#### **Effective Programming Practices for Economists**

## **Data Analysis in Python**

Cross-validation and hyperparameters in scikit-learn

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### The bias-variance trade-off

- For prediction, want to be as close to the values to be predicted as possible
- Very simple models, e.g. just an intercept and a couple of regressors
  - Large bias, low variance, no overfitting
- Very large models, e.g. including squares, interactions, ...
  - Small bias, high variance, danger of overfitting
- Typically, one or more parameters govern the bias variance trade-off

## **Example: Penalty in a logit model**

- Logistic regression is fit by maximizing a log likelihood function
- Can augment likelihood by a term that penalizes model complexity
- Typically, model complexity means many non-zero parameters
- Penalty is a function of the parameter vector

$$heta^* = rg \min_{ heta} \ell( heta; X, y) + \lambda \cdot p( heta)$$

### Different penalties

- lacksquare L1:  $p( heta) = \sum_i | heta_i|$ 
  - Penalizes all deviations from zero equally
  - Induces sparsity
  - Harder numerical optimization, not compatible with all optimizers
- lacksquare L2:  $p( heta) = \sum_i heta_i^2$ 
  - Penalizes values close to zero very weakly
  - Does not induce sparsity
  - Simpler numerical optimization

# Two splits are not enough

- Want to set tuning parameters optimally
- Naive approach:
  - Fit models with different parameters on training set
  - Evaluate performance on test set
  - Keep the best
- Problem: Hyperparameters are over-fit to the test set
- Use cross-validation to avoid this

#### K-fold cross validation

- Idea: Split the training data repeatedly into:
  - Data used for actual training
  - Data used for evaluation
- Repeat k times to get k scores
- Keep model that achieves best average score
- Use actual test set only once in the end to measure model quality

### **Cross-validaton**

```
>>> from sklearn.model_selection import cross_val_score
>>> scores = cross_val_score(
     LogisticRegression(max_iter=3000),
    X train.
    y_train,
     cv=5
>>> scores
array([
  0.84844291.
 0.84532872.
 0.85709343.
  0.84492904.
  0.86396677
>>> scores.mean()
0.8519521727205328
```

- Import and create instance as normal, do not call fit()
- L2 penalty is default
- Provide data to cross\_val\_score
- cv argument specifies number of folds
- cross\_val\_score Will call fit()
  repeatedly

# Systematic hyperparameter tuning

- Specify a combination of hyperparameters we want to try
- Calculate cross validation score for each set of parameters
- Keep model with best performance
- Re-fit best model on entire dataset
- Implement in GridSearchCV

#### **Grid Search**

```
>>> from sklearn.model_selection import GridSearchCV
>>> param_grid = {
... "penalty": ["12", "11"],
... "C": [0.1, 1, 10],
>>> grid = GridSearchCV(
    LogisticRegression(solver="liblinear"),
    param_grid,
\cdots cv=5.
>>> grid.fit(X_train, y_train)
>>> grid.best_params_
{'C': 10, 'penalty': 'l1'}
>>> grid.best_estimator_.score(
    X test.
     y_test
0.8430232558139535
```

- param\_grid keys are names of arguments of LogisticRegression
- param\_grid values are lists of possible values for the arguments
- Setting up the grid does not fit models yet
- grid.fit() takes some time and often produces warnings