

Solution 1:

1) Interpretation of the generalization error  $\text{GE}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}}, \rho)$

- $\text{GE}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}}, \rho)$  is the *expected future performance* of learner  $\mathcal{I}$  with configuration  $\boldsymbol{\lambda}$  trained on  $n_{\text{train}}$  observations and evaluated with performance measure  $\rho$ .
- In  $\text{GE}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}}, \rho) = \lim_{n_{\text{test}} \rightarrow \infty} \mathbb{E}_{\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{test}} \sim \mathbb{P}_{xy}} [\rho(\mathbf{y}, \mathbf{F}_{\mathcal{D}_{\text{test}}, \mathcal{I}(\mathcal{D}_{\text{train}}, \boldsymbol{\lambda})})]$ , the randomness comes from repeatedly sampling train and test sets  $\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{test}}$  from  $\mathbb{P}_{xy}$ .
- For each draw:
  - We train a model  $\mathcal{I}(\mathcal{D}_{\text{train}}, \boldsymbol{\lambda})$  on  $\mathcal{D}_{\text{train}}$ .
  - We evaluate its performance  $\rho(\mathbf{y}, \mathbf{F}_{\mathcal{D}_{\text{test}}, \mathcal{I}(\mathcal{D}_{\text{train}}, \boldsymbol{\lambda})})$  on an independent test set  $\mathcal{D}_{\text{test}}$ .
- Taking the expectation over all such draws and the limit  $n_{\text{test}} \rightarrow \infty$  removes randomness from the particular test set and yields the true expected performance of the learner for training size  $n_{\text{train}}$ .

2) Empirical estimation of  $\text{GE}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}} = 100, \rho)$  when we can sample from  $\mathbb{P}_{xy}$

- Repeat the following for  $k = 1, \dots, K$ :
  - Draw a training set  $\mathcal{D}_{\text{train}, k}$  of size  $n_{\text{train}} = 100$  from  $\mathbb{P}_{xy}$ .
  - Draw an independent test set  $\mathcal{D}_{\text{test}, k}$  of size  $n_{\text{test}}$  (large) from  $\mathbb{P}_{xy}$ .
  - Train the learner:  $\hat{f}^{[k]} = \mathcal{I}(\mathcal{D}_{\text{train}, k}, \boldsymbol{\lambda})$ .
  - Compute the performance on the test set:  $\rho(\mathbf{y}_{J_{\text{test}, k}}, \mathbf{F}_{J_{\text{test}, k}, \mathcal{I}(\mathcal{D}_{\text{train}, k}, \boldsymbol{\lambda})})$ .
- Average  $K$  values:  $\widehat{\text{GE}}_K(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}} = 100, \rho) = \frac{1}{K} \sum_{k=1}^K \rho(\mathbf{y}_{J_{\text{test}, k}}, \mathbf{F}_{J_{\text{test}, k}, \mathcal{I}(\mathcal{D}_{\text{train}, k}, \boldsymbol{\lambda})})$ .
- For  $K, n_{\text{test}} \rightarrow \infty$ , the estimator converges to the theoretical quantity  $\text{GE}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}} = 100, \rho)$ .

3) Effect of training size  $|J_{\text{train}}|$  on the bias of the hold-out estimator

- In practice we only have a fixed data set  $\mathcal{D}$  of size  $n$ . The target we care about is the generalization error of a learner trained on *all* available data, i.e.:

$$\text{GE}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}}, \rho) = \text{GE}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}} = n, \rho),$$

- Hold-out splitting uses only a subset  $\mathcal{D}_{\text{train}}$  of size  $|J_{\text{train}}| < n$  for training and a disjoint subset  $\mathcal{D}_{\text{test}}$  for testing. The empirical estimator is  $\widehat{\text{GE}}(\mathcal{I}, \boldsymbol{\lambda}, (J_{\text{train}}, J_{\text{test}}), \rho) = \rho(\mathbf{y}_{J_{\text{test}}}, \mathbf{F}_{J_{\text{test}}, \mathcal{I}(\mathcal{D}_{\text{train}}, \boldsymbol{\lambda})})$ .
- Because models trained on fewer points are typically worse on average than models trained on all  $n$  points, the estimator is *pessimistically biased*:

$$\mathbb{E}_{(J_{\text{train}}, J_{\text{test}})} [\widehat{\text{GE}}(\mathcal{I}, \boldsymbol{\lambda}, (J_{\text{train}}, J_{\text{test}}), \rho)] \geq \text{GE}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}}, \rho).$$

- For regression tasks with loss-based measures such as MSE or MAE, this inequality means we systematically *overestimate* the true expected loss of a model trained on all  $n$  observations.

4) Effect of training size  $|J_{\text{train}}|$  on the variance of the hold-out estimator

- We have the constraint  $|J_{\text{train}}| + |J_{\text{test}}| = n$ .
- **Large** training size  $|J_{\text{train}}|$ :
  - $|J_{\text{test}}|$  is small  $\Rightarrow \rho(\cdot)$  is computed on few test observations.
  - The estimator  $\widehat{\text{GE}}(\mathcal{I}, \boldsymbol{\lambda}, (J_{\text{train}}, J_{\text{test}}), \rho)$  has *high variance* across different splits.
- **Small** training size  $|J_{\text{train}}|$ :
  - $|J_{\text{test}}|$  is large  $\Rightarrow$  variance due to the test set is reduced.
  - But the model is trained on few data points, which increases pessimistic bias as in (3).
- There is a *trade-off* between bias and variance when choosing  $|J_{\text{train}}|$ : larger  $|J_{\text{train}}|$  decreases bias but increases variance; smaller  $|J_{\text{train}}|$  decreases variance but increases bias.