

# Mini-course Machine Learning in Empirical Economic Research

## Lecture 2: Introduction to supervised learning

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## Supervised learning

- outcome  $y$ , regressors/features  $x$
- $f(x)$  prediction of  $y$  using prediction rule  $f$
- loss function  $L(y, f(x))$
- quadratic loss

$$L(y, f(x)) = (y - f(x))^2$$

- function class  $\mathcal{F}$  of possible  $f$
- subclasses  $\mathcal{F}_\lambda \subset \mathcal{F}$
- $\lambda =$  tuning parameter

# Machine learning as data-driven model selection

## “Traditional” econometrics

- specify  $\mathcal{F}$
- $\mathcal{F}$  is typically very “small”
- fit “best”  $f \in \mathcal{F}$

## Machine Learning

- specify  $\mathcal{F}$  and  $\lambda \mapsto \mathcal{F}_\lambda$
- $\mathcal{F}$  is typically “large”
- use data to determine a “good”  $\hat{\lambda}$
- typically  $\mathcal{F}_{\hat{\lambda}}$  is “small” or at least well-behaved
- fit “best”  $f \in \mathcal{F}_{\hat{\lambda}}$

## Fitting $f \in \mathcal{F}_\lambda$

- training data  $\mathcal{T} = \{(y_i, x'_i)\}_{i=1}^n$
- *training error* = average loss on  $\mathcal{T}$

$$\overline{\text{err}}(f) = \frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i))$$

- fit  $f$  with minimal training error

$$\hat{f} = \hat{f}^\lambda = \arg \min_{f \in \mathcal{F}^\lambda} \overline{\text{err}}(f)$$

- conceptually this is the same as what we do in econometrics!
  - ▶ what loss functions do we use in econometrics?
  - ▶ how do we call the fitted training error?
  - ▶ estimation as constrained optimization?

## Intuition for $\lambda$

- assume  $\lambda \in \mathbb{R}$
- often  $\lambda$  performs *regularization*
- let  $\mathcal{C}(f)$  measure “complexity” of  $f$

$$\mathcal{F}_\lambda(f) = \{f \in \mathcal{F} : \mathcal{C}(f) \leq \lambda\}$$

- example: fitting a smooth curve over an interval

$$\mathcal{C}(f) = \int_{x \in [a,b]} |f''(x)|^2 dx$$

- implies nesting of classes: for  $\lambda_1 \leq \lambda_2 \leq \dots$

$$\mathcal{F}_{\lambda_1} \subset \mathcal{F}_{\lambda_2} \subset \dots$$

## Choice of $\lambda$ = trade-off

### small $\lambda$

- small  $\mathcal{F}_\lambda$
- consisting of “simple” models
- potentially poor approximation (high bias)
- easy to estimate (low variance)
- we order models according to the “Occam’s razor” principle

### large $\lambda$

- large  $\mathcal{F}_\lambda$
- consisting of “complex” models
- potentially better approximation (low bias)
- hard to estimate (high variance)

## Determining $\hat{\lambda}$

- our objective = prediction
- good  $\lambda$  leads to estimator with good predictive properties
- $\mathbb{E}_{\mathcal{T}}$  = expectation operator wrt training sample
- $E_{y,x}$  = integral wrt probability measure of a new  $(y, x')$  observation
- expected prediction error

$$EPE(\hat{f}^{\lambda}) = \mathbb{E}_{\mathcal{T}} E_{y,x} L(y, \hat{f}^{\lambda}(x))$$

## Training error does not estimate prediction error

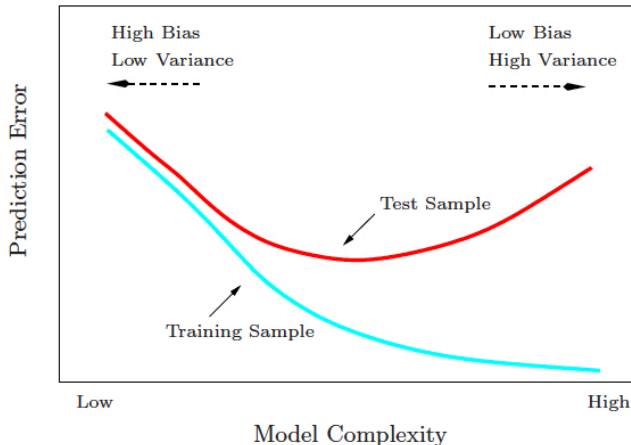


Figure: Figure 2.11 from Hastie, Tibshirani, and Friedman (2009)



# Overfitting

- $\overline{\text{err}}(f)$  is an *optimistic* estimate of prediction error
  - ▶ the training error does not account for cost of uncertainty (variance)
- minimizing training error  $\overline{\text{err}}(f)$  over all of  $\mathcal{F}$  leads to *overfitting*
- introductory econometrics courses often don't discuss overfitting, why?
- Two lessons:
  - ▶ estimation: fit  $\overline{\text{err}}(f)$  keeping  $\lambda$  fixed
  - ▶ model testing: in-sample fit (aka  $\overline{\text{err}}$  or  $R^2$ ) is not a good measurement of fit
    - even if you are interested in predictive power don't look at  $R^2$ !

## How do we validate fit in empirical economic research?

*“For many years, economists have reported in-sample goodness-of-fit measures using the excuse that we had small datasets. But now that larger datasets have become available, there is no reason not to use separate training and testing sets.” (Varian 2014)*

# Sample-splits in data-rich environments

Use independent samples for three distinct tasks:

**Training** fit  $f \in \mathcal{F}_\lambda$

- this is how we fit  $\hat{f}^\lambda$  for candidate  $\lambda$
- minimize training error

**Validation** estimate EPE for given  $\hat{f}^\lambda$

- this is how we evaluate suitability of  $\lambda$  candidates
- best candidate =  $\hat{\lambda}$

**Test** estimate predictive power of final model  $\hat{f}^{\hat{\lambda}}$

## Estimating EPE from independent validation data set

Validation data set

$$\{(y_i^*, (x_i^*)')\}_{i=1}^{n^*}$$

Estimated  $EPE$

$$\widehat{EPE}(f) = \frac{1}{n^*} \sum_{i=1}^{n^*} L(y_i, f(x_i^*))$$

- $\widehat{EPE}(\hat{f}^\lambda)$  estimates the *conditional* expected prediction error

$$EPE_{\mathcal{T}}(\hat{f}^\lambda) = E_{y,x} L(y, \hat{f}^\lambda(x))$$

## Estimating EPE using cross-validation

- validation step without need for validation data set
- $k$ -fold cross-validation (CV) based on sample split *of the training sample*
- example with  $k = 5$  folds

1	2	3	4	5
Train	Train	Validation	Train	Train

Figure: Figure from p242 of Hastie, Tibshirani, and Friedman (2009)

## $k$ -fold cross-validation

Random partition  $\{\kappa_j\}_{j=1}^k$

$$\bigcup_{j=1}^k \kappa_j = \{1, \dots, n\}$$

$\hat{f}_{-\kappa_j}^\lambda = \text{fit } f \in \mathcal{F}_\lambda \text{ on subsample}$

$$\{1, \dots, n\} \setminus \kappa_j$$

evaluate  $\hat{f}_{-\kappa_j}^\lambda$  on  $\kappa_j$

$$CV_j(\lambda) = \frac{1}{|\kappa_j|} \sum_{i \in \kappa_j} L(\hat{f}_{-\kappa_j}^\lambda(x_i), y_i)$$

## $k$ -fold cross-validation

Average over partitions

$$CV(\lambda) = \frac{1}{k} \sum_{j=1}^k CV_j(\lambda)$$

- $CV(\lambda)$  is an estimate of the *unconditional* expected prediction error

$$EPE(\hat{f}^\lambda) = \mathbb{E}_{\mathcal{T}} E_{y,x} L(\hat{f}^\lambda(x), y)$$

## Standard error of cross-validation

$$\begin{aligned} SE_{CV}(\lambda) &= \text{sample std of } \{CV_j(\lambda)\}_{j=1}^k / \sqrt{k} \\ &= \sqrt{\frac{1}{k} \sum_{j=1}^k (CV_j(\lambda) - CV(\lambda))^2} / \sqrt{k} \end{aligned}$$

- ad-hoc measure of the “sampling error” of cross-validation



## Choice of number of folds

- typically values  $k = 5, 10, n$
- $k = n$ : leave-one-out cross-validation

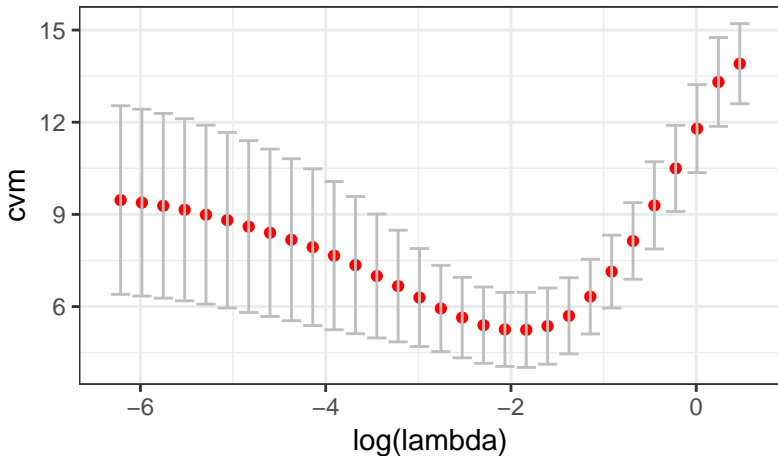
### few folds

- training step in CV uses *much less* observations than  $n$
- biased
- low variance (training sets not very similar)

### leave-one-out

- training step in CV almost  $n$  observations
- approximately unbiased
- high variance (training sets very similar)

## Example



**Figure:** Cross-validation  $CV(\lambda)$ ,  $k = 10$  folds. Here: small  $\lambda$  = complex model, large  $\lambda$  = simple model.

## Choice of $\lambda$ based on CV

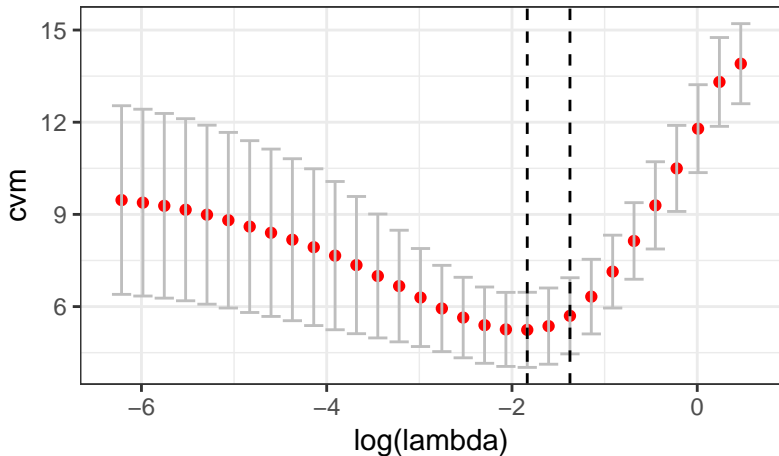
- optimize  $\lambda$  for prediction: minimal  $\lambda$

$$\hat{\lambda} = \hat{\lambda}_{\min} = \arg \min_{\lambda} CV(\lambda)$$

- suppose large  $\lambda$  = simpler model (more regularization)
- impose additional regularization: 1- $\sigma$  rule

$$\begin{aligned}\hat{\lambda} &= \hat{\lambda}_{1\sigma} \\ &= \max\{\lambda \in \mathbb{R} : CV(\lambda) \leq CV(\hat{\lambda}_{\min}) + SE_{CV}(\hat{\lambda}_{\min})\}\end{aligned}$$

## Example



**Figure:** Optimal choice of  $\lambda$ ,  $k = 10$  folds. Here: small  $\lambda$  = complex model, large  $\lambda$  = simple model.

# Applying a supervised learning method

- have to choose a *tuning parameter*  $\lambda$ 
  - ▶ regularization parameter
  - ▶ hyperparameter
- can be a vector

**Training the model**

- For given tuning parameter  $\lambda$ , fit the best model  $\hat{f}^\lambda$  using training data.
- $\hat{f}^\lambda$  is *learned*

**Hyperparameter optimization**

- choose  $\lambda$
- find the  $\lambda$  that gives  $\hat{f}^\lambda$  with the best generalization (= out-of-sample) performance
  - ▶ independent validation sample
  - ▶ cross-validation
  - ▶ other
- compute the training step many times



Figure: Source: <https://xkcd.com/1838/>