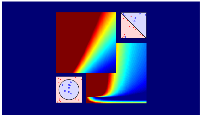
Machine Learning Foundations
(機器學習基石)



Lecture 15: Validation

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Roadmap

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn **Better**?

Lecture 14: Regularization

minimizes **augmented error**, where the added **regularizer** effectively **limits model complexity**

Lecture 15: Validation

- Model Selection Problem
- Validation
- Leave-One-Out Cross Validation
- V-Fold Cross Validation

So Many Models Learned

Even Just for Binary Classification . . .

$\mathcal{A} \in \{$ PLA, pocket, linear regression, logistic regression$\}$

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$T \in \{ 100, 1000, 10000\}$

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$\Omega(\mathbf{w}) \in \{$ L2 regularizer, L1 regularizer, symmetry regularizer$\}$

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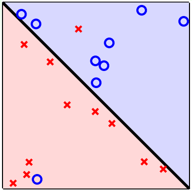
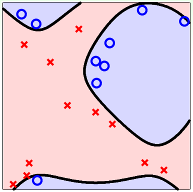
in addition to your **favorite** combination, may need to try other combinations to get a good g

Model Selection Problem



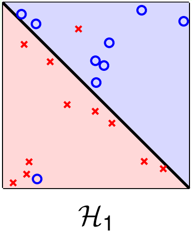
$\mathcal{H}_1$

which one do you prefer? :-)



$\mathcal{H}_2$

Model Selection Problem



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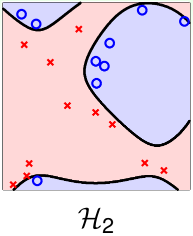

- given: M models $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_M$, each with corresponding algorithm $\mathcal{A}_1, \mathcal{A}_2, \ldots, \mathcal{A}_M$

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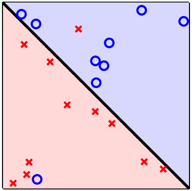

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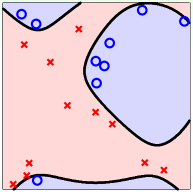

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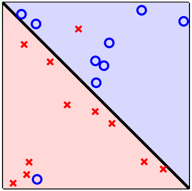
Model Selection Problem



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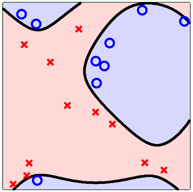

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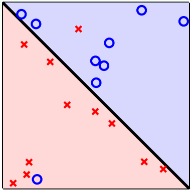
Model Selection Problem



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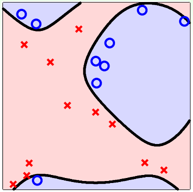

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- arguably the **most important** practical problem of ML

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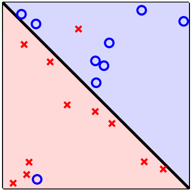

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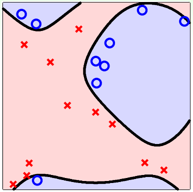

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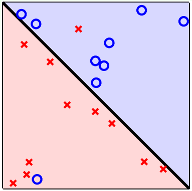
how to select?

Model Selection Problem



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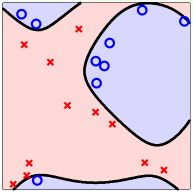

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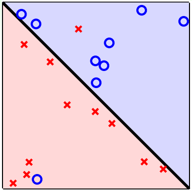
how to select? **visually?**

Model Selection Problem



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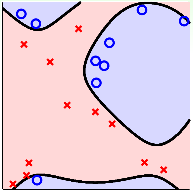

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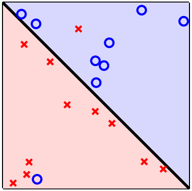
how to select? **visually?**
—no, remember Lecture 12? :-)

Model Selection by Best E_{in}



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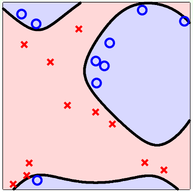
select by best E_{in}?

$$m^* = \underset{1 \le m \le M}{\operatorname{argmin}}(E_m = E_{\text{in}}(\mathcal{A}_m(\mathcal{D})))$$



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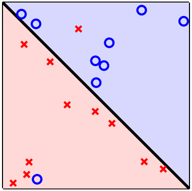

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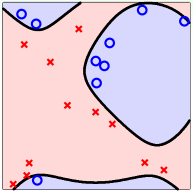

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- $\mathbf{\Phi}_{1126}$ always more preferred over $\mathbf{\Phi}_1$;
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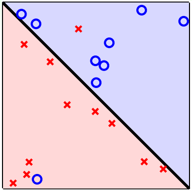

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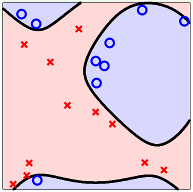

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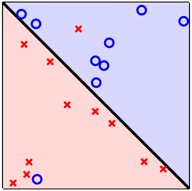

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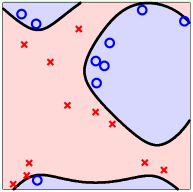

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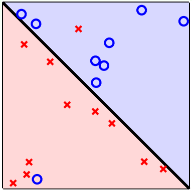

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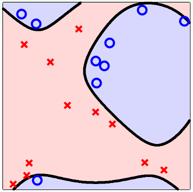

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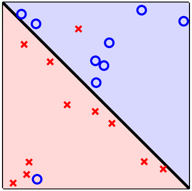
Model Selection by Best E_{in}



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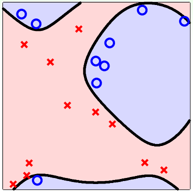

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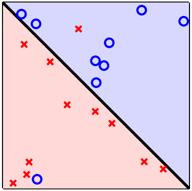
- if $\mathcal{A}_1$ minimizes E_{in} over $\mathcal{H}_1$ and $\mathcal{A}_2$ minimizes E_{in} over $\mathcal{H}_2$, $\Longrightarrow g_{m^*}$ achieves minimal E_{in} over $\mathcal{H}_1 \cup \mathcal{H}_2$

Model Selection by Best E_{in}



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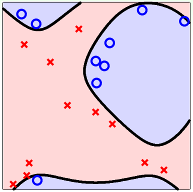

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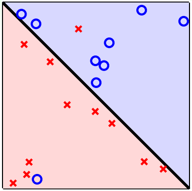
  $\Longrightarrow$ 'model selection + learning' pays $d_{\text{VC}}(\mathcal{H}_1 \cup \mathcal{H}_2)$

Model Selection by Best E_{in}



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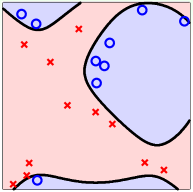

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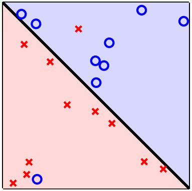
  —**bad generalization?**

Model Selection by Best E_{in}



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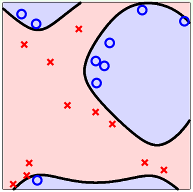

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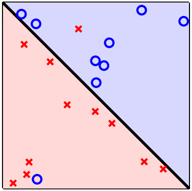
selecting by E_{in} is **dangerous**

Model Selection by Best E_{test}



$\mathcal{H}_1$

select by best E_{test}, which is evaluated on a fresh $\mathcal{D}_{\text{test}}$?

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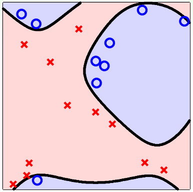

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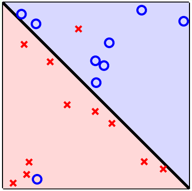
Model Selection by Best E_{test}



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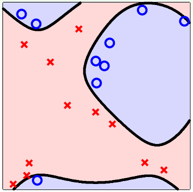
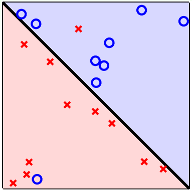


$\mathcal{H}_2$

- generalization guarantee (finite-bin Hoeffding):

Model Selection by Best E_{test}



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select by best E_{test}, which is evaluated on a fresh $\mathcal{D}_{\text{test}}$?

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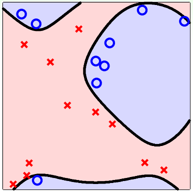

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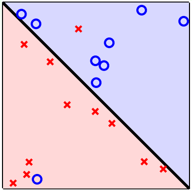

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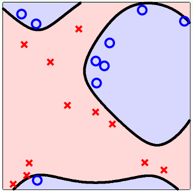

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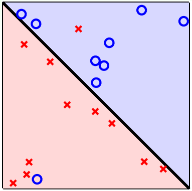

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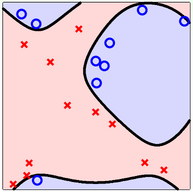

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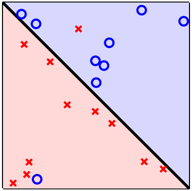

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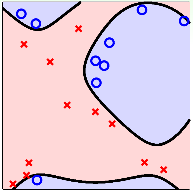

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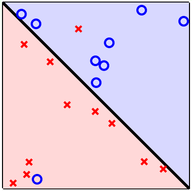

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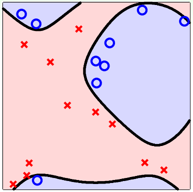

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selecting by E_{test} is **infeasible** and **cheating**

Comparison between E_{in} and E_{test}

in-sample error E_{in}

- calculated from $\mathcal{D}$

test error E_{test}

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Comparison between E_{in} and E_{test}

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- feasible on hand

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- **feasible** on hand

Comparison between E_{in} and E_{test}

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selecting by E_{val}: **legal cheating :-)**

Fun Time

For $\mathcal{X} = \mathbb{R}^d$, consider two hypothesis sets, $\mathcal{H}_+$ and $\mathcal{H}_-$. The first hypothesis set contains all perceptrons with $w_1 \geq 0$, and the second hypothesis set contains all perceptrons with $w_1 \leq 0$. Denote g_+ and g_- as the minimum-E_{in} hypothesis in each hypothesis set, respectively. Which statement below is true?

1. If $E_{\text{in}}(g_+) < E_{\text{in}}(g_-)$, then g_+ is the minimum-E_{in} hypothesis of all perceptrons in $\mathbb{R}^d$.
2. If $E_{\text{test}}(g_+) < E_{\text{test}}(g_-)$, then g_+ is the minimum-E_{test} hypothesis of all perceptrons in $\mathbb{R}^d$.
3. The two hypothesis sets are disjoint.
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4. None of the above

Reference Answer: ①

Note that the two hypothesis sets are not disjoint (sharing '$w_1 = 0$' perceptrons) but their union is all perceptrons.

Validation Set $\mathcal{D}_{\text{val}}$

$$\underbrace{\mathcal{D}}_{\text{size } N} \rightarrow \qquad \underbrace{\mathcal{D}_{\text{val}}}_{\text{size } K}$$

- $\mathcal{D}_{\text{val}} \subset \mathcal{D}$: called **validation set**—'on-hand' simulation of test set

Validation Set $\mathcal{D}_{\text{val}}$

$$\underbrace{\mathcal{D}}_{\text{size } N} \;\rightarrow\; \qquad \underbrace{\mathcal{D}_{\text{val}}}_{\text{size } K}$$

$E_{\text{in}}(h) \uparrow \mathcal{D}$ $\qquad$ $E_{\text{val}}(h) \uparrow \mathcal{D}_{\text{val}}$

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Validation Set $\mathcal{D}_{\text{val}}$

$$E_{\text{in}}(h) \qquad\qquad\qquad E_{\text{val}}(h)$$

$$\uparrow \qquad\qquad\qquad\qquad \uparrow$$

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- $\mathcal{D}_{\text{val}} \subset \mathcal{D}$: called **validation set**—'on-hand' simulation of test set
- to connect E_{val} with E_{out}:
  $\mathcal{D}_{\text{val}} \overset{iid}{\sim} P(\mathbf{x}, y) \Longleftarrow$ select K examples from $\mathcal{D}$ at random

Validation Set $\mathcal{D}_{\text{val}}$

$$\underbrace{\mathcal{D}}_{\text{size } N} \rightarrow \underbrace{\mathcal{D}_{\text{train}}}_{\text{size } N-K} \cup \underbrace{\mathcal{D}_{\text{val}}}_{\text{size } K}$$

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Validation Set $\mathcal{D}_{\text{val}}$

$$
\begin{array}{ccccc}
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\uparrow & & & & \uparrow \\
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\downarrow & & \downarrow & & \\
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$$m^* = \underset{1 \le m \le M}{\text{argmin}}\left(E_m = E_{\text{val}}(\mathcal{A}_m(\mathcal{D}_{\text{train}}))\right)$$

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—**learning curve, remember? :-)**

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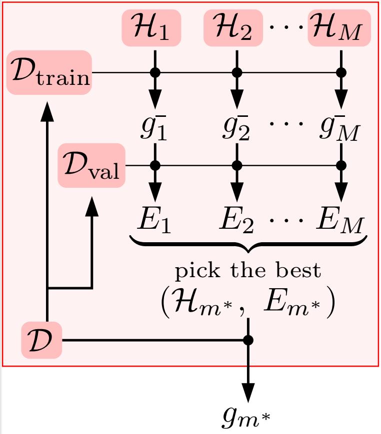

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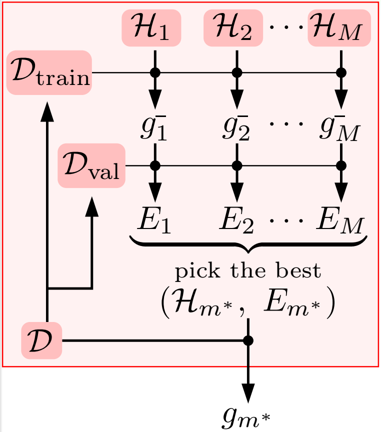

$$E_{\text{out}}(g_{m^*}) \le E_{\text{out}}(g_{m^*}^-) \le E_{\text{val}}(g_{m^*}^-) + O\left(\sqrt{\frac{\log M}{K}}\right)$$

Validation in Practice

use validation to select between $\mathcal{H}_{\mathbf{\Phi}_5}$ and $\mathcal{H}_{\mathbf{\Phi}_{10}}$

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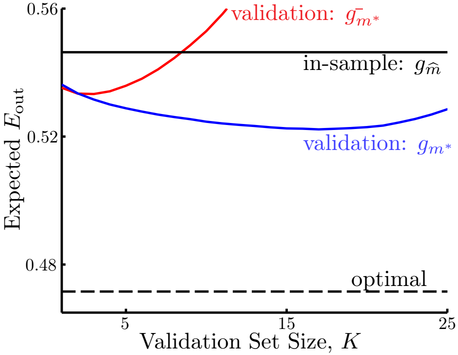

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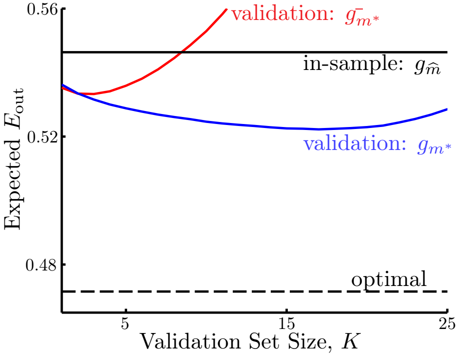

- in-sample: selection with E_{in}

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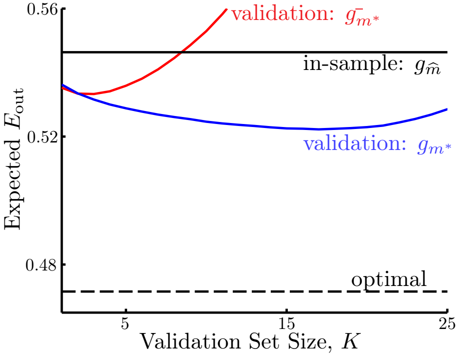

- in-sample: selection with E_{in}
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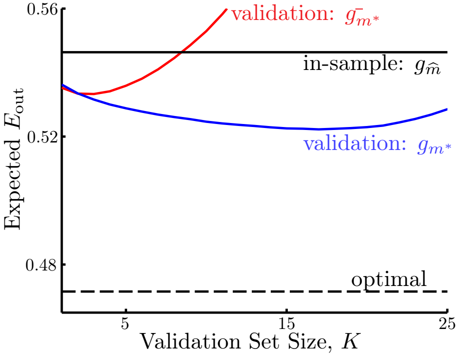

- in-sample: selection with E_{in}
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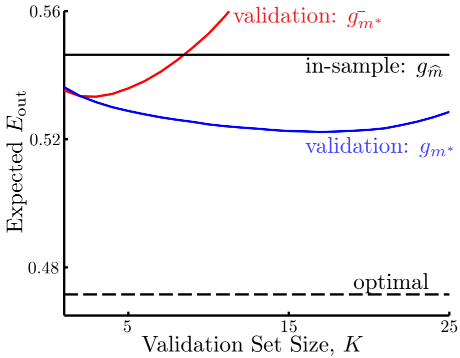

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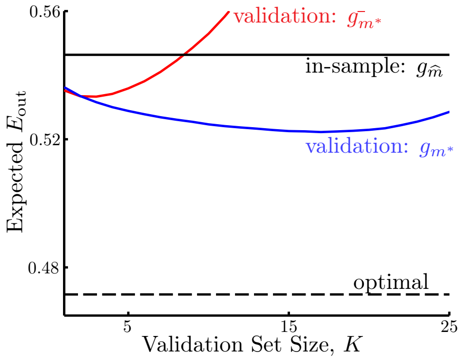

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  —$E_{\text{out}}(g_{m^*}) \le E_{\text{out}}(g^-_{m^*})$ indeed

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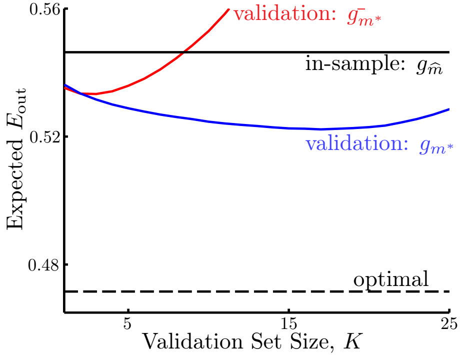

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why is sub-g worse than in-sample some time?

The Dilemma about K

reasoning of validation:

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

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- large K: **every** $E_{\text{val}} \approx E_{\text{out}}$,

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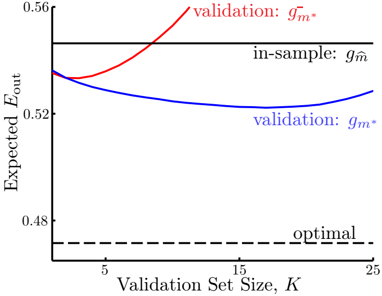

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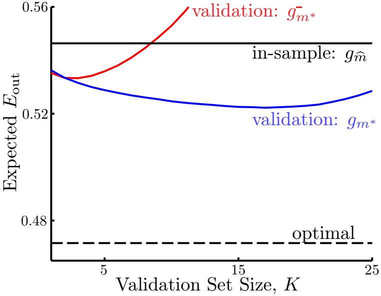
- small K: every $g_m^- \approx g_m$,



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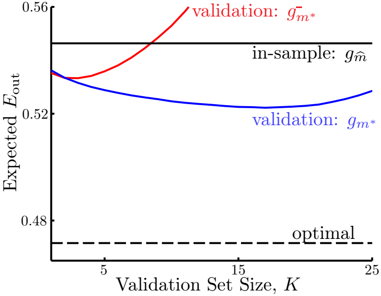
$$E_{out}(g) \underset{\text{(small } K)}{\approx} E_{out}(g^-) \underset{\text{(large } K)}{\approx} E_{val}(g^-)$$

- large K: **every** $E_{val} \approx E_{out}$, but all g_m^- much worse than g_m
- small K: every $g_m^- \approx g_m$, but E_{val} far from E_{out}



The Dilemma about K

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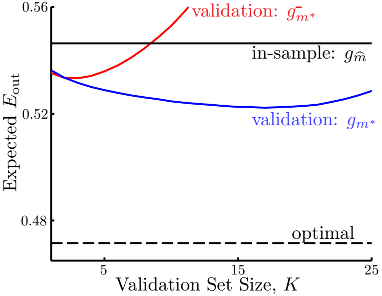

practical rule of thumb: $K = \frac{N}{5}$

Fun Time

For a learning model that takes N^2 seconds of training when using N examples, what is the total amount of seconds needed when running the whole validation procedure with $K = \frac{N}{5}$ on 25 such models with different parameters to get the final g_{m^*}?

1. $6N^2$
2. $17N^2$
3. $25N^2$
4. $26N^2$

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Reference Answer: 2

To get all the g_m^-, we need $\frac{16}{25}N^2 \cdot 25$ seconds.
Then to get g_{m^*}, we need another N^2 seconds.
So in total we need $17N^2$ seconds.

Extreme Case: $K = 1$

reasoning of validation:

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

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Extreme Case: $K = 1$

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- make e_n closer to $E_{\text{out}}(g)$?

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- leave-one-out cross validation estimate:

$$E_{\text{loocv}}(\mathcal{H}, \mathcal{A}) = \frac{1}{N}\sum_{n=1}^{N} e_n = \frac{1}{N}\sum_{n=1}^{N} \text{err}(g_n^-(\mathbf{x}_n), y_n)$$

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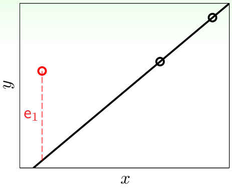
hope: $E_{\text{loocv}}(\mathcal{H}, \mathcal{A}) \approx E_{\text{out}}(g)$

Illustration of Leave-One-Out



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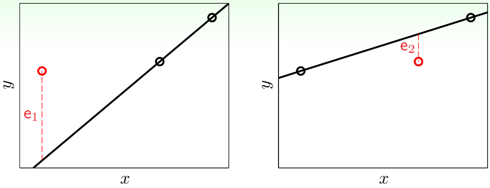

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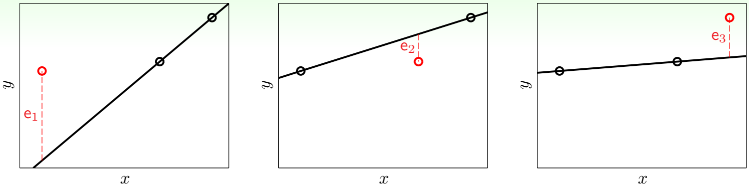

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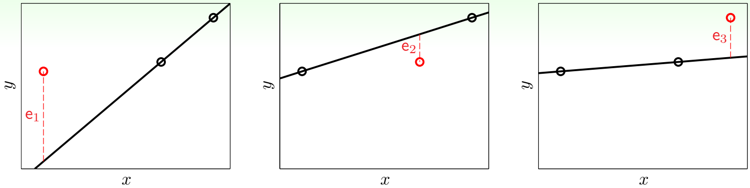

$$E_{\text{loocv}}(\text{linear}) = \frac{1}{3}(e_1 + e_2 + e_3)$$

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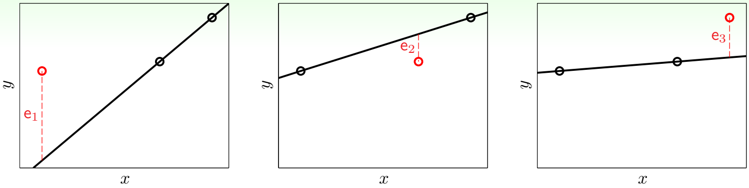

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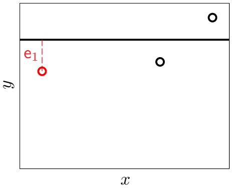

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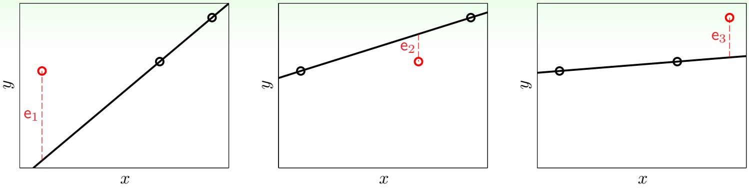

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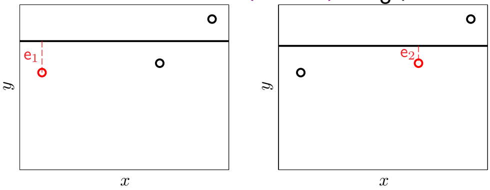

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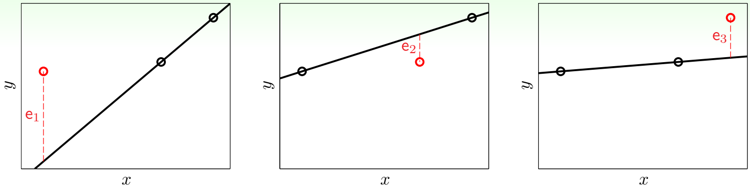

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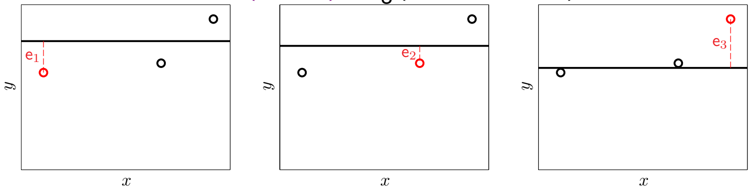

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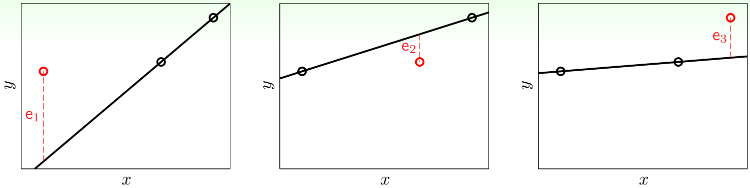

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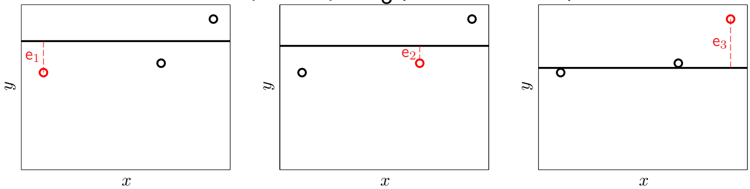

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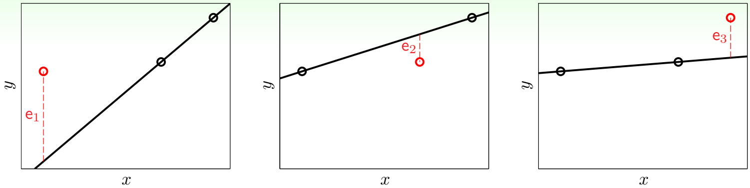

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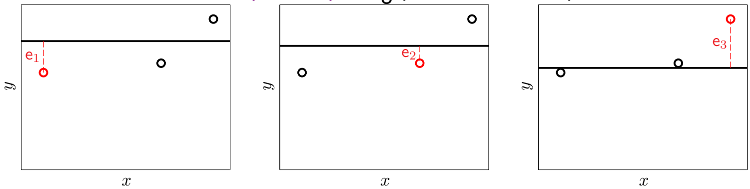

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which one would you choose?

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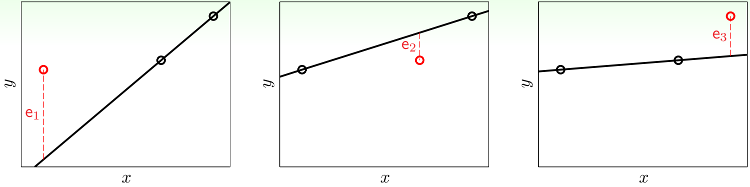

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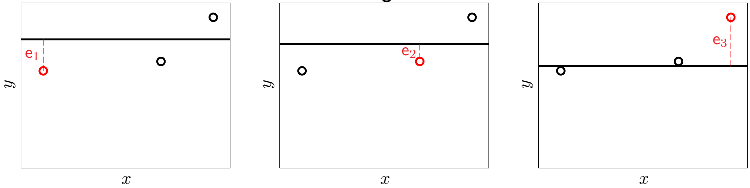

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which one would you choose?

$$m^* = \underset{1 \le m \le M}{\text{argmin}}(E_m = E_{\text{loocv}}(\mathcal{H}_m, \mathcal{A}_m))$$

Theoretical Guarantee of Leave-One-Out Estimate

does $E_{\text{loocv}}(\mathcal{H}, \mathcal{A})$ say something about $E_{\text{out}}(g)$?

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$$= \overline{E_{\text{out}}}(N-1)$$

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$$= \quad \frac{1}{N}\sum_{n=1}^{N} \underset{\mathcal{D}_n}{\mathcal{E}}$$

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$$
\begin{aligned}
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&= \quad \frac{1}{N} \sum_{n=1}^{N} \mathop{\mathcal{E}}_{\mathcal{D}_n} E_{\text{out}}(g_n^-) \\
&= \quad \frac{1}{N} \sum_{n=1}^{N} \qquad\qquad = \overline{E_{\text{out}}}(N-1)
\end{aligned}
$$

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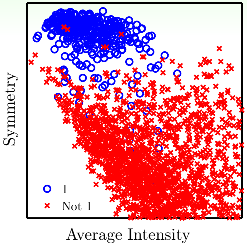
$$= \frac{1}{N}\sum_{n=1}^{N} \overline{E_{\text{out}}}(N-1) = \overline{E_{\text{out}}}(N-1)$$

expected $E_{\text{loocv}}(\mathcal{H}, \mathcal{A})$ says something about expected $E_{\text{out}}(g^-)$
—often called 'almost unbiased estimate of $E_{\text{out}}(g)$'

Leave-One-Out in Practice



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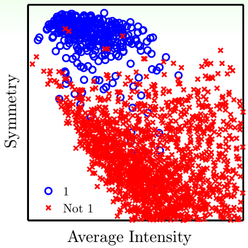
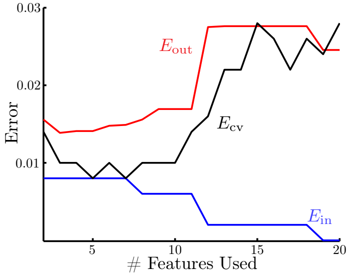
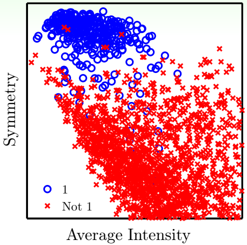
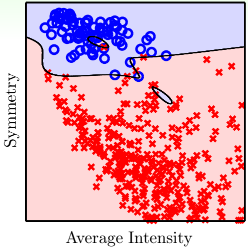


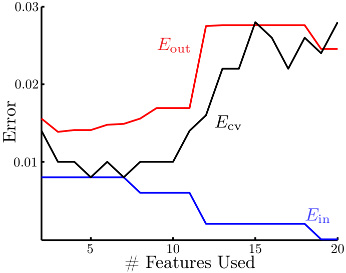


Leave-One-Out in Practice





select by E_{in}



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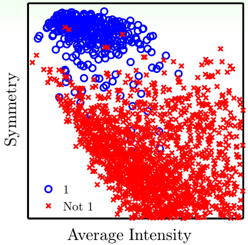

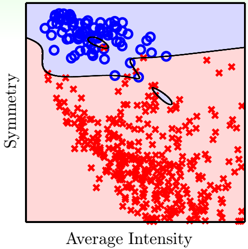

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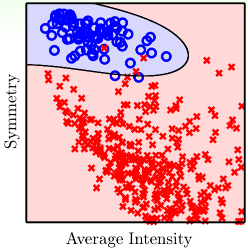
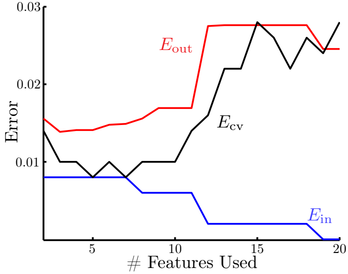
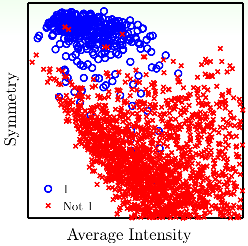
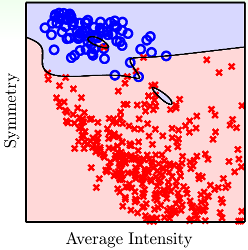


select by E_{loocv}



Leave-One-Out in Practice





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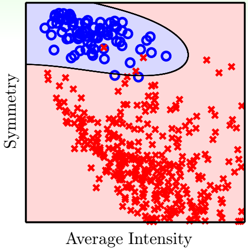
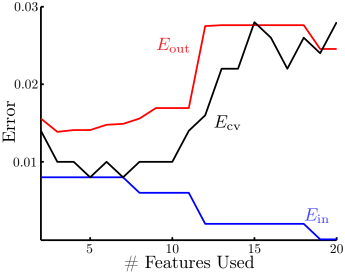


select by E_{loocv}



E_{loocv} much better than E_{in}

Fun Time

Consider three examples $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), (\mathbf{x}_3, y_3)$ with $y_1 = 1$, $y_2 = 5$, $y_3 = 7$. If we use E_{loocv} to estimate the performance of a learning algorithm that predicts with the average y value of the data set—the optimal constant prediction with respect to the squared error. What is E_{loocv} (squared error) of the algorithm?

1. 0
2. $\frac{56}{9}$
3. $\frac{60}{9}$
4. 14

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4. 14

Reference Answer: ④

This is based on a simple calculation of $e_1 = (1 - 6)^2, e_2 = (5 - 4)^2, e_3 = (7 - 3)^2$.

Disadvantages of Leave-One-Out Estimate

Computation

$$E_{\text{loocv}}(\mathcal{H}, \mathcal{A}) = \frac{1}{N} \sum_{n=1}^{N} e_n = \frac{1}{N} \sum_{n=1}^{N} \text{err}(g_n^-(\mathbf{x}_n), y_n)$$

- *N* 'additional' training per model, not always feasible in practice

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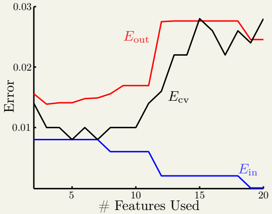

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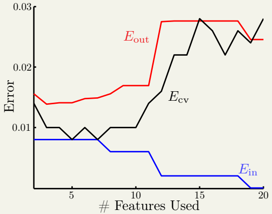

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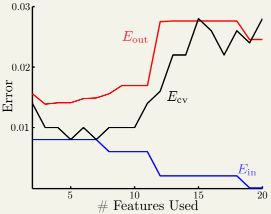

E_{loocv}: not often used practically

V-fold Cross Validation

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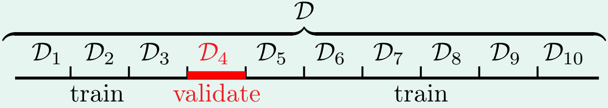

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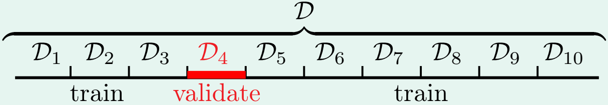

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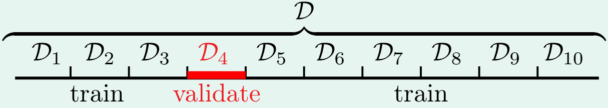

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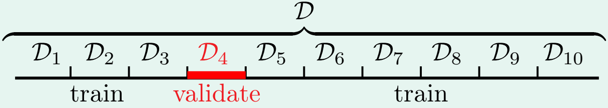

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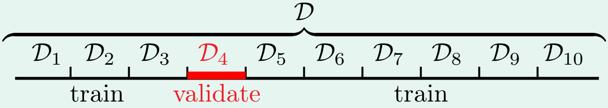

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practical rule of thumb: $V = 10$

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‘Selecting’ Validation Tool

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do not fool yourself and others **:-)**, report test result, not best validation result

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For a learning model that takes N^2 seconds of training when using N examples, what is the total amount of seconds needed when running 10-fold cross validation on 25 such models with different parameters to get the final g_{m^*}?

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Reference Answer: 3

To get all the E_{cv}, we need $\frac{81}{100}N^2 \cdot 10 \cdot 25$ seconds. Then to get g_{m^*}, we need another N^2 seconds. So in total we need $\frac{407}{2}N^2$ seconds.

Summary

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn **Better**?

Lecture 14: Regularization

Lecture 15: Validation

- Model Selection Problem
  dangerous by E_{in} and dishonest by E_{test}
- Validation
  select with $E_{\text{val}}(\mathcal{A}_m(\mathcal{D}_{\text{train}}))$ while returning $\mathcal{A}_{m^*}(\mathcal{D})$
- Leave-One-Out Cross Validation
  huge computation for almost unbiased estimate
- V-Fold Cross Validation
  reasonable computation and performance

- **next: something 'up my sleeve'**