Learning From Data
Lecture 13
Validation and Model Selection

The Validation Set
Model Selection
Cross Validation

M. Magdon-Ismail
CSCI 4100/6100

RECAP: # Regularization

Regularization combats the effects of noise by putting a leash on the algorithm.

$$E_{\text{aug}}(h) = E_{\text{in}}(h) + \frac{\lambda}{N}\Omega(h)$$

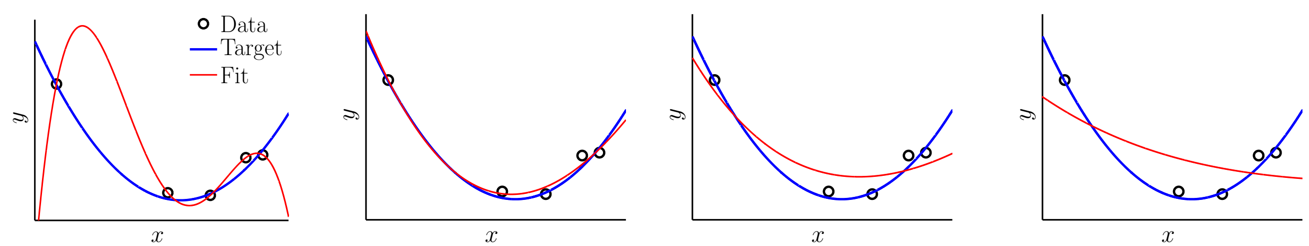
$\Omega(h) \rightarrow$ smooth, simple h

noise is rough, complex.

Different regularizers give different results

can choose λ, the **amount** of regularization.

$\lambda = 0$ $\quad$ $\lambda = 0.0001$ $\quad$ $\lambda = 0.01$ $\quad$ $\lambda = 1$



Overfitting $\rightarrow$ $\rightarrow$ **Underfitting**

Optimal λ balances approximation and generalization, bias and variance.

Validation: A Sneak Peek at E_{out}

$$E_{\text{out}}(g) = E_{\text{in}}(g) + \underbrace{\text{overfit penalty}}$$

VC bounds this using a complexity error bar $\Omega(\mathcal{H})$

regularization estimates this through a heuristic complexity penalty $\Omega(g)$

Validation: A Sneak Peek at E_{out}

$$E_{\text{out}}(g) = E_{\text{in}}(g) + \underbrace{\text{overfit penalty}}_{\substack{\text{VC bounds this using a complexity error bar } \Omega(\mathcal{H}) \\ \text{regularization estimates this through a heuristic complexity penalty } \Omega(g)}}$$

Validation goes directly for the jugular:

$$\underbrace{E_{\text{out}}(g)}_{\text{validation estimates this directly}} = E_{\text{in}}(g) + \text{overfit penalty}.$$

Validation: A Sneak Peek at E_{out}

$$E_{\text{out}}(g) = E_{\text{in}}(g) + \underbrace{\text{overfit penalty}}$$

VC bounds this using a complexity error bar $\Omega(\mathcal{H})$

regularization estimates this through a heuristic complexity penalty $\Omega(g)$

Validation goes directly for the jugular:

$$\underbrace{E_{\text{out}}(g)} = E_{\text{in}}(g) + \text{overfit penalty}.$$

validation estimates this directly

In-sample estimate of E_{out} is the Holy Grail of learning from data.

The Test Set

$$
\begin{tikzcd}
\underset{(N\text{ data points})}{\mathcal{D}} \arrow[d] & \underset{(K\text{ test points})}{\mathcal{D}_{\text{test}}} \arrow[d] \\
g \arrow[r, "\mathsf{e}_k = \mathsf{e}(g(\mathbf{x}_k),\, y_k)"] \arrow[d] & \mathsf{e}_1, \mathsf{e}_2, \ldots, \mathsf{e}_K \arrow[d] \\
\boxed{g} \arrow[d] & \boxed{E_{\text{test}} = \frac{1}{K}\sum_{k=1}^{K} \mathsf{e}_k} \\
\boxed{E_{\text{out}}(g)} &
\end{tikzcd}
$$

E_{test} is an estimate for $E_{\text{out}}(g)$

$$\mathbb{E}_{\mathcal{D}_{\text{test}}}[\mathsf{e}_k] = E_{\text{out}}(g)$$

$$
\begin{aligned}
\mathbb{E}[E_{\text{test}}] &= \frac{1}{K}\sum_{k=1}^{K} \mathbb{E}[\mathsf{e}_k] \\
&= \frac{1}{K}\sum_{k=1}^{K} E_{\text{out}}(g) = E_{\text{out}}(g)
\end{aligned}
$$

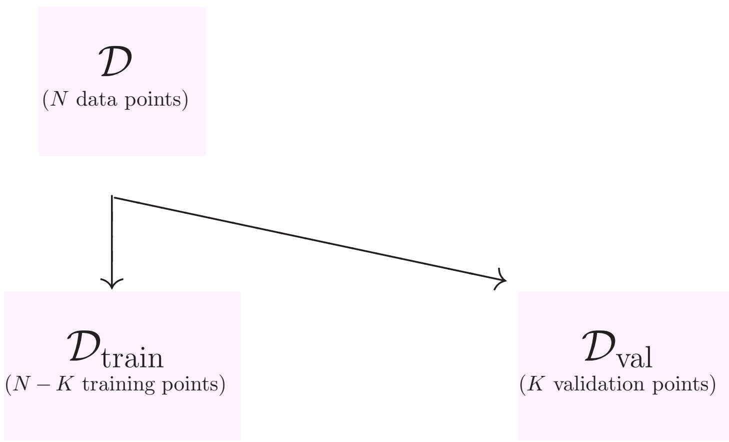
$\mathsf{e}_1, \ldots, \mathsf{e}_K$ are *independent*

$$
\begin{aligned}
\operatorname{Var}[E_{\text{test}}] &= \frac{1}{K^2}\sum_{k=1}^{K} \operatorname{Var}[\mathsf{e}_k] \\
&= \frac{1}{K}\operatorname{Var}[e]
\end{aligned}
$$

decreases like $\frac{1}{K}$

bigger $K \implies$ more reliable E_{test}.

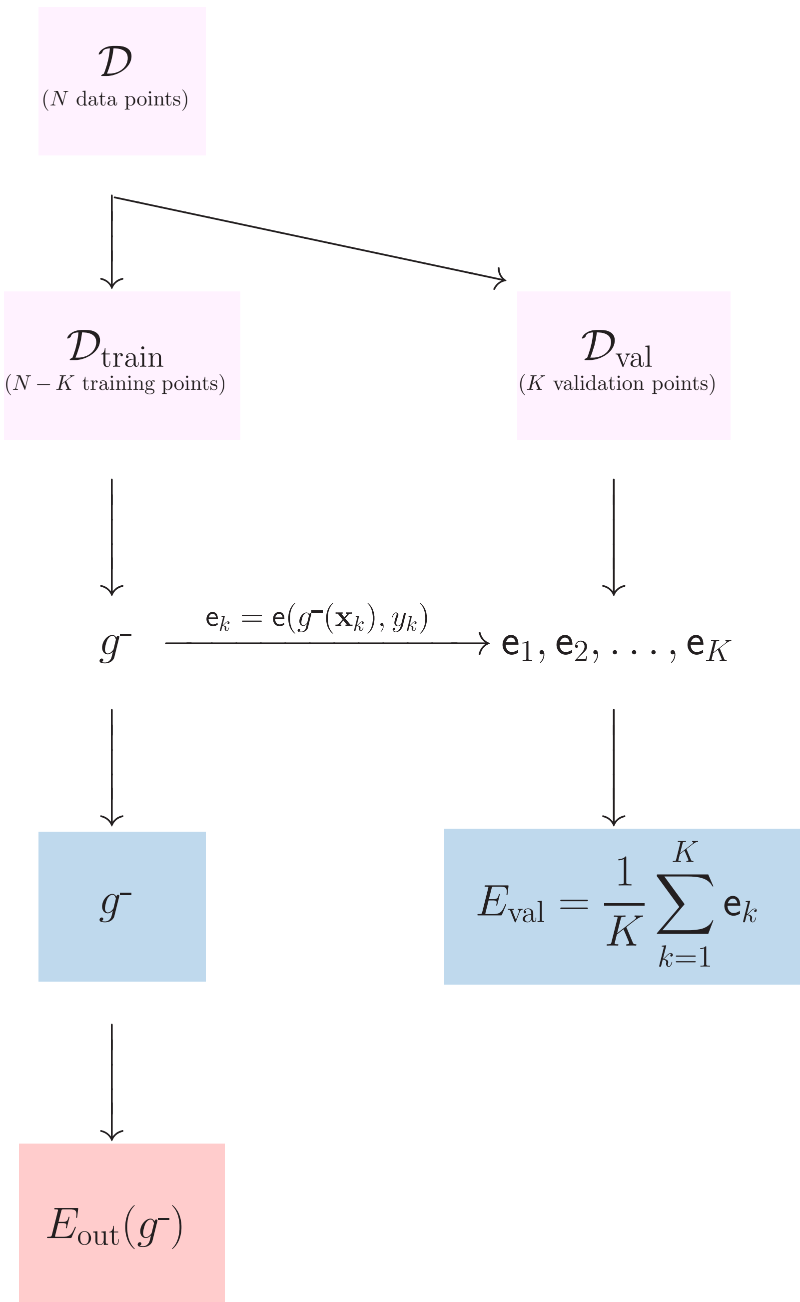
The Validation Set



1. Remove K points from $\mathcal{D}$

$$\mathcal{D} = \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{val}}.$$

The Validation Set



1. Remove K points from $\mathcal{D}$

$$\mathcal{D} = \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{val}}.$$

2. Learn using $\mathcal{D}_{\text{train}} \longrightarrow g^-$.

3. Test g^- on $\mathcal{D}_{\text{val}} \longrightarrow E_{\text{val}}$.

4. Use error E_{val} to estimate $E_{\text{out}}(g^-)$.

The Validation Set

$$
\begin{tikzcd}
\underset{(N\text{ data points})}{\mathcal{D}} \arrow[d] \arrow[dr] & \\
\underset{(N-K\text{ training points})}{\mathcal{D}_{\text{train}}} \arrow[d] & \underset{(K\text{ validation points})}{\mathcal{D}_{\text{val}}} \arrow[d] \\
g^{-} \arrow[r, "\mathsf{e}_k = \mathsf{e}(g^{-}(\mathbf{x}_k),\, y_k)"] \arrow[d] & \mathsf{e}_1, \mathsf{e}_2, \ldots, \mathsf{e}_K \arrow[d] \\
g^{-} \arrow[d] & E_{\text{val}} = \dfrac{1}{K}\displaystyle\sum_{k=1}^{K} \mathsf{e}_k \\
E_{\text{out}}(g^{-}) &
\end{tikzcd}
$$

E_{val} is an estimate for $E_{\text{out}}(g^{-})$

$$\mathbb{E}_{\mathcal{D}_{\text{val}}}[\mathsf{e}_k] = E_{\text{out}}(g^{-})$$

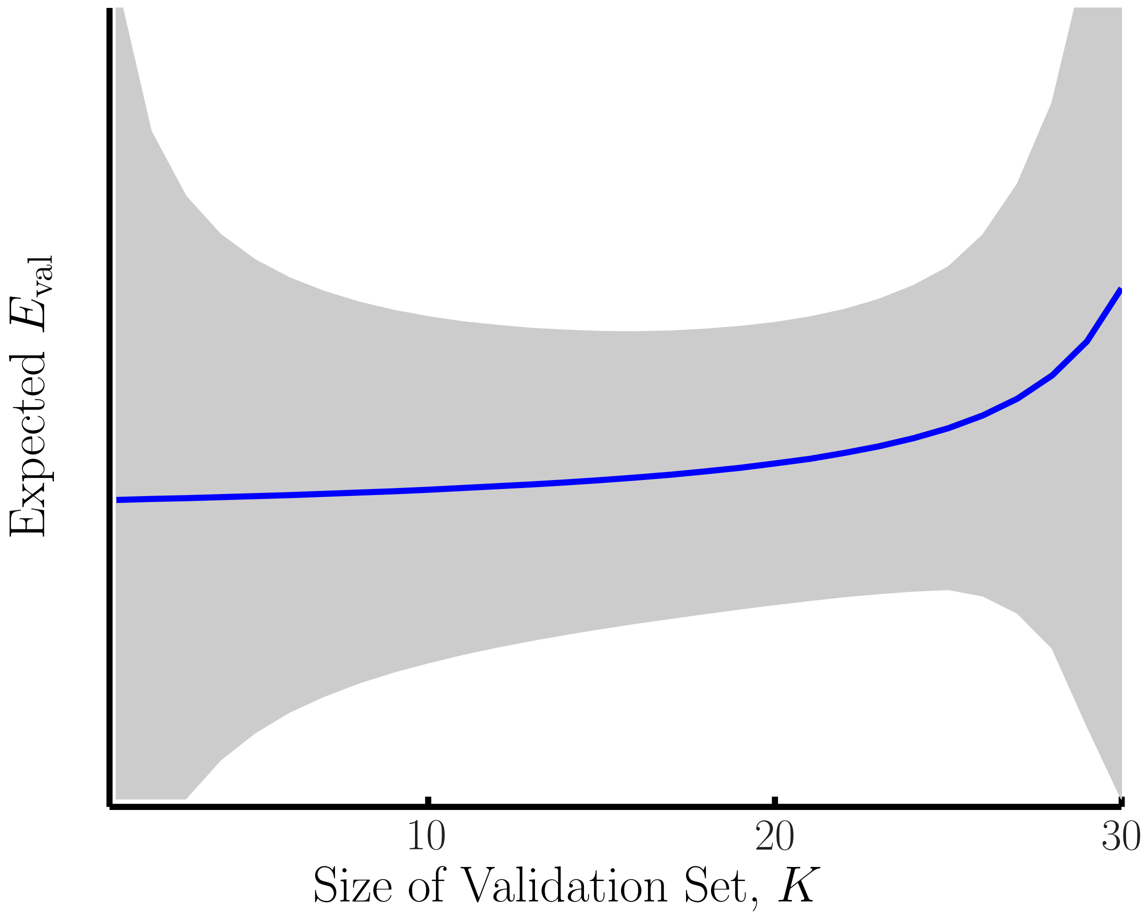
$$
\begin{aligned}
\mathbb{E}[E_{\text{test}}] &= \frac{1}{K}\sum_{k=1}^{K} \mathbb{E}[\mathsf{e}_k] \\
&= \frac{1}{K}\sum_{k=1}^{K} E_{\text{out}}(g^{-}) = E_{\text{out}}(g^{-})
\end{aligned}
$$

$\mathsf{e}_1, \ldots, \mathsf{e}_K$ are *independent*

$$
\begin{aligned}
\text{Var}[E_{\text{val}}] &= \frac{1}{K^2}\sum_{k=1}^{K} \text{Var}[\mathsf{e}_k] \\
&= \frac{1}{K}\text{Var}[e(g^{-})]
\end{aligned}
$$

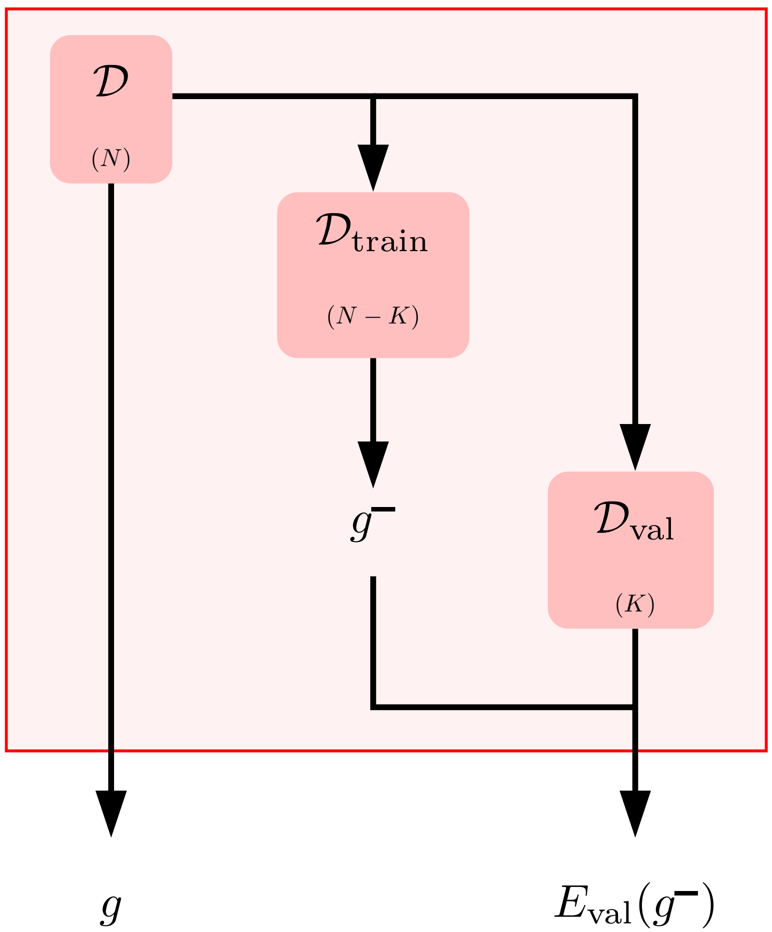
decreases like $\frac{1}{K}$
depends on g^{-}, not $\mathcal{H}$
bigger $K \implies$ more reliable E_{val}?

Choosing K



Rule of thumb: $K^* = \frac{N}{5}$.

Restoring $\mathcal{D}$



CUSTOMER

Primary goal: output best hypothesis.

g was trained on *all* the data.

Secondary goal: estimate $E_{\text{out}}(g)$.

g^- is behind closed doors.

$$\begin{array}{cc} E_{\text{out}}(g) & E_{\text{out}}(g^-) \\ \downarrow & \downarrow \\ \underbrace{E_{\text{in}}(g) \qquad E_{\text{val}}(g^-)}_{\text{which should we use?}} & \end{array}$$

E_{val} Versus E_{in}

Biased error bar depends on $\mathcal{H}$.

$$E_{\text{out}}(g) \;\le\; E_{\text{in}}(g) + O\left(\sqrt{\frac{d_{\text{VC}}}{N}\log N}\right)$$

$$E_{\text{out}}(g) \;\le\; E_{\text{out}}(g^{-}) \le E_{\text{val}}(g^{-}) + O\left(\frac{1}{\sqrt{K}}\right)$$

learning curve is decreasing
(a practical truth, not a theorem)

Unbiased error bar depends on g^{-}.

$E_{\text{val}}(g)$ usually wins as an estimate for $E_{\text{out}}(g)$, especially when the learning curve is not steep.

Model Selection

The most important use of validation

$$\begin{array}{ccccc} \boxed{\mathcal{H}_1} & \boxed{\mathcal{H}_2} & \boxed{\mathcal{H}_3} & \cdots & \boxed{\mathcal{H}_M} \\ \downarrow & \downarrow & \downarrow & & \downarrow \\ g_1 & g_2 & g_3 & \cdots & g_M \end{array}$$

Validation Estimate for $(\mathcal{H}_1, g_1)$

The most important use of validation

Validation Estimate for $(\mathcal{H}_1, g_1)$

The most important use of validation

Compute Validation Estimates for All Models

The most important use of validation

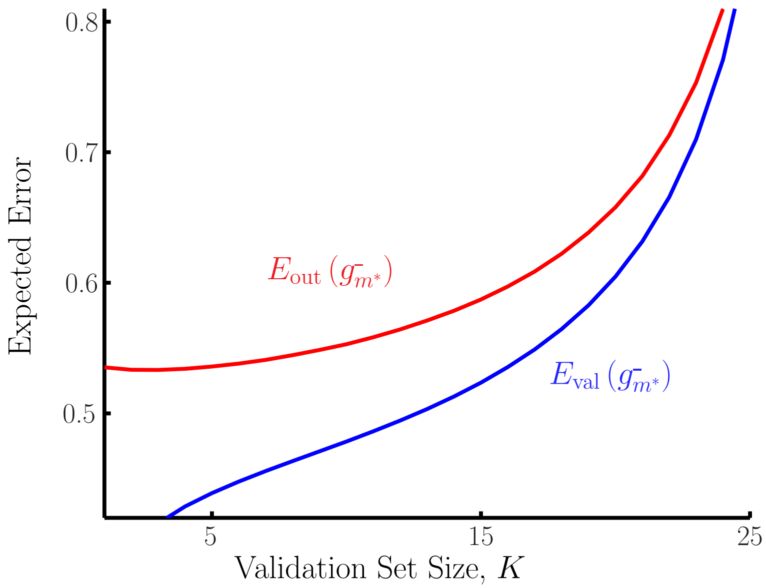
$$
\begin{array}{rccccc}
 & \mathcal{H}_1 & \mathcal{H}_2 & \mathcal{H}_3 & \cdots & \mathcal{H}_M \\
\mathcal{D}_{\text{train}} \longrightarrow & \downarrow & \downarrow & \downarrow & & \downarrow \\
 & g_1^- & g_2^- & g_3^- & \cdots & g_M^- \\
\mathcal{D}_{\text{val}} \longrightarrow & \downarrow & \downarrow & \downarrow & & \downarrow \\
 & E_1 & E_2 & E_3 & \cdots & E_M
\end{array}
$$

Pick The Best Model According to Validation Error

The most important use of validation

$$
\begin{tikzcd}
 & \boxed{\mathcal{H}_1} \arrow[d] & \boxed{\mathcal{H}_2} \arrow[d] & \boxed{\mathcal{H}_3} \arrow[d] & \cdots & \boxed{\mathcal{H}_M} \arrow[d] \\
\mathcal{D}_{\text{train}} \arrow[r] & g_1^- \arrow[d] & g_2^- \arrow[d] & g_3^- \arrow[d] & \cdots & g_M^- \arrow[d] \\
\mathcal{D}_{\text{val}} \arrow[r] & E_1 & E_2 & E_3 & \cdots & E_M
\end{tikzcd}
$$

$E_{\text{val}}(g^-_{m^*})$ is not Unbiased For $E_{\text{out}}(g^-_{m^*})$



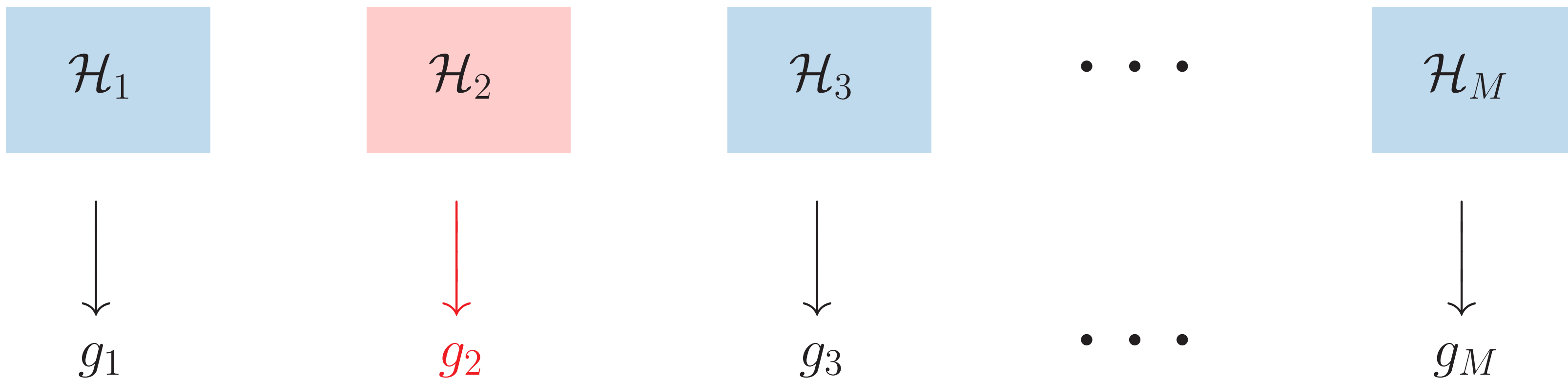
…because we *choose* one of the M finalists.

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

$\uparrow$

VC error bar for selecting a hypothesis from M using a data set of size K.

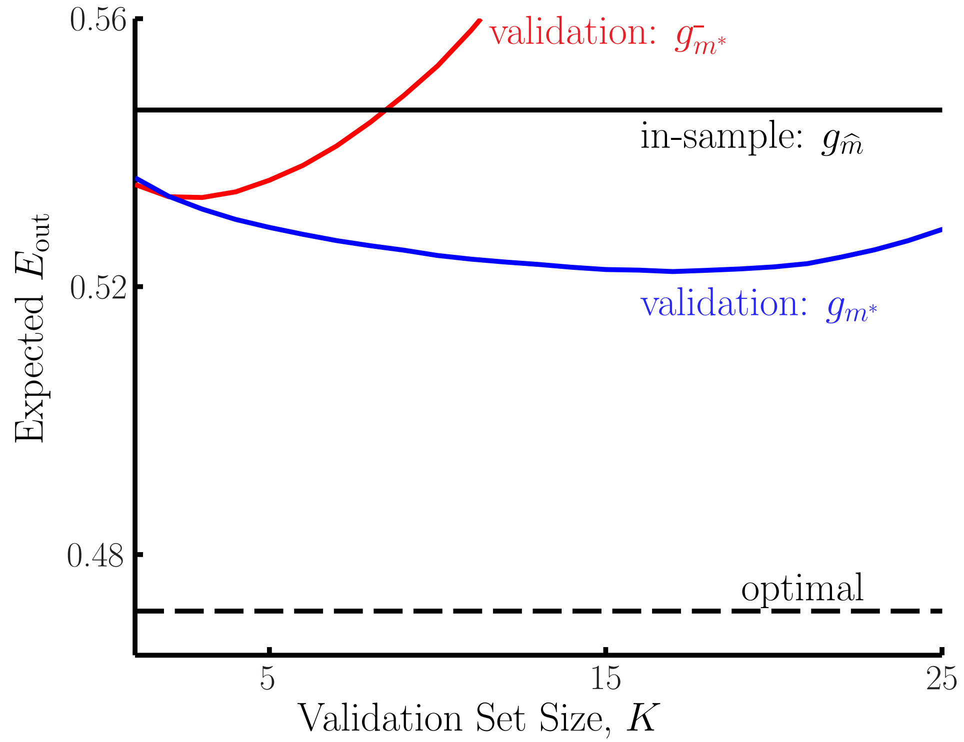
Restoring $\mathcal{D}$

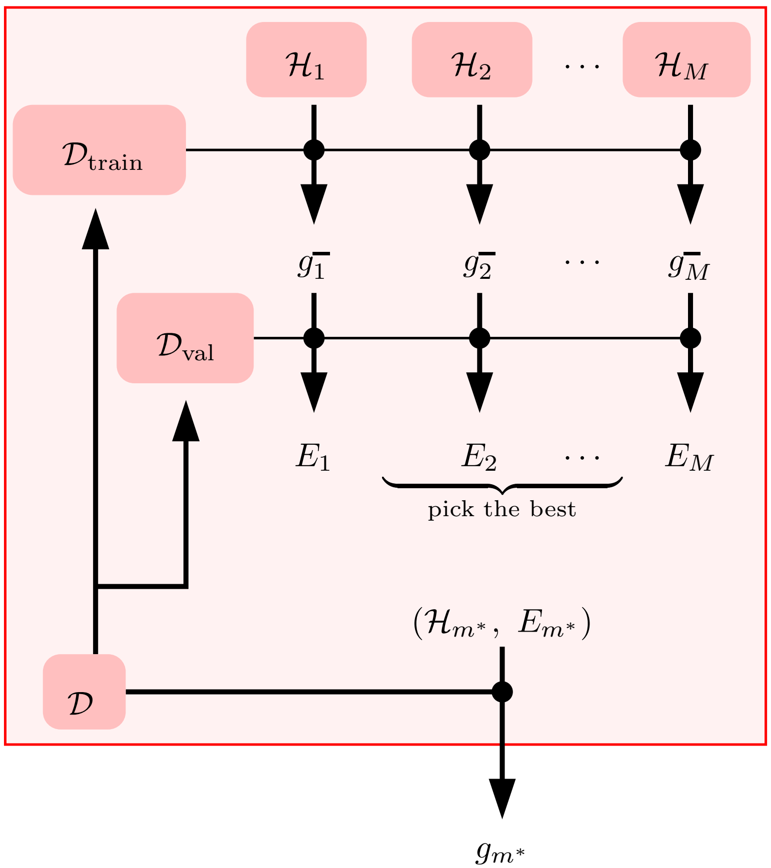


Model with best g also has best g^- ← leap of faith

We can find model with best g^- using validation ← true modulo E_{val} error bar

Comparing E_{in} and E_{val} for Model Selection





Application to Selecting λ

Which regularization parameter to use?

$$\lambda_1, \lambda_2, \ldots, \lambda_M.$$

This is a special case of *model selection* over M models,

$$\begin{array}{ccccc} (\mathcal{H}, \lambda_1) & (\mathcal{H}, \lambda_2) & (\mathcal{H}, \lambda_3) & \cdots & (\mathcal{H}, \lambda_M) \\ \downarrow & \downarrow & \downarrow & & \downarrow \\ g_1 & g_2 & g_3 & \cdots & g_M \end{array}$$

Picking a model amounts to chosing the optimal λ

The Dilemma When Choosing K

Validation relies on the following chain of reasoning,

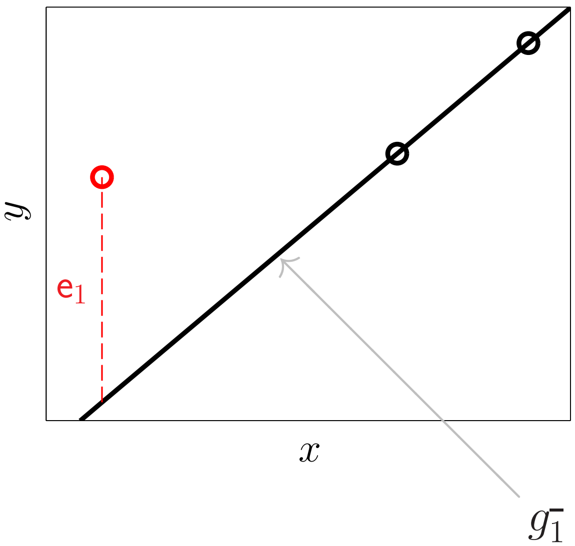
$$E_{\text{out}}(g) \approx E_{\text{out}}(g^-) \approx E_{\text{val}}(g^-)$$

(small K) (large K)

Can we get away with $K = 1$?

Yes, almost!

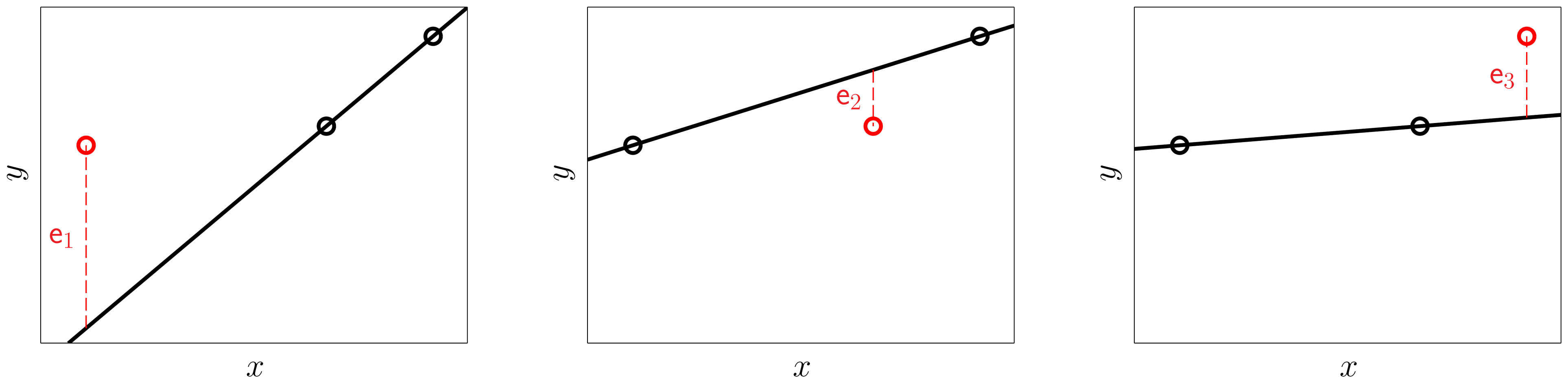
The Leave One Out Error ($K = 1$)



$$\mathbb{E}[\mathsf{e}_1] = E_{\text{out}}(g_1^-)$$

…but it is a **wild** estimate

The Leave One Our Errors



$$E_{\text{cv}} = \frac{1}{N}\sum_{n=1}^{N} \mathsf{e}_n$$

Cross Validation is Unbiased

Theorem. E_{cv} is an unbiased estimate of $\bar{E}_{\text{out}}(N-1)$.

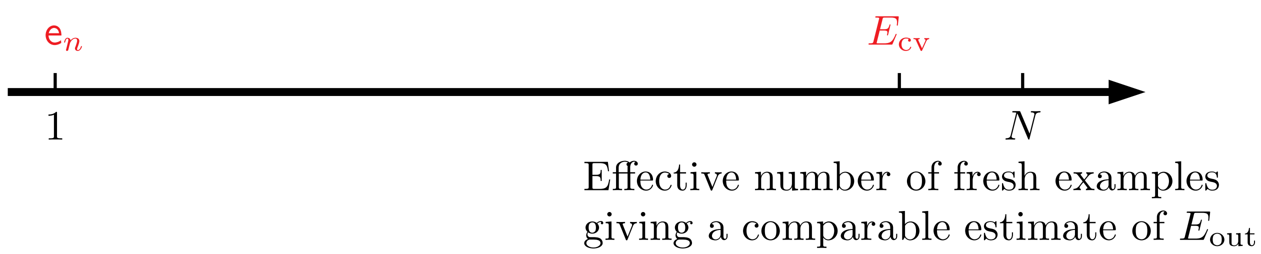
Expected E_{out} when learning with $N-1$ points.

Reliability of E_{cv}

e_n and e_m are not independent.

e_n depends on g_n^- which was trained on $(\mathbf{x}_m, y_m)$.

e_m is evaluated on $(\mathbf{x}_m, y_m)$.



Cross Validation is Computationally Intensive

N epochs of learning each on a data set of size $N-1$.

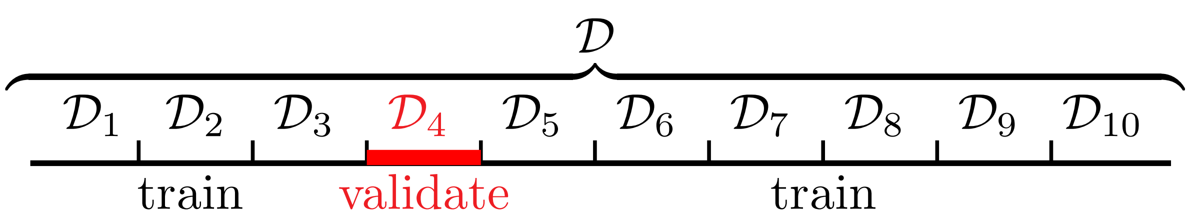
- Analytic approaches, for example linear regression with weight decay

$$\mathbf{w}_{\text{reg}} = (\mathrm{Z}^{\mathrm{T}}\mathrm{Z} + \lambda \mathrm{I})^{-1}\mathrm{Z}^{\mathrm{T}}\mathbf{y}$$

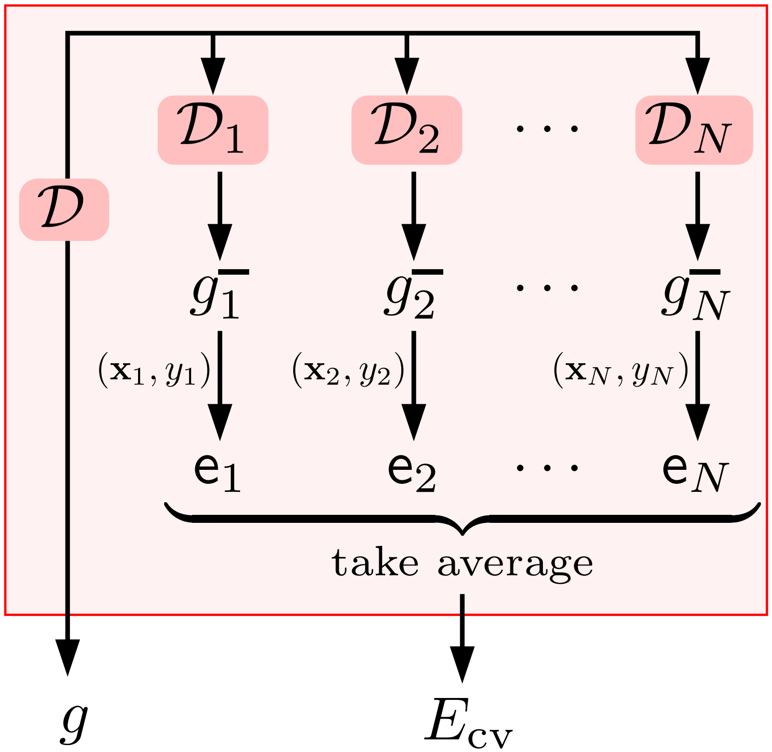
$$E_{\text{cv}} = \frac{1}{N}\sum_{n=1}^{N}\left(\frac{\hat{y}_n - y_n}{1 - \mathrm{H}_{nn}(\lambda)}\right)^2$$

$\mathrm{H}(\lambda) = \mathrm{Z}(\mathrm{Z}^{\mathrm{T}}\mathrm{Z} + \lambda \mathrm{I})^{-1}\mathrm{Z}^{\mathrm{T}}$.

- 10-fold cross validation



Restoring $\mathcal{D}$



CUSTOMER

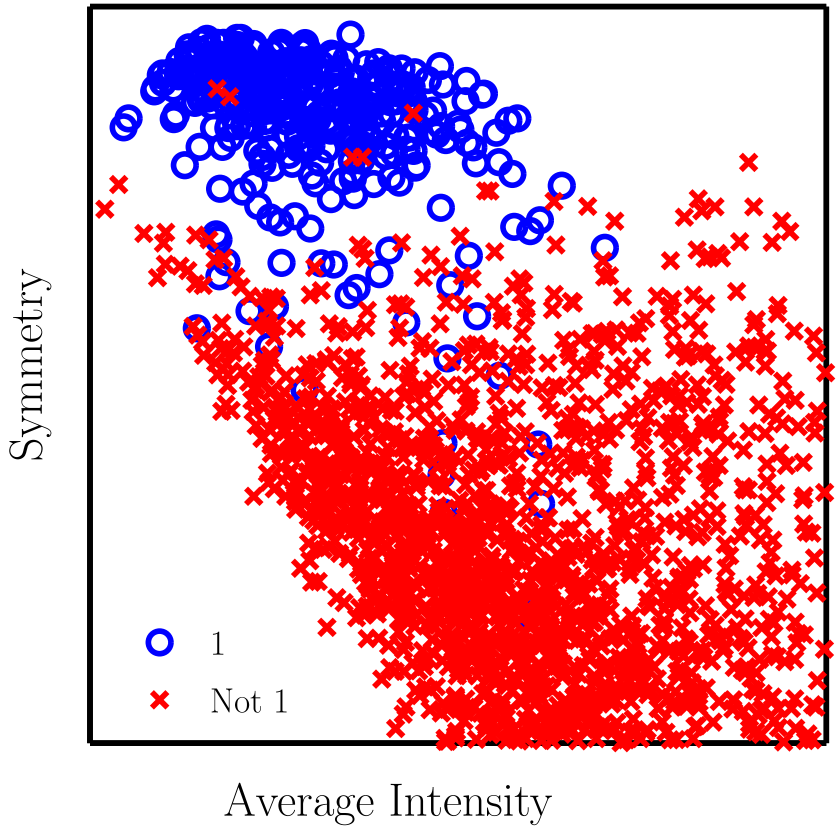
$$E_{\text{out}}(g^{(N)}) \le \bar{E}_{\text{out}}(N-1) \le E_{\text{cv}} + O\left(\frac{1}{\sqrt{N}}\right).$$

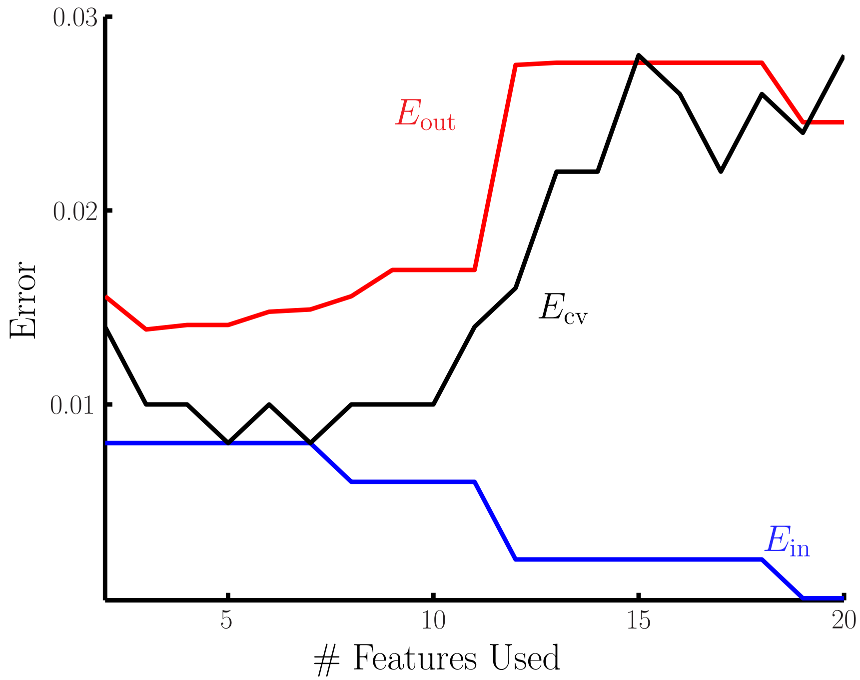
learning curve

nearly independent e_n

E_{cv} can be used for model selection just as E_{val}, for example to choose λ.

Digits Problem: ‘1’ Versus ‘Not 1’

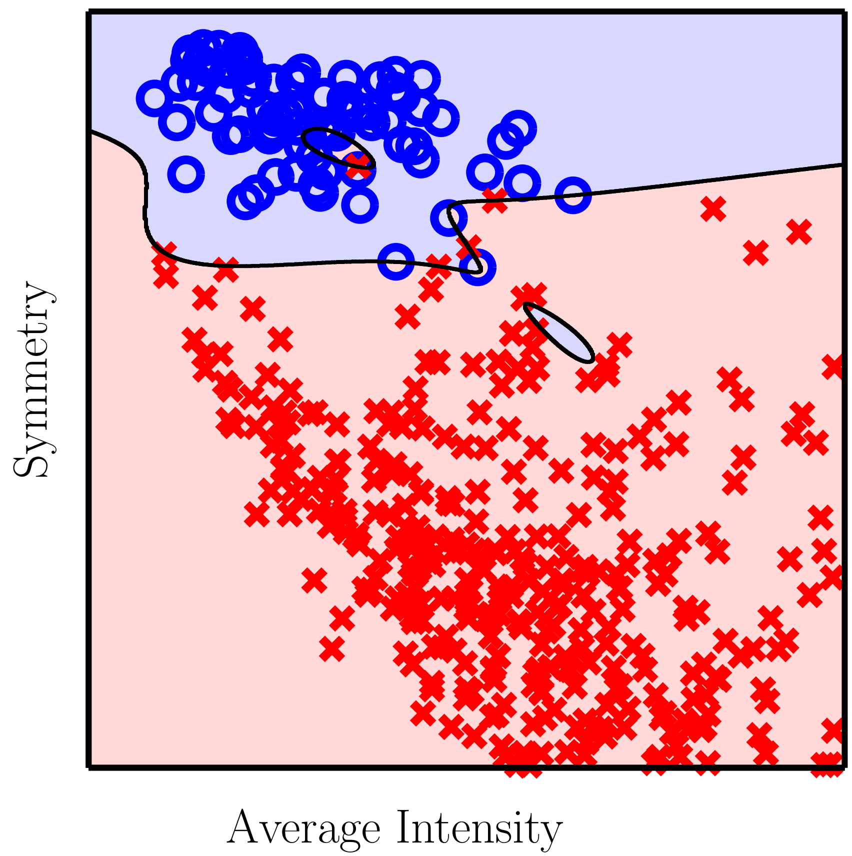




$$\mathbf{x} = (1, x_1, x_2)$$

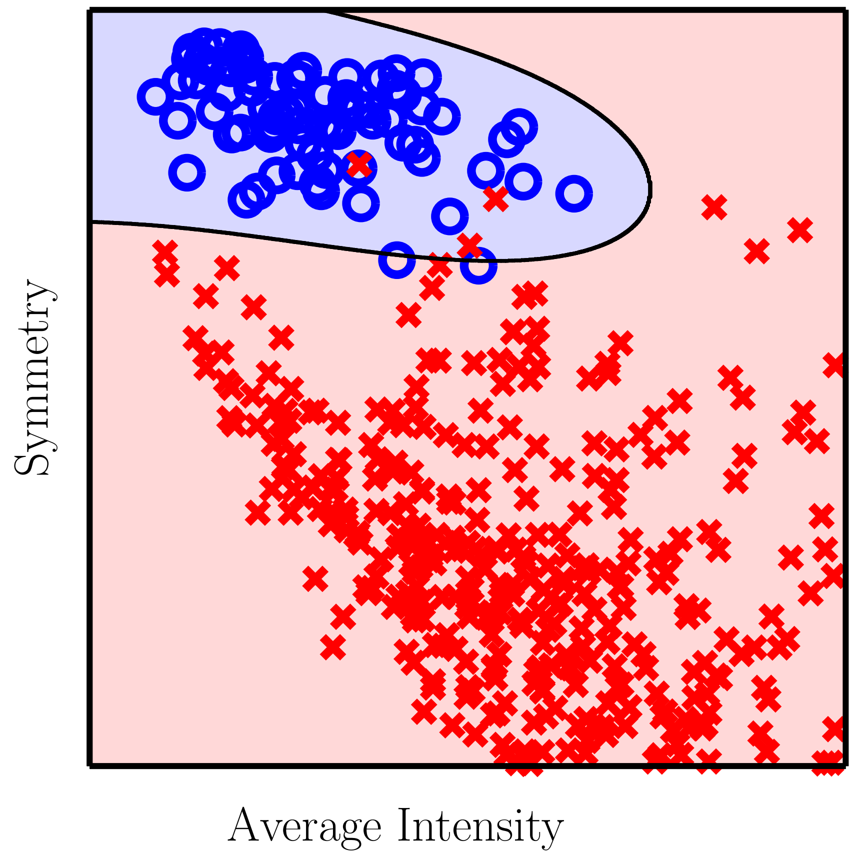
$$\mathbf{z} = \underbrace{(1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3, x_1^2x_2, x_1x_2^2, x_2^3, \ldots, x_1^5, x_1^4x_2, x_1^3x_2^2, x_1^2x_2^3, x_1x_2^4, x_2^5)}_{\text{5th order polynomial transform} \longrightarrow \text{20 dimensional non linear feature space}}$$

Validation Wins In the Real World



no validation (20 features)

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



cross validation (6 features)

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