

Regularization and Validation 6

CS 3244
Machine Learning

A




NUS | Computing

Recap from Week 05

Bias

The difference between the average prediction and the true value.



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Bias and Variance

In-Lecture Activity

$$\mathbb{E}_{\mathcal{D}}[(h_{\mathcal{D}}(x) - f(x))^2] = \underbrace{\mathbb{E}_{\mathcal{D}}[(h_{\mathcal{D}}(x) - \bar{h}(x))^2]}_{\text{Q4}} + \underbrace{(\bar{h}(x) - f(x))^2}_{\text{Q5}}$$

Quick Quiz: Which is which?

- Bias
- Variance
- I give up

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Lesson learned

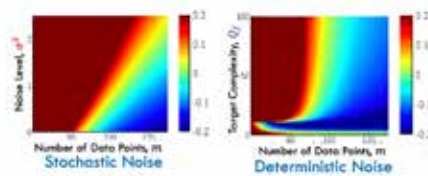
Match the 'model complexity' to the

data resources, not to the **target complexity**.

Quality and Quantity

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Overfit measure: $L_{test}(h_{10}) - L_{test}(h_2)$



Number of Data Points, m

Stochastic Noise

Deterministic Noise

Number of data points	↑	Overfitting	↓
Stochastic Noise	↑	Overfitting	↑
Deterministic Noise	↑	Overfitting	↑

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Upcoming Milestones



Midterm

- 60-minute, 60 marks midterm, on first day of Week 07.
- Open lecture notes, mostly MCQ/MRQ
- Multiple Response Questions that correct for random chance scoring.

Projects

- Project Proposals due on Tue.
- Project Mentors to be assigned after proposal deadline.
- Peer review due next Tue. Done via Google Forms.

Multiple Response Question (MRQ)

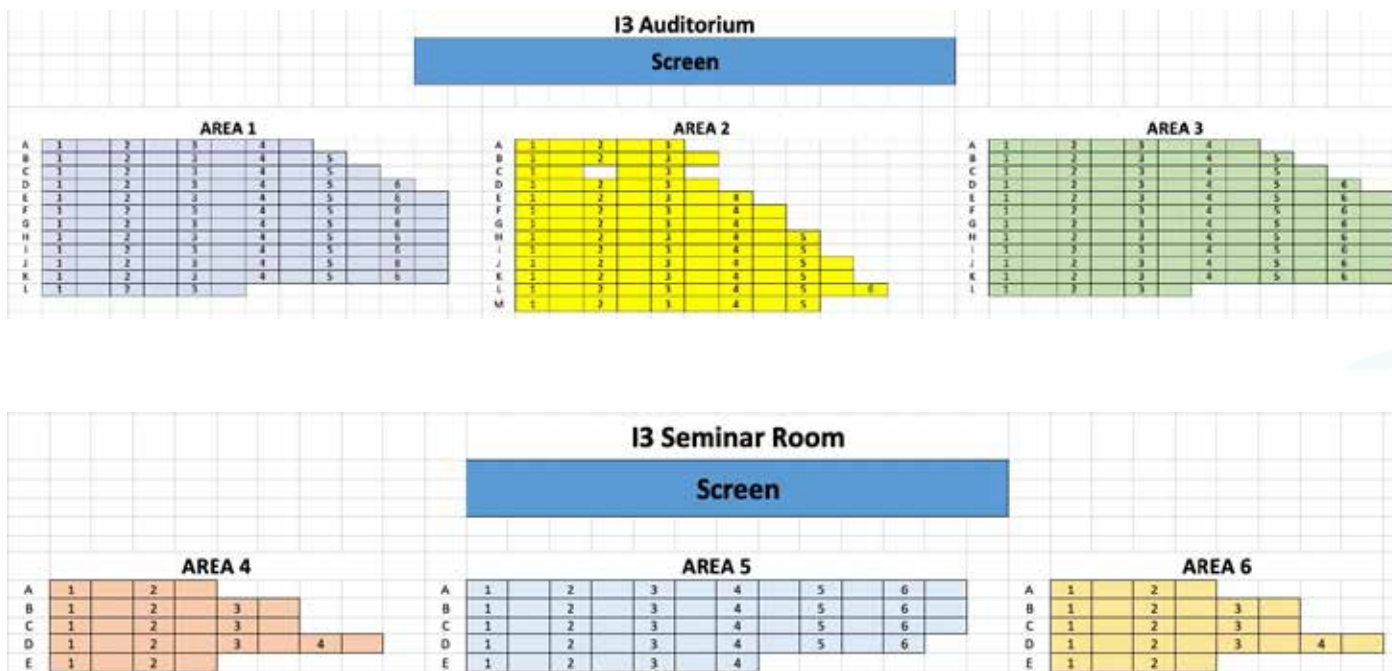


Example:

- 5 option, 4 mark question. Note that leaving all options blank may be a valid entry.
- You marked A, B, C but correct answer was B, C, D.

Treated as a set of binary questions, where random chance agreement, rounded down, is subtracted away.

- 5 options: expected # of binary questions correct: 2.5, rounded to 2.
- You got B, C and E correct, but A, D incorrect: 3 of 5 binary questions correct.
- After chance agreement: 1 of 3 correct = awarded 1.33 marks out of 4 marks.




Forecast for Week 06



Learning Outcomes for this week:

- Understand **Regularization** as a means of restraining the model.
- Choose appropriate doses of regularization for a model.
- Understand and execute **Validation**, as a reality check by peeking (at the bottom line).
- Understand the different forms extending validation to encompass additional estimation.
- Understand how validation and regularization complement each other and their roles in affecting learning.



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Regularization

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Two Cures

In one form or another, $L_{test}(h) = L_{train}(h) + \text{overfit penalty}$

1. **Regularization:** Restrain the model

$$L_{test}(h) = L_{train}(h) + \text{overfit penalty}$$

Regularization estimates this quantity

2. **Validation:** Reality check by peeking (at the bottom line)

$$L_{test}(h) = L_{train}(h) + \text{overfit penalty}$$

Restraining the model

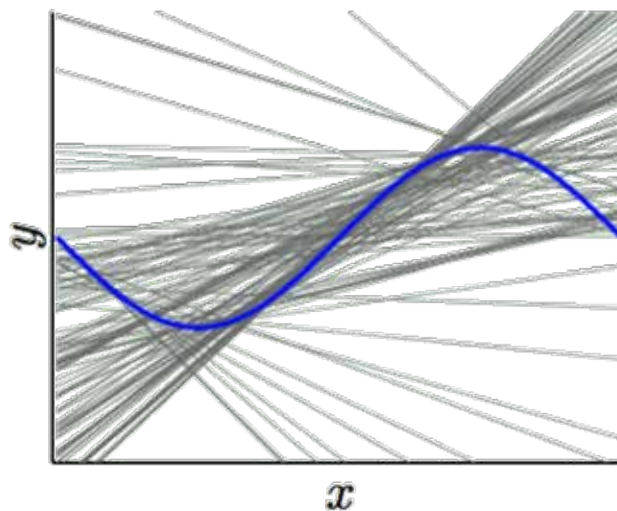


Regularization

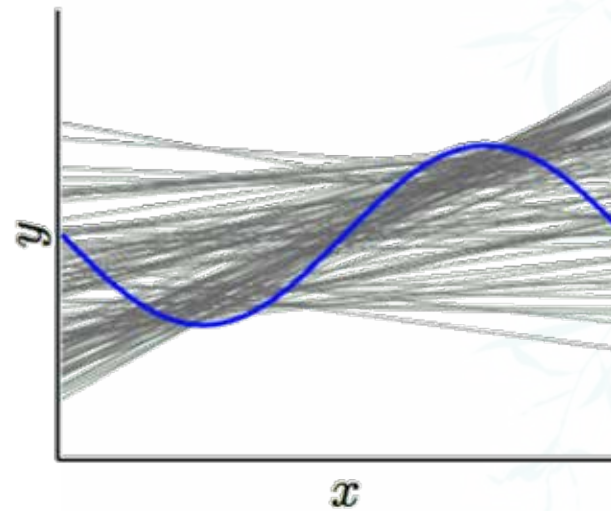
- What is it: A cure for our tendency to fit (get distracted by) the noise, hence improving L_{test} .
- How does it work?
By constraining the model so that we cannot fit the noise.
- Side effect: if we cannot fit the noise, maybe we cannot fit the signal f .

A familiar example

Without regularization



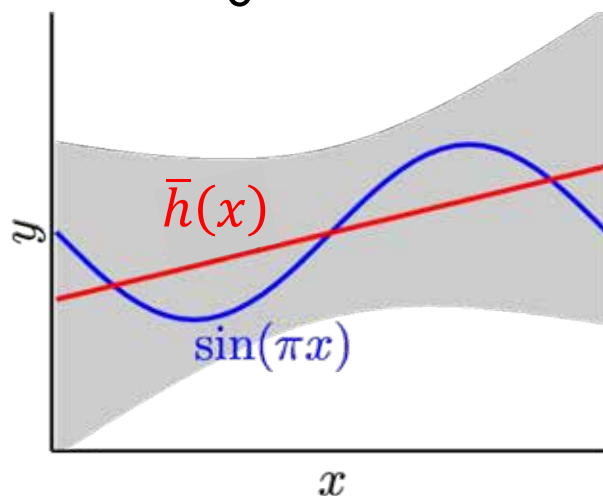
With regularization



Constrain weights to be a bit smaller

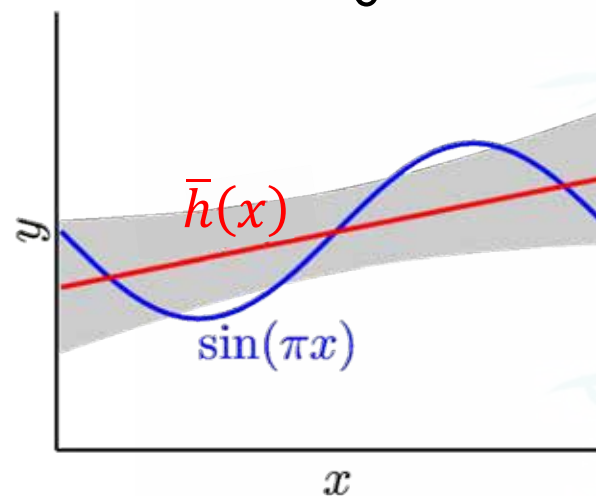
Bias goes up a little

Without regularization



Bias = 0.21
Variance = 1.69

With regularization



Bias = 0.23
Variance = 0.33


Side
Effect

Constraining the model: \mathcal{H}_2 versus \mathcal{H}_{10}

$$\mathcal{H}_{10} = \{h(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10}\}$$

$$\mathcal{H}_2 = \{h(x) = \theta_0 + \theta_1 x + \cdots + \theta_{10} x^{10} \}$$

such that $\theta_3 = \theta_4 = \cdots = \theta_{10} = 0$



A “hard” order constraint that sets
some weights to zero.

$$\mathcal{H}_2 \subset \mathcal{H}_{10}$$

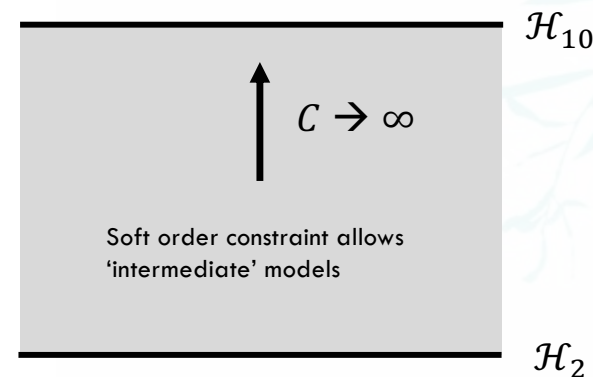
Soft Order Constraint



Don't set weights explicitly to zero.

Re-use loss optimization by giving a budget and let the learning process choose. Introduce a regularization function $\Omega(h)$.

$$\Omega(h) \equiv \sum_{q=0}^Q \theta_q^2 \leq C$$



Soft Order Constrained Model



$$\mathcal{H}_{10} = \{h(x) = \theta_0 + \theta_1 x + \dots + \theta_{10} x^{10}\}$$

$$\mathcal{H}_C = \{h(x) = \theta_0 + \theta_1 x + \dots + \theta_{10} x^{10} \}$$

such that $\sum_{q=0}^{10} \theta_q^2 \leq C$

N.B. \mathcal{H}_2 and $\mathcal{H}_{C=2}$
are unrelated!

$$\mathcal{H}_2 = \{h(x) = \theta_0 + \theta_1 x + \dots + \theta_{10} x^{10}\}$$

such that $\theta_3 = \theta_4 = \dots = \theta_{10} = 0$

\mathcal{H} is
larger

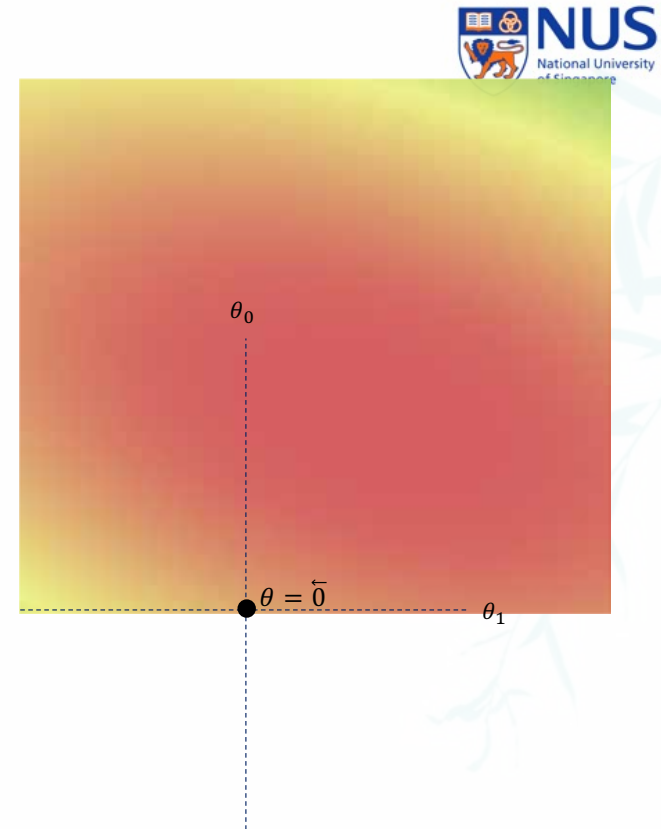


\mathcal{H} is
smaller

Solving for θ_{reg}

Minimize $L_{train} = \frac{1}{m}(\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^\top(\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$

Subject to a regularization function $\Omega(h) \equiv \boldsymbol{\theta}^\top \boldsymbol{\theta} \leq C$



Solving for θ_{reg}

Minimize $L_{train} = \frac{1}{m}(\mathbf{X}\theta - \mathbf{y})^\top(\mathbf{X}\theta - \mathbf{y})$

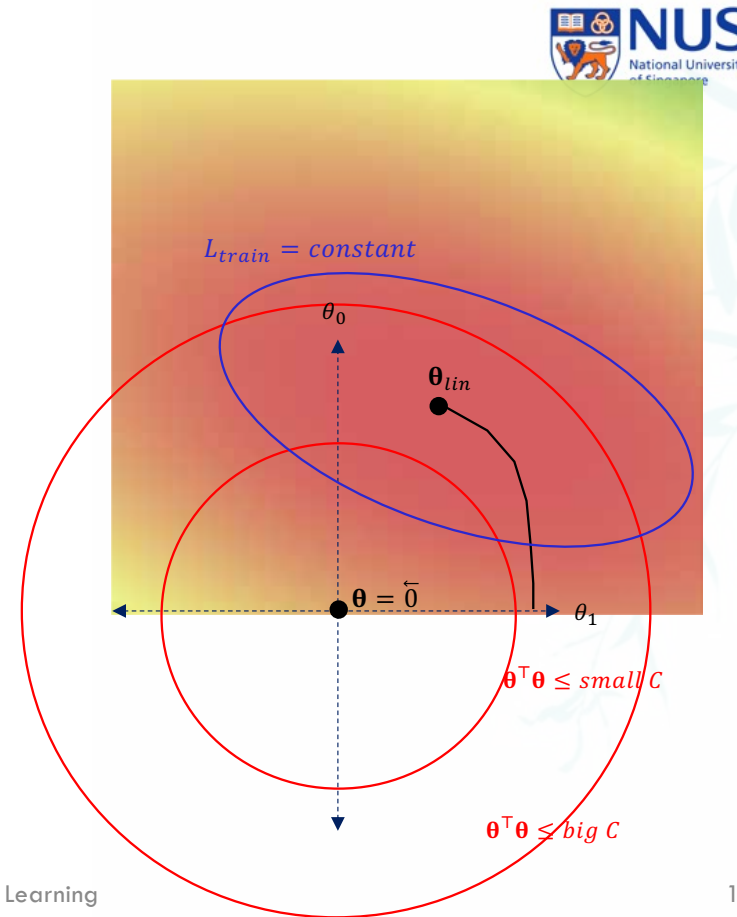
Subject to $\theta^\top \theta \leq C$










Pictorially with 2 weights θ_0, θ_1 :

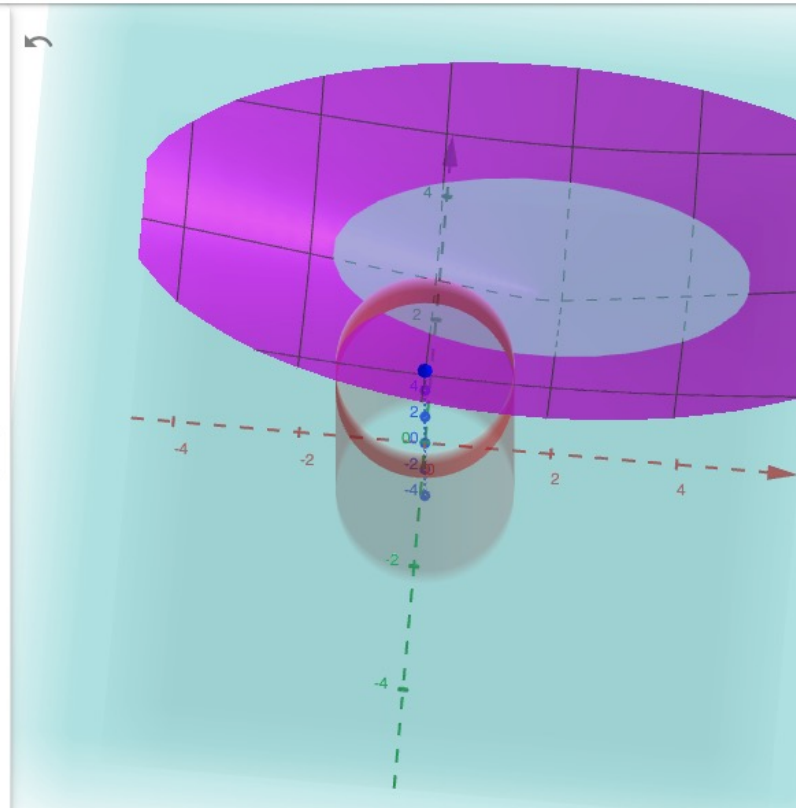
L_{train} gradient as heatmap.

Blue oval is a contour where L_{train} is a constant value (same color)

Red disc defines uniform weight decay region where $\theta^\top \theta \leq C$.



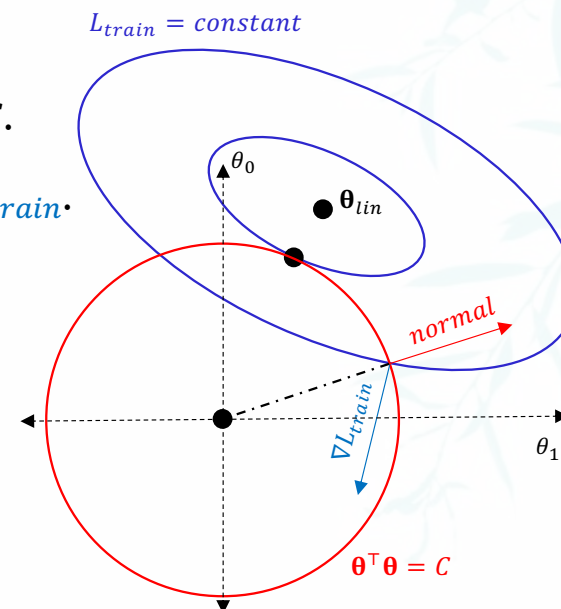
	Cone : $z = 0.2 \sqrt{(3x - 5)^2 + (7y - 15)^2} + 2$	
	l1: $\text{abs}(\text{abs}(x) + \text{abs}(y)) = 2$	
	l2: $x^2 + y^2 = 2$	
	f : $z = 4$	
	Input...	



Solving for θ_{reg}

Observations:

1. Optimal θ tries to get as 'close' to θ_{lin} as possible
Optimal θ will use full budget and be on the surface $\theta^T \theta = C$.
2. Surface $\theta^T \theta = C$, at optimal θ , must be perpendicular to ∇L_{train} .
Otherwise can move along the surface and decrease L_{train} .
3. **Normal** to surface $\theta^T \theta = C$ is the vector θ .
4. Surface is $\perp \nabla L_{train}$; surface is \perp **normal**.
 ∇L_{train} is parallel to **normal** (but in the opposite direction).



Solving for θ_{reg}

Minimize $L_{train} = \frac{1}{m}(\mathbf{X}\theta - \mathbf{y})^\top(\mathbf{X}\theta - \mathbf{y})$

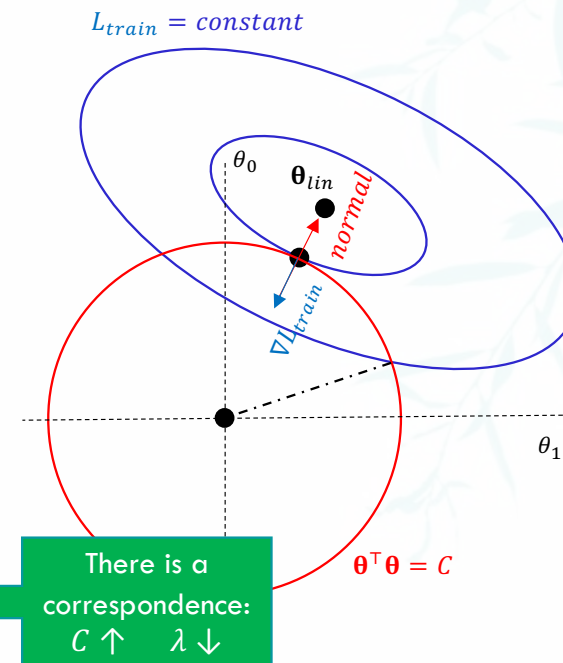
Subject to $\theta^\top \theta \leq C$

Observations:

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Optimal θ will use full budget and be on the surface $\theta^\top \theta = C$.
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Otherwise can move along the surface and decrease L_{train} .
3. **Normal** to surface $\theta^\top \theta = C$ is the vector θ .
4. Surface is $\perp \nabla L_{train}$; surface is \perp **normal**.
 ∇L_{train} is parallel to **normal** (but in the opposite direction).

$$\nabla L_{train}(\theta_{reg}) \propto -\theta_{reg}$$

Constant of proportionality. Chosen for convenience $\rightarrow = -2 \frac{\lambda}{m} \theta_{reg}$



Comparison with Linear Regression



Unconstrained

$$\min L_{train} = \frac{1}{m} \sum_{j=1}^m (\boldsymbol{\theta}^\top \mathbf{x}^{(j)} - y^{(j)})^2$$

$$\min L_{train} = \frac{1}{m} (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^\top (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$$

$$\boldsymbol{\theta}_{lin} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

Constrained:

$$\min L_{train} = \frac{1}{m} (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^\top (\mathbf{X}\boldsymbol{\theta} - \mathbf{y}), \text{ subject to: } \boldsymbol{\theta}^\top \boldsymbol{\theta} \leq C$$

$$\boldsymbol{\theta}_{reg} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

Augmented Error L_{aug}



Unconstrained

$$\min L_{train} = \frac{1}{m} \sum_{j=1}^m (\boldsymbol{\theta}^\top \mathbf{x}^{(j)} - y^{(j)})^2$$

$$\min L_{train} = \frac{1}{m} (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^\top (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$$

$$\boldsymbol{\theta}_{lin} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

Constrained:

$$\min L_{train} = \frac{1}{m} (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^\top (\mathbf{X}\boldsymbol{\theta} - \mathbf{y}), \text{ subject to: } \boldsymbol{\theta}^\top \boldsymbol{\theta} \leq C$$

|||

$$\min L_{aug}(\boldsymbol{\theta}) = L_{train}(\boldsymbol{\theta}) + \frac{\lambda}{m} \boldsymbol{\theta}^\top \boldsymbol{\theta}$$

$$= \frac{1}{m} ((\mathbf{X}\boldsymbol{\theta} - \mathbf{y})^\top (\mathbf{X}\boldsymbol{\theta} - \mathbf{y}) + \lambda \boldsymbol{\theta}^\top \boldsymbol{\theta})$$

Compare
versus
implicit
constraint

Take derivatives:

$$\text{Set } \nabla L_{aug}(\boldsymbol{\theta}) = \bar{\mathbf{0}} \Rightarrow$$

$$= \mathbf{X}^\top (\mathbf{X}\boldsymbol{\theta} - \mathbf{y}) + \lambda \boldsymbol{\theta}$$

$$= (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}) \boldsymbol{\theta} - \mathbf{X}^\top \mathbf{y}$$

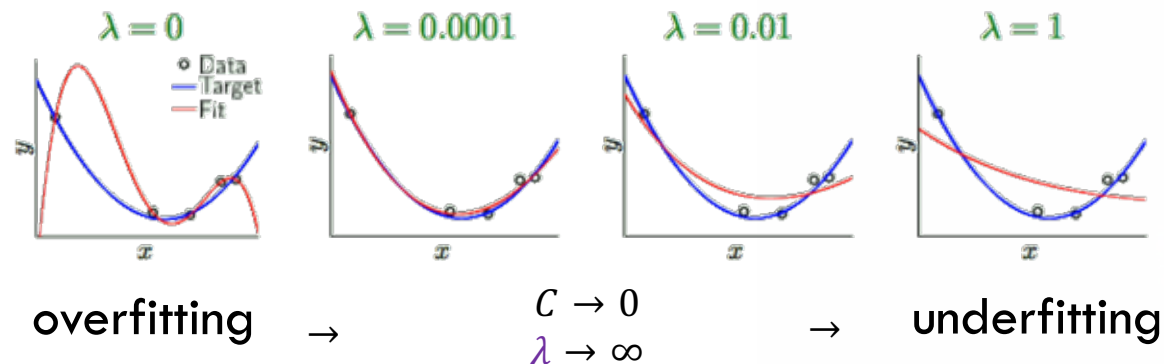
$$\boldsymbol{\theta}_{reg} = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

Still 1 step learning!
 λ determines the amount
of regularization.

Take the right λ amount of medicine



Minimizing $[L_{train}(\theta) + \frac{\lambda}{m} \theta^T \theta]$ for different λ 's:



Q1: What happens to θ in the limit as $\lambda \rightarrow \infty$?

An aerial photograph of a city grid, likely New York City, with individual blocks color-coded in shades of yellow, orange, red, and blue. The colors are applied in a somewhat irregular, hand-painted style.

Regularization Variants

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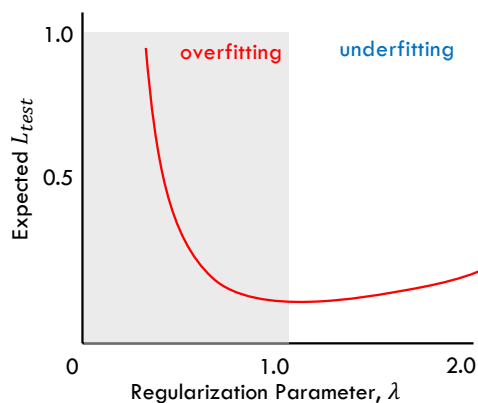
Regularizer variations $\Omega(h)$

Uniform weight decay

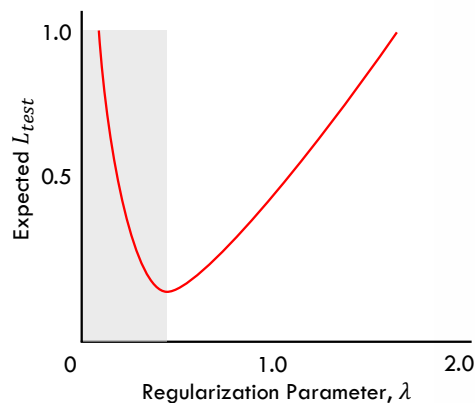
Why is it called
"weight decay"?
We'll see in
neural networks.

Low Order Fit

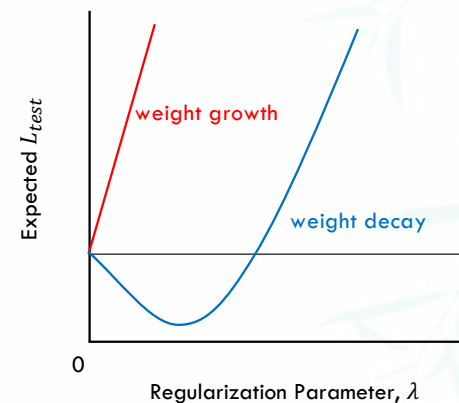
Weight growth



$$\ell^2 = \sum_{q=0}^Q \theta_q^2$$



$$\sum_{q=0}^Q q \theta_q^2$$



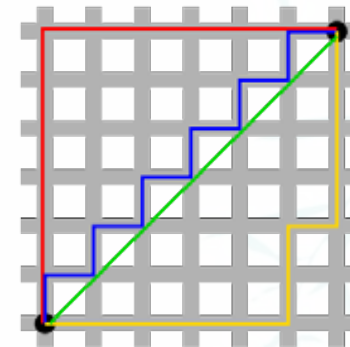
$$\sum_{q=0}^Q \frac{1}{\theta_q^2}$$

Geometry of ℓ^p norms

$$||\theta||_p \equiv \left(\sum_{i=1}^n |\theta_i|^p \right)^{\frac{1}{p}}$$

ℓ^1 = Manhattan (Taxicab) distance
 $\sum_{i=1}^n |\theta_i|$

ℓ^2 = Euclidean distance (weight decay)
 $\sqrt{\sum_{i=1}^n |\theta_i|^2}$

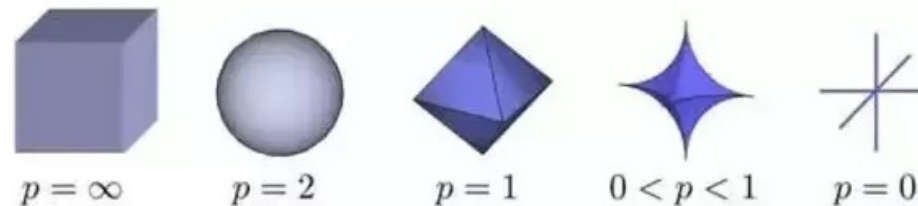


ℓ^p ball visualized



As the value of p decreases, the size of the corresponding space also decreases.

In 3 equally weighted dimensions (e.g., $\theta_1, \theta_2, \theta_3$):

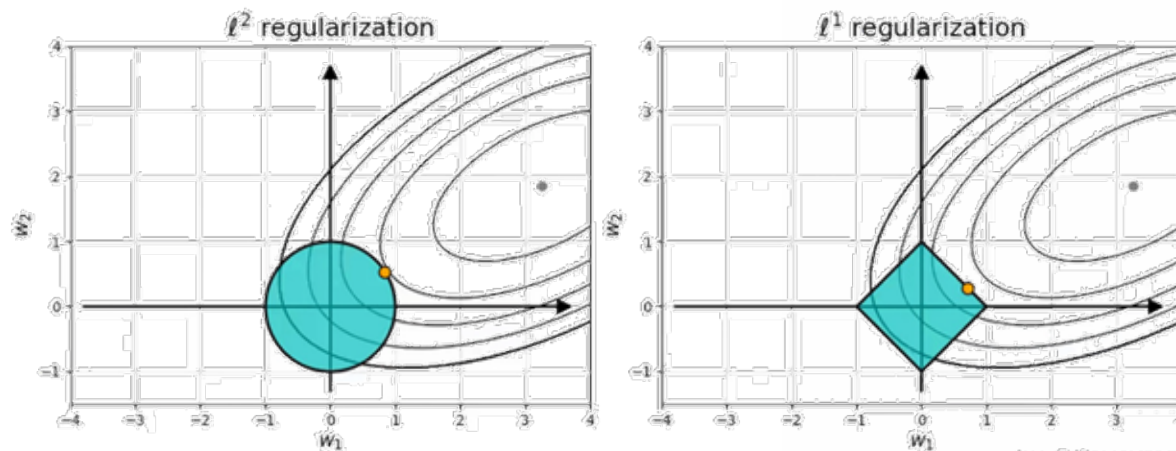


Properties from geometry

ℓ^1 encourages sparse solutions; akin to feature selection.

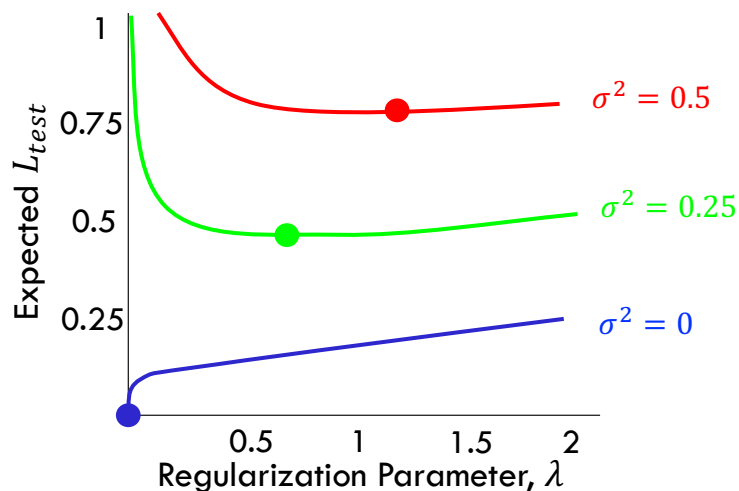
ℓ^2 can be used for homogenous data.

ℓ^1 induces sparse solutions for least squares

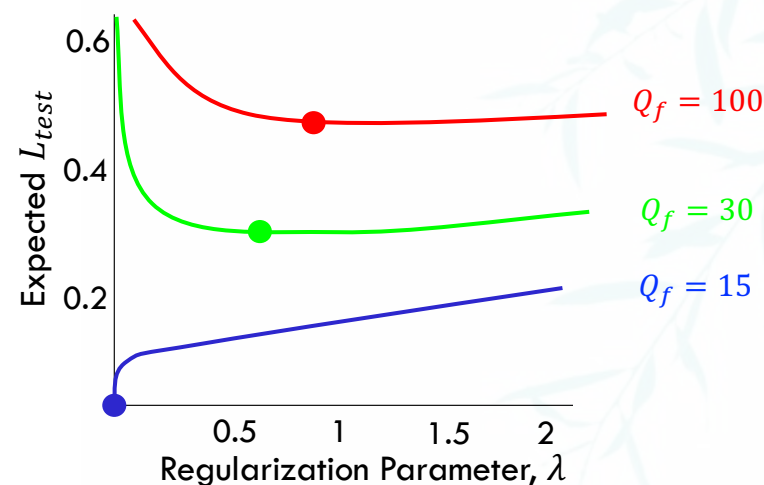


Getting the right dose

Recall the bias-variance experiment varying σ^2 (noise) and Q_f (target complexity) from last week:



Stochastic Noise
(high frequency)



Deterministic Noise (Bias)
(also non-smooth w.r.t. to \mathcal{H})

Regularization – Summary

Give up modeling a subset of \mathcal{H} to lower variance error.

$$L_{aug}(\boldsymbol{\theta}) \equiv L_{train}(\boldsymbol{\theta}) + \frac{\lambda}{m} \Omega(h)$$

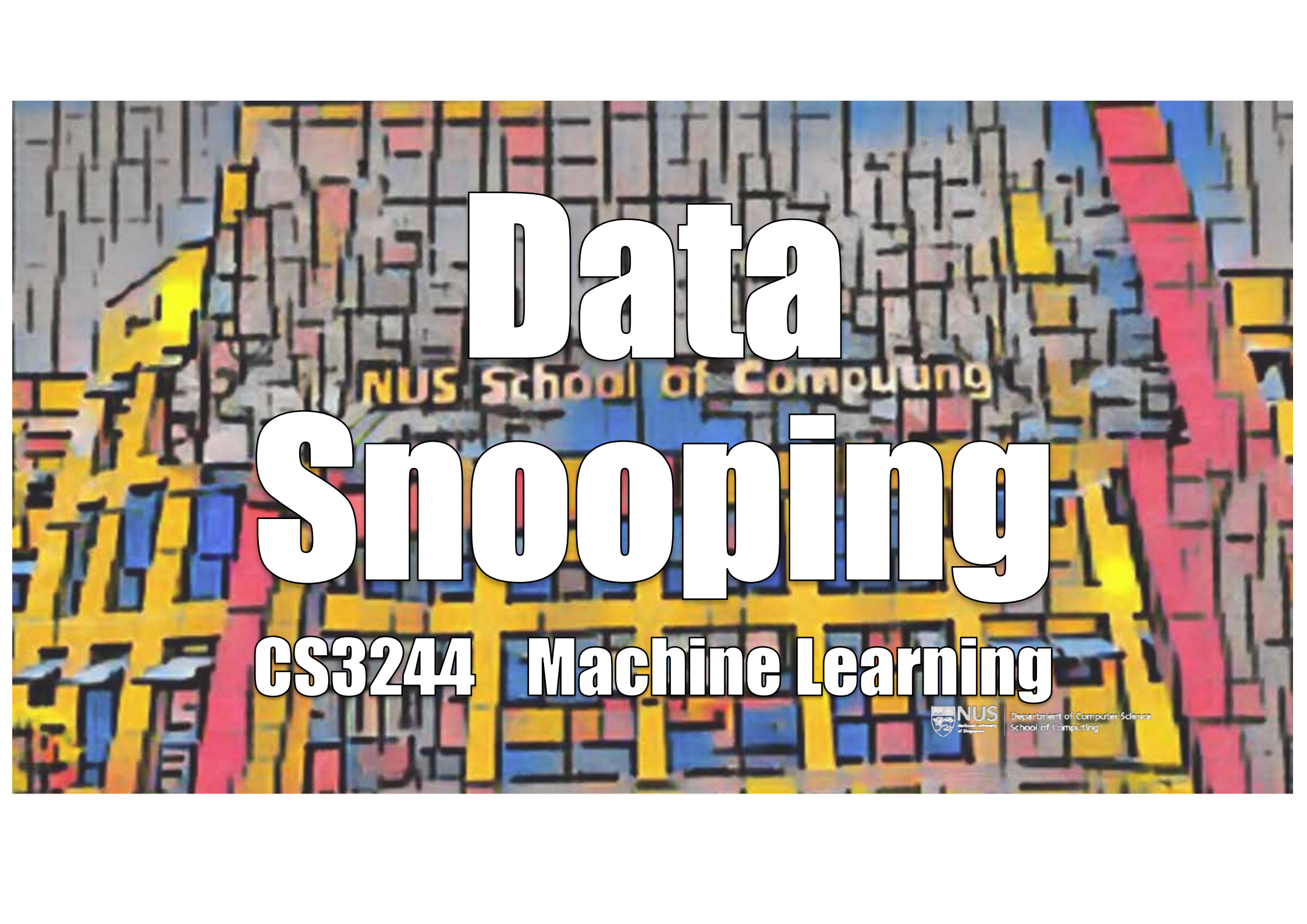
λ is the dose of regularization:

the higher the dose, the smaller the budget C .

Choosing a regularizer $\Omega(h)$:

Weight decay is common $\sum_{q=0}^Q \theta_q^2 \equiv \boldsymbol{\theta}^\top \boldsymbol{\theta}$ (ℓ^2 regularization)

Choose λ by validation ...



Data Snooping

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Data Snooping

Predict USD versus GBP

Normalize data, split randomly:
 $\mathbf{X}_{train}, \mathbf{X}_{test}$

Train only on \mathbf{X}_{train} ,
Test h_{θ} on \mathbf{X}_{test}

Got great performance!
Let's invest!



$$\Delta r_{-20}, \Delta r_{-19}, \dots, \Delta r_{-1} \rightarrow \Delta r_0$$

Chart credits: Monaneko @ [Wikimedia Commons](#)

Data Snooping

In Zoom breakout or physical subgroups,

(5 mins): Answer why we lost our money 💰💵💵

Ask one member to write it to the [#lectures](#) thread. Upvote others that you like.



$$\Delta r_{-20}, \Delta r_{-19}, \dots, \Delta r_{-1} \rightarrow \Delta r_0$$

Chart credits: Monaneko @ [Wikimedia Commons](#)

Data Snooping

Lost our \$\$\$\$. Why?

If a data set has affected any step in the learning process, its ability to assess the outcome has been compromised.



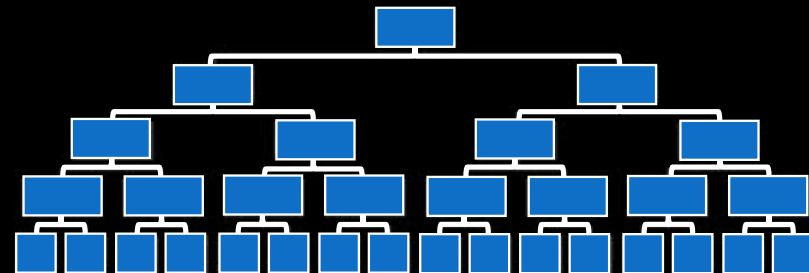
Most common trap for practitioners – many ways to slip.

Chart credits: Monaneko @ [Wikimedia Commons](#)

Perfect Forecasting — or luck of the draw?

There always is that political pundit, stock picker and other high-value forecaster that nails all of their predictions.

Is this person to be trusted?





Validation

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Two Cures

In one form or another, $L_{test}(h) = L_{train}(h) + \text{overfit penalty}$

1. **Regularization:** Restrain the model

$$L_{test}(h) = L_{train}(h) + \text{overfit penalty}$$

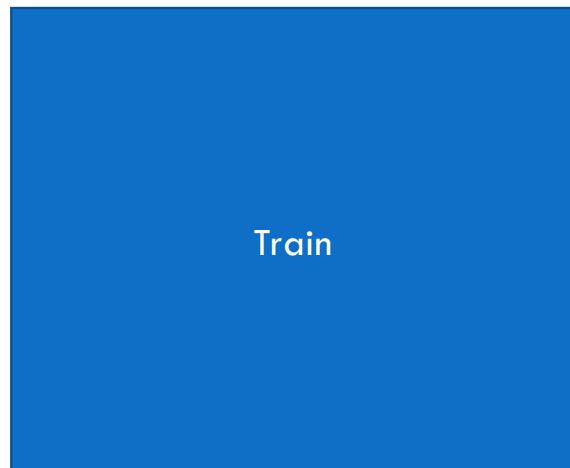
2. **Validation:** Reality check by peeking (at the bottom line)

$$L_{test}(h) = L_{train}(h) + \text{overfit penalty}$$



Validation estimates this quantity

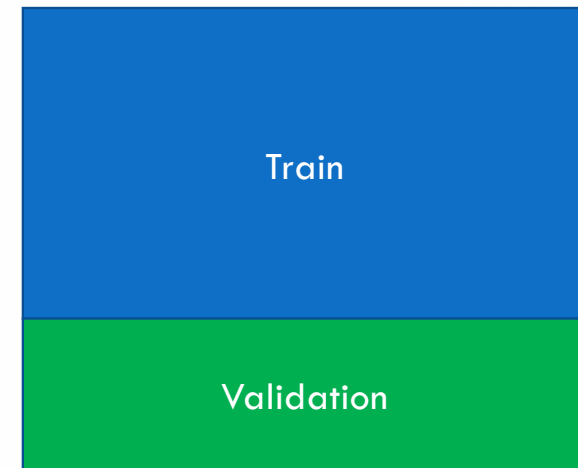
What is validation?



🤔 How can I
estimate L_{test} ?

Now I can!
 L_{val}

“Mock Test”



Analyzing the estimated loss

On a test point (x, y) , the cost $l(h_\theta(x), y)$ is:

Squared error: $(h_\theta(x) - y)^2$

Binary error: $[h_\theta(x) \neq y]$

$$\mathbb{E}[l(h_\theta(x), y)] = L_{test}(h_\theta)$$

$$Var[l(h_\theta(x), y)] = \sigma^2$$

From a point to a set

On a validation set $(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(K)}, y^{(K)})$,
the cost is $L_{val}(h) = \frac{1}{K} \sum_{k=1}^K l(h(\mathbf{x}^{(k)}), y^{(k)})$

$$\mathbb{E}[L_{val}(h)] = \frac{1}{K} \sum_{k=1}^K \mathbb{E}[l(h(\mathbf{x}^{(k)}), y^{(k)})] = L_{test}(h)$$

$$\text{Var}[L_{val}(h)] = \frac{1}{K^2} \sum_{k=1}^K \text{Var}[l(h(\mathbf{x}^{(k)}), y^{(k)})] = \frac{\sigma^2}{K}$$

← Our K points
are i.i.d.
Covariance is 0.

$$L_{val}(h) = L_{test}(h) \pm O\left(\frac{1}{\sqrt{K}}\right)$$

← Standard
Deviation

K is taken out of m

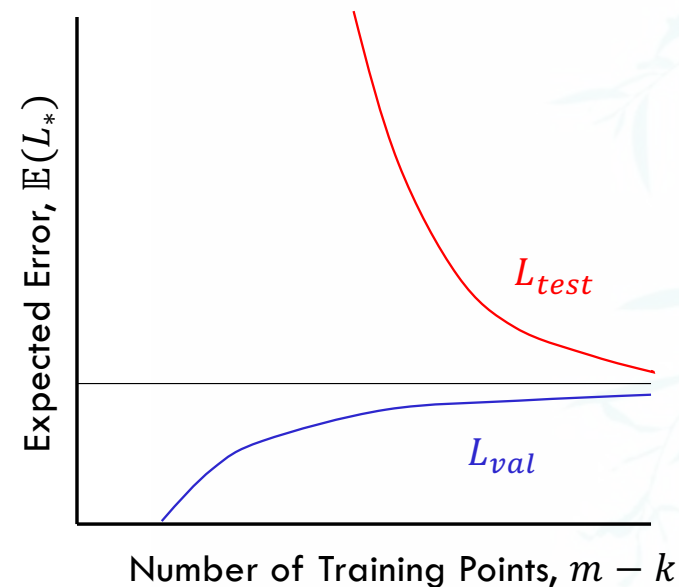
Given the data set \mathcal{D} , separate:

1. K points for validation
2. $m - K$ points for training

$O\left(\frac{1}{\sqrt{K}}\right)$:

Small K = bad estimate

Large K = ?



K is put back into m

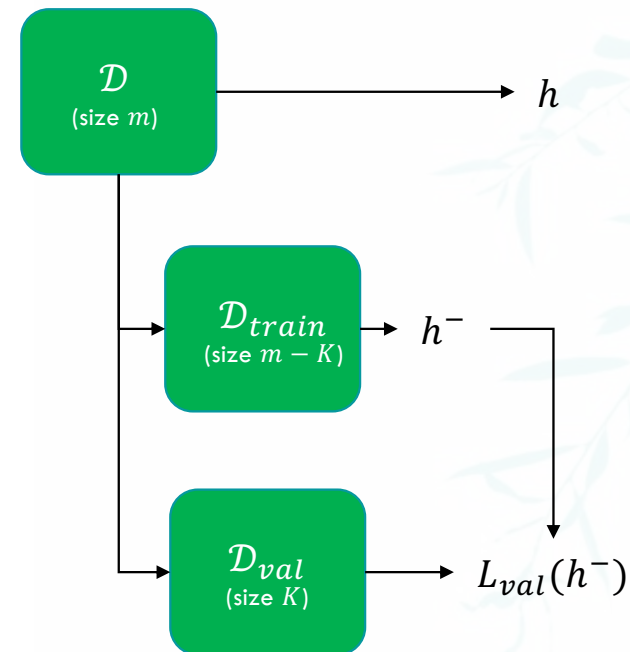
1. Train on \mathcal{D}_{train} to yield h^-
2. Test h^- on \mathcal{D}_{val} to yield L_{val}
3. Use cost L_{val} to estimate $L_{test}(h^-)$
4. Use h (not h^- !) in the end

Large K ?

h^- trained on too few examples.

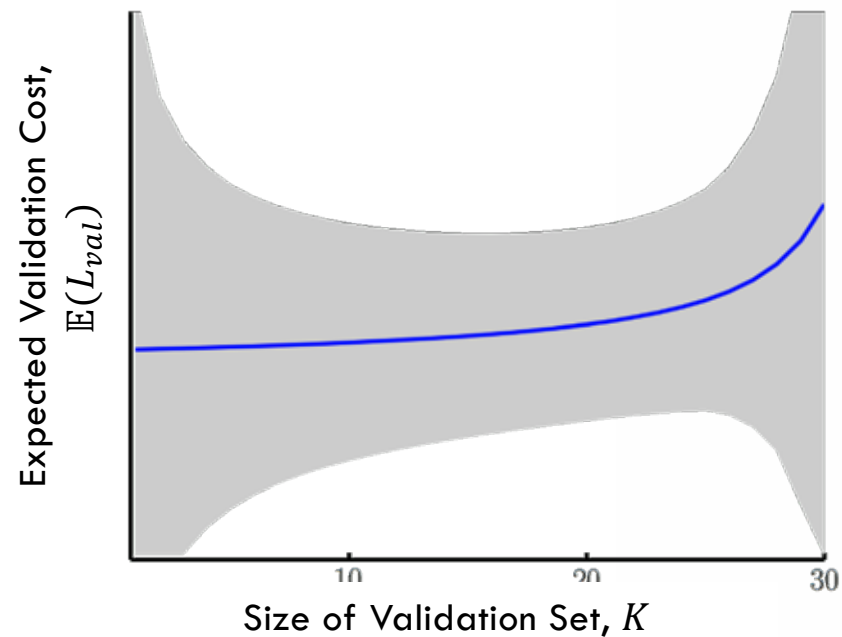
Leads to bad h^- , poor estimate.

Rule of Thumb: $K = \frac{m}{5}$



Expected Validation Error for \mathcal{H}_2

With $m = 40$, and noise level = 0.4





Cleanliness of Validation

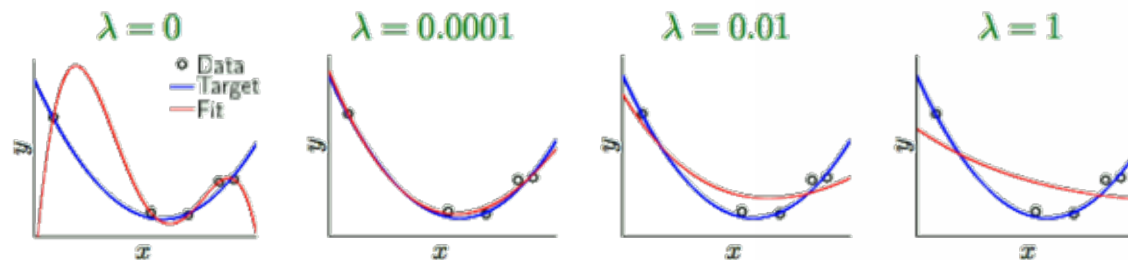
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Why 'validation'?

Because \mathcal{D}_{val} is used to make learning choices,
e.g. choosing the level of regularization to minimize L_{val}



If an estimate L_{test} affects learning:

The set is no longer a test set, it becomes a **validation** set!

What's the difference?

We know that the test set is unbiased.
But what about the validation set?

Your Turn: Does the validation set have an **optimistic** or **pessimistic bias**?

Two hypotheses h_a and h_b with $L_{test}(h_a) = L_{test}(h_b) = 0.5$

Error estimates l_a and l_b uniform on $[0,1]$

We **pick** $h \in \{h_a, h_b\}$ by virtue of its $l = \min(l_a, l_b)$.

What then, is the value of $\mathbb{E}(l)$?

Q4

leading to

Q5

bias.

What's the difference?

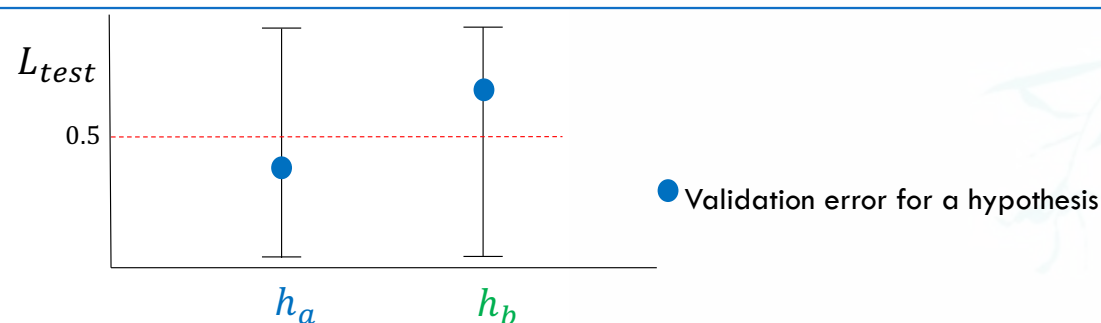
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Error estimates l_a and l_b uniform on $[0,1]$

We **pick** $h \in \{h_a, h_b\}$ by virtue of its $l = \min(l_a, l_b)$.

What then, is the value of $\mathbb{E}(l)$?

$\mathbb{E}(l) < 0.5$, leading to an optimistic bias.



Hypothesis Selection: Using \mathcal{D}_{val} more than once

Θ models $\mathcal{H}_1, \dots, \mathcal{H}_\Theta$

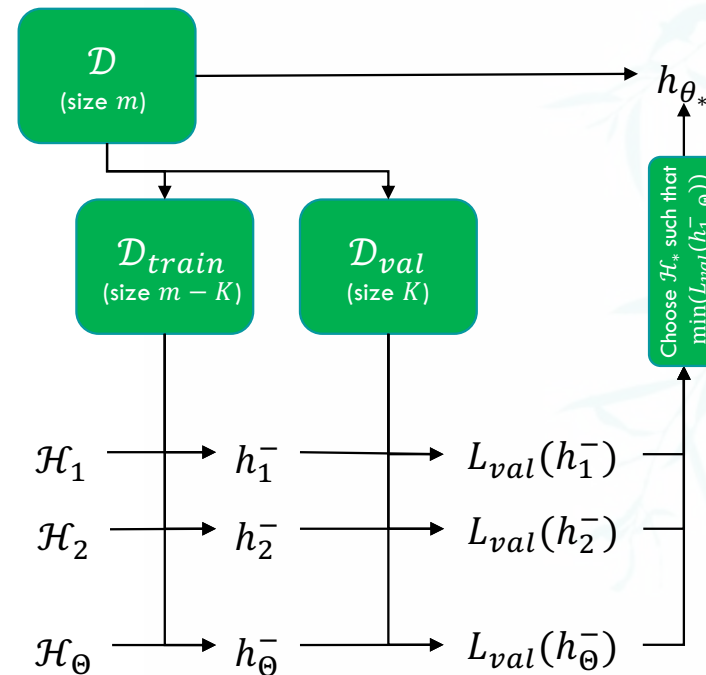
Use \mathcal{D}_{train} to learn h_θ^- for each model

Evaluate h_θ^- using \mathcal{D}_{val} :

$$L_\theta = L_{val}(h_\theta^-); \quad \theta = 1, \dots, \Theta$$

Pick model $\theta = \theta_*$ with **smallest** L_θ

Uh oh!
Biased!



Data contamination

Error estimates: L_{train} , L_{test} , L_{val}

Contamination: optimistic (deceptive) bias in estimating L_{test}

- Training set: totally contaminated
- Validation set: slightly contaminated
- Test set: totally 'clean'

Time Out: Check your understanding

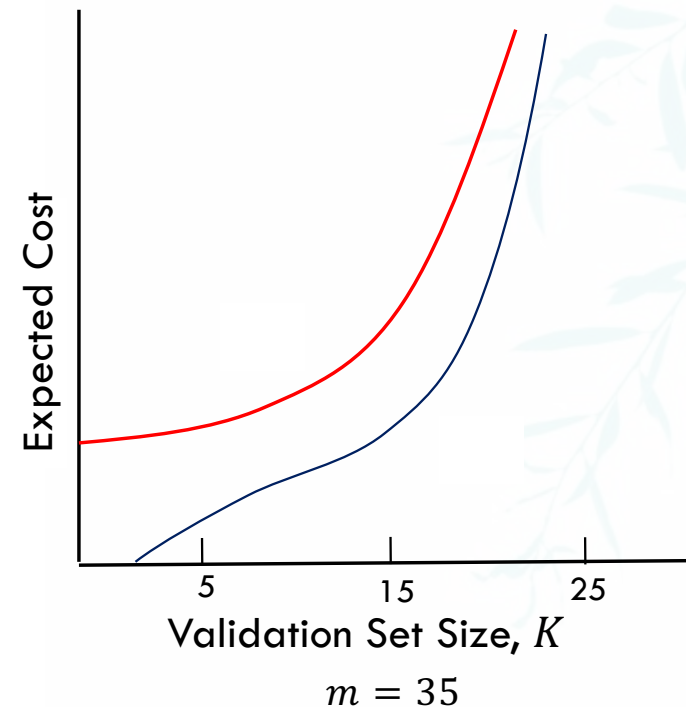
We **selected** the model \mathcal{H}_{θ^*} **using** \mathcal{D}_{val} . We can think of validation as training among the set of Θ models.

$L_{val}(h_{\theta^*})$ is a biased estimate of $L_{test}(h_{\theta^*})$

Your Turn:

One curve is L_{val} , and the other L_{test}

1. Which curve is L_{val} ? ● or ●
2. Why are the curves going up?
3. Why do the curves get closer together?





Cross Validation

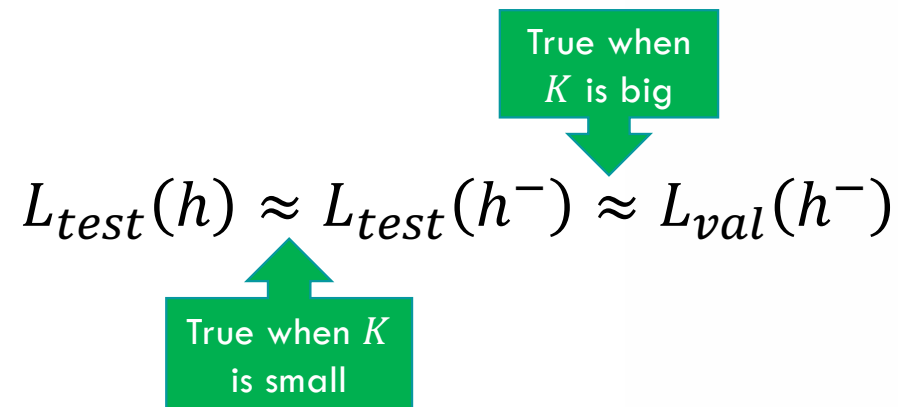
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The dilemma about K

Validation relies on the following chain of reasoning:



Can we have both K being both big and small?

Yes, we can!

Leave out out cross validation

$m - 1$ points for training and **1 point** for validation

(Sounds familiar? It was at the beginning of the pre validation lecture)

$\mathcal{D}_{cv} = (\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(cv)}, y^{(cv)}), \dots, (\mathbf{x}^{(m)}, y^{(m)})$ validation

Final hypothesis learned from \mathcal{D}_{cv} is h_{cv}^- .

$$l_{cv} = l_{val}(h_{cv}^-) = l(h_{cv}^-(\mathbf{x}^{(cv)}), y^{(cv)})$$

Caveat: Hypothesis learned will be highly correlated.

As most points are identical: The 1st hypothesis will use points 2, 3, ..., m and the 2nd will use 1, 3, ..., m .

Leave out out cross validation

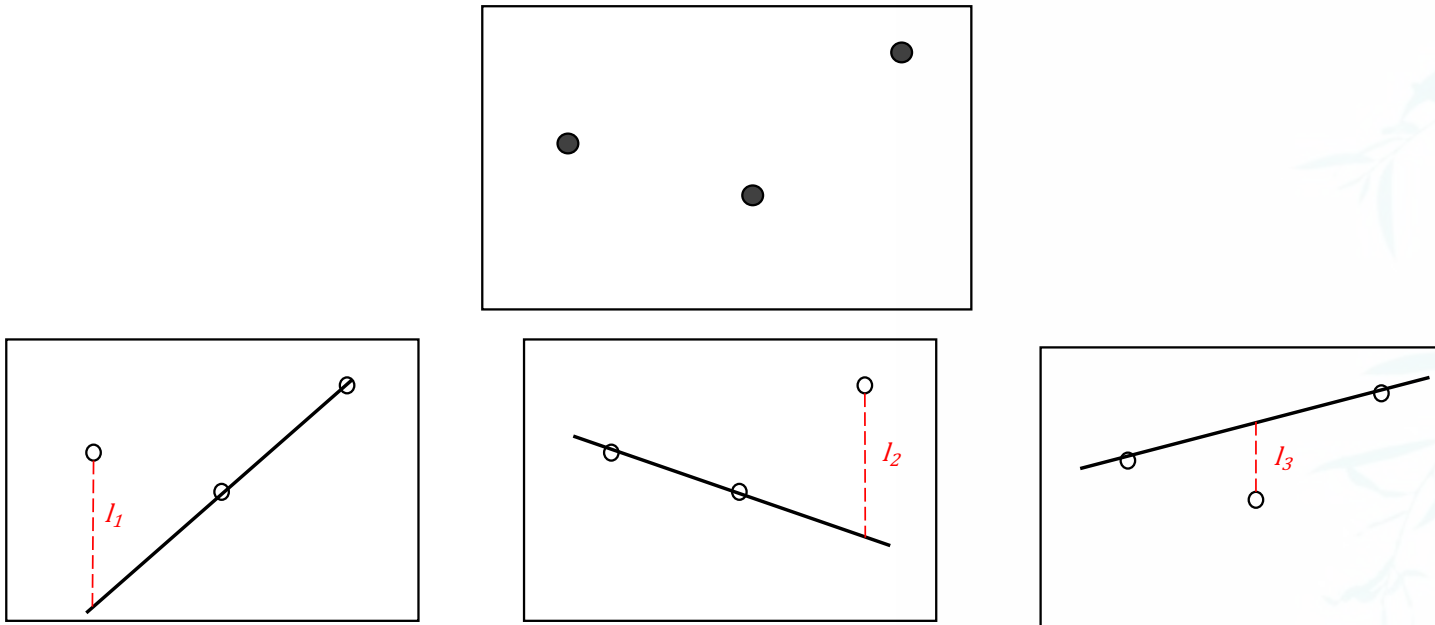
Final hypothesis learned from \mathcal{D}_{cv} is h_{cv}^- .

$$l_{cv} = l_{val}(h_{cv}^-) = l(h_{cv}^-(\mathbf{x}^{(cv)}), y^{(cv)})$$

Cross validation cost: $L_{loocv} = \frac{1}{m} \sum_{cv=1}^m l_{cv}$.

(Almost) using m examples for K .

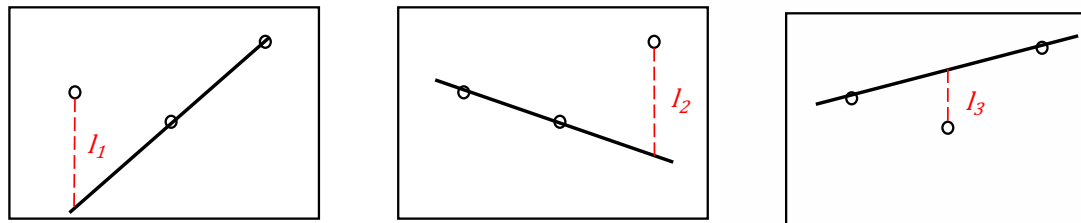
Illustration of cross validation



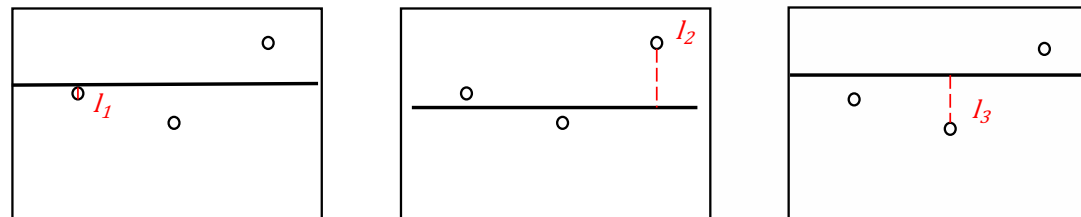
$$L_{loocv} = \frac{1}{3}(l_1 + l_2 + l_3)$$

Model selection using CV

Linear



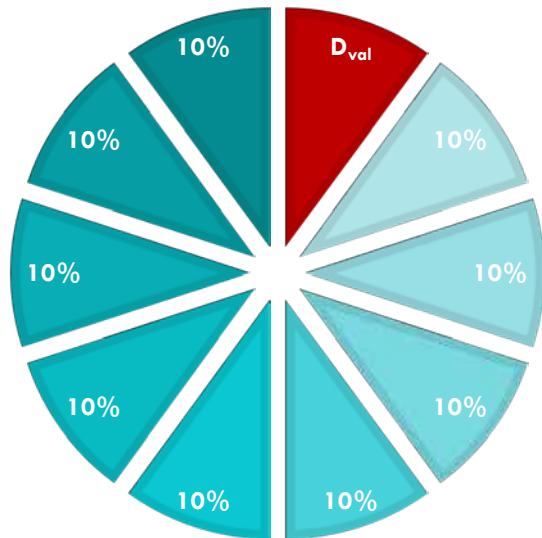
Constant



L_{cv} empirically shows that the constant model is a better fit for this dataset

Have your cake and eat it too: K fold cross validation

10 FOLD C.V.



LOOCV can be very expensive for large datasets. Why?

Instead, use K fold cross validation: i.e.,
 K training sessions on $\frac{m}{K}$ points each.

Recommend: 10-fold CV

Assigned Task (due before next Mon)



Read the post <https://www.kaggle.com/alexisbcook/cross-validation>
(10 mins)

Post a 1–2 sentence answer to the topic in your tutorial group: **#tg-xx**

How does cross validation relate to variance?

[There's an optional exercise with this course page, using random forest and MAE, you're welcomed to do it if you'd like]



Cross-validation can help to reduce variance



Cross-validation helps improve the model to reduce variance with unseen data samples



Cross-validation is able to reduce variance as all the data points will get to be used as both the training and validation sets. As long as the sets are not too small, there will be less impact from noise.



Cross validation is a method to gauge the performance of a machine learning model. In the case of how cross variance affects the variance, the number of folds impacts how the variance and the bias of the model would vary. The lower the number of folds, the greater bias and lower the variance and the greater the number of folds, the greater the variance. This is because the more folds there are the smaller the sample size of the training data set, leading to a greater influence of random chances/data points on the model.

How does cross validation relate to variance?



If cross-validation were averaging independent estimates: LOOCV should see lower variance, since training sets overlap substantially.

This is not true when training sets are highly correlated: Then, LOOCV may be blind to instabilities that may not be triggered by changing a single point in the training data. This makes it highly variable to the realization of the training set, hence high variance.

A more definitive answer to the paraphrase is here:

<https://stats.stackexchange.com/questions/61783/bias-and-variance-in-leave-one-out-vs-k-fold-cross-validation>

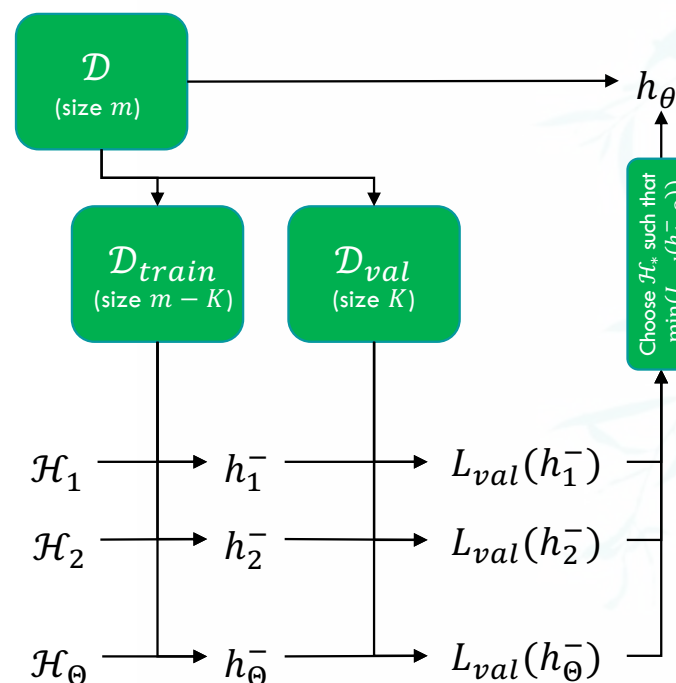
Cross Validation – Summary

Estimate L_{val} multiple times

Breaks independence assumption:
performance is correlated.

Introduces the factor of **efficiency**
as a tradeoff.

To think about: How else can we
produce estimates of L_{test} ?





Wrapping up Week 06

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What did we learn this week?



Understand **Regularization** as a means of restraining the model.

Choose appropriate doses of regularization for a model.

Understand and execute **Validation**, as a reality check by peeking (at the bottom line).

Understand the different forms extending validation to encompass additional estimation.

Understand how validation and regularization complement each other and their roles in affecting learning.

Outlook for next week



**IF YOU
NEVER KNOW
FAILURE**

**YOU WILL
NEVER KNOW
SUCCESS**

—Sugar Ray Leonard

Assigned Task (due before next Mon)



Take a break, you deserve it!