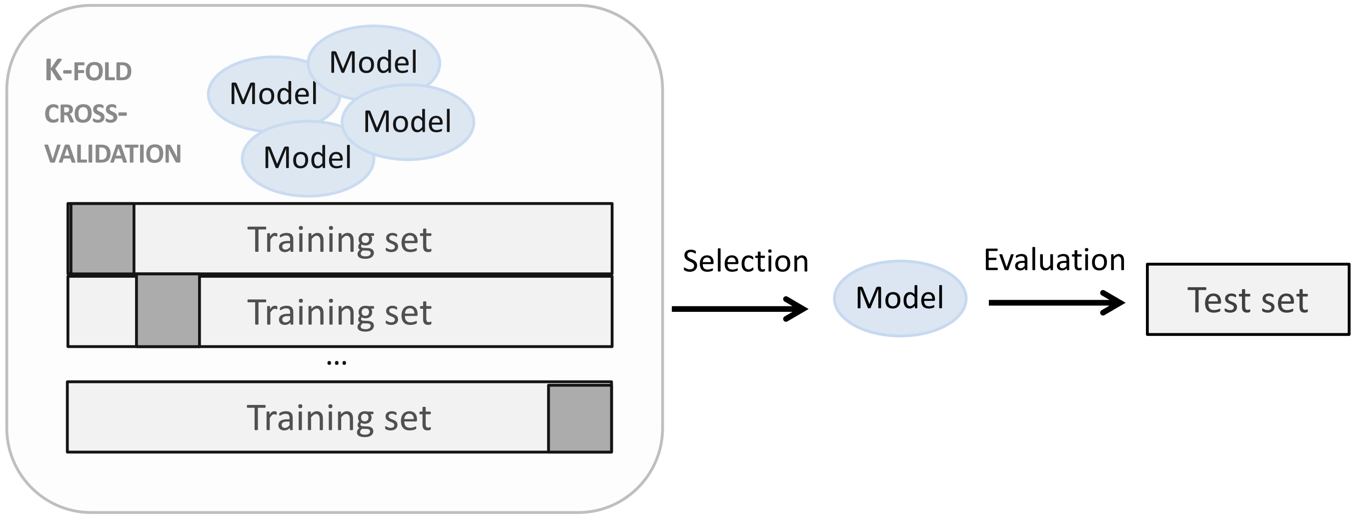
2) ✗



3) ✓



4) ✓✓

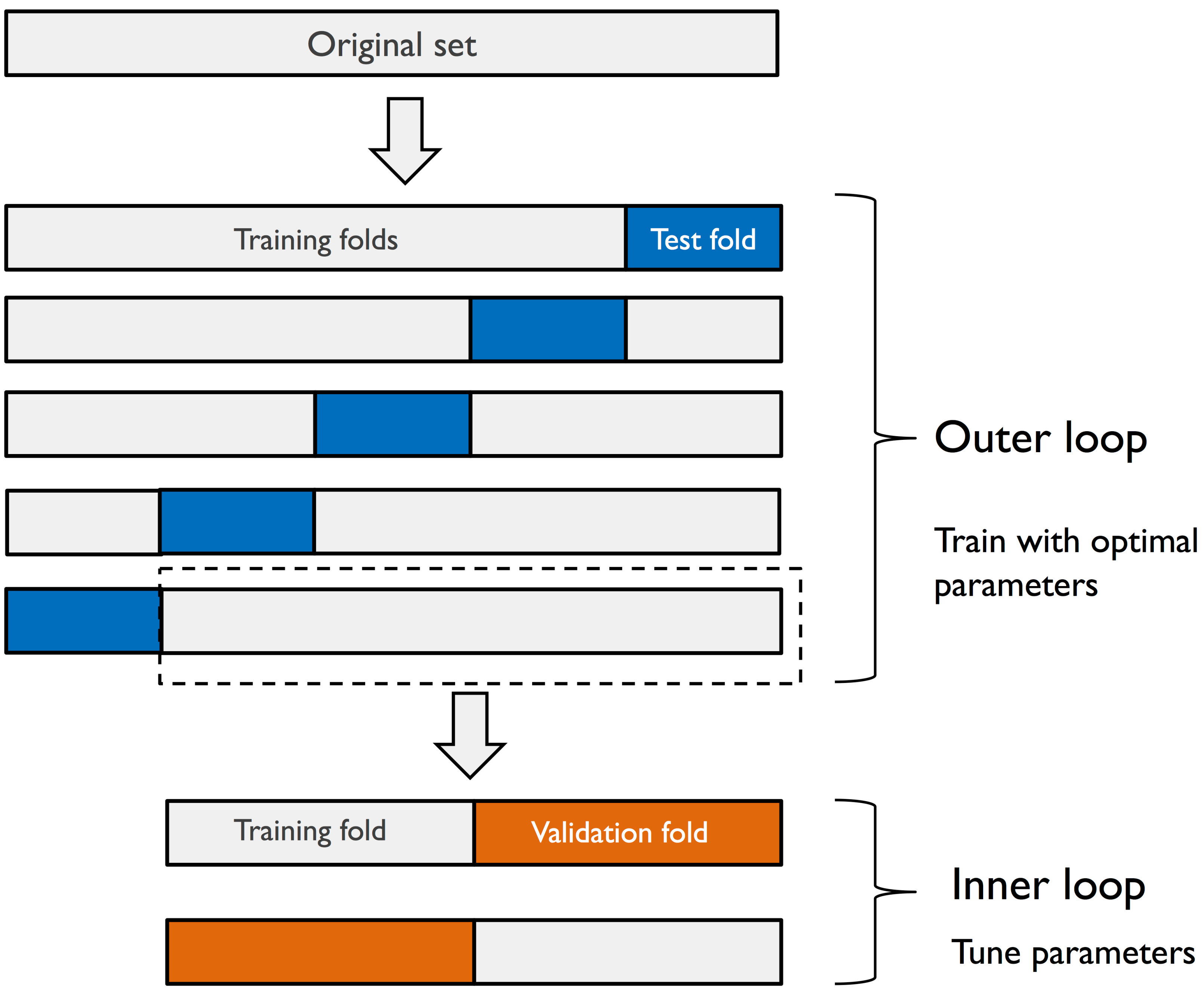


Nested Cross-Validation for Algorithm Selection

Main Idea:

- Outer loop: purpose related to train/test split
- Inner loop: like k-fold cross-validation for tuning

Nested Cross-Validation

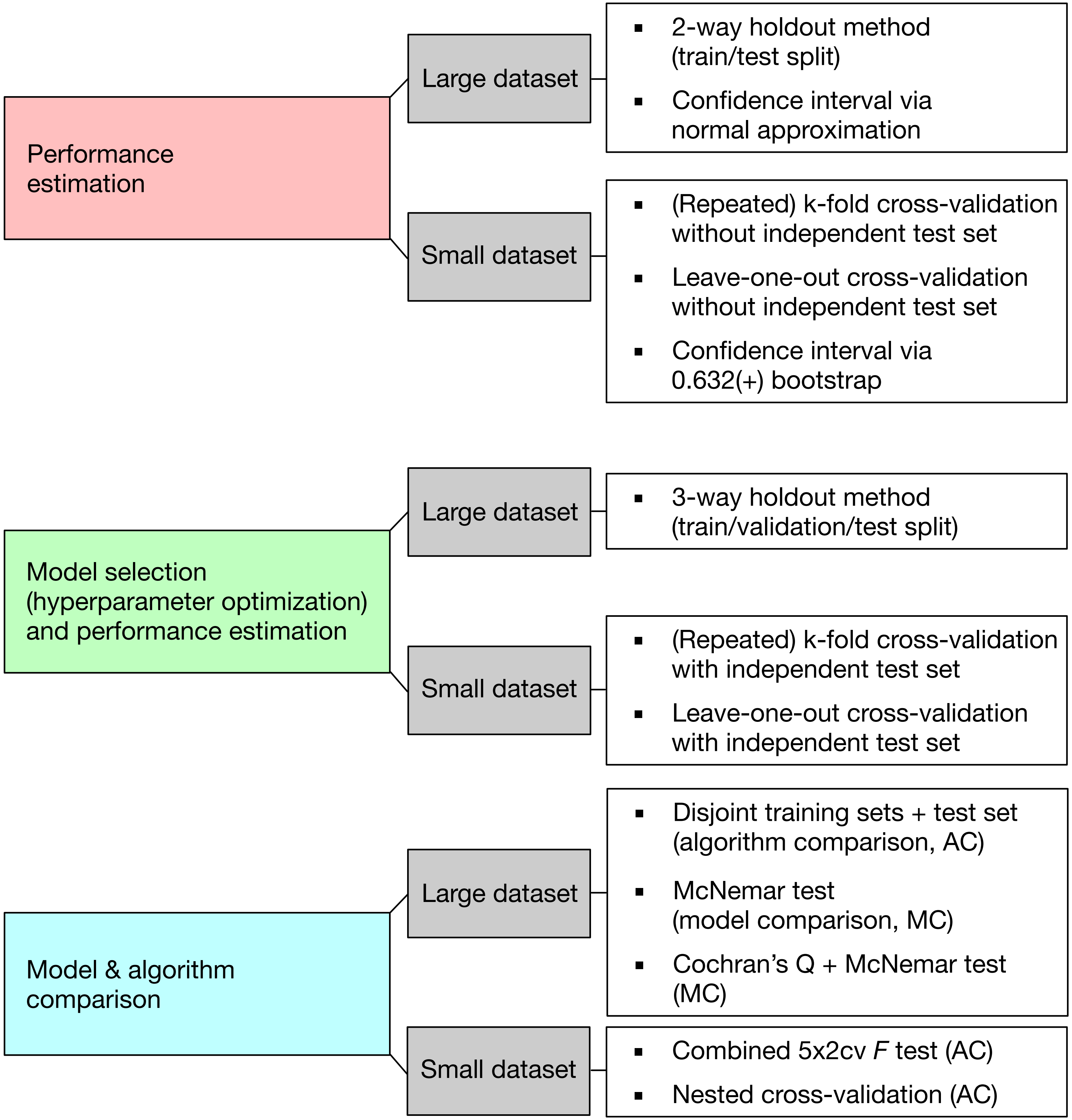


Nested Cross-Validation for Algorithm Selection

- Outer loop:
  use average performance as generalization performance
  check for "model stability"

- Finally:
  as usual, fit model on whole dataset for deployment

Conclusions, (my) "recommendations"



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Model selection (hyperparameter optimization) and performance estimation

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Model & algorithm comparison

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  - McNemar test (model comparison, MC)
  - Cochran’s Q + McNemar test (MC)
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Code Examples

(Coding will be part of your homework)

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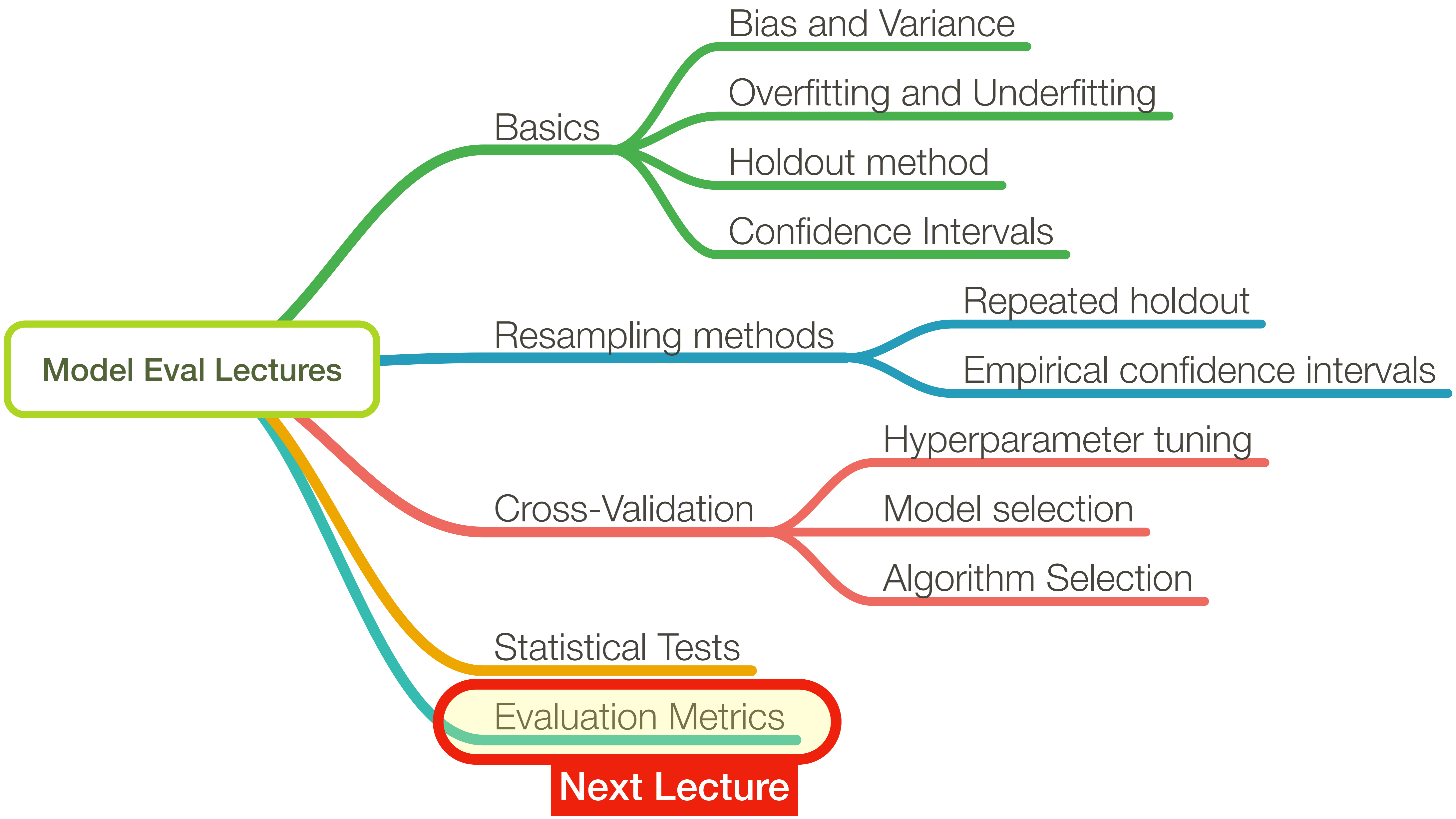
Model Eval Lectures
Basics
Bias and Variance
Overfitting and Underfitting
Holdout method
Confidence Intervals
Resampling methods
Repeated holdout
Empirical confidence intervals
Cross-Validation
Hyperparameter tuning
Model selection
Algorithm Selection
Statistical Tests
Evaluation Metrics
Next Lecture