Fine-tuning the hyper parameters for a classifier in HEP

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3rd COMCHA lectures

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Training + validation

Test

Apply

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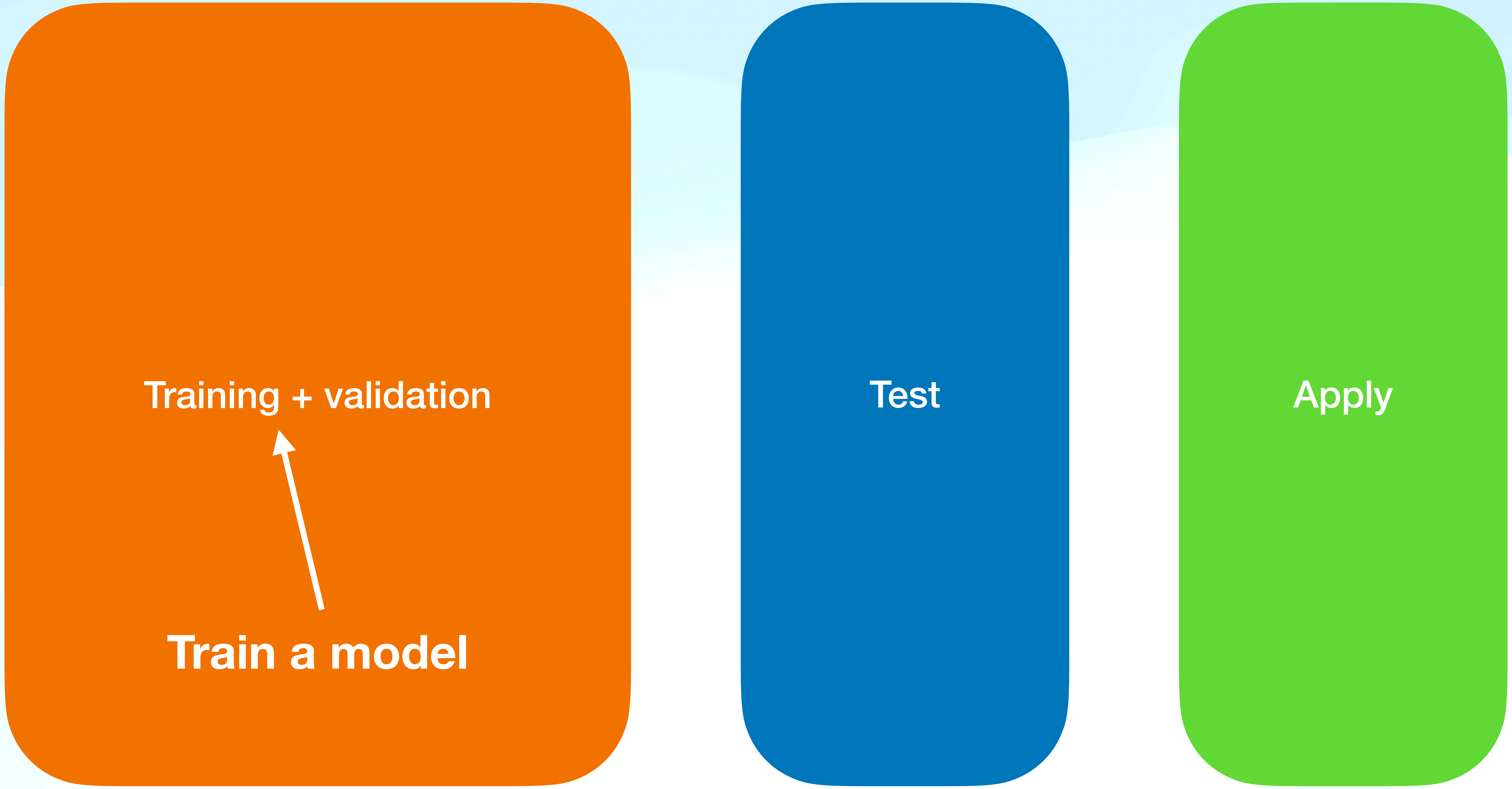

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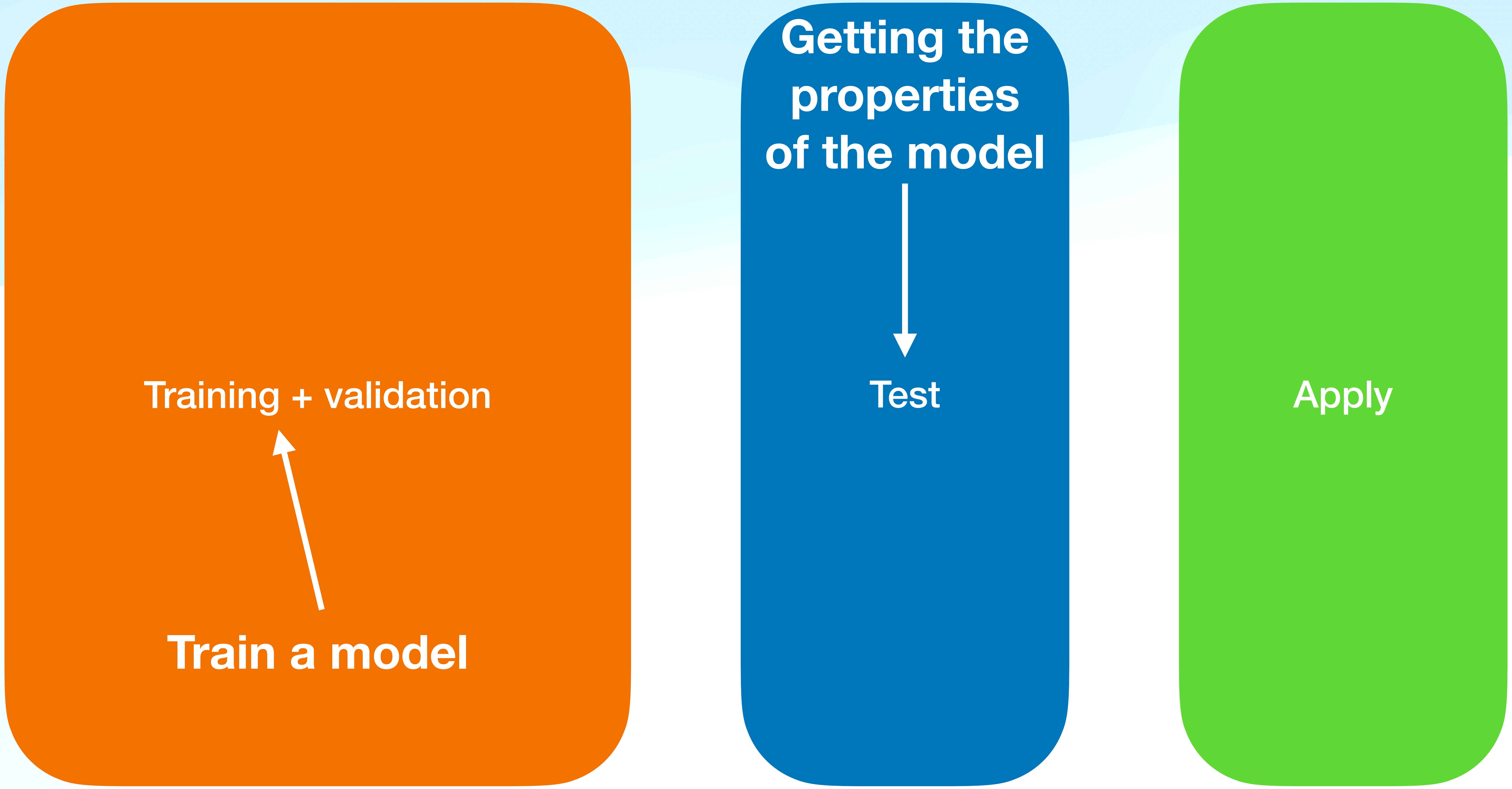

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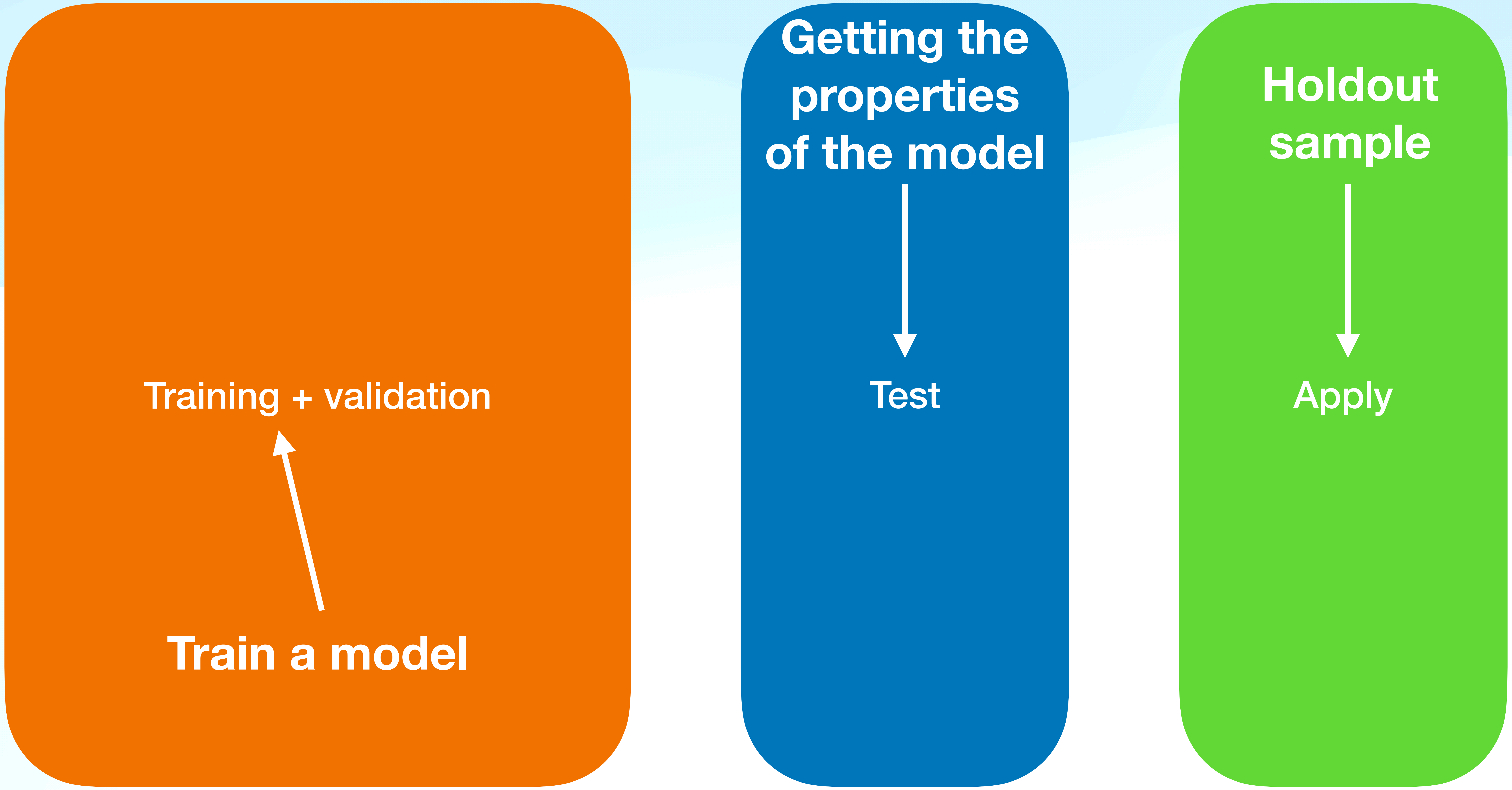

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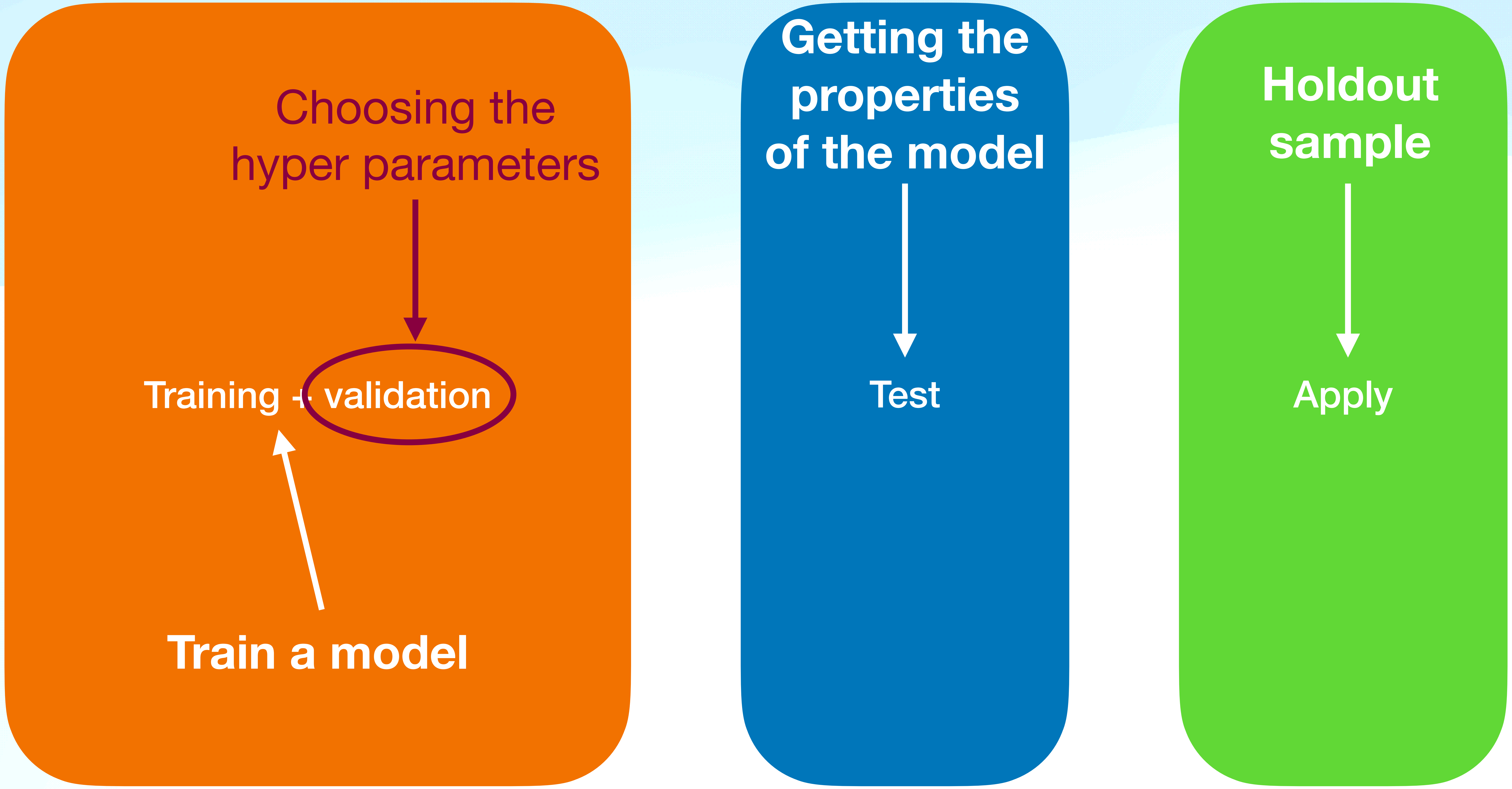

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    - AUC
    - Other metrics (precision, recall, specificity, etc.)

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- Successive halving allows us to allocate more and more resources to the models that are working best

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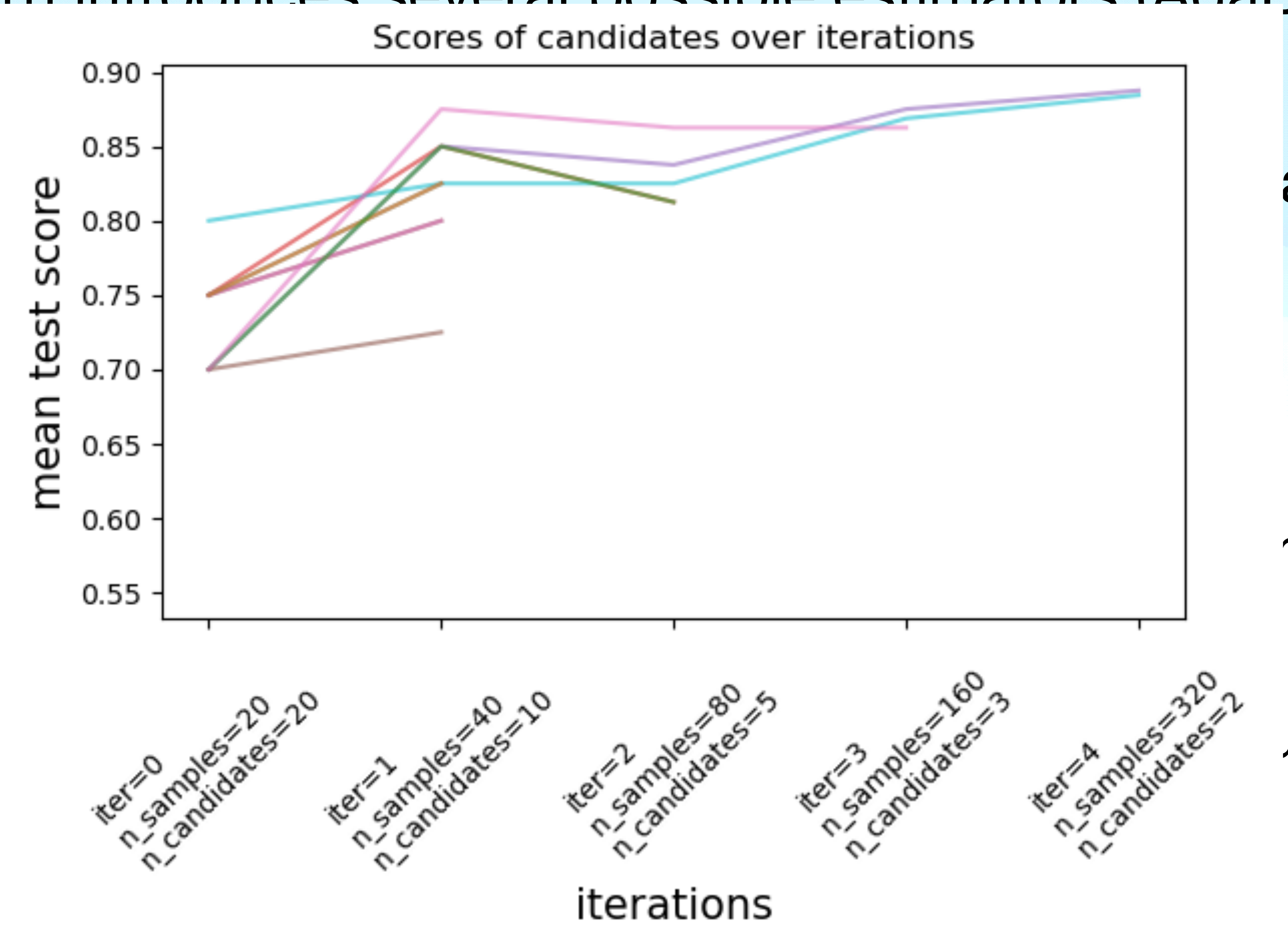

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$$q = \min\left(2 \times n_c \times k \times f^i,\, n\right);\ f = 3 \text{ (default)}$$

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- Notice: In the end, N doesn't really matter for random halving

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$$i = 0$$

$$N = 17, \quad q = 100$$

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$i = 2$ | $N = 2, \quad q = 900$

HalvingRandomSearchCV

sklearn.model_selection.HalvingRandomSearchCV

class `sklearn.model_selection.`**`HalvingRandomSearchCV`**(*estimator, param_distributions, *, n_candidates='exhaust', factor=3, resource='n_samples', max_resources='auto', min_resources='smallest', aggressive_elimination=False, cv=5, scoring=None, refit=True, error_score=nan, return_train_score=True, random_state=None, n_jobs=None, verbose=0*) ¶ [source]

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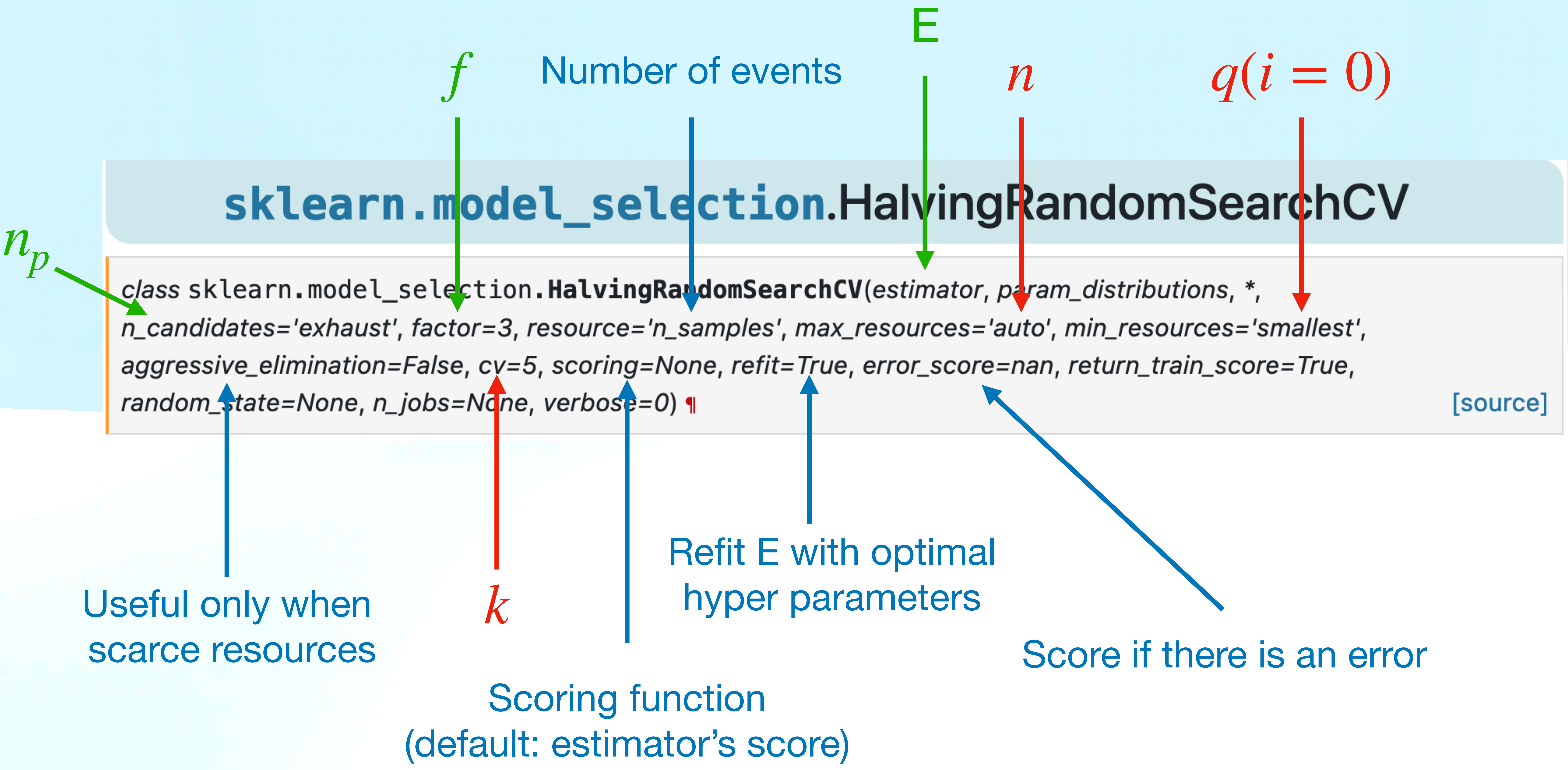

HalvingRandomSearchCV

f

Number of events

E

n

$q(i = 0)$

n_p

sklearn.model_selection.HalvingRandomSearchCV

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Useful only when scarce resources

k

Scoring function (default: estimator's score)

Refit E with optimal hyper parameters

Score if there is an error

Practical examples

- Two simple examples on sklearn's digits dataset:

https://github.com/miguel-fernandez/comcha23/blob/main/halving.py

https://github.com/miguel-fernandez/comcha23/blob/main/halving2.py

Optuna

- Optuna is a more generic approach to the search of hyper parameters
- It can also implement successive halving inside
- General concept:
  - Define a function to maximize or minimise (e.g., the accuracy)
  - Define a hyper parameter space (can be even more generic than in sklearn)
  - Do random approaches, exploiting the areas where the function looks more promising

Optuna’s language

- Every hyperparameter search is called a *study*
- We define an *objective function* to minimize/maximize
- Each study is comprised of several *tries*
  - Each try is a random sampling on the hyperparameter space
  - A hyperparameter combination is chosen
  - The objective function outputs a value, which optuna uses to learn in subsequent trials

Optuna example

- Basic example:

  https://github.com/miguel-fernandez/comcha23/blob/main/optuna_test.py

- Challenge:
  - Implement halving2.py on optuna

Backup

Some minor gripes with sklearn…

- No easy implementation of a holdout sample (very easy to train-test split)
- No easy implementation of spectator variables

- This, combined with the desire to create easier access to Hyperparameter fine-tuning led me to putting together a still-in-development package:

https://github.com/miguel-fernandez/hep-mva