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 $\mathcal{T}$

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

- 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?
  - estimation as constrained optimization?

Intuition for λ

- assume $\lambda \in \mathbb{R}$
- often λ 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 $\lambda_1 \leq \lambda_2 \leq \cdots$

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

Choice of λ = trade-off

small λ

- small $\mathcal{F}_\lambda$
- consisting of "simple" models
- potentially poor approximation (high bias)
- easy to estimate (low variance)

large λ

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

- we order models according to the "Occam's razor" principle

Determining $\hat{\lambda}$

- our objective = prediction
- good λ 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

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

Training error does not estimate prediction error

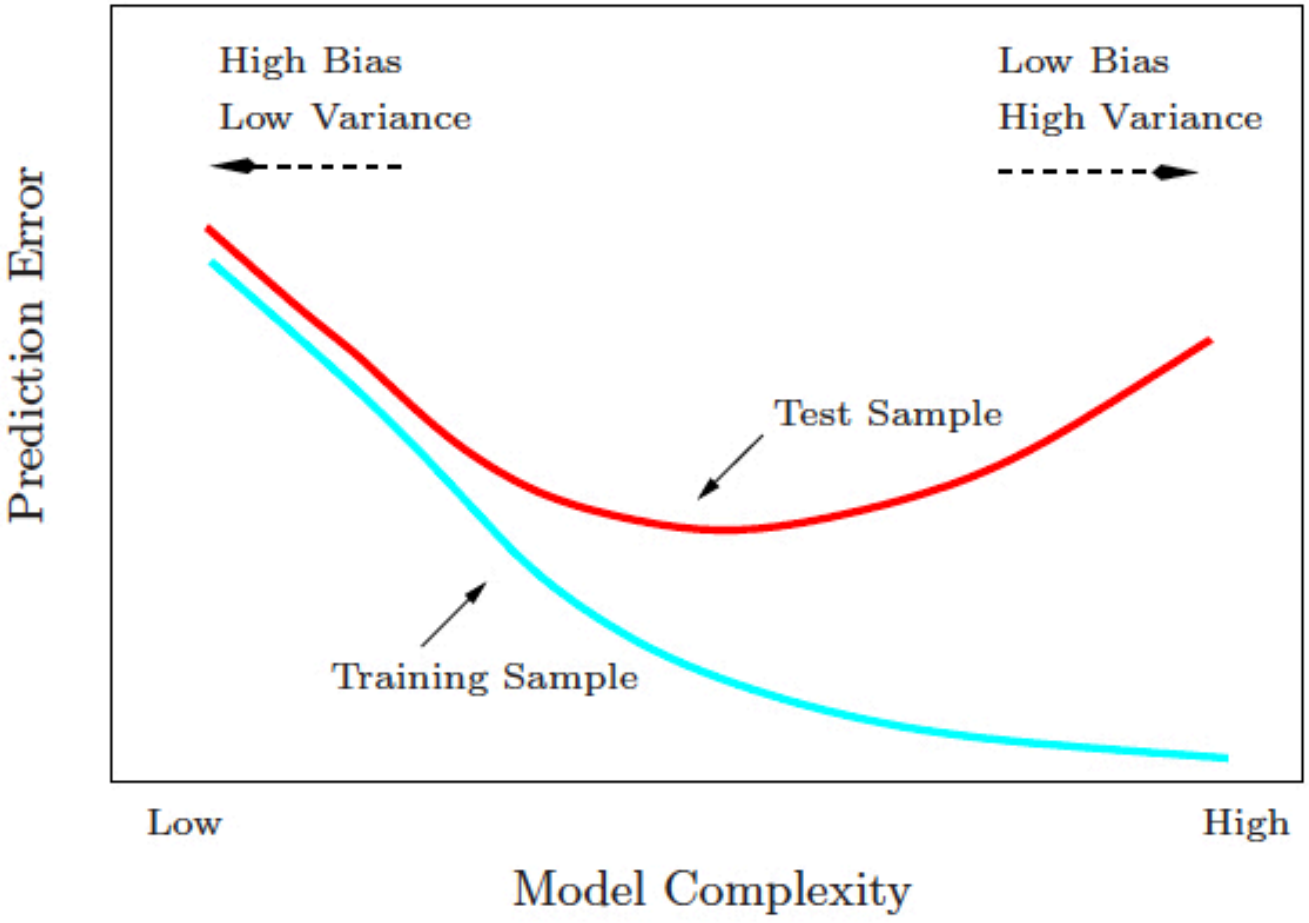

Figure: Figure 2.11 from Hastie, Tibshirani, and Friedman (2009)

Overfitting

- minimizing training error $\overline{\text{err}}(f)$ over all of $\mathcal{F}$ leads to *overfitting*
- $\overline{\text{err}}(f)$ is an *optimistic* estimate of prediction error
  - the training error does not account for cost of uncertainty (variance)

Overfitting

- minimizing training error $\overline{\text{err}}(f)$ over all of $\mathcal{F}$ leads to *overfitting*
- $\overline{\text{err}}(f)$ is an *optimistic* estimate of prediction error
  - the training error does not account for cost of uncertainty (variance)
- Two lessons:
  - estimation: fit $\overline{\text{err}}(f)$ keeping λ 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 $f \in \mathcal{F}_\lambda$

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

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*

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

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

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

Estimating EPE using cross-validation

- no need for validation data set
- k-fold cross-validation (CV) based on sample split *of the training sample*
- example with $k = 5$ folds

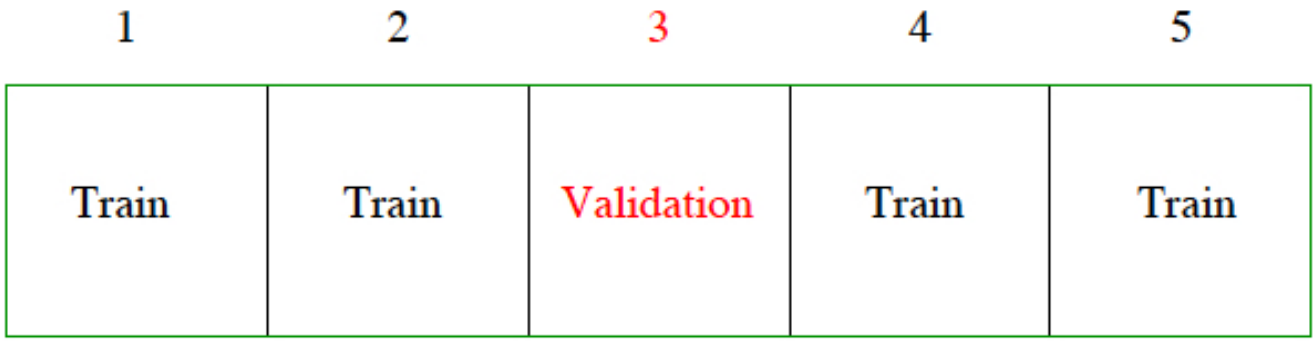

Figure: Figure from p242 of Hastie, Tibshirani, and Friedman (2009)

k-fold cross-validation

Random partition

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

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

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

evaluate $\hat{f}_{-\kappa_j}$ on κ_j

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

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

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

Standard error of cross-validation

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

- ad-hoc measure of the "sampling error" of cross-validation

Choice of number of folds

- typically values $k = 5, 10, n - 1$
- $k = n - 1$: 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

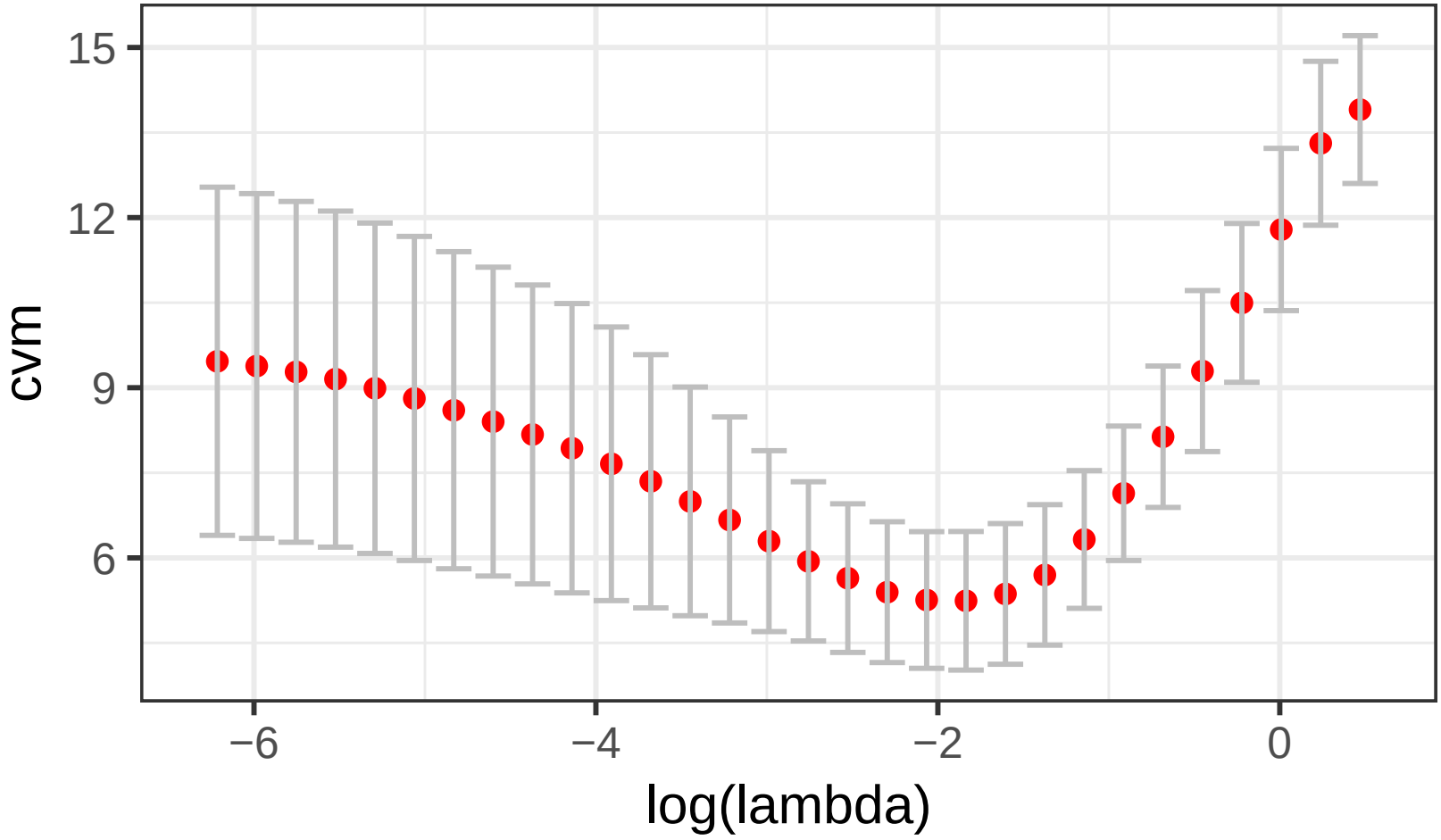

Figure: Cross-validation $CV(\lambda)$, $k = 10$ folds

Choice of λ based on CV

minimizing λ

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

- optimize λ for prediction

1-σ rule

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

- impose additional regularization

Example

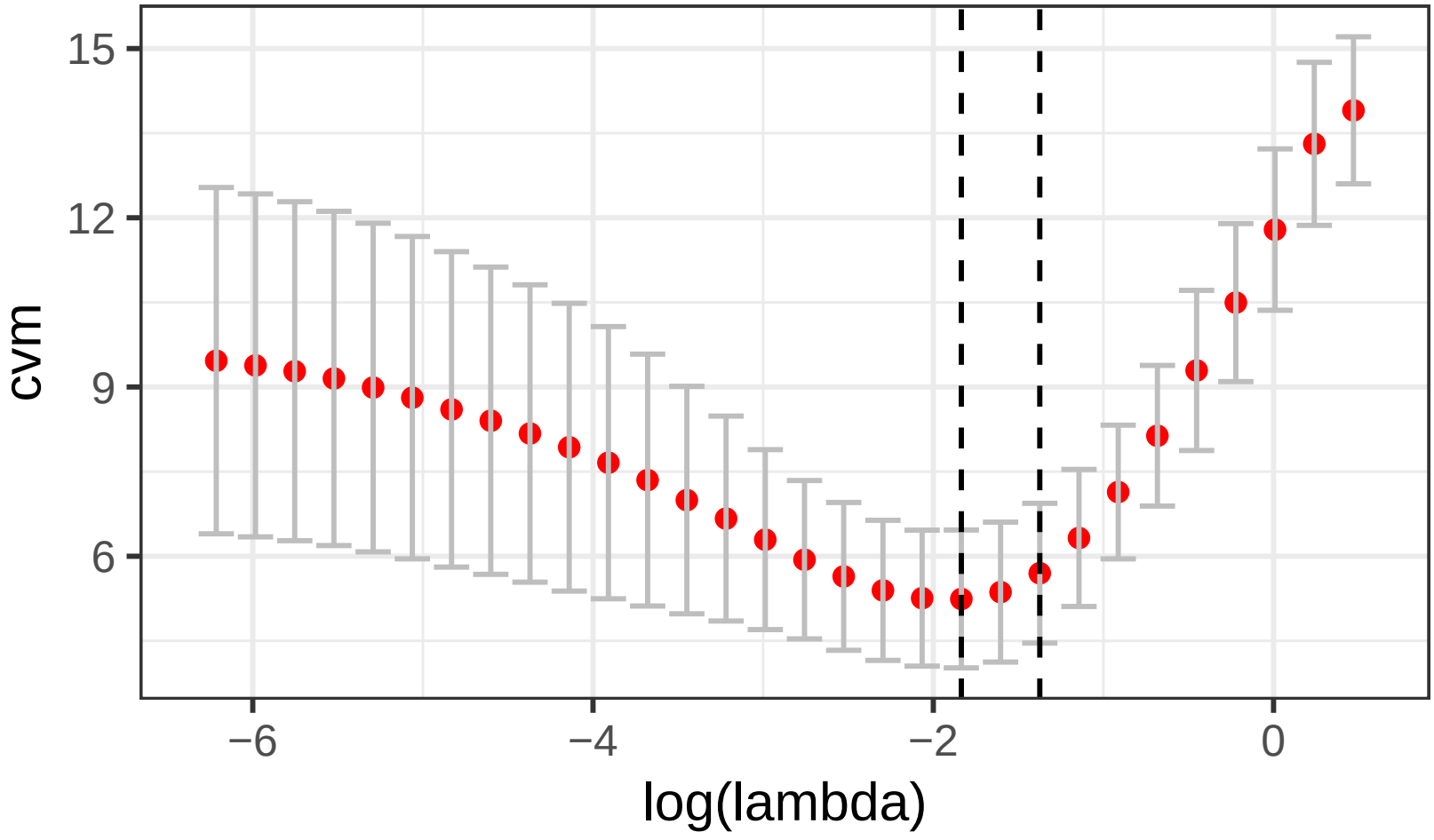

Figure: Optimal choice of λ, $k = 10$ folds