

Machine Learning Foundations

(機器學習基石)



Lecture 15: Validation

Hsuan-Tien Lin (林軒田)

htlin@csie.ntu.edu.tw

Department of Computer Science
& Information Engineering

National Taiwan University
(國立台灣大學資訊工程系)



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 . . .

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

×

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

×

$\eta \in \{ 1, 0.01, 0.0001 \}$

×

$\Phi \in \{ \text{linear, quadratic, poly-10, Legendre-poly-10} \}$

×

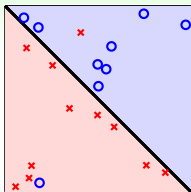
$\Omega(\mathbf{w}) \in \{ \text{L2 regularizer, L1 regularizer, symmetry regularizer} \}$

×

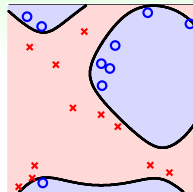
$\lambda \in \{ 0, 0.01, 1 \}$

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

模型选择 Model Selection Problem

 \mathcal{H}_1

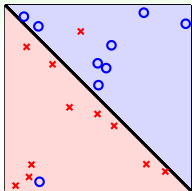
which one do you prefer? :-)

 \mathcal{H}_2

- given: M models $\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_M$, each with corresponding algorithm $\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_M$
- goal: select \mathcal{H}_{m^*} such that $g_{m^*} = \mathcal{A}_{m^*}(\mathcal{D})$ is of low $E_{\text{out}}(g_{m^*})$
- **unknown** E_{out} due to unknown $P(\mathbf{x})$ & $P(y|\mathbf{x})$, as always :-)
- arguably the **most important** practical problem of ML

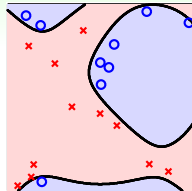
how to select? **visually?**
—no, remember Lecture 12? :-)

Model Selection by Best E_{in}

 \mathcal{H}_1

select by best E_{in} ?

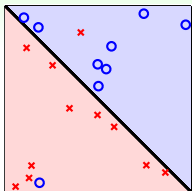
$$m^* = \operatorname{argmin}_{1 \leq m \leq M} (E_m = E_{in}(\mathcal{A}_m(\mathcal{D})))$$

 \mathcal{H}_2

- Φ_{1126} always more preferred over Φ_1 ;
 $\lambda = 0$ always more preferred over $\lambda = 0.1$ —**overfitting?**
- if \mathcal{A}_1 minimizes E_{in} over \mathcal{H}_1 and \mathcal{A}_2 minimizes E_{in} over \mathcal{H}_2 ,
 $\implies g_{m^*}$ achieves minimal E_{in} over $\mathcal{H}_1 \cup \mathcal{H}_2$
 \implies ‘**model selection** + learning’ pays $d_{vc}(\mathcal{H}_1 \cup \mathcal{H}_2)$
 —**bad generalization?**

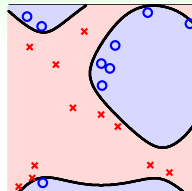
selecting by E_{in} is **dangerous**

Model Selection by Best E_{test}

 \mathcal{H}_1

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

$$m^* = \operatorname{argmin}_{1 \leq m \leq M} (E_m = E_{\text{test}}(\mathcal{A}_m(\mathcal{D})))$$

 \mathcal{H}_2

- generalization guarantee (finite-bin Hoeffding):

$$E_{\text{out}}(g_{m^*}) \leq E_{\text{test}}(g_{m^*}) + O\left(\sqrt{\frac{\log M}{N_{\text{test}}}}\right)$$

—**yes! strong guarantee :-)**

- but where is $\mathcal{D}_{\text{test}}$?—**your boss's safe, maybe? :-)**

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

Comparison between E_{in} and E_{test}

in-sample error E_{in}

- calculated from \mathcal{D}
- **feasible** on hand
- ‘contaminated’ as \mathcal{D} also used by \mathcal{A}_m to ‘select’ g_m

test error E_{test}

- calculated from $\mathcal{D}_{\text{test}}$
- **infeasible** in boss’s safe
- ‘clean’ as $\mathcal{D}_{\text{test}}$ never used for selection before

something in between: E_{val}

- calculated from $\mathcal{D}_{\text{val}} \subset \mathcal{D}$
- **feasible** on hand
- ‘clean’ **if** \mathcal{D}_{val} never used by \mathcal{A}_m before

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.
- 4 None of the above

Fun Time

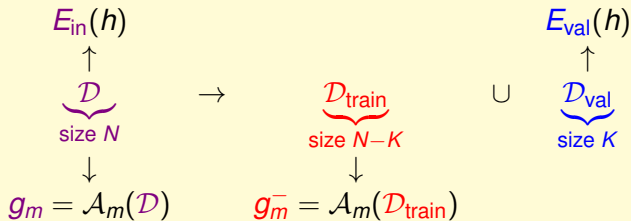
For $\mathcal{X} = \mathbb{R}^d$, consider two hypothesis sets, \mathcal{H}_+ and \mathcal{H}_- . The first hypothesis set contains all perceptrons with $w_1 \geq 0$, and the second hypothesis set contains all perceptrons with $w_1 \leq 0$. Denote g_+ and g_- as the minimum- E_{in} hypothesis in each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



- $\mathcal{D}_{\text{val}} \subset \mathcal{D}$: called **validation set**—‘on-hand’ simulation of test set
- to connect E_{val} with E_{out} :
 $\mathcal{D}_{\text{val}} \stackrel{iid}{\sim} P(\mathbf{x}, y) \iff$ select K examples from \mathcal{D} at random
- to make sure \mathcal{D}_{val} ‘clean’:
 feed only $\mathcal{D}_{\text{train}}$ to \mathcal{A}_m for model selection

$$E_{\text{out}}(g_m^-) \leq E_{\text{val}}(g_m^-) + O\left(\sqrt{\frac{\log M}{K}}\right)$$

Model Selection by Best E_{val}

$$m^* = \underset{1 \leq m \leq M}{\operatorname{argmin}} (E_m = E_{\text{val}}(\mathcal{A}_m(\mathcal{D}_{\text{train}})))$$

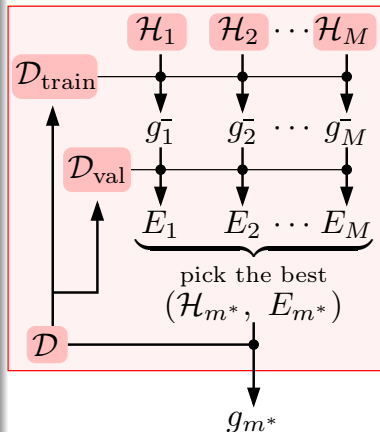
- generalization guarantee for all m :

$$E_{\text{out}}(\mathbf{g}_m^-) \leq E_{\text{val}}(\mathbf{g}_m^-) + O\left(\sqrt{\frac{\log M}{K}}\right)$$

- heuristic gain from $N - K$ to N :

$$E_{\text{out}}\left(\underbrace{\mathbf{g}_{m^*}}_{\mathcal{A}_{m^*}(\mathcal{D})}\right) \leq E_{\text{out}}\left(\underbrace{\mathbf{g}_{m^*}^-}_{\mathcal{A}_{m^*}(\mathcal{D}_{\text{train}})}\right)$$

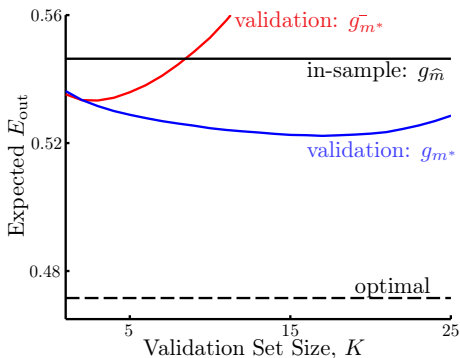
—learning curve, remember? :-)



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

Validation in Practice

use validation to select between \mathcal{H}_{Φ_5} and $\mathcal{H}_{\Phi_{10}}$



- in-sample: selection with E_{in}
- optimal: cheating-selection with E_{test}
- **sub- g** : selection with E_{val} and report \bar{g}_m^*
- **full- g** : selection with E_{val} and report g_m^*
 — $E_{\text{out}}(g_m^*) \leq E_{\text{out}}(\bar{g}_m^*)$ indeed

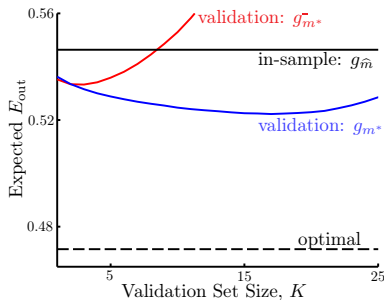
why is **sub- g** worse than in-sample some time?

The Dilemma about K

reasoning of validation:

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

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



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 $26N^2$

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 $26N^2$

只需要计算training阶段以及最后选择最小的g在全部数据集上的计算即可。

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:

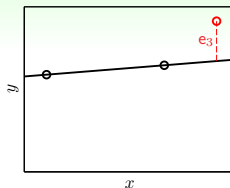
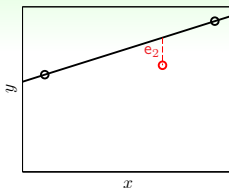
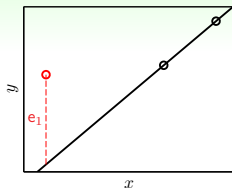
$$E_{\text{out}}(\textcolor{violet}{g}) \underset{\text{(small } K\text{)}}{\approx} E_{\text{out}}(\textcolor{red}{g}^-) \underset{\text{(large } K\text{)}}{\approx} E_{\text{val}}(\textcolor{red}{g}^-)$$

- take $K = 1$? $\mathcal{D}_{\text{val}}^{(n)} = \{(\mathbf{x}_n, y_n)\}$ and $E_{\text{val}}^{(n)}(\textcolor{red}{g}^-) = \text{err}(\textcolor{red}{g}^-(\mathbf{x}_n), y_n) = \textcolor{violet}{e}_n$
- make $\textcolor{violet}{e}_n$ closer to $E_{\text{out}}(\textcolor{violet}{g})$?—average over possible $E_{\text{val}}^{(n)}$
- leave-one-out cross validation estimate:
留一交叉验证法

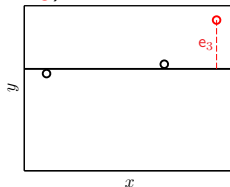
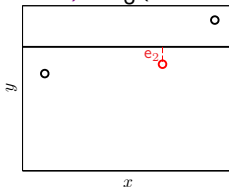
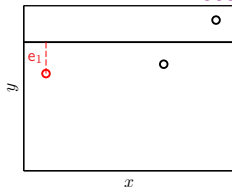
$$E_{\text{loocv}}(\mathcal{H}, \mathcal{A}) = \frac{1}{N} \sum_{n=1}^N \textcolor{violet}{e}_n = \frac{1}{N} \sum_{n=1}^N \text{err}(\textcolor{red}{g}^-(\mathbf{x}_n), y_n)$$

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

Illustration of Leave-One-Out



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



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

which one would you choose?

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

Theoretical Guarantee of Leave-One-Out Estimate

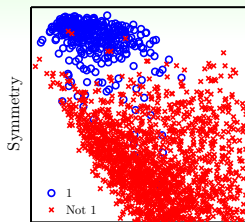
does $E_{\text{loocv}}(\mathcal{H}, \mathcal{A})$ say something about $E_{\text{out}}(g)$?

yes, for average E_{out} on size- $(N - 1)$ data

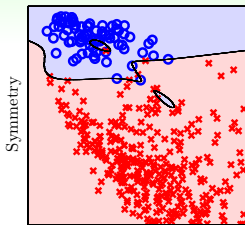
$$\begin{aligned}
 \mathcal{E}_{\mathcal{D}} E_{\text{loocv}}(\mathcal{H}, \mathcal{A}) &= \mathcal{E}_{\mathcal{D}} \frac{1}{N} \sum_{n=1}^N e_n = \frac{1}{N} \sum_{n=1}^N \mathcal{E}_{\mathcal{D}} e_n \\
 &= \frac{1}{N} \sum_{n=1}^N \mathcal{E}_{\mathcal{D}_n(\mathbf{x}_n, y_n)} \text{err}(\mathbf{g}_n^-(\mathbf{x}_n), y_n) \\
 &= \frac{1}{N} \sum_{n=1}^N \mathcal{E}_{\mathcal{D}_n} E_{\text{out}}(\mathbf{g}_n^-) \\
 &= \frac{1}{N} \sum_{n=1}^N \overline{E_{\text{out}}(N-1)} = \overline{E_{\text{out}}(N-1)}
 \end{aligned}$$

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

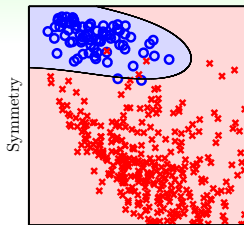
Leave-One-Out in Practice



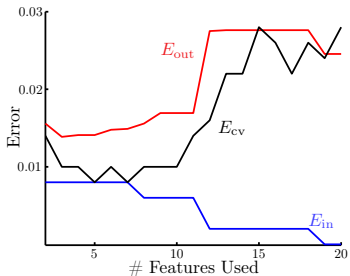
Average Intensity



Average Intensity

select by E_{in} 

Average Intensity

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

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

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

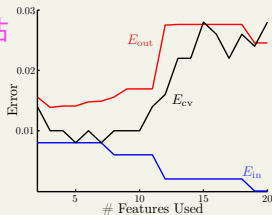
LOO花费的代价很大。一般在实践中不会使用

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

- N ‘additional’ training per model, not always feasible in practice
- except ‘special case’: 线性回归有解析解，所以可以用 LOO

Stability—due to variance of single-point estimates

不稳定，由于单个点估计的方差导致

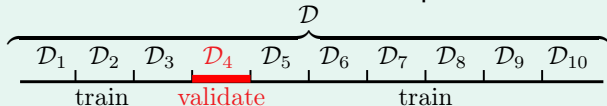


E_{loocv} : not often used practically

V-fold Cross Validation

how to **decrease computation need** for cross validation?

- essence of leave-one-out cross validation: partition \mathcal{D} to N parts, taking $N - 1$ for training and 1 for validation orderly
- V-fold cross-validation: random-partition of \mathcal{D} to **V equal parts**,



take $V - 1$ for training and 1 for validation orderly

选取 $V-1$ 份用来训练，剩下的1份用来作为验证

$$E_{cv}(\mathcal{H}, \mathcal{A}) = \frac{1}{V} \sum_{v=1}^V E_{val}^{(v)}(\mathbf{g}_v^-)$$

LOO可以看做V折交叉验证的特例：此时 $V=N$ ，每份有1个样本

- selection by E_{cv} : $m^* = \operatorname{argmin}_{1 \leq m \leq M} (E_m = E_{cv}(\mathcal{H}_m, \mathcal{A}_m))$

practical rule of thumb: $V = 10$

Final Words on Validation

'Selecting' Validation Tool

- **V-Fold** generally preferred over single validation if computation allows
- **5-Fold or 10-Fold** generally works well:
not necessary to trade V-Fold with Leave-One-Out

Nature of Validation

- all training models: select among hypotheses “初赛”
- all validation schemes: **select among finalists** “复赛”
- all testing methods: just **evaluate** “决赛”

validation still **more optimistic than testing**

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

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 10-fold cross validation on 25 such models with different parameters to get the final g_{m^*} ?

- ① $\frac{47}{2} N^2$
- ② $47 N^2$
- ③ $\frac{407}{2} N^2$
- ④ $407 N^2$

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 10-fold cross validation on 25 such models with different parameters to get the final g_{m^*} ?

- ① $\frac{47}{2} N^2$
- ② $47 N^2$
- ③ $\frac{407}{2} N^2$
- ④ $407 N^2$

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'**