Learning From Data

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Lecture 13: Validation

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Outline

- The validation set

- Model selection

- Cross validation

Validation versus regularization

In one form or another, $$E_{\text{out}}(h) \;=\; E_{\text{in}}(h) \;+\; \text{overfit penalty}$$

Regularization:

$$E_{\text{out}}(h) \;=\; E_{\text{in}}(h) + \underbrace{\text{overfit penalty}}_{\text{regularization estimates this quantity}}$$

Validation:

$$\underbrace{E_{\text{out}}(h)}_{\text{validation estimates this quantity}} = \; E_{\text{in}}(h) \;+\; \text{overfit penalty}$$

Analyzing the estimate

On out-of-sample point $(\mathbf{x}, y)$, the error is $\quad \mathbf{e}(h(\mathbf{x}), y)$

Squared error: $\quad \big(h(\mathbf{x}) - y\big)^2$

Binary error: $\quad [\![h(\mathbf{x}) \neq y]\!]$

$$\mathbb{E}\left[\mathbf{e}(h(\mathbf{x}), y)\right] = E_{\text{out}}(h)$$

$$\text{var}\left[\mathbf{e}(h(\mathbf{x}), y)\right] = \sigma^2$$

From a point to a set

On a validation set $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_K, y_K)$, the error is $E_{\text{val}}(h) = \frac{1}{K} \sum_{k=1}^{K} \mathbf{e}(h(\mathbf{x}_k), y_k)$

$$\mathbb{E}\left[E_{\text{val}}(h)\right] = \frac{1}{K} \sum_{k=1}^{K} \mathbb{E}\left[\mathbf{e}(h(\mathbf{x}_k), y_k)\right] = E_{\text{out}}(h)$$

$$\text{var}\left[E_{\text{val}}(h)\right] = \frac{1}{K^2} \sum_{k=1}^{K} \text{var}\left[\mathbf{e}(h(\mathbf{x}_k), y_k)\right] = \frac{\sigma^2}{K}$$

$$E_{\text{val}}(h) = E_{\text{out}}(h) \pm O\left(\frac{1}{\sqrt{K}}\right)$$

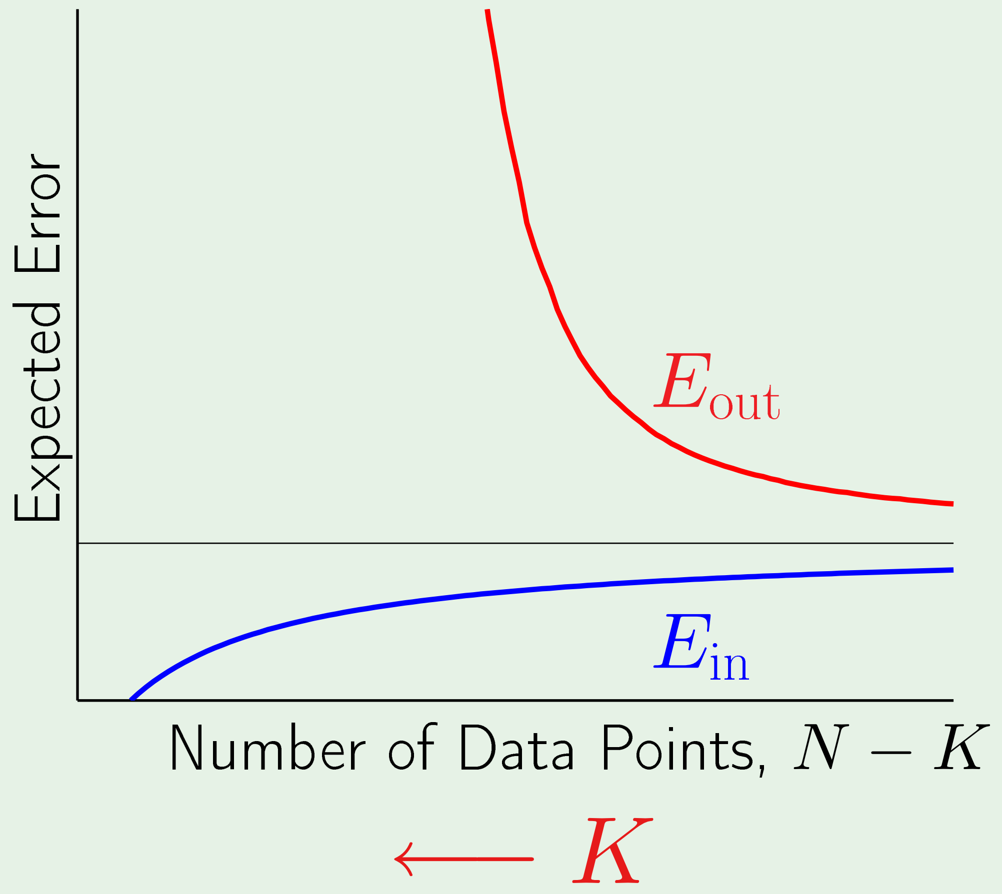
K is taken out of N

Given the data set $\mathcal{D} = (\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$

$\underbrace{K \text{ points}}_{\mathcal{D}_{\text{val}}} \rightarrow$ validation $\qquad \underbrace{N-K \text{ points}}_{\mathcal{D}_{\text{train}}} \rightarrow$ training

$O\left(\frac{1}{\sqrt{K}}\right)$: Small $K \implies$ bad estimate

Large $K \implies$?



K is put back into N

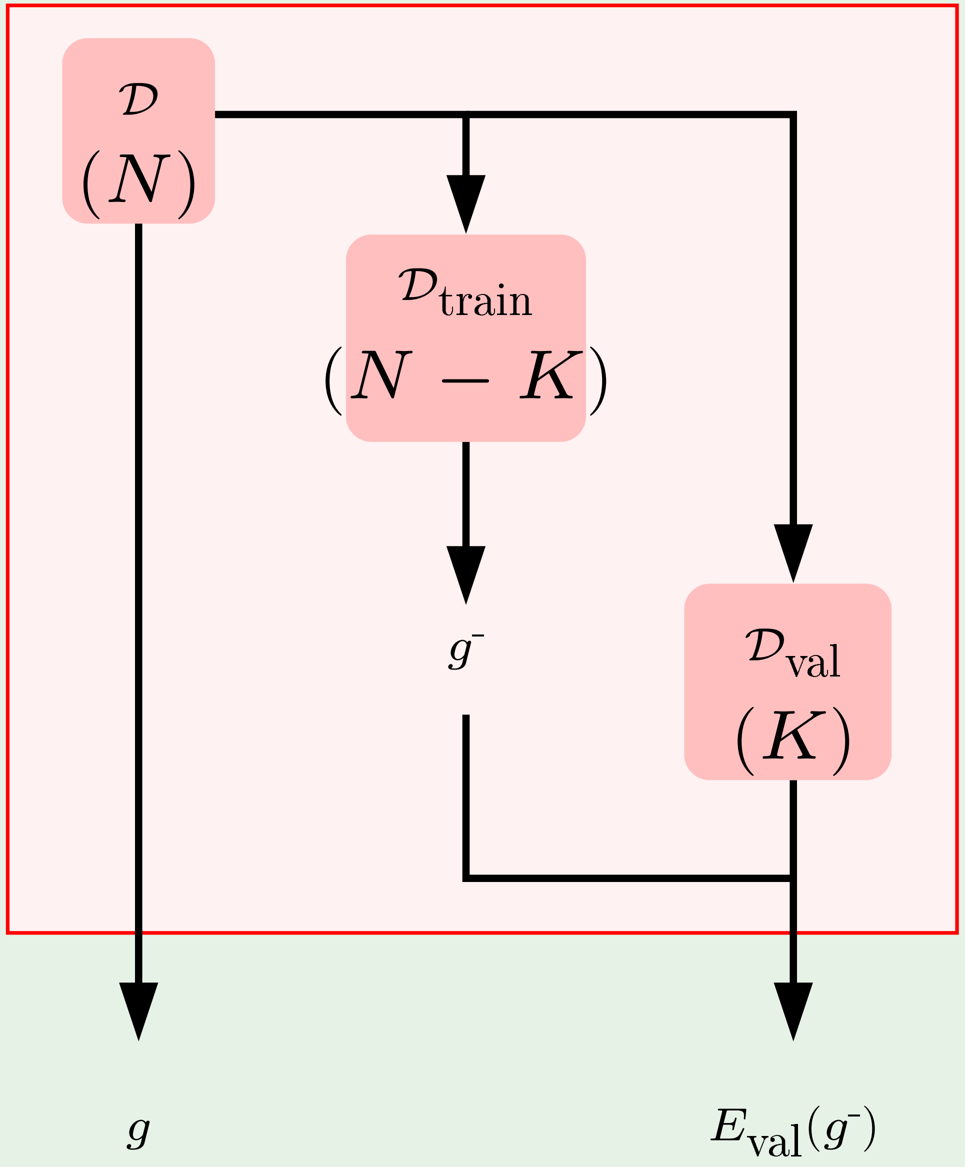
$$\begin{array}{ccc} \mathcal{D} & \longrightarrow & \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{val}} \\ \downarrow & & \downarrow \qquad \downarrow \\ N & & N-K \quad K \end{array}$$

$$\mathcal{D} \Longrightarrow g \qquad \mathcal{D}_{\text{train}} \Longrightarrow g^{-}$$

$E_{\text{val}} = E_{\text{val}}(g^{-})$ Large $K \Longrightarrow$ bad estimate!

Rule of Thumb:

$$K = \frac{N}{5}$$



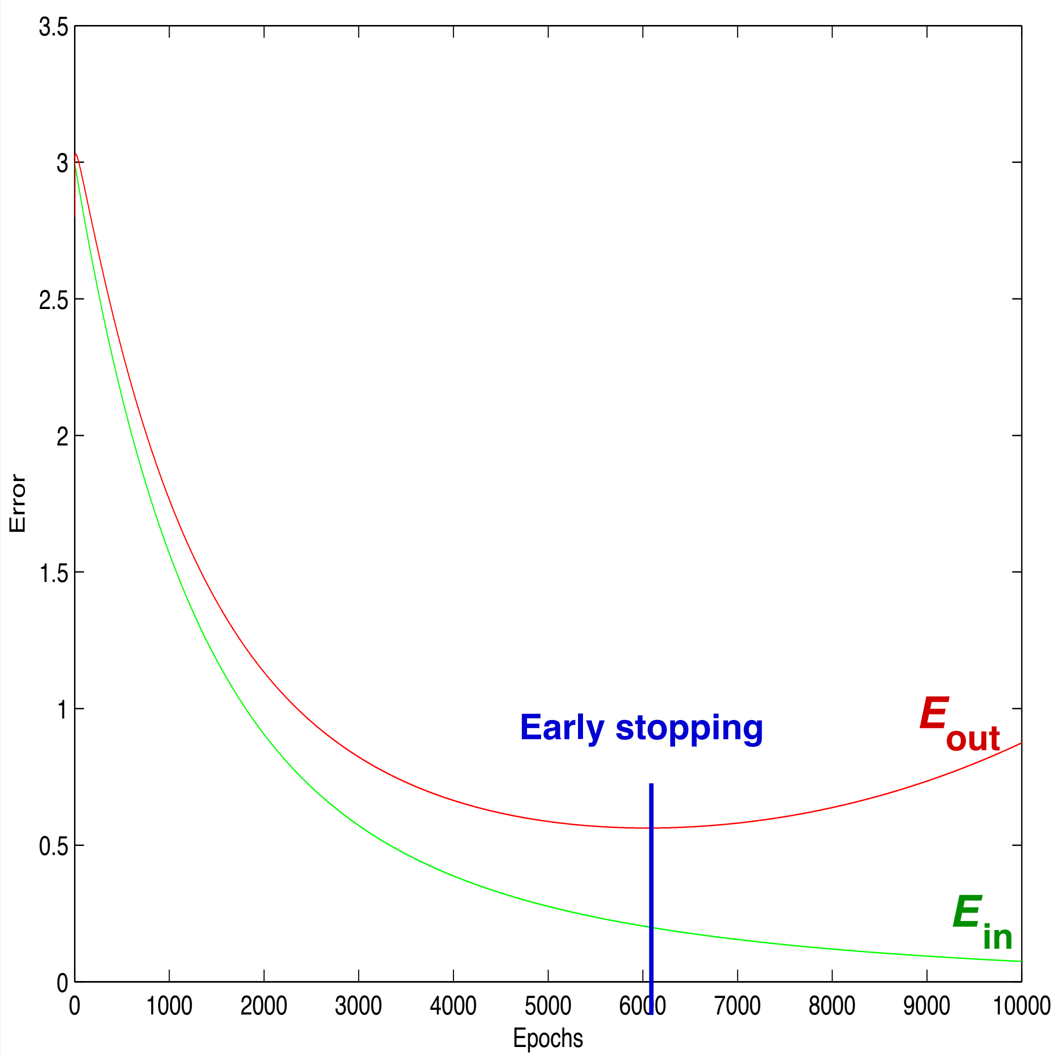
Why 'validation'

$\mathcal{D}_{\text{val}}$ is used to make learning choices

If an estimate of E_{out} affects learning:

the set is no longer a **test** set!

It becomes a validation set



What's the difference?

Test set is unbiased; validation set has optimistic bias

Two hypotheses h_1 and h_2 with $E_{\text{out}}(h_1) = E_{\text{out}}(h_2) = 0.5$

Error estimates $\mathbf{e}_1$ and $\mathbf{e}_2$ uniform on $[0, 1]$

Pick $h \in \{h_1, h_2\}$ with $\mathbf{e} = \min(\mathbf{e}_1, \mathbf{e}_2)$

$\mathbb{E}(\mathbf{e}) < 0.5$ optimistic bias

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Using $\mathcal{D}_{\text{val}}$ more than once

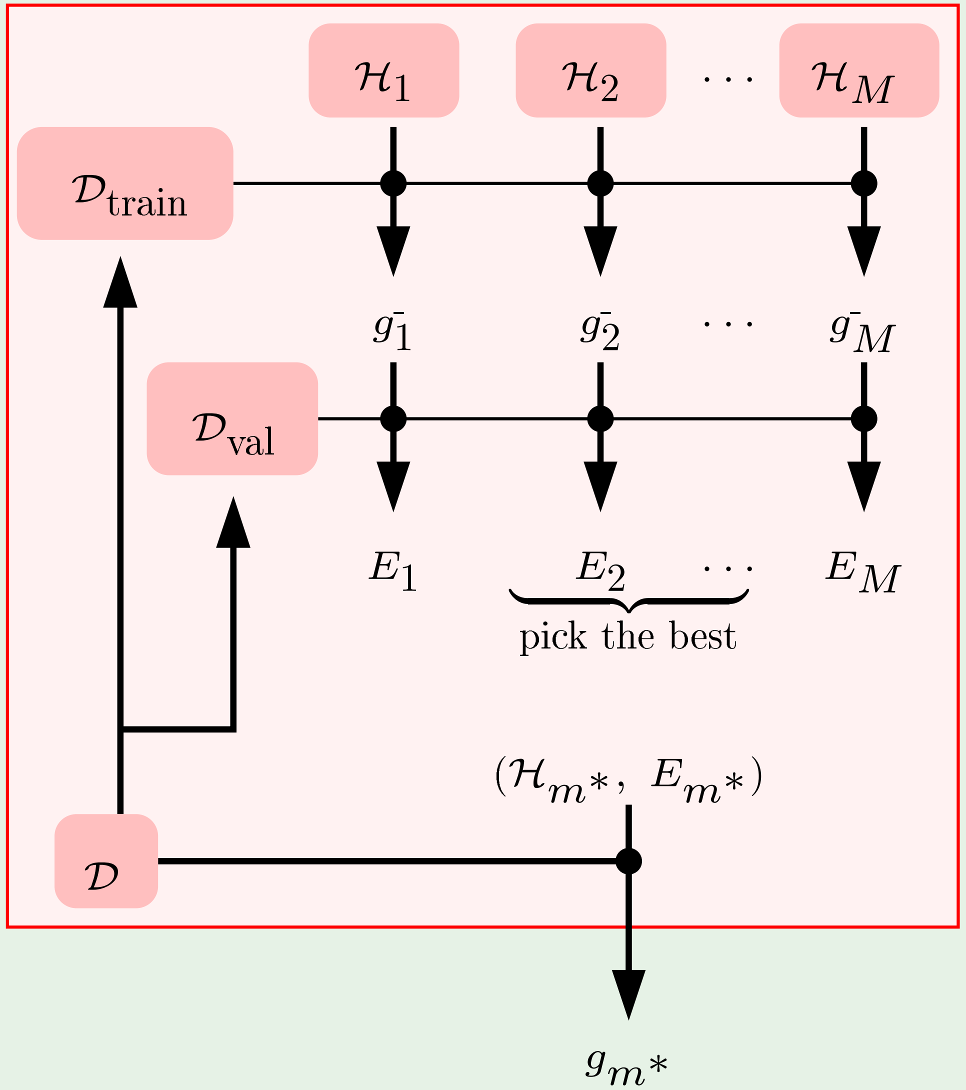
M models $\mathcal{H}_1, \ldots, \mathcal{H}_M$

Use $\mathcal{D}_{\text{train}}$ to learn g_m^- for each model

Evaluate g_m^- using $\mathcal{D}_{\text{val}}$:

$$E_m = E_{\text{val}}(g_m^-); \quad m = 1, \ldots, M$$

Pick model $m = m^*$ with smallest E_m

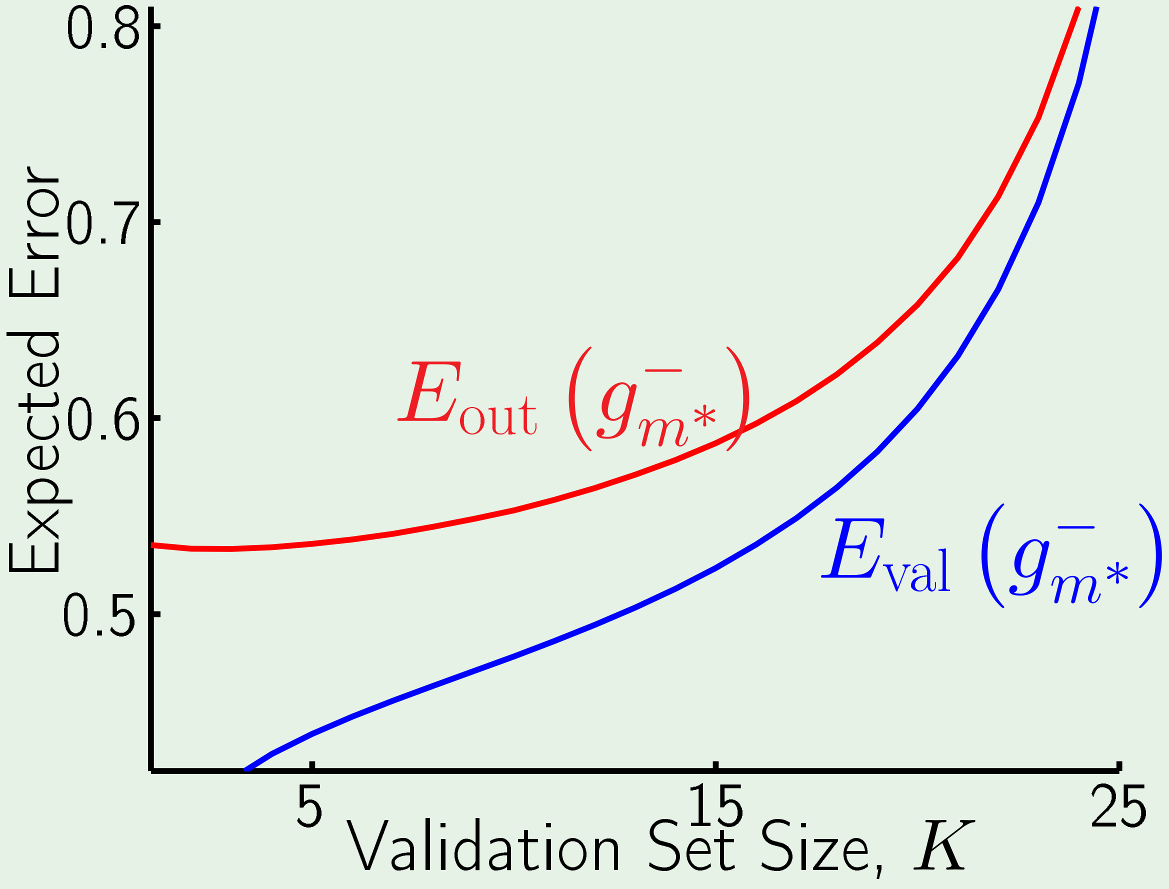


The bias

We selected the model $\mathcal{H}_{m^*}$ using $\mathcal{D}_{\text{val}}$

$E_{\text{val}}(g^-_{m^*})$ is a biased estimate of $E_{\text{out}}(g^-_{m^*})$

Illustration: selecting between 2 models



How much bias

For M models: $\mathcal{H}_1, \ldots, \mathcal{H}_M$

$\mathcal{D}_{\text{val}}$ is used for "training" on the **finalists model**:

$$\mathcal{H}_{\text{val}} = \{g_1^-, g_2^-, \ldots, g_M^-\}$$

Back to Hoeffding and VC!

$$E_{\text{out}}(g_{m^*}^-) \le E_{\text{val}}(g_{m^*}^-) + O\left(\sqrt{\frac{\ln M}{K}}\right)$$

regularization λ early-stopping T

Data contamination

Error estimates: $E_{\text{in}}, \ E_{\text{test}}, \ E_{\text{val}}$

Contamination: Optimistic (deceptive) bias in estimating E_{out}

Training set: totally contaminated

Validation set: slightly contaminated

Test set: totally 'clean'

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The dilemma about K

The following chain of reasoning:

$$E_{\text{out}}(g) \underset{\text{(small } K)}{\approx} E_{\text{out}}(g^-) \underset{\text{(large } K)}{\approx} E_{\text{val}}(g^-)$$

highlights the dilemma in selecting K:

Can we have K both small and large? ☺

Leave one out

$N-1$ points for training, and 1 point for validation!

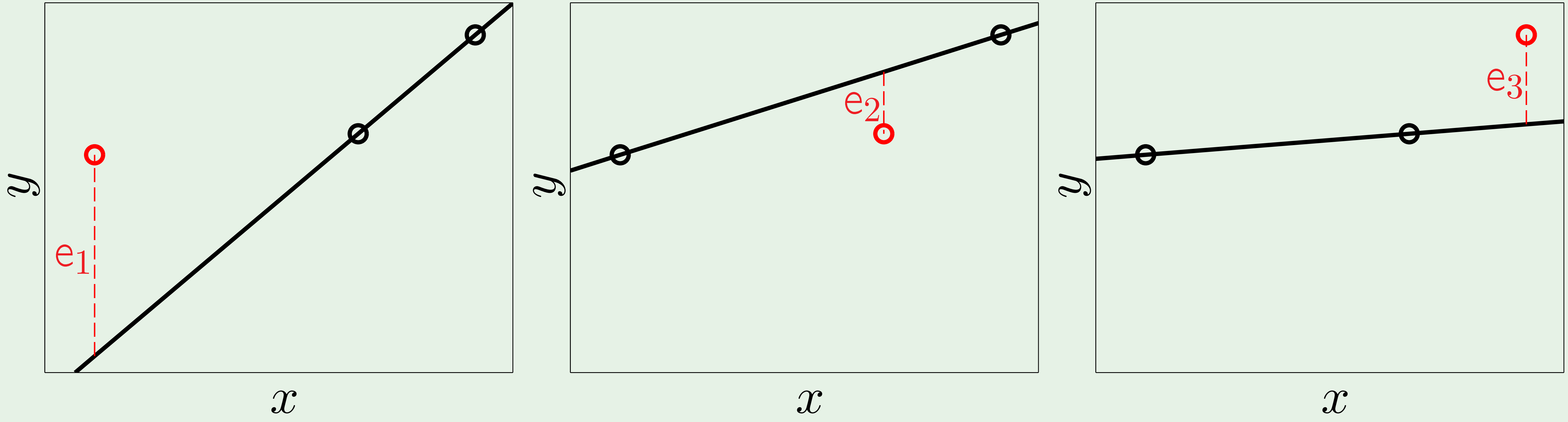
$$\mathcal{D}_n = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_{n-1}, y_{n-1}), \cancel{(\mathbf{x}_n, y_n)}, (\mathbf{x}_{n+1}, y_{n+1}), \ldots, (\mathbf{x}_N, y_N)$$

Final hypothesis learned from $\mathcal{D}_n$ is g_n^-

$$\mathbf{e}_n = E_{\text{val}}(g_n^-) = \mathbf{e}\left(g_n^-(\mathbf{x}_n), y_n\right)$$

cross validation error: $E_{\text{cv}} = \dfrac{1}{N} \displaystyle\sum_{n=1}^{N} \mathbf{e}_n$

Illustration of cross validation

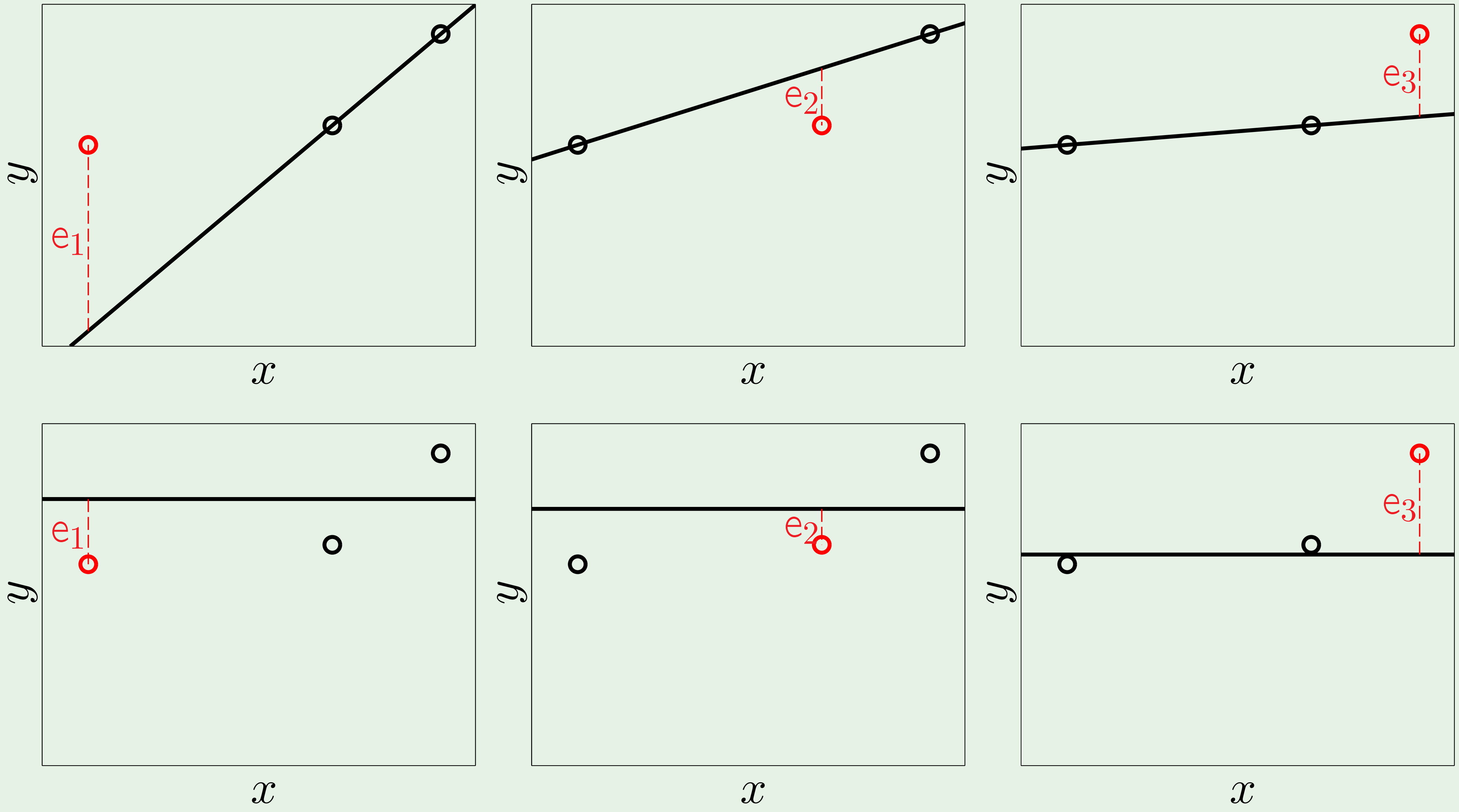


$$E_{\text{cv}} = \frac{1}{3}\left(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3 \right)$$

Model selection using CV

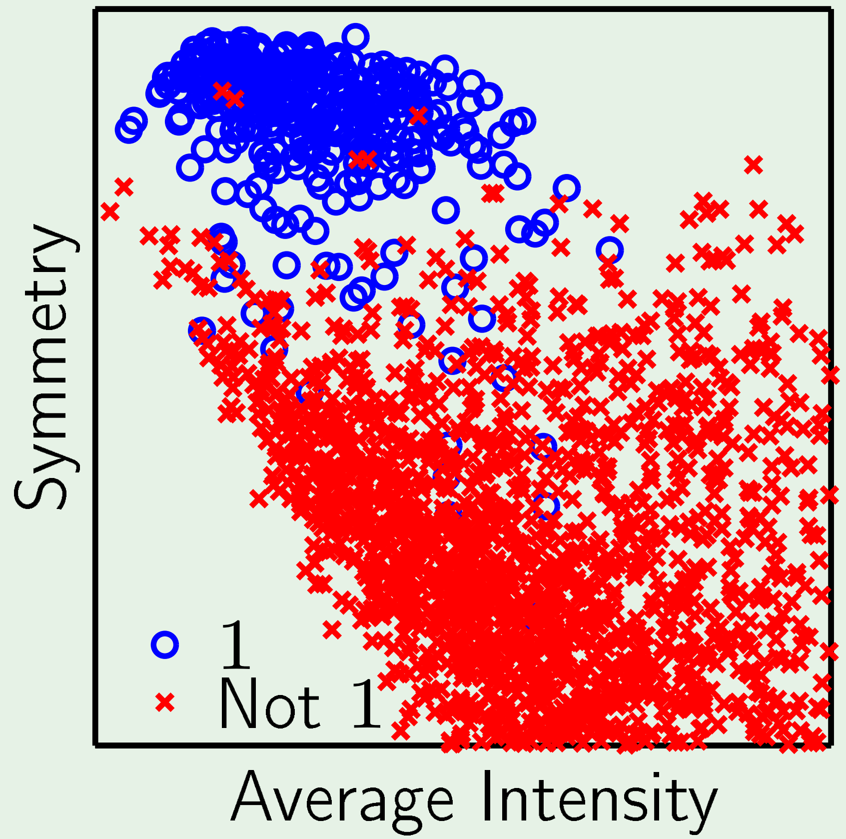
Linear:

Constant:

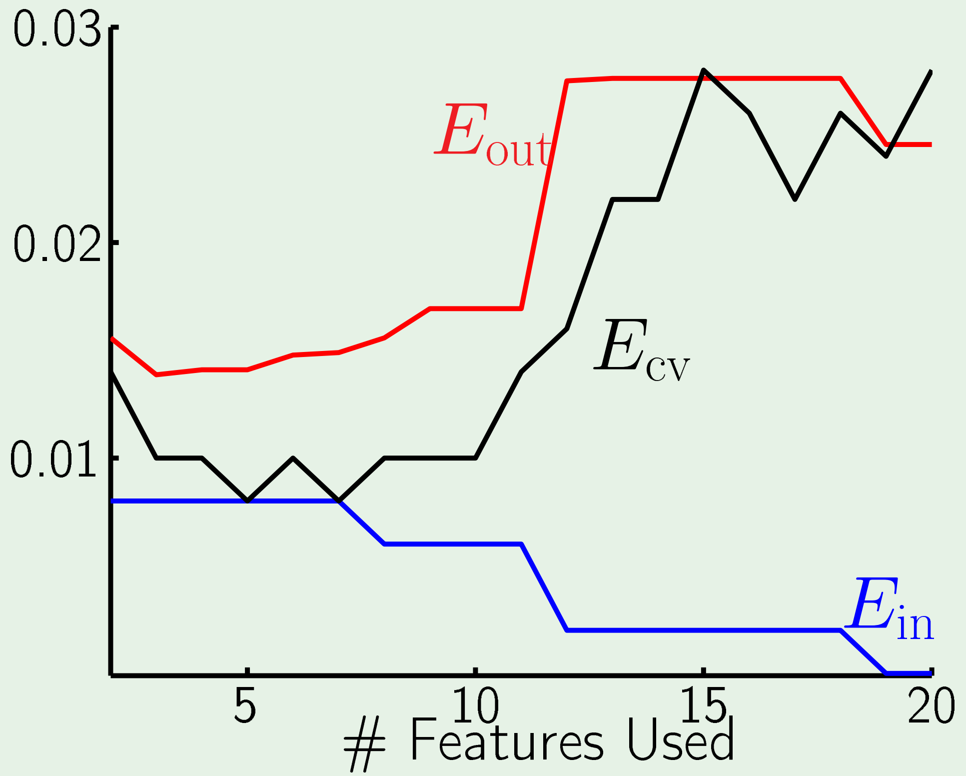


Cross validation in action

Digits classification task



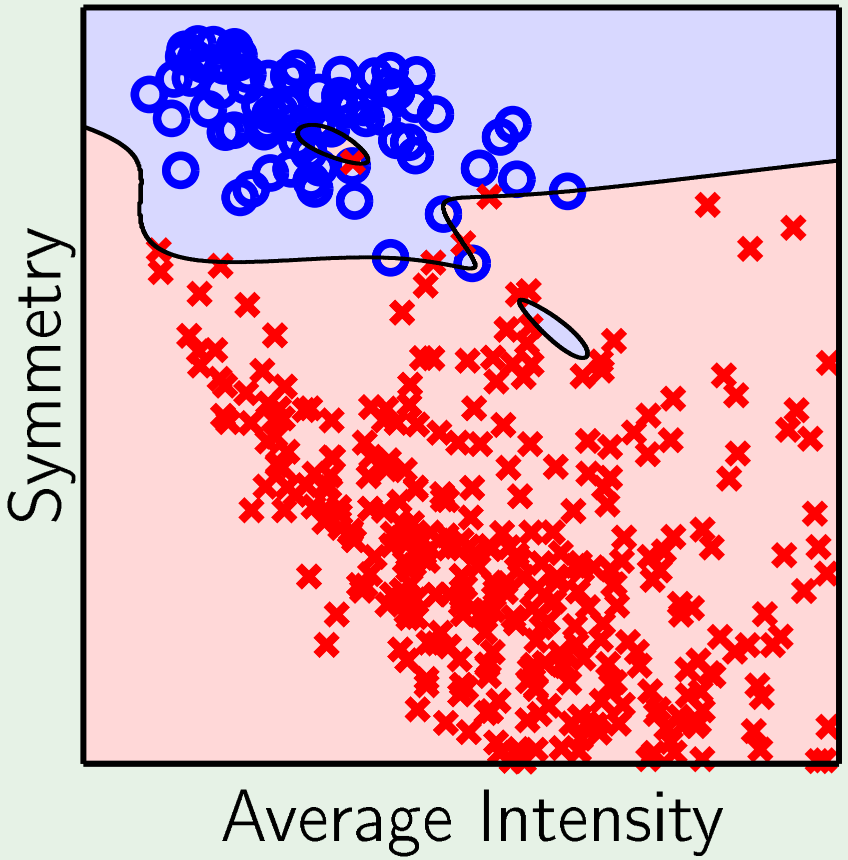
Different errors



$$(1, x_1, x_2) \rightarrow (1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3, x_1^2x_2, \ldots, x_1^5, x_1^4x_2, x_1^3x_2^2, x_1^2x_2^3, x_1x_2^4, x_2^5)$$

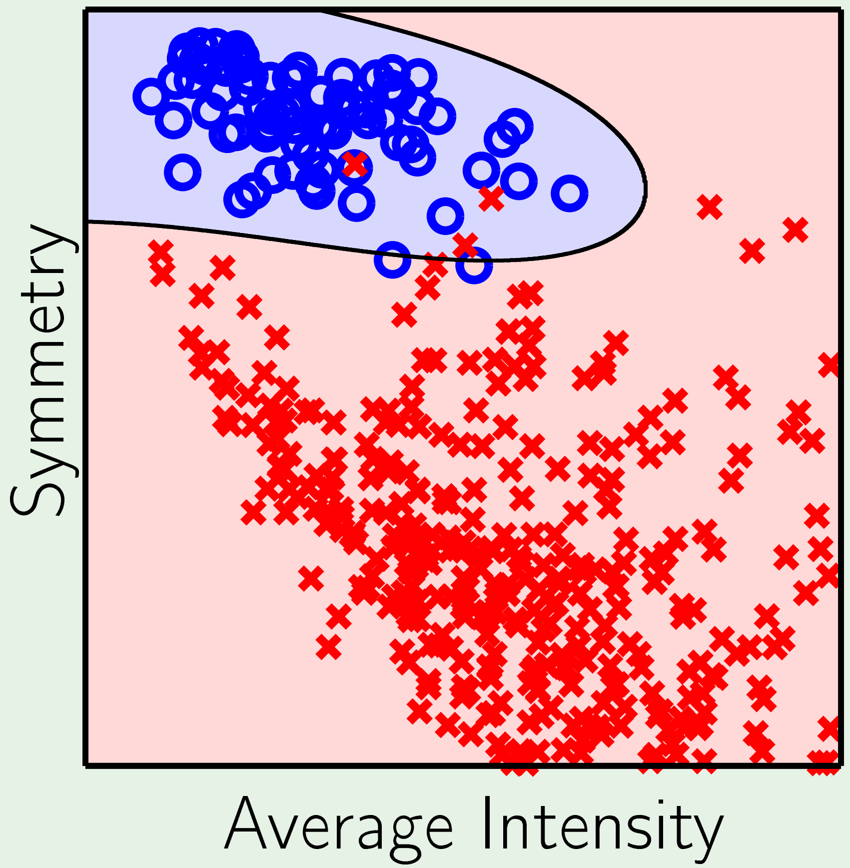
The result

without validation



$E_{\text{in}} = 0\% \qquad E_{\text{out}} = 2.5\%$

with validation

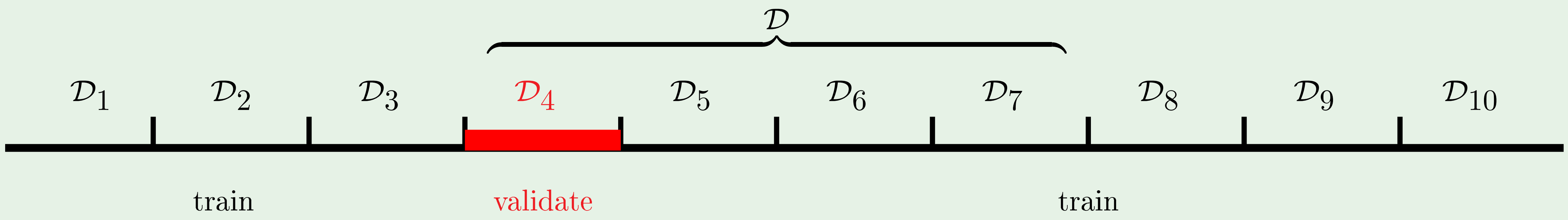


$E_{\text{in}} = 0.8\% \qquad E_{\text{out}} = 1.5\%$

Leave more than one out

Leave one out: N training sessions on $N-1$ points each

More points for validation?



$\frac{N}{K}$ training sessions on $N-K$ points each

10-fold cross validation: $K = \frac{N}{10}$