Model selection

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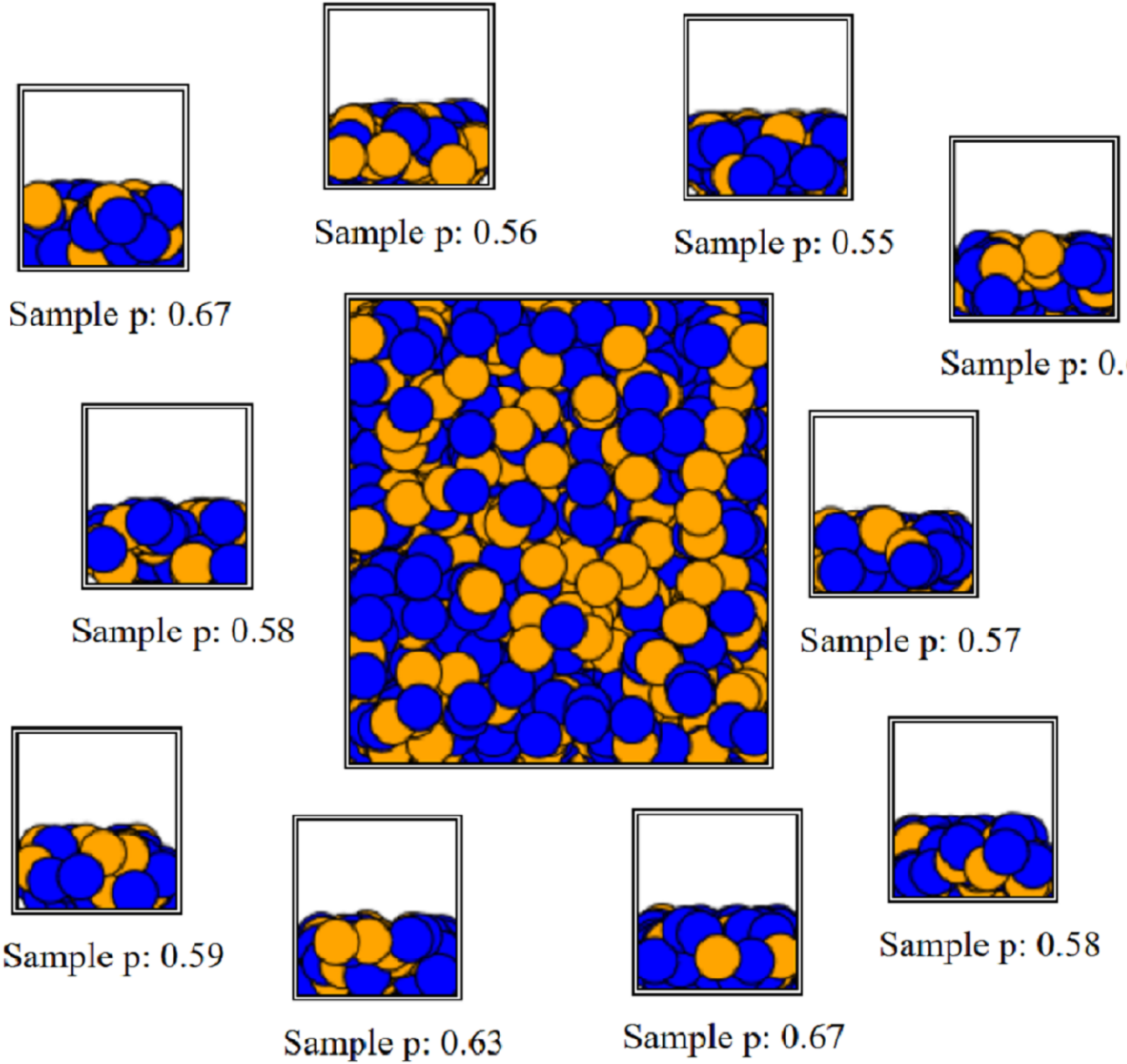
Slides in this presentation are from material kindly provided by Sebastian Rashka



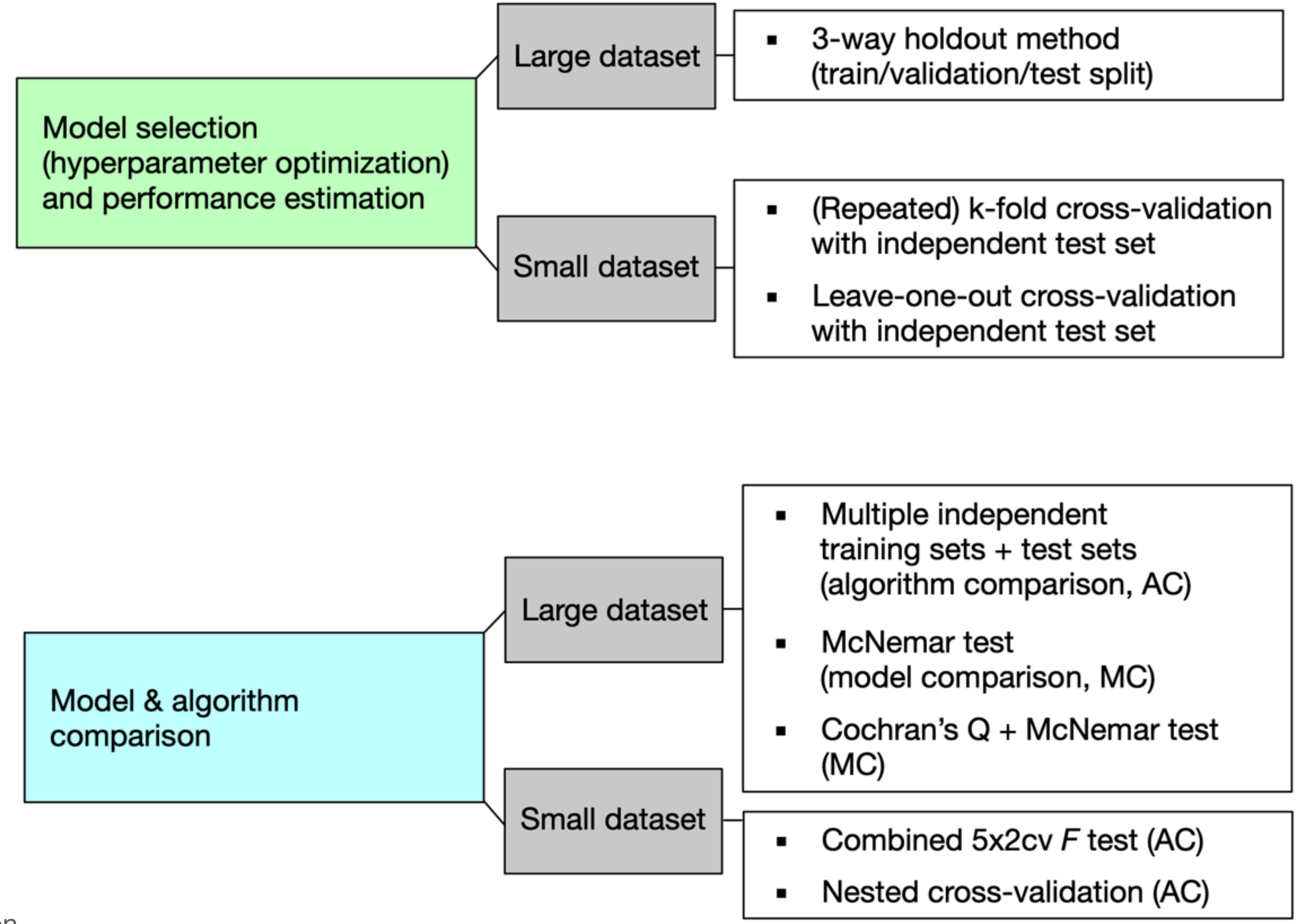
One of the hold out folds

Or one trial of model selection via cross-val

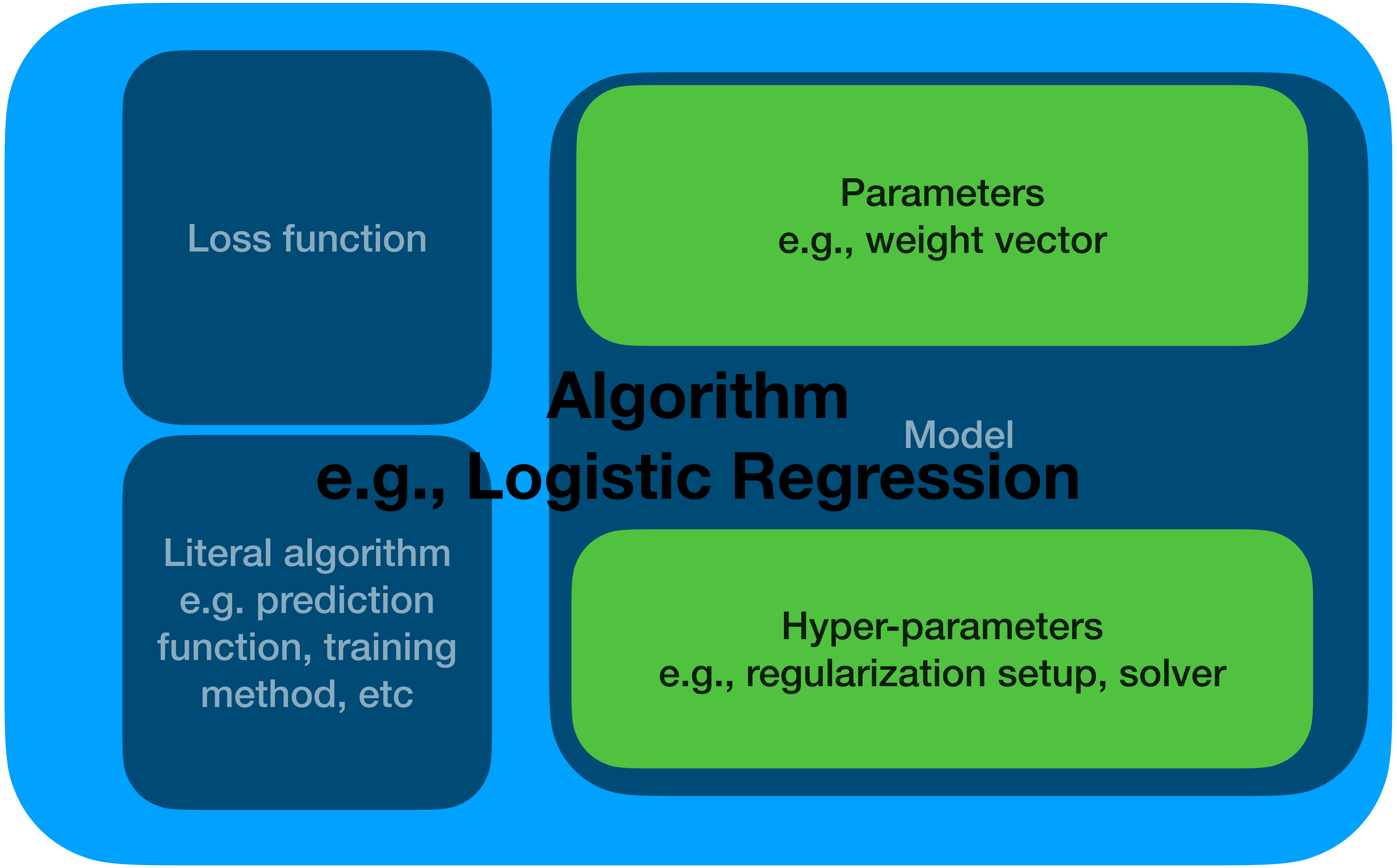
Estimation of performance

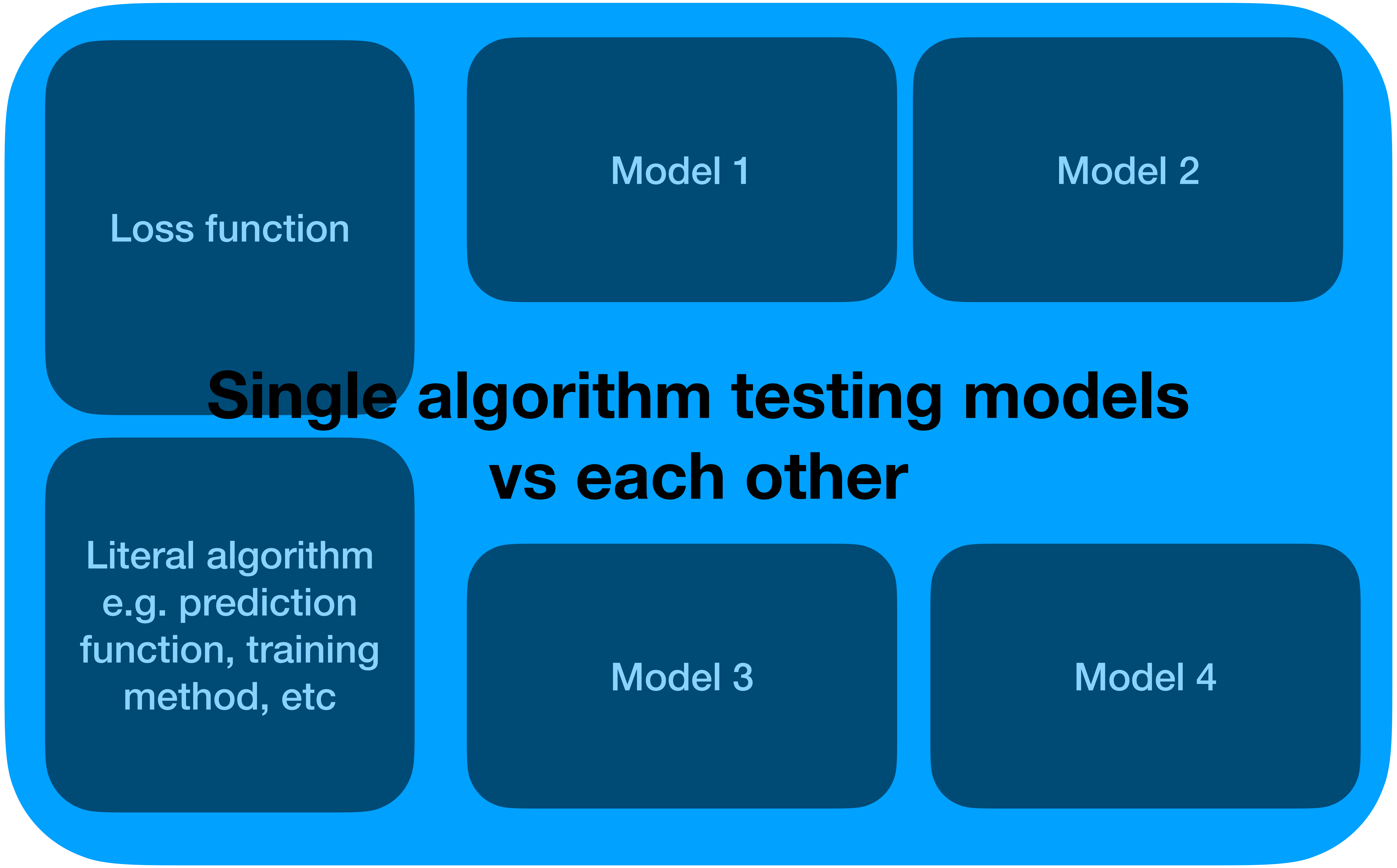
Many methods, two use cases, one reason

- THE ONE REASON: every measure is a random draw from a distribution of performances… What if the data was a bit different? What if the random seed is different? Etc.
- TWO USE CASES:
  - To estimate how well the system will generalize (test)
  - To perform model selection or algorithm selection (validation)
- MANY METHODS:
  - See Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning, Sebatian Rashkha, https://arxiv.org/pdf/1811.12808.pdf for a good intro (but there are more out there!)



Model Evaluation, Model Selection,
and Algorithm Selection in Machine Learning
Sebatian Rashkha
https://arxiv.org/pdf/1811.12808.pdf


Loss function
Parameters
e.g., weight vector
Algorithm
e.g., Logistic Regression
Model
Literal algorithm
e.g. prediction
function, training
method, etc
Hyper-parameters
e.g., regularization setup, solver



“Model selection”

“Algorithm selection”

Method #1 - Train/Validate/Test sets

For either Model or Algorithm selection using HUGE datasets

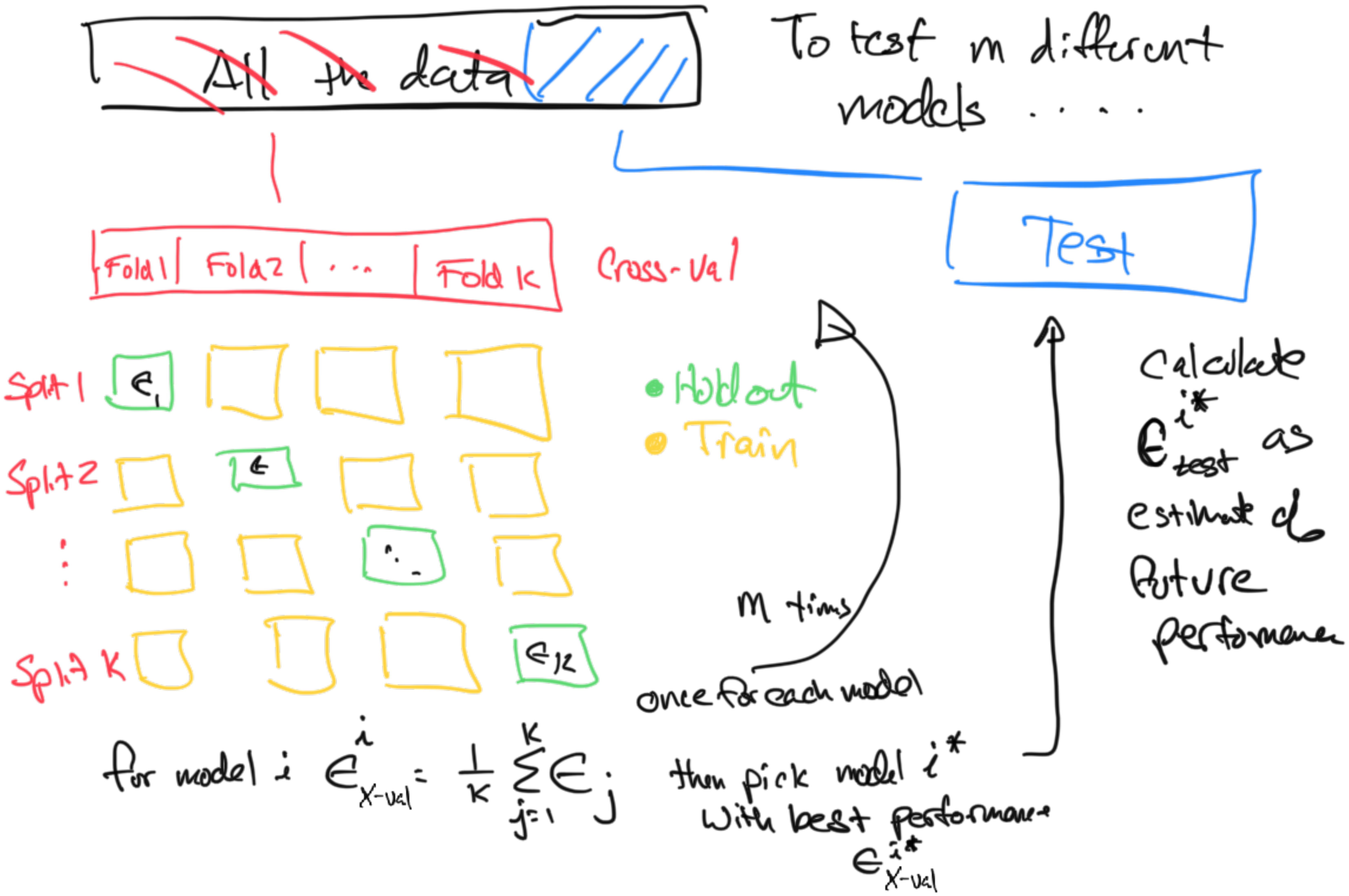
- Split data into train, validate, test
- [OPTIONAL] Outer loop… do this T times:
  - do this M times, once for each model in the hyper-parameter search space or each algorithm-model combination:
    - Train it on the same training set
    - Predict on the same validation set
- Pick the best model or algorithm based on its performance on [OPTIONAL the mean across trials] of the validation set
- Train the best version on the whole of training set + validation set
- Test it on the test set to estimate its ability to generalize

METHOD 1 - with enough data to have a good test set

Let's say you had around 8k samples in a dataset

For each trial:

- training set ~ sample 5k (with or w/o) replacement from entire dataset
- Grid search of hyper parameters using k-fold cross validation on the training set
- Select best model from grid, train on entire training set
- Evaluate best model on the test set (everything not sampled for training)



Method #2 - Cross validation

For either model or algorithm selection using medium sized datasets

- Split data into cross-validation and test sets
- [OPTIONAL] Outer loop… do this T times:
  - do this M times, once for each model in the hyper-parameter search space or each algorithm-model combination:
    - Use k-fold cross validation to estimate validation error
- Pick the best model or algorithm based on its performance on [OPTIONAL the mean across trials] of the validation sets
- Train the best version on the whole of cross validation set
- Test it on the test set to estimate its ability to generalize

Set aside detailed coverage of Nested CV for after exam

METHOD 3 - AC or data efficient MC

Nested Cross-validation

For **algorithm comparison** if done the time/memory efficient way: store metrics on inner cv, pick best model, then store metrics of best model on outer cv for AC

…can be used for **model comparison** if done the inefficient way: metrics stored on inner and outer cv, calc best model post hoc on inner, use outer cv as test metric for best model

This for when you've got only ~2000 samples, which is barely enough to fit the data well let alone test

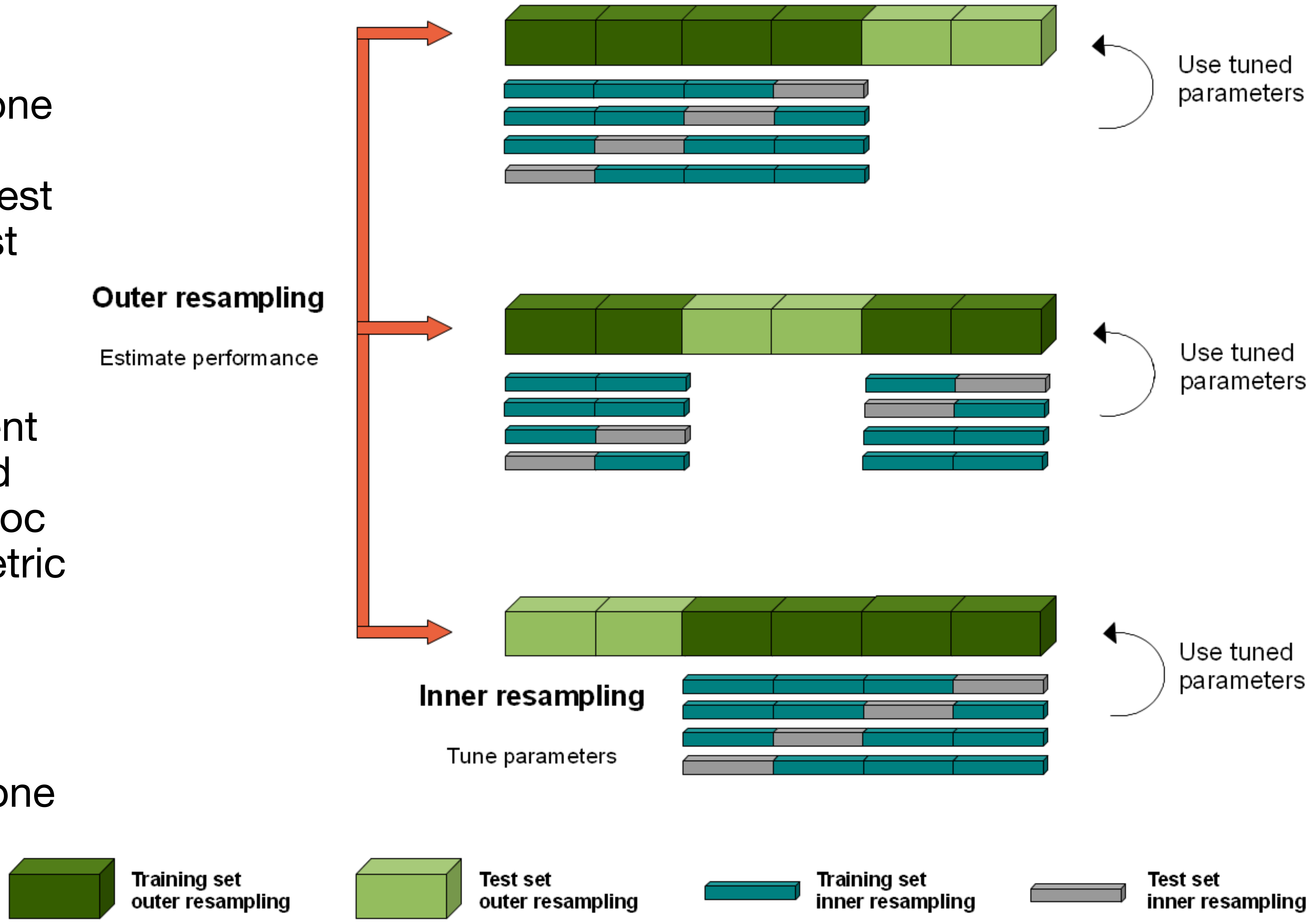


Figure from mlr R package docs

Method 3a - Nested CV

For doing algorithm selection

- Split off a test set for later
- [OPTIONAL] Outer loop… do this T times:
    - Do this M times, once for each algorithm
        - Use nested k-fold cross validation…
            - Inner CV estimates validation error for all the hyperparams tested for a given model
            - Outer CV estimates validation error for the best hyperparams from inner CV for a given algorithm.
- Pick the best algorithm based on its performance on the mean across [OPTIONAL trials and] the outer cross validation folds
- Train the chosen algorithm on entire nested CV dataseet. Use test set to estimate generalization performance
- Reasonably time/memory efficient as outer loop is only done once per algorithm and you don't have to store the inner loop results

Method 3b - Nested CV

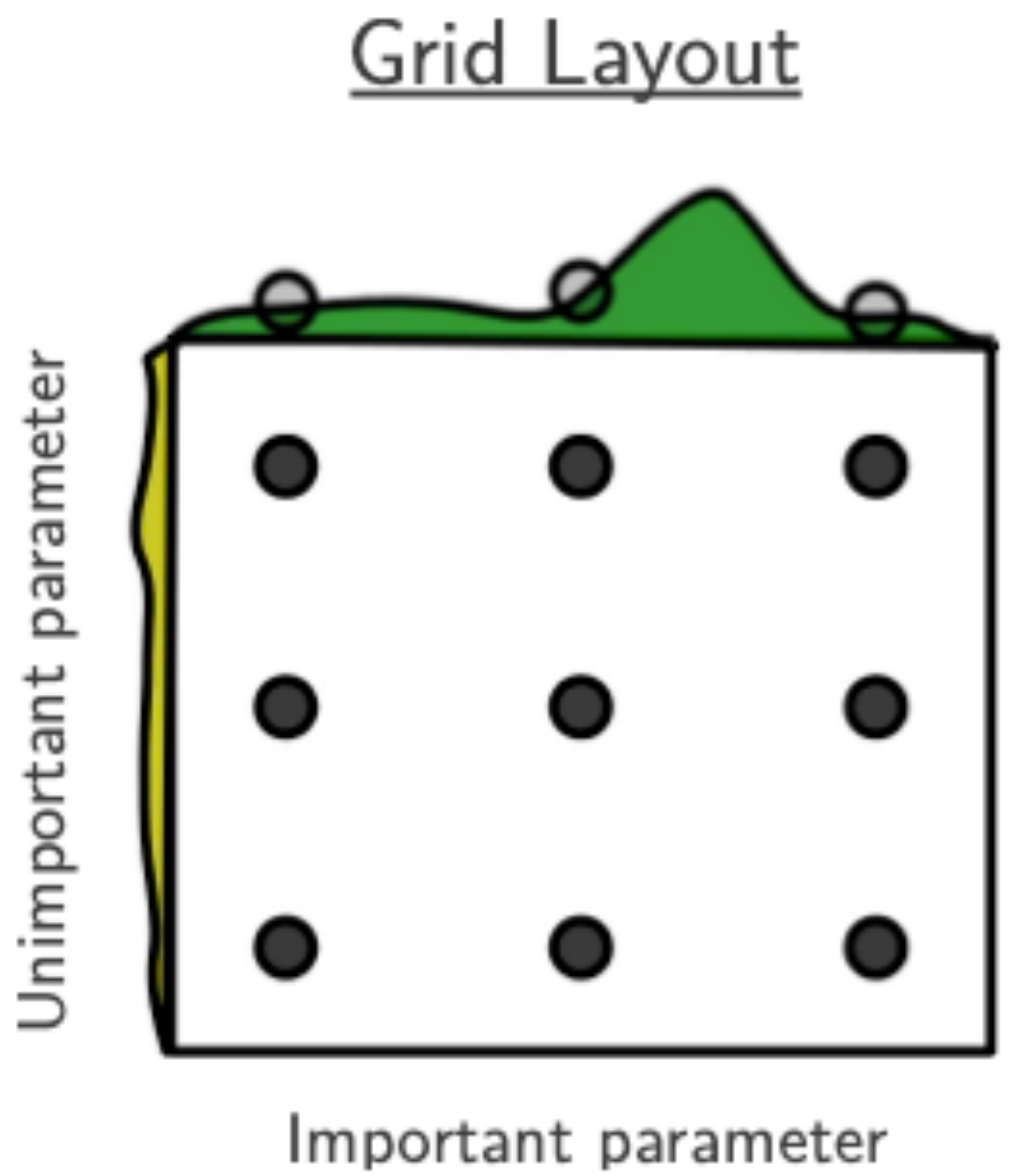
For model selection on small datasets

- Do not split off a test set! This is why its data efficient.
- [OPTIONAL] Outer loop… do this T times:
    - Do this M times, once for each algorithm
        - Use nested k-fold cross validation…
            - Inner CV estimates validation error for all the hyperparams tested for a given model
            - Outer CV estimates test error for all the hyperparams tested for a given model
- Pick the best model based on its performance on the mean across [OPTIONAL trials and] folds of the inner cross validations and report its generalization performance on the mean across [OPTIONAL trials and] folds of the outer cross validation. This is post-hoc… you don't know which model is best until all the trials are done, so you have to calculate and store both inner and outer fold performance on every model.

But how do you organize your search of the hyper parameter space?

Grid Search

- Exhaustive search
- Thorough but expensive
- Specify grid for parameter search
- Can be run in parallel
- Can suffer from poor coverage
- Often run with multiple resolutions



Bergstra, J., & Bengio, Y. (2012). Random search for hyper-parameter optimization. *The Journal of Machine Learning Research*, *13*(1), 281-305.

Randomized Search

- Search based on a time budget
- Preferred if there are many hyperparameters (e.g. > 3 distinct ones)
- specify distribution for parameter search
- can be run in parallel

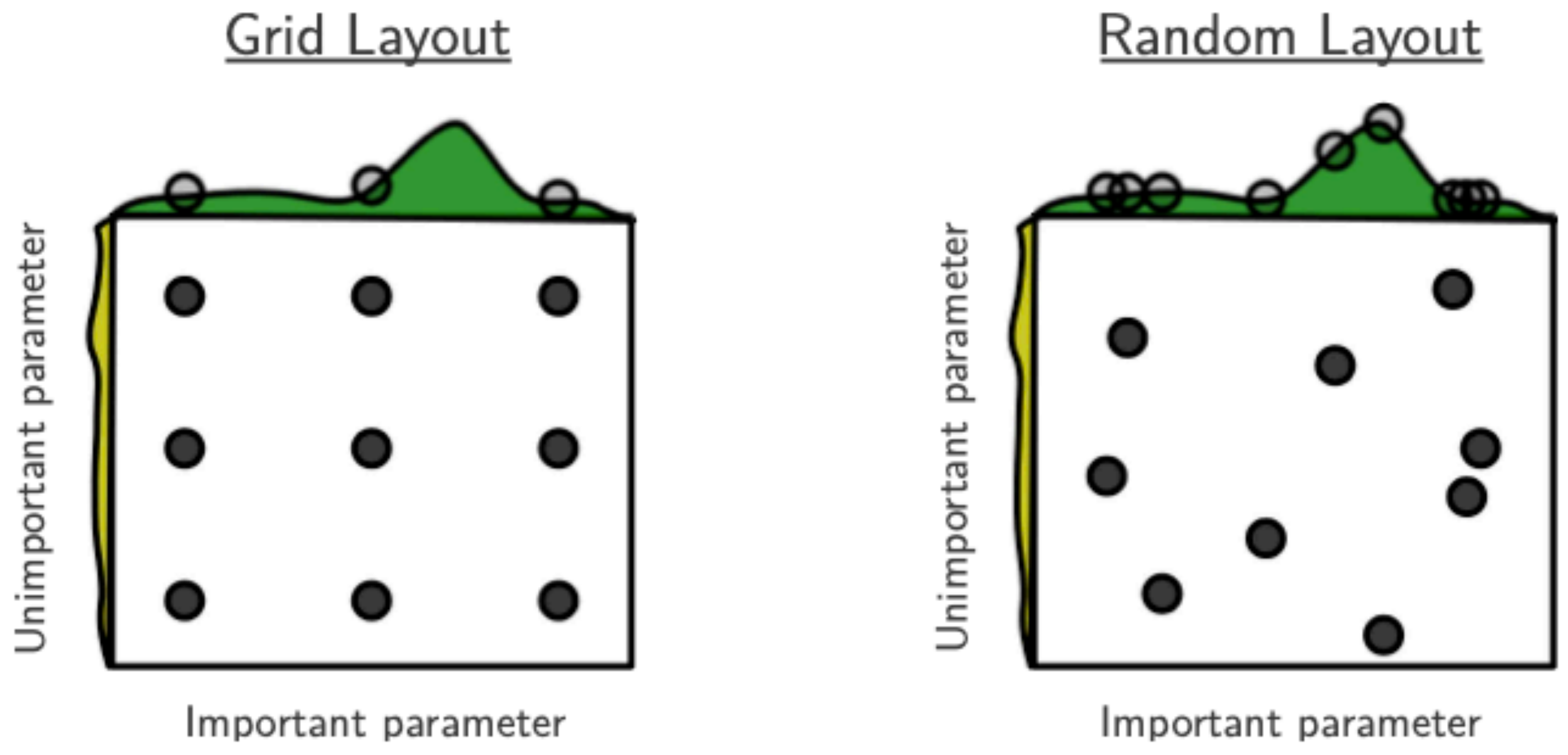


Figure 1: Grid and random search of nine trials for optimizing a function $f(x,y) = g(x) + h(y) \approx g(x)$ with low effective dimensionality. Above each square $g(x)$ is shown in green, and left of each square $h(y)$ is shown in yellow. With grid search, nine trials only test $g(x)$ in three distinct places. With random search, all nine trials explore distinct values of g. This failure of grid search is the rule rather than the exception in high dimensional hyper-parameter optimization.

Bergstra, J., & Bengio, Y. (2012). Random search for hyper-parameter optimization. *The Journal of Machine Learning Research*, *13*(1), 281-305.

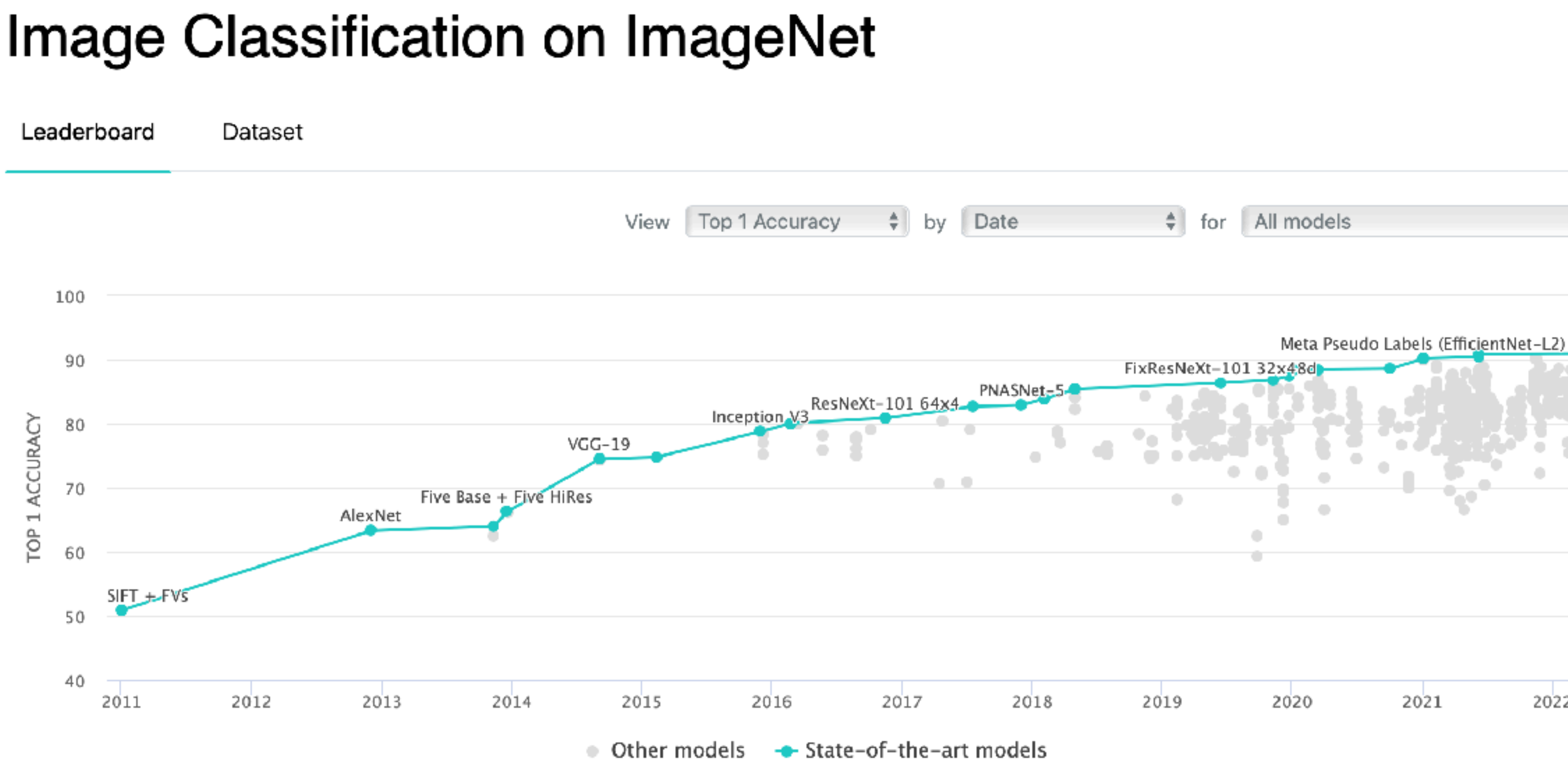
Stopped here for time

Statistical testing

https://sebastianraschka.com/pdf/lecture-notes/stat479fs18/11_eval-algo_notes.pdf

Statistical testing on model performance

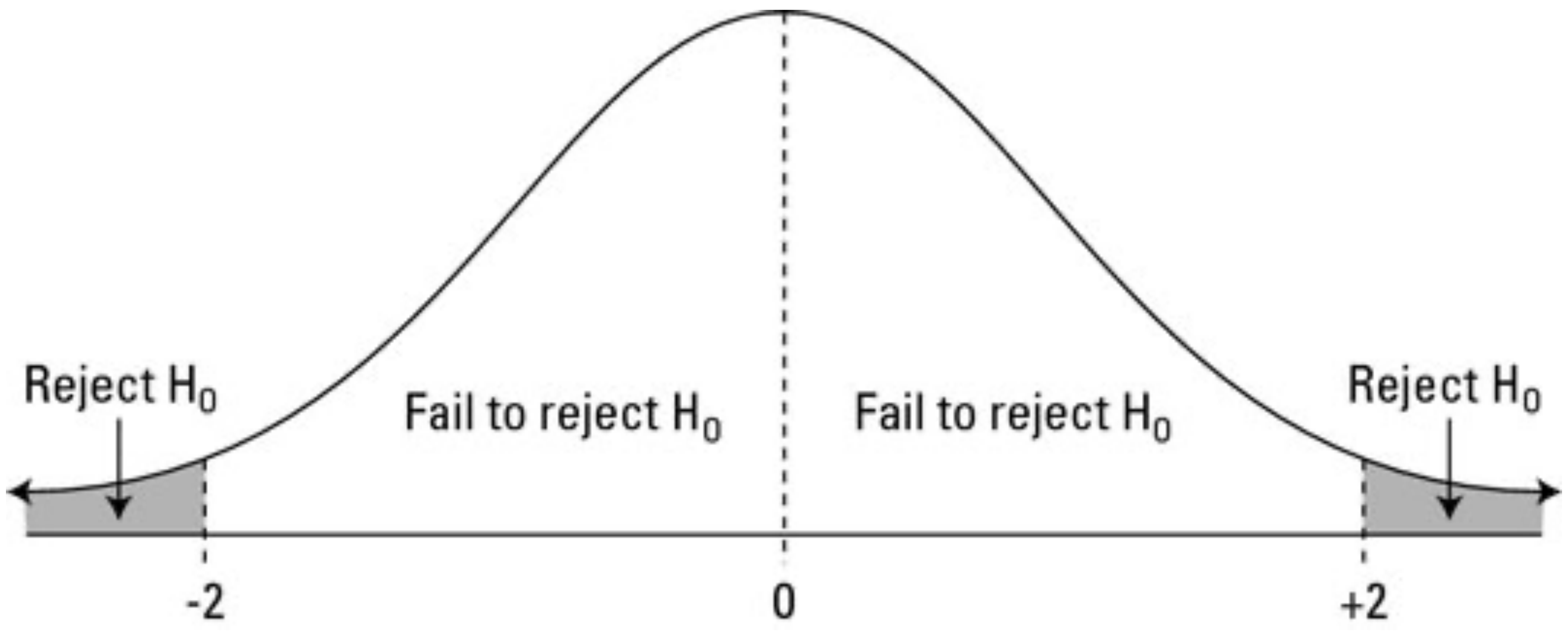
- Testing is almost always paired (over folds of cross validation)
- Distinguish between tests appropriate for algorithm comparison vs model selection (hyperparameter settings)
- Distinguish between test that are computationally efficient vs those that are not
- Distinguish between pair-wise and group-wise tests



Jason gets grumpy about blindly following methods you don’t understand fully

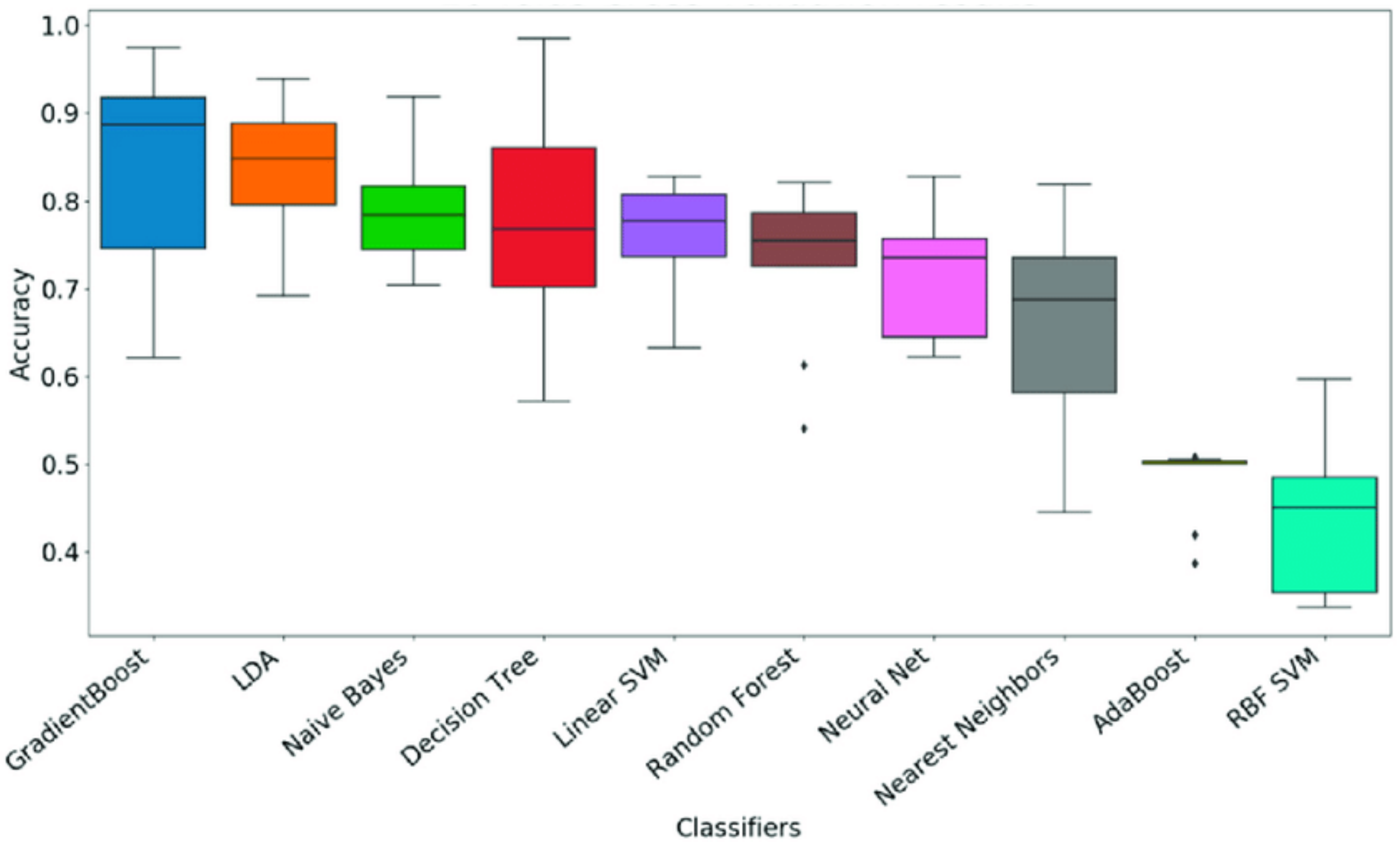
The p-value

- In range 0,1
- Smaller is support for alternative hypothesis
- Larger is inconclusive
- Ignores effect size!!!@!!! Is the difference practically important?
- Assumes conditions on data
- $P(H|D) = \frac{P(D|H)P(H)}{P(D)}$



Maybe you don’t need a statistical test

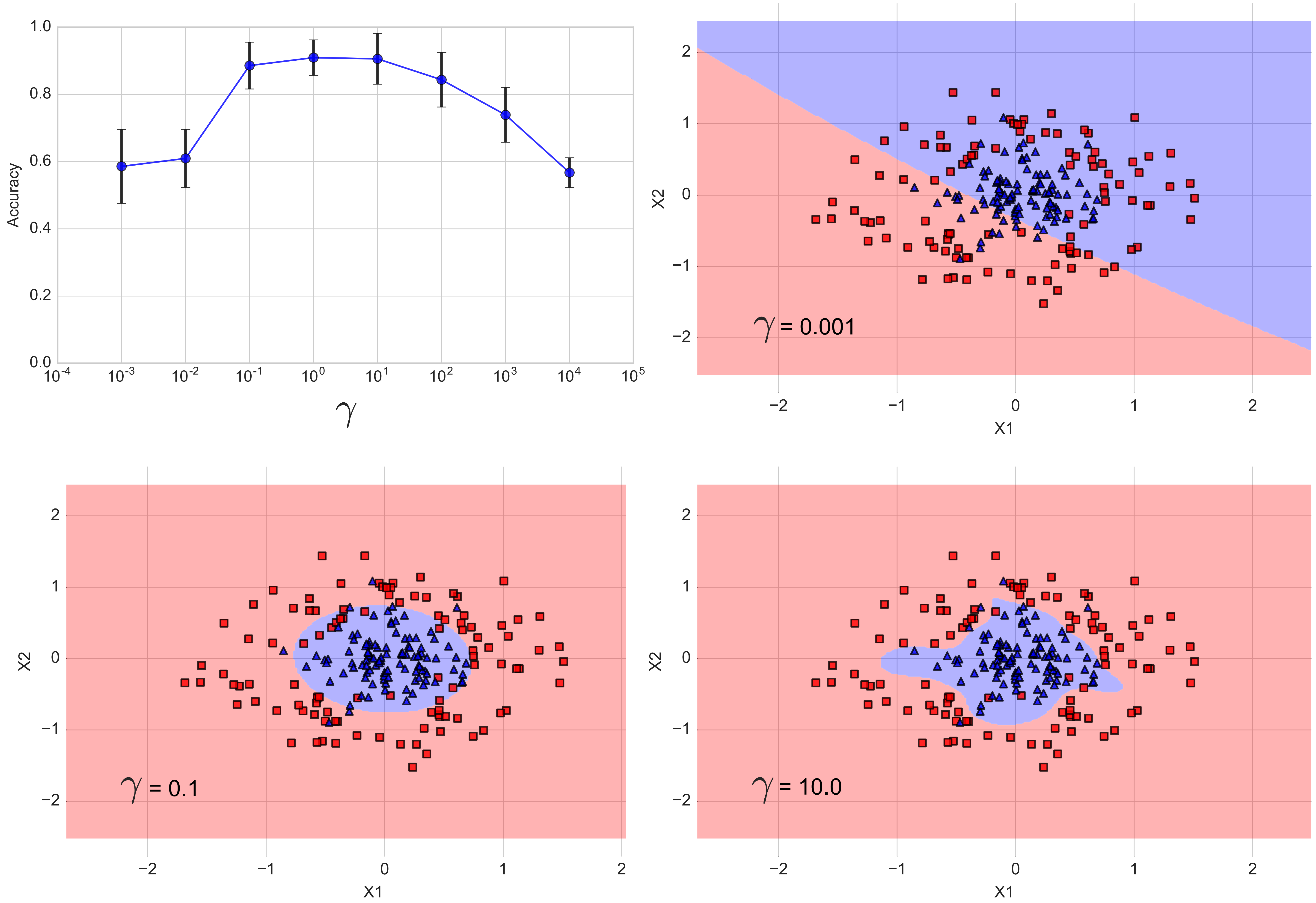
3x5 repeated cross validation results



Parsimony Principle

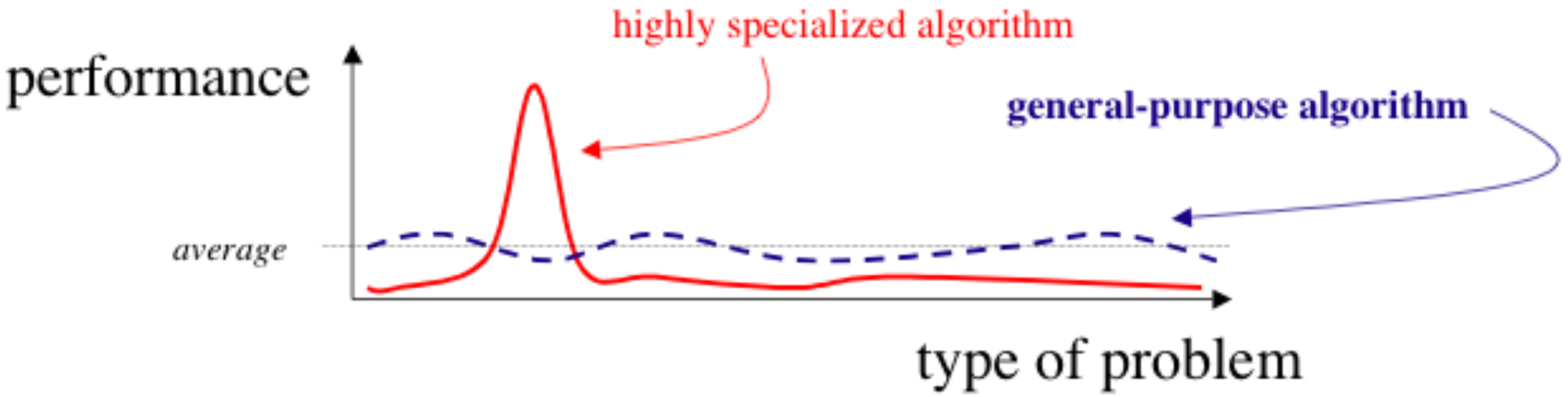
Choose the simplest w/in 1 std error of optimal

Which parameter would you select?



No free lunch theorem

Why even bother??



Wolpert, D. H.; Macready, W. G. (1995). "No Free Lunch Theorems for Search" (PDF). *Technical Report SFI-TR-95-02-010*. Santa Fe Institute.

http://www.no-free-lunch.org