METIS

Validation And Testing: Selecting Models And Estimating Their Quality

LEARNING GOALS

1. Understand the importance of estimating model generalization error (testing) and practical methodologies for doing so
2. Learn validation/cross-validation strategies for model selection
3. Recognize the difference between validation and testing

Testing: Estimating Generalization Error

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TESTING

Generalization Error: How well can we expect a model to perform on new data from the same distribution as the training data?

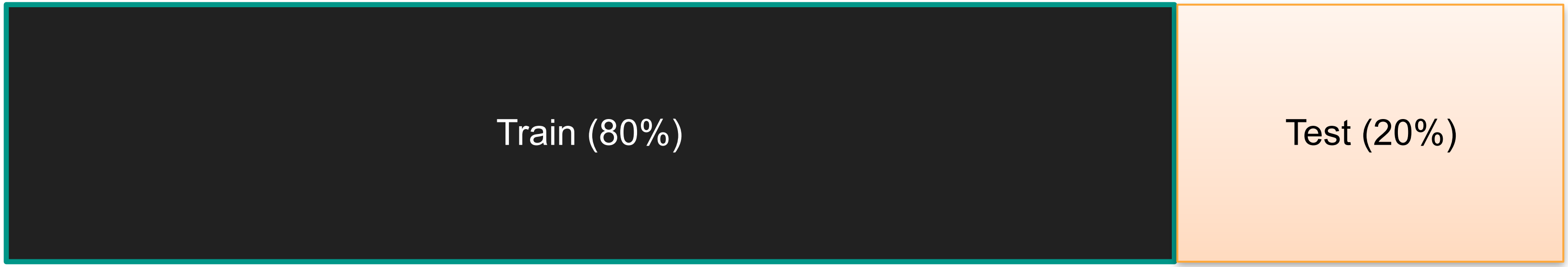
- Predictive models are only *useful* if they can give us good target approximations for samples that we haven't seen before
- <u>Example</u>: Zillow predicts the market value of a home before it's listed for sale, training a model on known listing prices
- So when evaluating models, we should attempt to measure how well they *generalize,* i.e. estimate performance on samples we didn't train on. We call this **testing**.

TESTING, IN PRACTICE

Simulate generalization: We can *hold out* a portion of our labeled dataset to simulate the real-world challenge of unseen samples

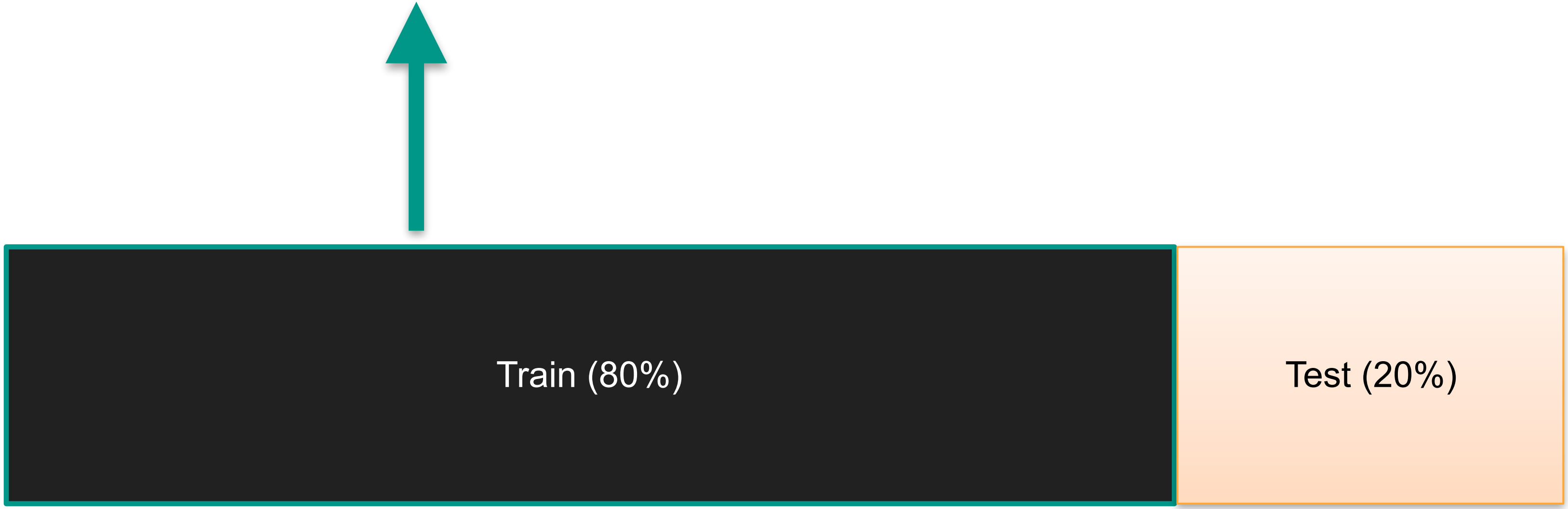
We call this a **test set**, and exclude it from the data we train on

We then *estimate generalization error* by making predictions on test, and scoring those predictions against the ground truth (our test labels)



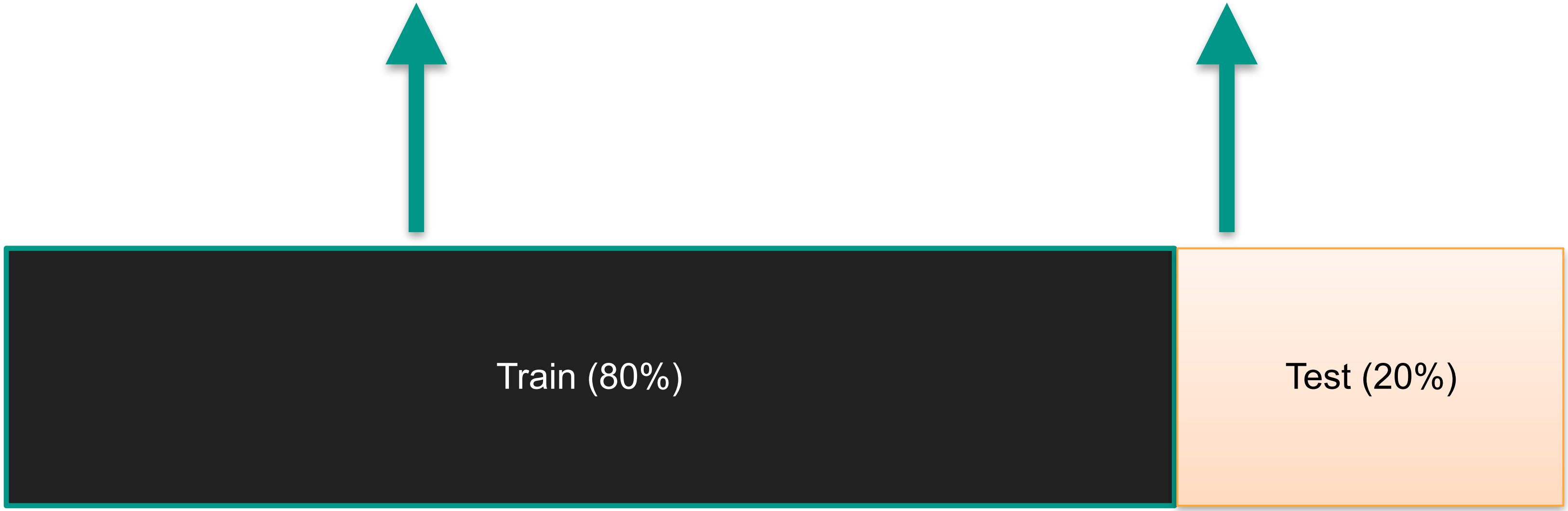
TESTING, IN PRACTICE; cont.

1. Fit model to training data



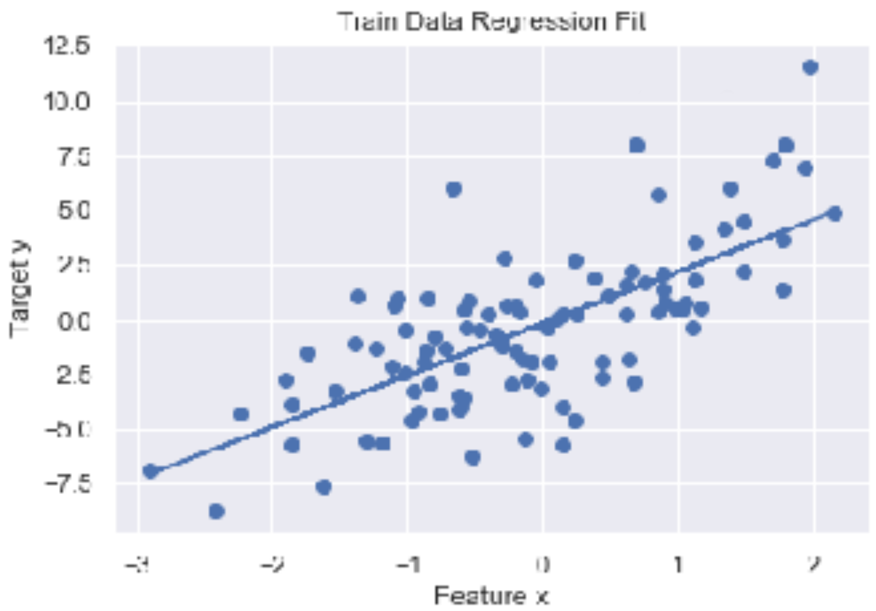
TESTING, IN PRACTICE; cont.

1. Fit model to training data
2. Score model on testing data

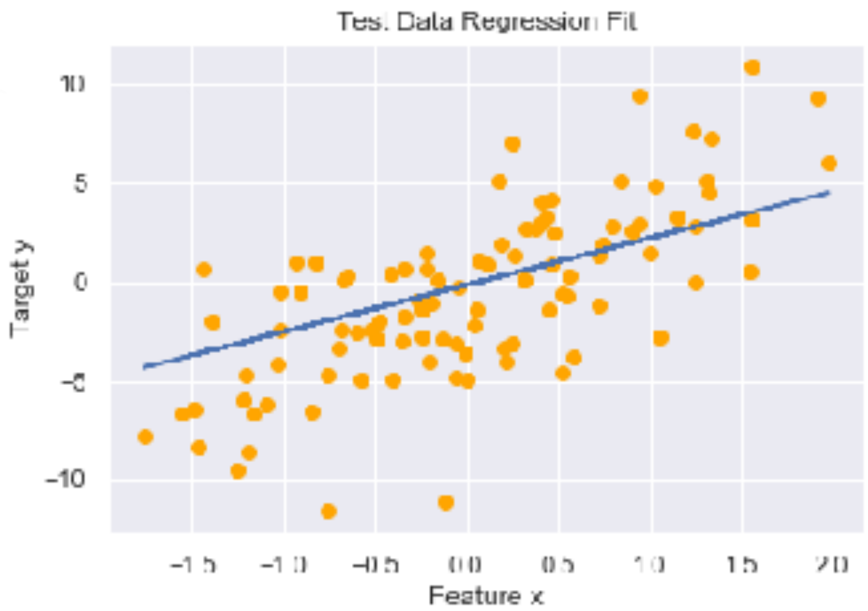


TEST USUALLY UNDERPERFORMS TRAIN

Model is optimized to perform as well as possible on train, so it’s no surprise that it tends to have a worse evaluation score on test (though this is not guaranteed).



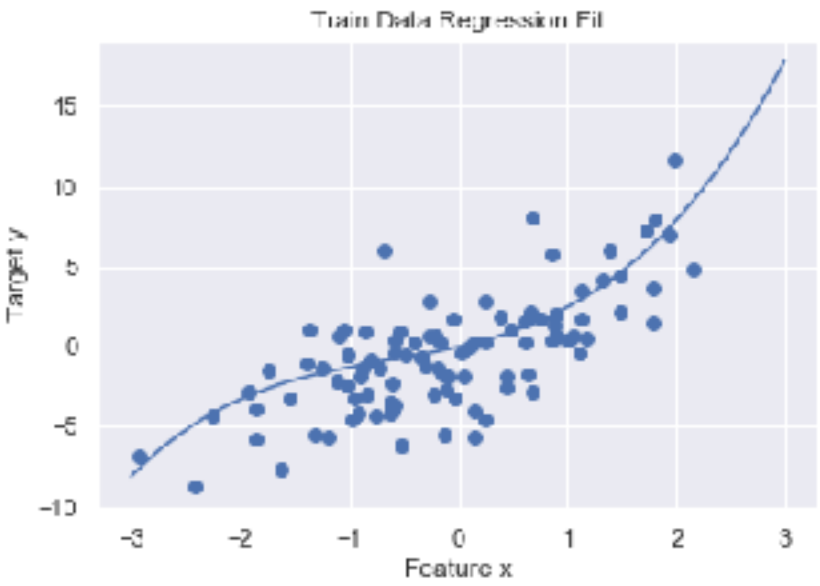
$\rightarrow$ R^2: .49



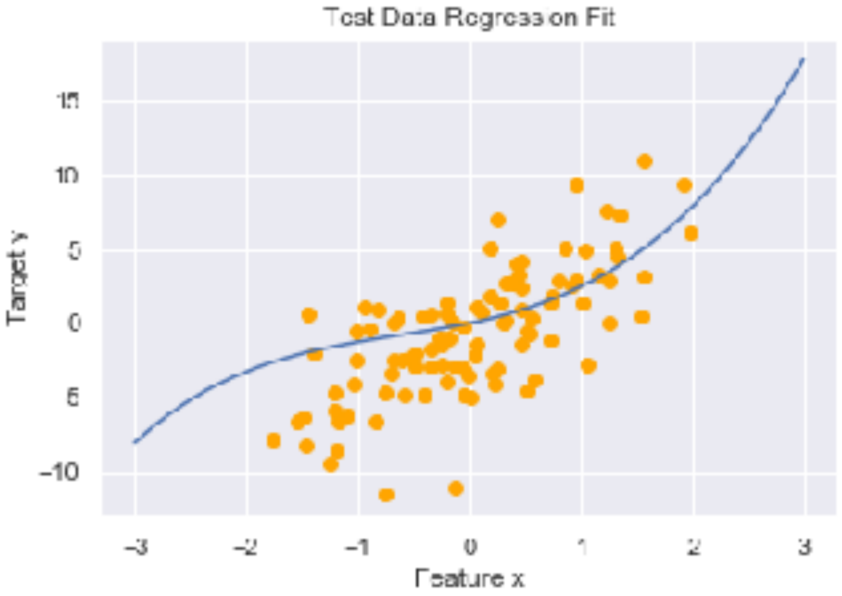
$\rightarrow$ R^2: .43

THE RISK OF OVERFITTING

Out of sample evaluations let us check for overfitting: more complex models can get arbitrarily better at predicting the train data, but will start to fit to spurious patterns and generalize more poorly



Degree 4 R^2: .54



Degree 4 R^2: .42

Validation: Optimizing Our Modeling Choices

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VALIDATION: OPTIMIZING CHOICES

When we construct predictive models, we typically have **many choices**:

- Features: which data columns do we include/exclude or engineer?
- Preprocessing: how should we handle nulls? Should we standardized the scale of the features?
- Hyper-parameters: What degree polynomial regression should we fit? What regularization strength should we use? How does a random forest model compare to a linear regression model?

VALIDATION IN PRACTICE

We can make some choices using our domain knowledge and good instincts, but a **validation framework** gives us an empirical way to choose and avoid over/under-fitting

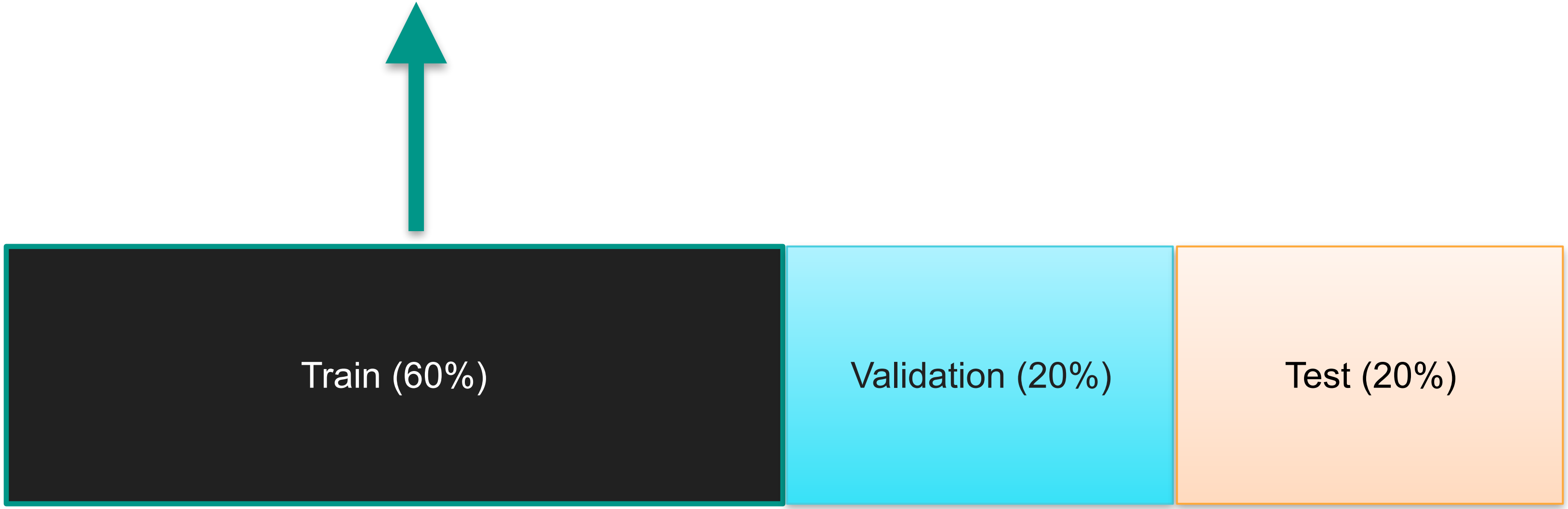
We validate with the usual *best generalization* end-goal in mind: we exclude validation data from training, and use it to <u>score predictions across a range of model choices</u>

We can then *select* a choice of model based on the strongest validation score - i.e., this score gives us **direct feedback on a possible choice**. Once we've chosen a model, we can combine our train and validation sets, retrain the model, and get the test score

VALIDATION IN PRACTICE; cont.

1. Train candidate models

- Linear Regression
- Polynomial Regression
- Ridge Regression



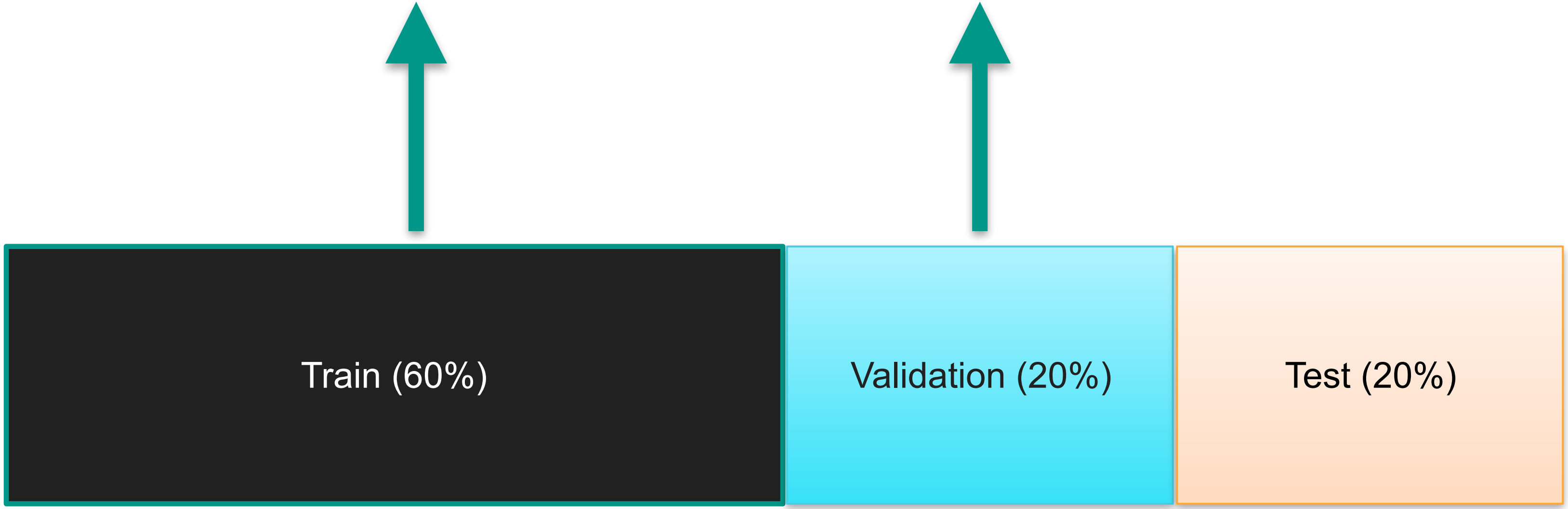
VALIDATION IN PRACTICE; cont.

1. Train candidate models

- Linear Regression
- Polynomial Regression
- Ridge Regression

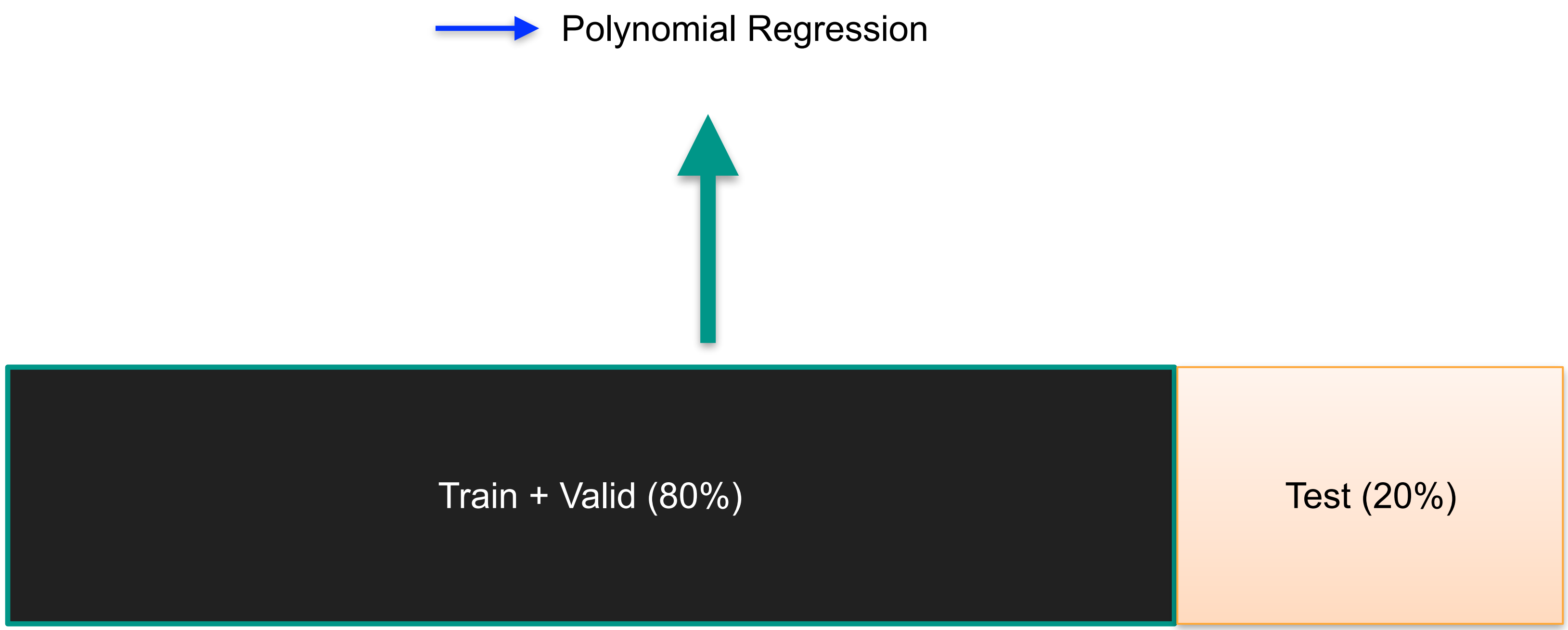
2. Score candidates

- R^2: .35
- $\boxed{R^2\text{: .50}}$
- R^2: .25



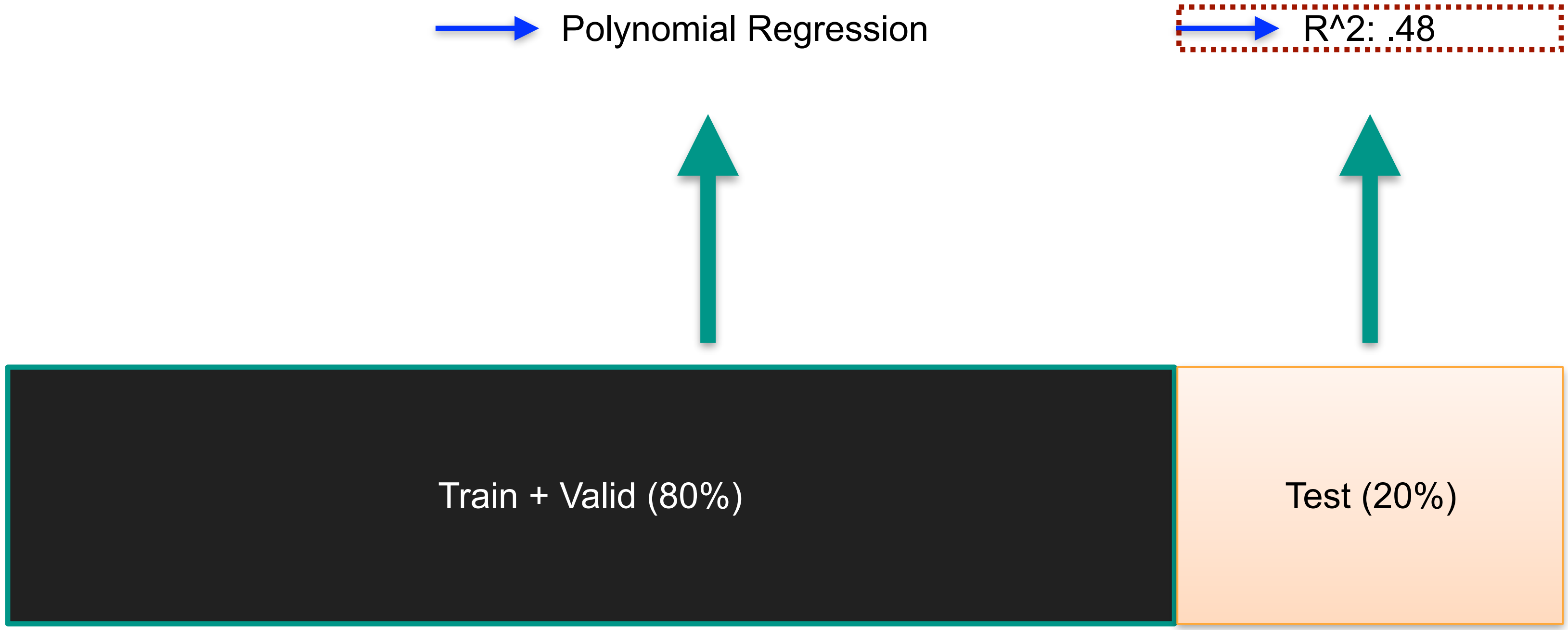
VALIDATION IN PRACTICE; cont.

3. Retrain best candidate on train + validation



VALIDATION IN PRACTICE; cont.

4. Score final model on test



VALIDATION: KEY CONSIDERATIONS

Validation is not testing: This is a very common pitfall. Once you've used a data set to influence your model choices through direct feedback, it can't be used to give an unbiased estimate of generalization error

Fair comparisons: Candidate models should be compared against the same validation scheme

Data efficiency: after we use a portion of our data for validation, we should reuse it as training data to improve the final model

Cross Validation: Optimizing Our Optimization Of Choices

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CROSS VALIDATION: ADDING MORE RIGOR

Cross-validation is about reliability and efficiency: what if we overfit to an unlucky validation set? Can we use more of our data than just one hold-out for validation?

K-Fold partitioning: randomly divide our non-test data into *K* equal-sized groups. Each group will be used as a validation set once, and we'll compare candidate models via mean scores across all validation scores.

K is usually 5 or 10: depends on problem and size of data, but these are common choices

CROSS VALIDATION IN PRACTICE

Train data: divided into 5 folds

Do the following, <u>for each candidate model</u>

Test, held out

CROSS VALIDATION IN PRACTICE

Train data:
divided into
5 folds

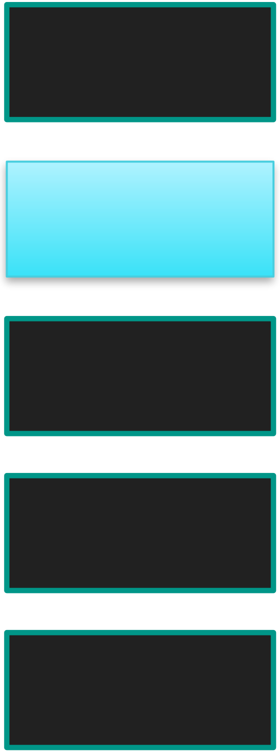
Train on
black folds

Validate on
cyan fold

Validation R^2 scores: .45,

CROSS VALIDATION IN PRACTICE

Train data:
divided into
5 folds



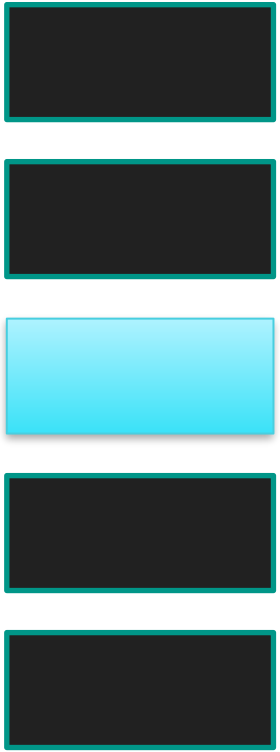
Train on
black folds

Validate on
cyan fold

Validation R^2 scores: .45, .39,

CROSS VALIDATION IN PRACTICE

Train data:
divided into
5 folds



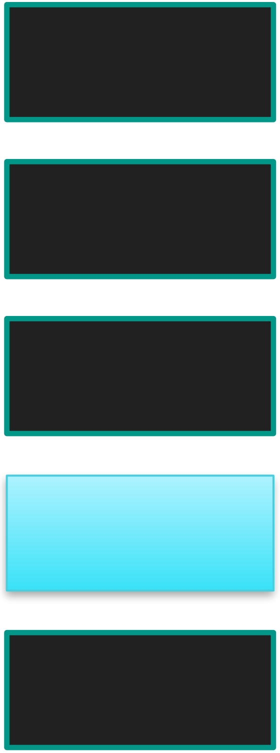
Train on
black folds

Validate on
cyan fold

Validation R^2 scores: .45, .39, .57,

CROSS VALIDATION IN PRACTICE

Train data:
divided into
5 folds



Train on
black folds

Validate on
cyan fold

Validation R^2 scores: .45, .39, .57, .49,

CROSS VALIDATION IN PRACTICE

Train data:
divided into
5 folds

Train on
black folds

Validate on
cyan fold

Validation R^2 scores: .45, .39, .57, .49, .50

CROSS VALIDATION IN PRACTICE

Train data: divided into 5 folds

Produces a set of results for each candidate model

Linear regression

Validation R^2 scores: .45, .39, .57, .49, .50

Poly regression

Validation R^2 scores: .53, .43, .67, .55, .51

CROSS VALIDATION IN PRACTICE

Train data:
divided into
5 folds

Summarize candidates by mean score, select best

Linear regression

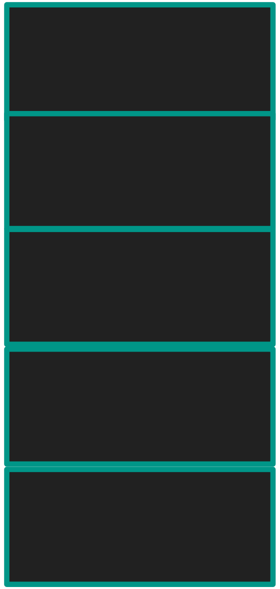
5-Fold validation mean R^2 score: .48

Poly regression

5-Fold validation mean R^2 score: .54

CROSS VALIDATION IN PRACTICE

Train data: recombined



Polynomial regression selected as best candidate model

Test, held out

Poly regression, retrained on all data, final score on test

→ R^2: .48

Validation And Testing: Recap

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WORKFLOW METHOD 1: Train/Valid/Test

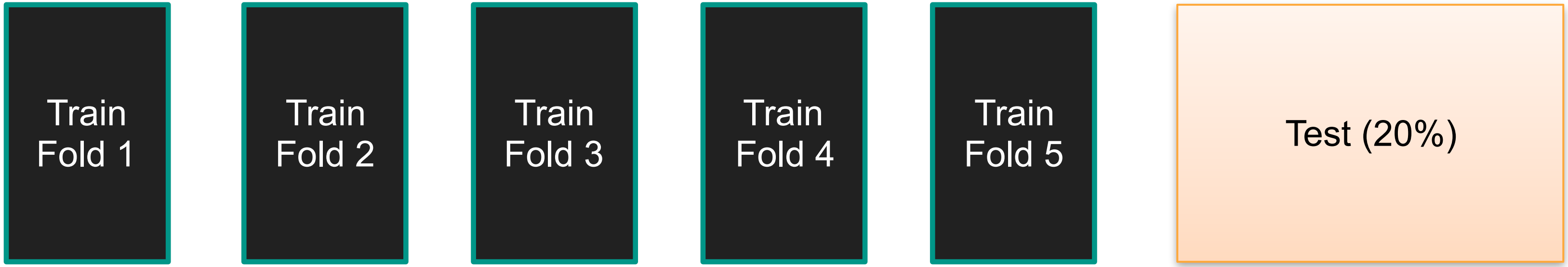
Collect set of candidate models. Fit each on train, score on validation, select final model via best validation score

Retrain final model on train + validation, report score on test as estimate of generalization error

WORKFLOW METHOD 2: CV/Test

Collect set of candidate models. Run each through a K-fold CV loop, select final model via best mean validation score

Retrain final model on combined folds, report score on test as estimate of generalization error



VALIDATION VS. CV - WHEN TO USE?

Simple validation is significantly faster and often representative enough when working with very large samples (~millions+)

Cross validation is more appropriate with small-medium size data or when variance in results between different validation sets is high

CAN WE PUSH EVEN FURTHER?

There's nothing stopping us from doing **repeated rounds of CV** with different random K-folds for even more rigor

- Also an alternate form of testing: run CV on all data to select, then run another K-Fold loop to get multiple/mean out of sample scores

We usually take means across validation folds in CV to compare model candidates, but we can also gain information from **distributions of scores across folds** (e.g. variance)

Nested CV is another advanced technique for a more robust combination of CV and testing: see here for detail.

WHAT ABOUT TIME SERIES DATA?

For certain data (e.g. data with a time series component), a more specialized validation and testing setup may be called for

In **time-based validation**, validation/testing data should chronologically follow training data: this simulates the model's **generalization into the future**

Example: when using historical stock market data to predict future returns, try to make sure that past patterns continue to be predictive in the future

SUMMARY

Training	Validation	Testing
In sample	Out of sample	Out of sample
Model building	Feedback to model selection	No feedback to model selection
Optimize model parameters (fit)	Optimize choices: features and model hyper-parameters	Final estimate of model generalization error


VALIDATION SO WOW
SUCH MODEL SELECTION
VERY NOT ESTIMATE
OF GENERALIZATION ERROR
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