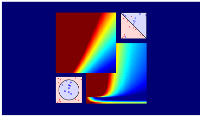
Machine Learning Foundations
(機器學習基石)



Lecture 16: Three Learning Principles

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National Taiwan University
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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 15: Validation

(**crossly**) reserve **validation data** to simulate testing procedure for **model selection**

Lecture 16: Three Learning Principles

- Occam's Razor
- Sampling Bias
- Data Snooping
- Power of Three

Occam's Razor

> *An explanation of the data should be made as simple as possible, but no simpler.*—Albert Einstein**?** (1879-1955)

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(entities must not be multiplied **beyond necessity**)
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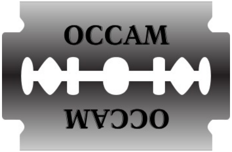
'**Occam's razor**' for trimming down unnecessary explanation



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Occam's Razor for Learning

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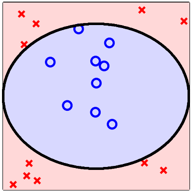
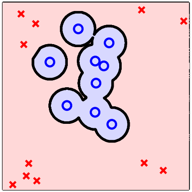


which one do you prefer? :-)



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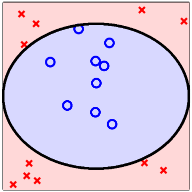

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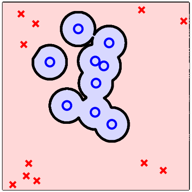

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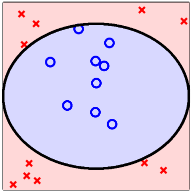

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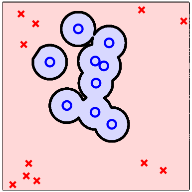

two questions:

1. What does it mean for a model to be simple?
2. How do we know that simpler is better?

Simple Model

simple hypothesis h

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simple: **small hypothesis/model complexity**

Simple is Better

in addition to **math proof** that you have seen, philosophically:

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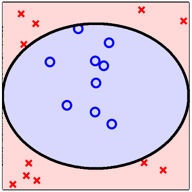

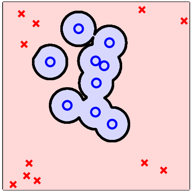

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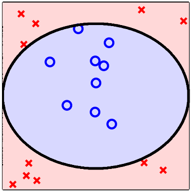

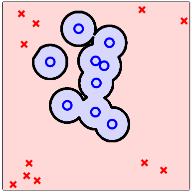

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direct action: **linear first**;
always ask whether **data over-modeled**

Fun Time

Consider the decision stumps in $\mathbb{R}^1$ as the hypothesis set $\mathcal{H}$. Recall that $m_{\mathcal{H}}(N) = 2N$. Consider 10 different inputs $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{10}$ coupled with labels y_n generated iid from a fair coin. What is the probability that the data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{10}$ is separable by $\mathcal{H}$?

1. $\frac{1}{1024}$
2. $\frac{10}{1024}$
3. $\frac{20}{1024}$
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Reference Answer: 3

Of all 1024 possible $\mathcal{D}$, only $2N = 20$ of them is separable by $\mathcal{H}$.

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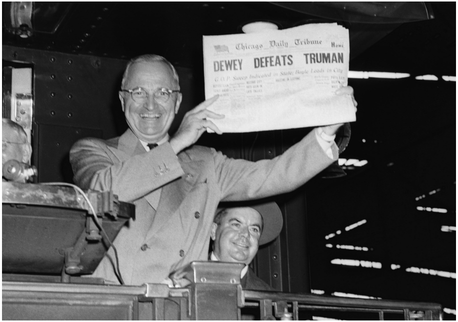
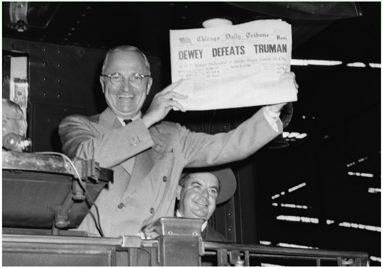


who is this? :-)

The Big Smile Came from . . .



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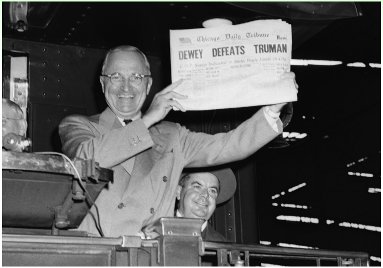

Truman, and **yes he won**

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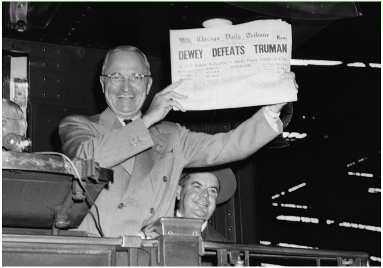

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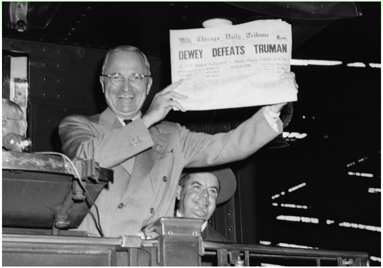

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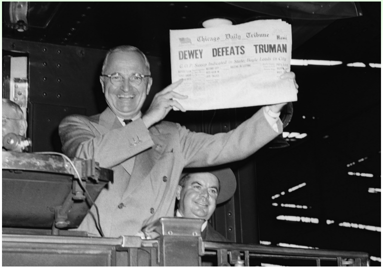

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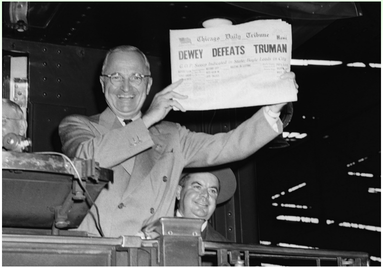

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hint: phones were **expensive :-)**

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'minor' VC assumption:
data and testing **both iid from** P

Sampling Bias in Learning

A True Personal Story

- Netflix competition for movie recommender system:
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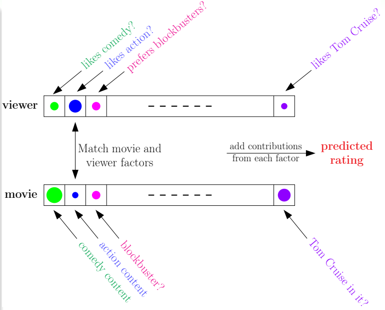

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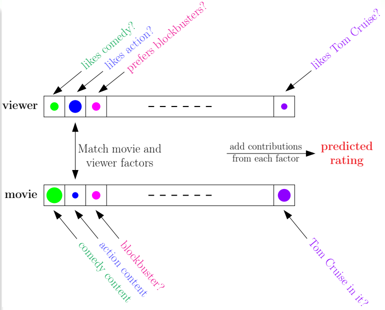

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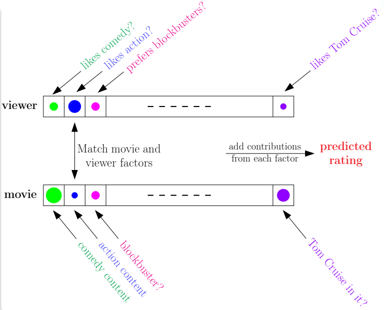

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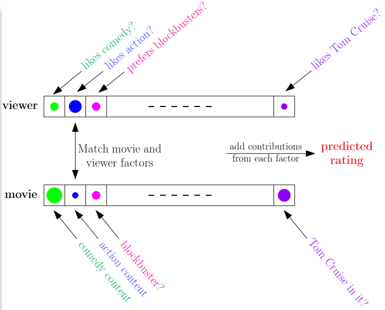

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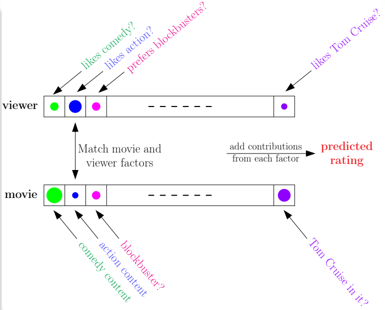

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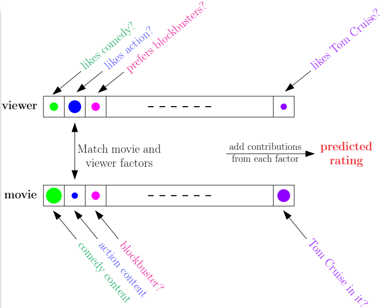

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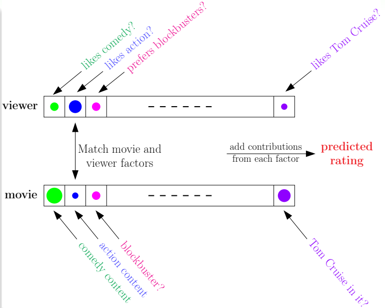

validation: random examples within $\mathcal{D}$;
test: 'last' user records 'after' $\mathcal{D}$

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last puzzle:

danger when learning 'credit card approval' with existing bank records?

Fun Time

If the data $\mathcal{D}$ is an unbiased sample from the underlying distribution P for binary classification, which of the following subset of $\mathcal{D}$ is also an unbiased sample from P?

1. all the positive ($y_n > 0$) examples
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Reference Answer: 2

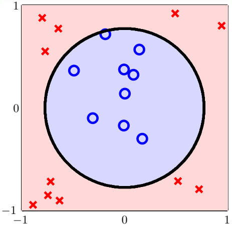
That's how we form the validation set, remember? :-)

Visual Data Snooping

Visualize $\mathcal{X} = \mathbb{R}^2$

- full $\mathbf{\Phi}_2$: $\mathbf{z} = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$, $d_{\text{VC}} = 6$
- or $\mathbf{z} = (1, x_1^2, x_2^2)$, $d_{\text{VC}} = 3$, **after visualizing**?
- or better $\mathbf{z} = (1, x_1^2 + x_2^2)$, $d_{\text{VC}} = 2$?
- or even better $\mathbf{z} = \left(\text{sign}(0.6 - x_1^2 - x_2^2)\right)$?

—careful about **your brain's 'model complexity'**



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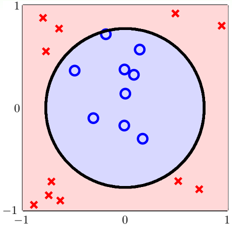

for VC-safety, $\mathbf{\Phi}$ shall be decided **without 'snooping'** data

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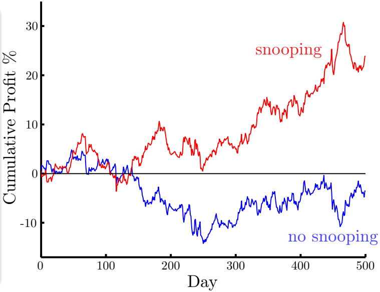

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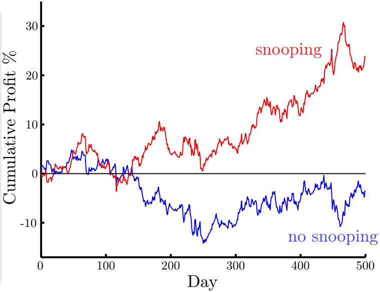

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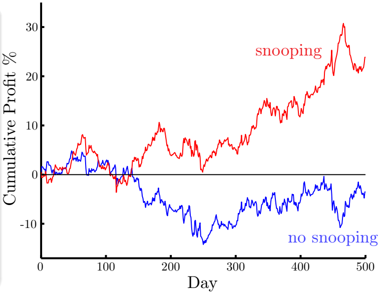

- snooping: shift-scale all values by training + testing
- no snooping: shift-scale all values by training only

Data Snooping by Data Reusing

Research Scenario

benchmark data $\mathcal{D}$

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Data Snooping by Data Reusing

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if you torture the data long enough, it will confess :-)

Dealing with Data Snooping

- truth—**very hard to avoid**, unless being extremely honest

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one secret to winning KDDCups:

careful balance between
data-driven modeling (snooping) and
validation (no-snooping)

Fun Time

Which of the following can result in unsatisfactory test performance in machine learning?

1. data snooping
2. overfitting
3. sampling bias
4. all of the above

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Which of the following can result in unsatisfactory test performance in machine learning?

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Reference Answer: 4

A professional like you should be aware of those! :-)

Three Related Fields

Power of Three

Data Mining

- use **(huge)** data to **find property** that is interesting
- difficult to distinguish ML and DM in reality

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Artificial Intelligence

- compute something that shows **intelligent behavior**
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Three Related Fields

Power of Three

Data Mining

- use **(huge)** data to **find property** that is interesting
- difficult to distinguish ML and DM in reality

Artificial Intelligence

- compute something that shows **intelligent behavior**
- ML is one possible route to realize AI

Statistics

- use data to **make inference** about an unknown process
- statistics contains many useful tools for ML

Three Theoretical Bounds

Power of Three

Hoeffding

$$P[\text{BAD}] \leq 2\exp(-2\epsilon^2 N)$$

- **one** hypothesis
- useful for **verifying/testing**

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VC

$$P[\text{BAD}] \leq 4m_{\mathcal{H}}(2N)\exp(\ldots)$$

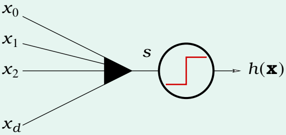
- all $\mathcal{H}$
- useful for **training**

Three Linear Models

Power of Three

PLA/pocket

$$h(\mathbf{x}) = \text{sign}(s)$$



plausible err = 0/1
(small flipping noise)
minimize **specially**

Three Linear Models

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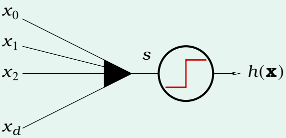

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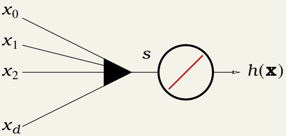
linear regression

$$h(\mathbf{x}) = s$$



friendly err = squared

(easy to minimize)

minimize **analytically**

Three Linear Models

Power of Three

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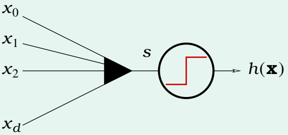

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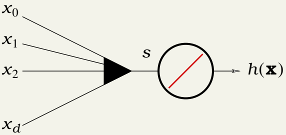


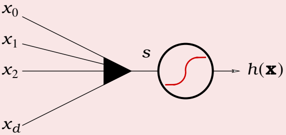
friendly err = squared

(easy to minimize)

minimize **analytically**

logistic regression

$$h(\mathbf{x}) = \theta(s)$$



plausible err = CE

(maximum likelihood)

minimize **iteratively**

Three Key Tools

Power of Three

Feature Transform

$$E_{\text{in}}(\mathbf{w}) \rightarrow E_{\text{in}}(\tilde{\mathbf{w}})$$
$$d_{\text{VC}}(\mathcal{H}) \rightarrow d_{\text{VC}}(\mathcal{H}_{\boldsymbol{\Phi}})$$

- by using **more complicated $\boldsymbol{\Phi}$**
- **lower E_{in}**
- higher d_{VC}

Three Key Tools

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Regularization

$$E_{\text{in}}(\mathbf{w}) \rightarrow E_{\text{in}}(\mathbf{w}_{\text{REG}})$$
$$d_{\text{VC}}(\mathcal{H}) \rightarrow d_{\text{EFF}}(\mathcal{H}, \mathcal{A})$$

- by augmenting **regularizer Ω**
- **lower d_{EFF}**
- higher E_{in}

Three Key Tools

Power of Three

Feature Transform

$$\begin{aligned} E_{\text{in}}(\mathbf{w}) &\rightarrow E_{\text{in}}(\tilde{\mathbf{w}}) \\ d_{\text{VC}}(\mathcal{H}) &\rightarrow d_{\text{VC}}(\mathcal{H}_{\boldsymbol{\Phi}}) \end{aligned}$$

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- by augmenting **regularizer Ω**
- **lower d_{EFF}**
- higher E_{in}

Validation

$$\begin{aligned} E_{\text{in}}(h) &\rightarrow E_{\text{val}}(h) \\ \mathcal{H} &\rightarrow \{g_1^-, \ldots, g_M^-\} \end{aligned}$$

- by reserving K examples as $\mathcal{D}_{\text{val}}$
- **fewer choices**
- fewer examples

Three Learning Principles

Power of Three

Occam's Razer

simple is good

Three Learning Principles

Power of Three

Occam's Razer

simple is good

Sampling Bias

class matches exam

Three Learning Principles

Power of Three

Occam's Razer
simple is good

Sampling Bias
class matches exam

Data Snooping
honesty is best policy

Three Future Directions

Power of Three

More Transform

Three Future Directions

Power of Three

More Transform

More Regularization

Three Future Directions

Power of Three

More Transform	More Regularization	Less Label

Three Future Directions

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More Transform	More Regularization	Less Label

bagging decision tree support vector machine **neural network** *kernel*

AdaBoost aggregation *sparsity* autoencoder **coordinate descent**

dual uniform blending deep learning nearest neighbor decision stump

kernel LogReg large-margin *prototype* quadratic programming **SVR**

GBDT **PCA** `random forest` *matrix factorization* **Gaussian kernel**

soft-margin *k-means* OOB error **RBF network** probabilistic SVM

ready for the **jungle**!

Fun Time

What are the magic numbers that repeatedly appear in this class?

1. 3
2. 1126
3. both 3 and 1126
4. neither 3 nor 1126

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Reference Answer: 3

3 as illustrated, and **you may recall** 1126 **somewhere :-)**

Summary

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

Lecture 15: Validation

Lecture 16: Three Learning Principles

- Occam's Razor
  simple, simple, simple!
- Sampling Bias
  match test scenario as much as possible
- Data Snooping
  any use of data is 'contamination'
- Power of Three
  relatives, bounds, models, tools, principles

- **next: ready for jungle!**