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6.390 Intro to Machine Learning

Lecture 2: Linear regression and regularization

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(many slides adapted from Tamara Broderick)

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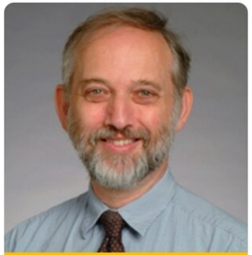
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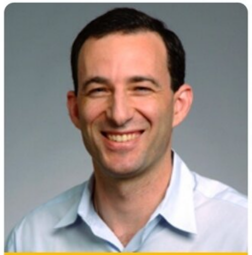
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Logistical issues? Personal concerns?
We'd love to help out!

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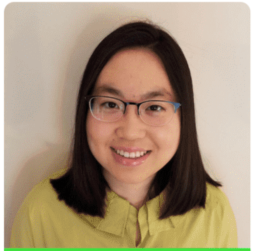
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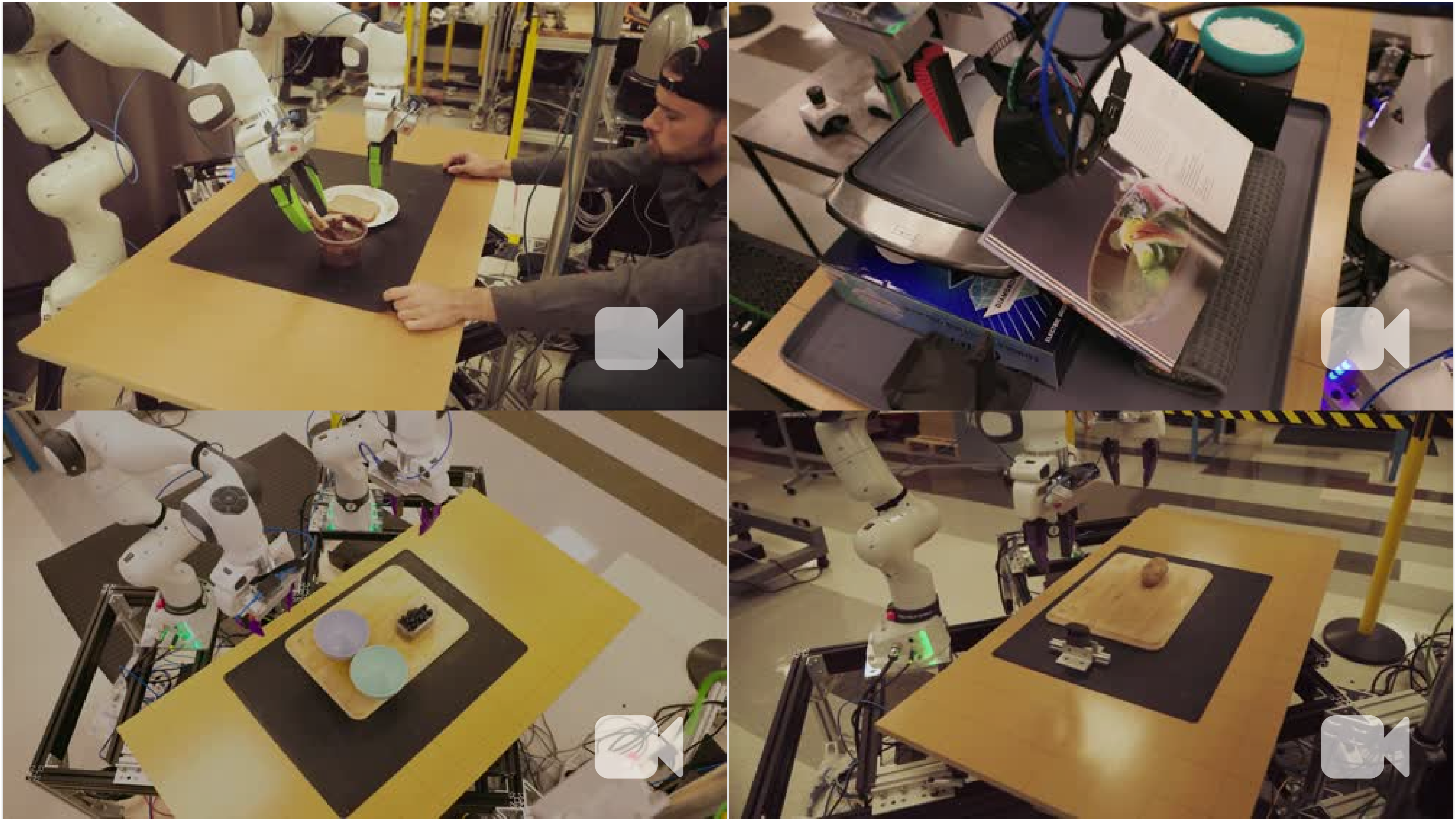
https://shenshen.mit.edu/demos/gifs/atlas_darpa_overall.gif

Optimization + first-principle physics



https://www.youtube.com/embed/fn3KWM1kuAw?start=1&enablejsapi=1

Outline

- Recap: ML set up, terminology
- Ordinary least-square regression
    - Closed-form solutions (when exists)
    - Cases when closed-form solutions don't exist
        - mathematically, practically, visually
- Regularization
- Hyperparameter and cross-validation

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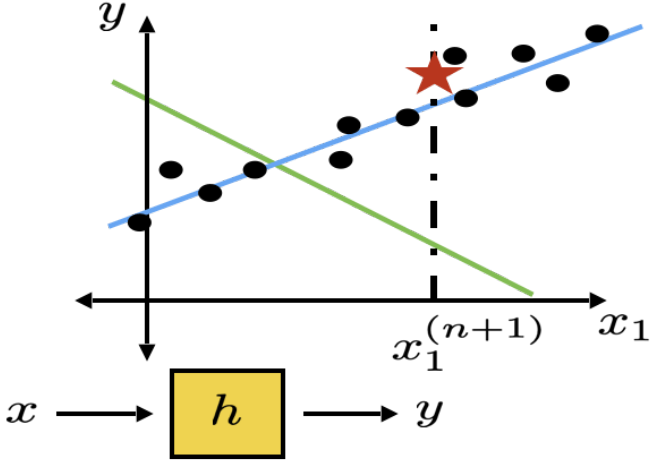
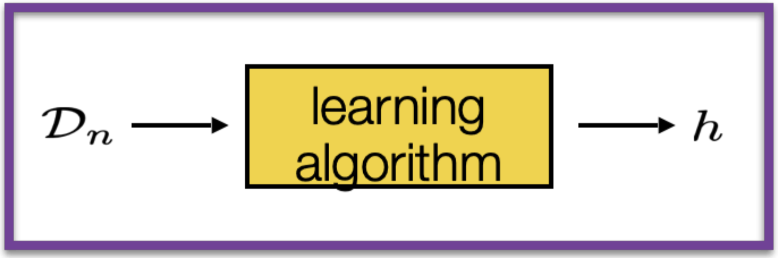
Recall lab1 intro

How do we learn?

- Have data; have hypothesis class
- Want to choose (learn) a good hypothesis h (or more concretely, a set of parameters)



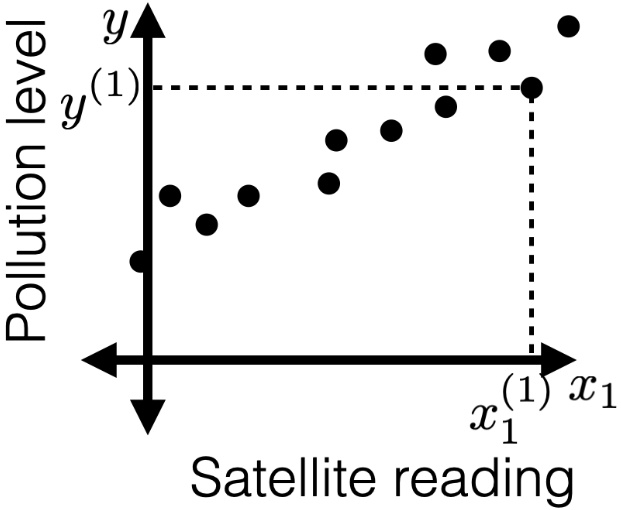
How to get it:
(Next time!)



Example: predict pollution level

(Training) data

- *n* training data points
- For data point $i \in \{1, \dots, n\}$
  - Feature vector $x^{(i)} = (x_1^{(i)}, \dots, x_d^{(i)})^\top \in \mathbb{R}^d$
  - Label $y^{(i)} \in \mathbb{R}$
- Training data $\mathcal{D}_n = \{(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})\}$



What do we want? A good way to label new points

How to label? Hypothesis $h : \mathbb{R}^d \to \mathbb{R}$

$x \rightarrow \boxed{h} \rightarrow y$

Is this a ***good*** hypothesis?

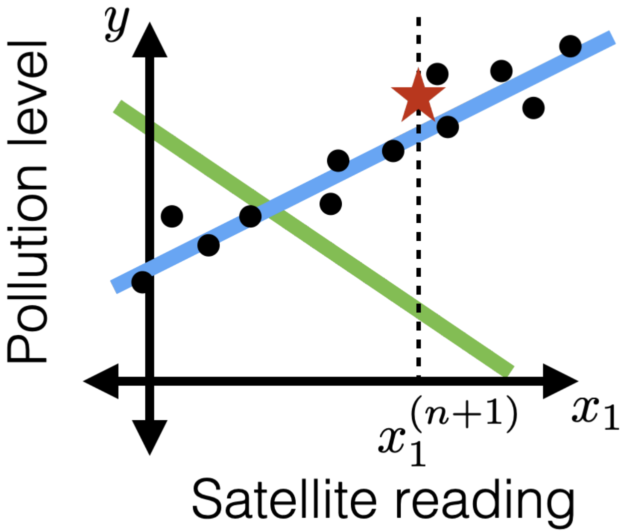
- Example *h*: For any *x*, *h*(*x*) = 1,000,000

How good is a regression hypothesis?

- Should predict well on future data
- How good is a regressor at one point?
- Loss $L(g, a)$
  - Ex: squared loss

g: guess,
a: actual

$$L(g, a) = (g - a)^2$$



- Training error: $\mathcal{E}_n(h) = \frac{1}{n}\sum_{i=1}^{n} L(h(x^{(i)}), y^{(i)})$
- Test error (n' new points): $\mathcal{E}(h) = \frac{1}{n'}\sum_{i=n+1}^{n+n'} L(h(x^{(i)}), y^{(i)})$
- One idea: prefer h to $\tilde{h}$ if $\mathcal{E}_n(h) < \mathcal{E}_n(\tilde{h})$

Recall lab1 Q1

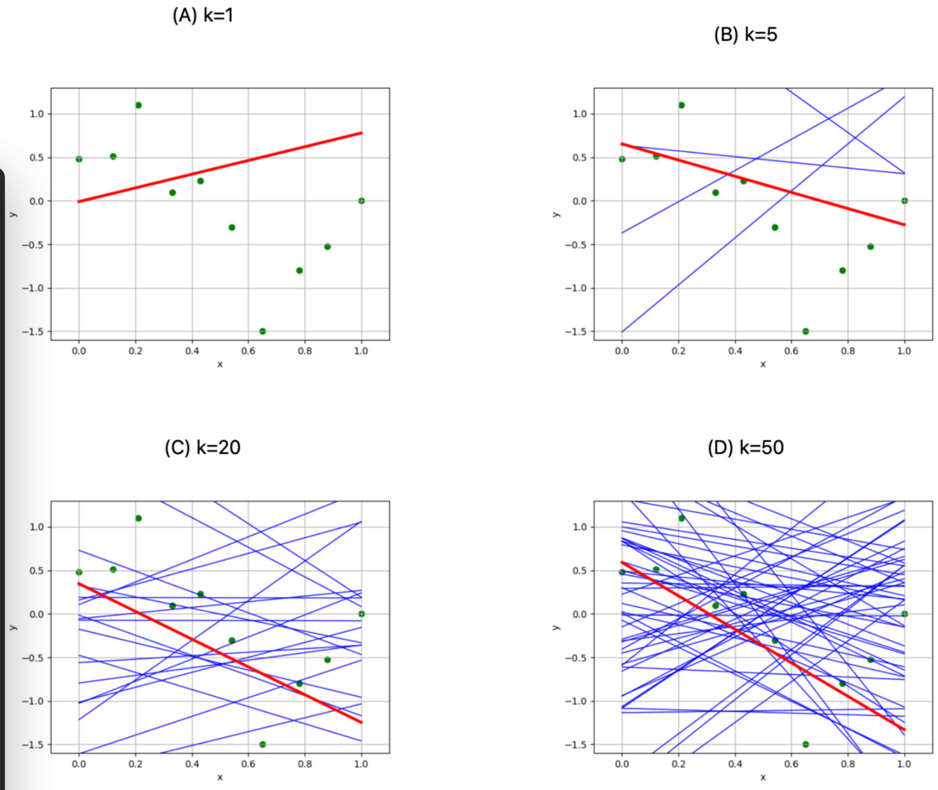
```
def random_regress(X, Y, k):
    d, n = X.shape

    # generate k random hypotheses
    ths = np.random.randn(d, k)
    th0s = np.random.randn(1, k)

    # compute the mean squared error of each
hypothesis on the data set
    errors = lin_reg_err(X, Y, ths, th0s.T)

    # Find the index of the hypotheses with the
lowest error
    i = np.argmin(errors)

    # return the theta and theta0 parameters
that define that hypothesis
    theta, theta0 = ths[:,i:i+1], th0s[:,i:i+1]
    return (theta, theta0), errors[i]
```



- Will this method eventually get arbitrarily close to the best solution? What do you think about the efficiency of this method?

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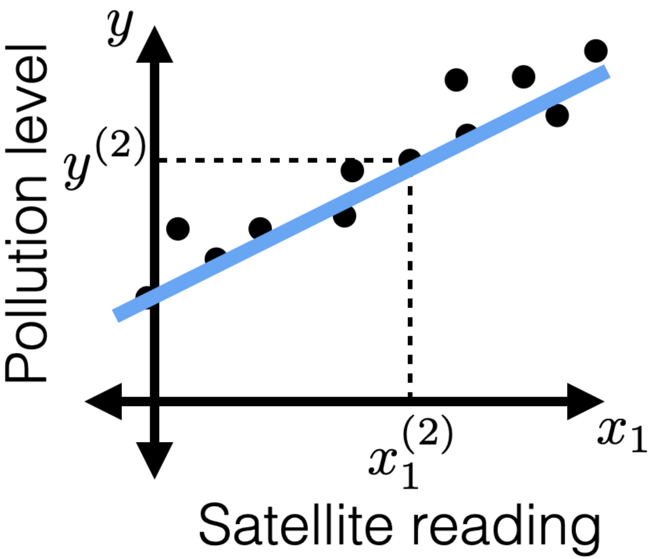
Linear regression: the analytical way

- How about we just consider all hypotheses in our class and choose the one with lowest training error?
- We'll see: not typically straightforward
- But for linear regression with square loss: can do it!
- In fact, sometimes, just by plugging in an equation!

Linear regressors

- Hypothesis class $\mathcal{H}$: set of h
- A linear regression hypothesis when d=1:

$$h(x) = \theta x + \theta_0$$



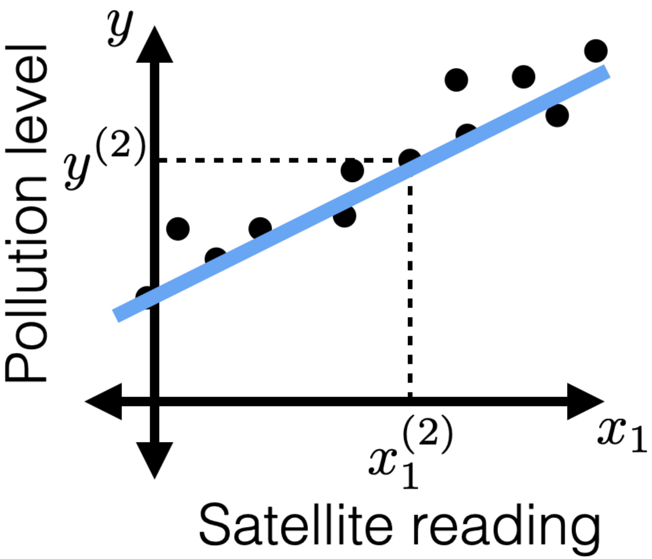
Linear regressors

- Hypothesis class $\mathcal{H}$: set of h

- A linear regression hypothesis when *d*=1:

$$h(x;\theta,\theta_0) = \theta x + \theta_0$$

parameters



Linear regressors

- Hypothesis class $\mathcal{H}$: set of h
- A linear regression hypothesis when *d*=1:

$$h(x; \theta, \theta_0) = \theta x + \theta_0$$

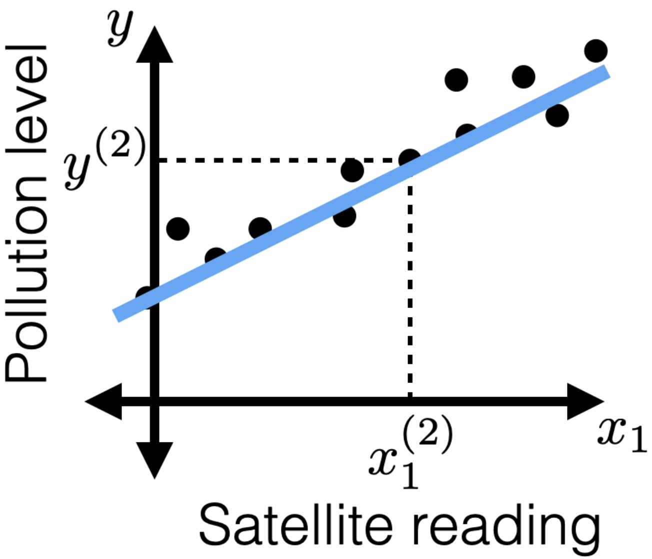
parameters

- A linear reg. hypothesis when *d*≥1:

$$h(x; \theta, \theta_0) = \theta_1 x_1 + \cdots + \theta_d x_d + \theta_0$$
$$= \theta^\top x + \theta_0$$

OR

$$h(x) = \theta_1 x_1 + \cdots + \theta_d x_d + (\theta_0)(1)$$
$$= \theta^\top x$$



- A linear reg. hypothesis when $d \geq 1$:

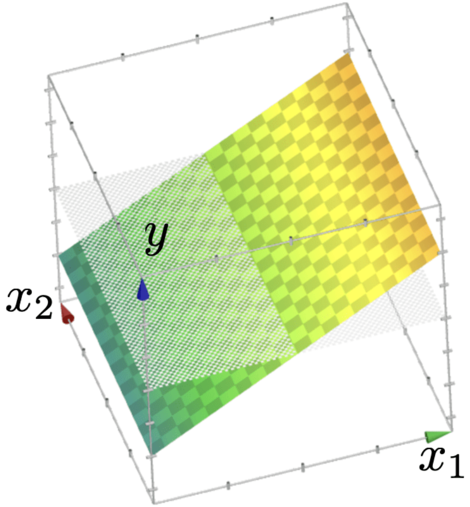
$$h(x;\theta,\theta_0) = \theta_1 x_1 + \cdots + \theta_d x_d + \theta_0$$
$$= \theta^\top x + \theta_0$$

1x2,2x1

OR

$$h(x) = \theta_1 x_1 + \cdots + \theta_d x_d + (\theta_0)(1)$$
$$= \theta^\top x$$

1x3,3x1



Notational trick: *not* the same θ & x!

- Our hypothesis class in linear regression will be the set of all such *h*

Hypothesis is a "hyperplane"

- Recall: training loss:

$$\frac{1}{n} \sum_{i=1}^{n} L\left(h\left(x^{(i)}\right), y^{(i)}\right)$$

- With squared loss:

$$\frac{1}{n} \sum_{i=1}^{n}\left(h\left(x^{(i)}\right)-y^{(i)}\right)^{2}$$

- Using linear hypothesis (with extra "1" feature):

$$\frac{1}{n} \sum_{i=1}^{n}\left(\theta^{\top} x^{(i)}-y^{(i)}\right)^{2}$$

- With given data, the error only depends on θ, so let's call the loss $J(\theta)$

Now training loss:

$$J(\theta) = \frac{1}{n} \sum_{i=1}^{n} \left(\theta^\top x^{(i)} - y^{(i)}\right)^2$$

$$= \frac{1}{n}(\tilde{X}\theta - \tilde{Y})^\top(\tilde{X}\theta - \tilde{Y})$$

Define

$$\tilde{X} = \begin{bmatrix} x_1^{(1)} & \cdots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(n)} & \cdots & x_d^{(n)} \end{bmatrix}$$

nxd

$$\tilde{Y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

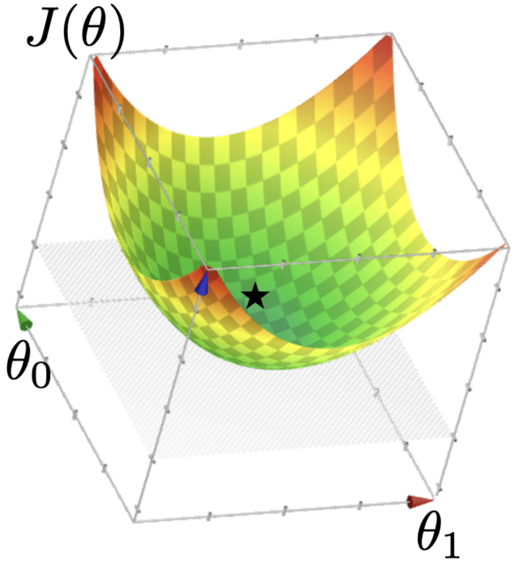
nx1

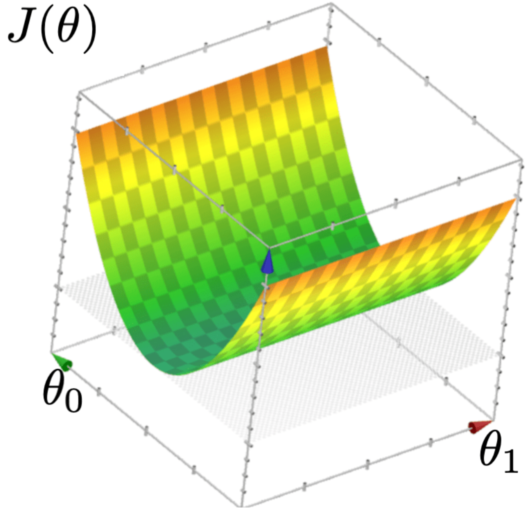
- Goal: find θ to minimize

$$J(\theta) = \frac{1}{n}(\tilde{X}\theta - \tilde{Y})^\top(\tilde{X}\theta - \tilde{Y})$$

- Q: what kind of function is $J(\theta)$ and what does it look like?

- A: Quadratic function. Looks like either a "bowl" or "half-pipe"



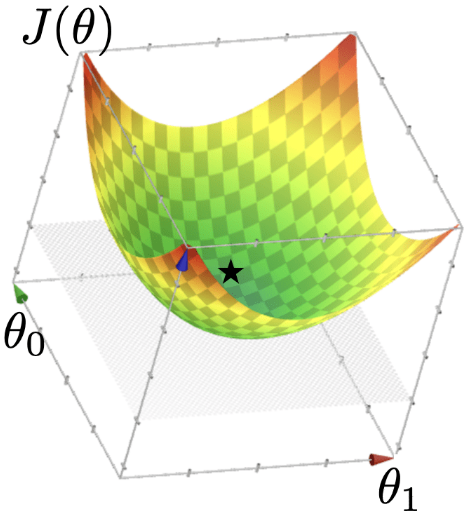


- When

$$J(\theta) = \frac{1}{n}(\tilde{X}\theta - \tilde{Y})^\top(\tilde{X}\theta - \tilde{Y})$$

looks a "bowl" (typically does)

- Uniquely minimized at a point if gradient at that point is zero and function "curves up" [see linear algebra]

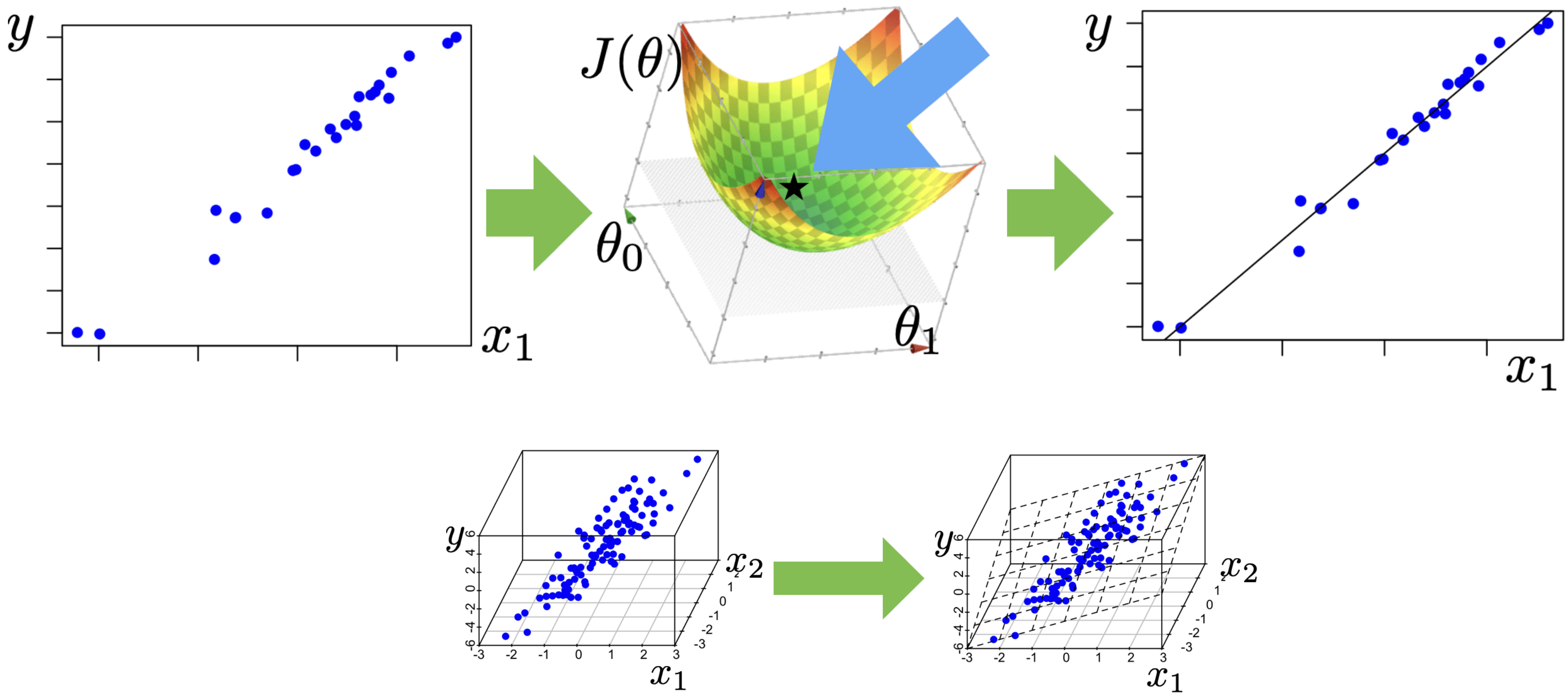


dx1

Set Gradient $\nabla_\theta J(\theta) \overset{\text{set}}{=} 0$

$$\theta^* = \left(\tilde{X}^\top \tilde{X}\right)^{-1} \tilde{X}^\top \tilde{Y}$$

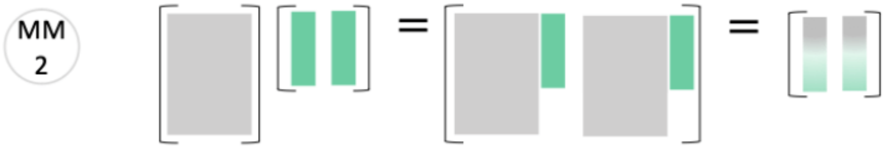
The beauty of $\theta^* = \left(\tilde{X}^\top \tilde{X}\right)^{-1} \tilde{X}^\top \tilde{Y}$: simple, general, unique minimizer



- Now, the catch (we'll see, all lead to half-pipe case)

- $\theta^* = \left(\tilde{X}^\top \tilde{X}\right)^{-1} \tilde{X}^\top \tilde{Y}$ is not well-defined if $\left(\tilde{X}^\top \tilde{X}\right)$ is not invertible

- Indeed, $\left(\tilde{X}^\top \tilde{X}\right)$ is not invertible if and only if $\tilde{X}$ is not full column rank



$A\boldsymbol{x}$ and $A\boldsymbol{y}$ are linear combinations of columns of A.

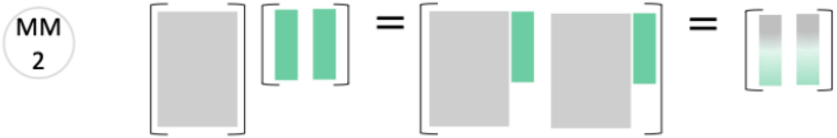
$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \end{bmatrix} = A[\boldsymbol{x} \quad \boldsymbol{y}] = [A\boldsymbol{x} \quad A\boldsymbol{y}]$$

- Indeed, $\left(\tilde{X}^\top \tilde{X}\right)$ is not invertible if and only if $\tilde{X}$ is not full column rank
- Recall

$$\underset{\text{nxd}}{\tilde{X}} = \begin{bmatrix} x_1^{(1)} & \cdots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(n)} & \cdots & x_d^{(n)} \end{bmatrix}$$

$\tilde{X}$ is not full column rank

1. if $n<d$
2. if columns (features) in $\tilde{X}$ have linear dependency

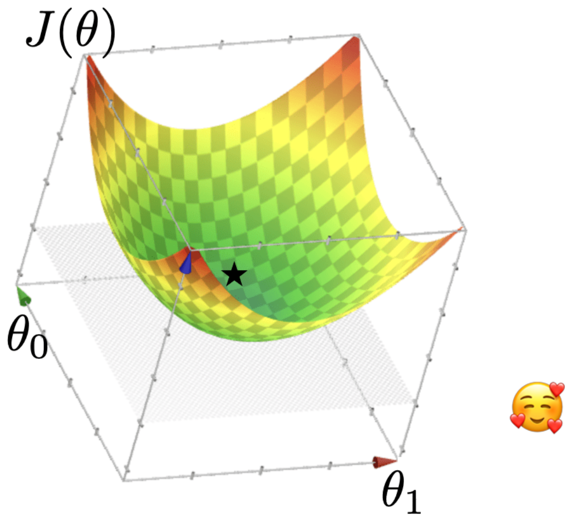


Ax and Ay are linear combinations of columns of A.

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \end{bmatrix} = A[\mathbf{x} \quad \mathbf{y}] = [A\mathbf{x} \quad A\mathbf{y}]$$

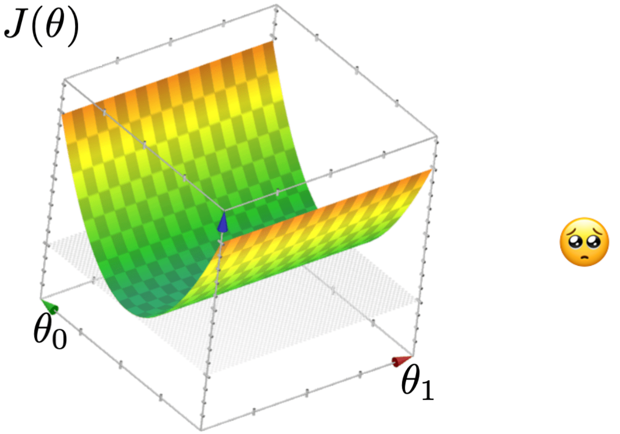
Quick Summary:

Typically $\theta^* = \left(\tilde{X}^\top \tilde{X}\right)^{-1} \tilde{X}^\top \tilde{Y}$



1. if $n<d$ (i.e. not enough data)
2. if columns (features) in $\tilde{X}$ have linear dependency (aka co-linearity)

- This formula 👈 is not well-defined
- Infinitely many optimal hyperplanes



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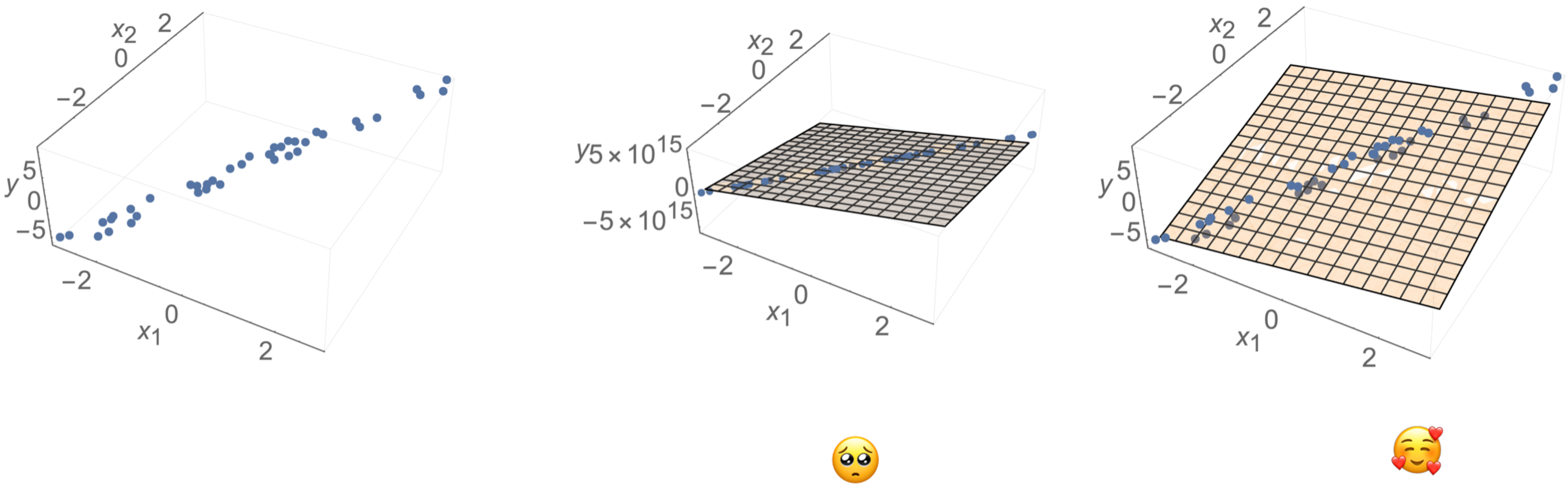
- Sometimes, noise can resolve the invertibility issue
- but still lead to undesirable results



- How to choose among hyperplanes?
- Prefer θ with small magnitude

Ridge Regression

- Add a square penalty on the magnitude
- $J_{\text{ridge}}(\theta) = \frac{1}{n}(\tilde{X}\theta - \tilde{Y})^\top(\tilde{X}\theta - \tilde{Y}) + \lambda\|\theta\|^2$ $(\lambda > 0)$
- λ is a so-called "hyperparameter"
- Setting $\nabla_\theta J_{\text{ridge}}(\theta) = 0$ we get
- $\theta^* = \left(\tilde{X}^\top \tilde{X} + n\lambda I\right)^{-1} \tilde{X}^\top \tilde{Y}$
- θ^* always exists, and is always the unique optimal parameters
- (If there's an offset, see recitation/hw for discussion.)

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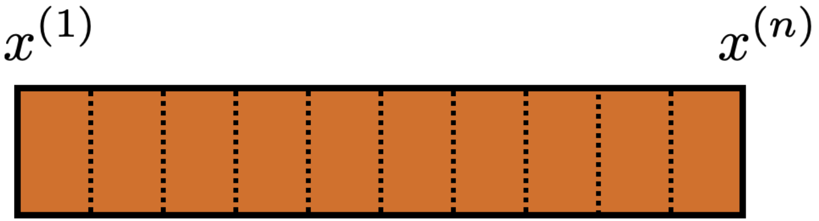
Cross-validation

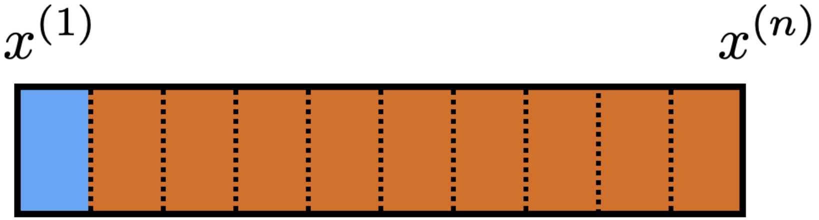



```
Cross-validate( 𝒟_n , k )
  Divide 𝒟_n into k chunks 𝒟_{n,1},...,𝒟_{n,k} (of
  roughly equal size)
```

Cross-validate($\mathcal{D}_n$, k)

Divide $\mathcal{D}_n$ into k chunks $\mathcal{D}_{n,1}, \ldots, \mathcal{D}_{n,k}$ (of roughly equal size)

Cross-validation

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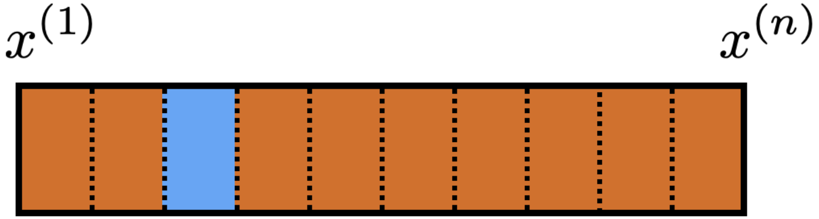
```

Cross-validation

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```
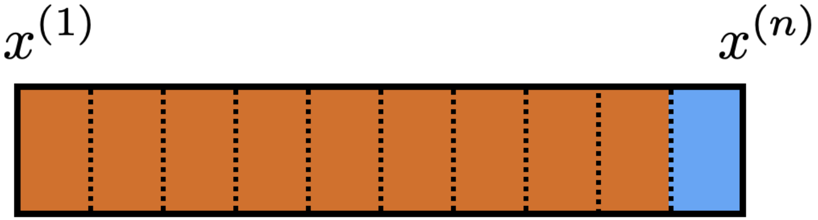
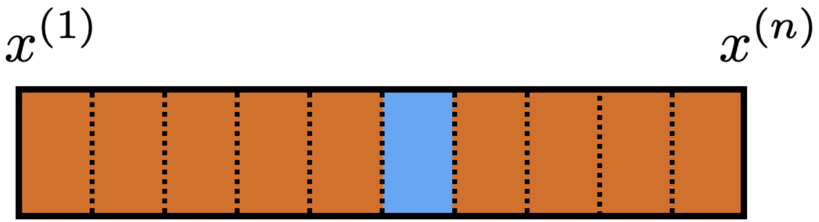

...

Cross-validation




```
Cross-validate( 𝒟ₙ , k )
  Divide 𝒟ₙ into k chunks 𝒟ₙ,₁,...,𝒟ₙ,ₖ (of
  roughly equal size)
  for i = 1 to k
```

Cross-validation




```
Cross-validate( 𝒟_n , k )
  Divide 𝒟_n into k chunks 𝒟_{n,1},...,𝒟_{n,k} (of
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  for i = 1 to k
    train h_i on 𝒟_n\𝒟_{n,i} (i.e. except chunk i)
```
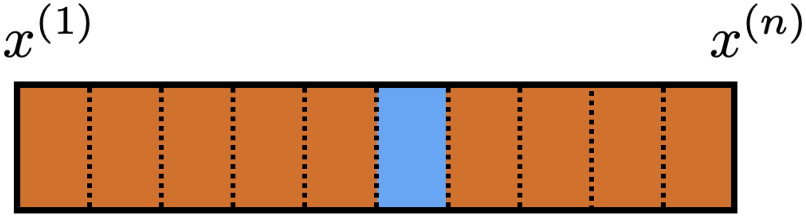
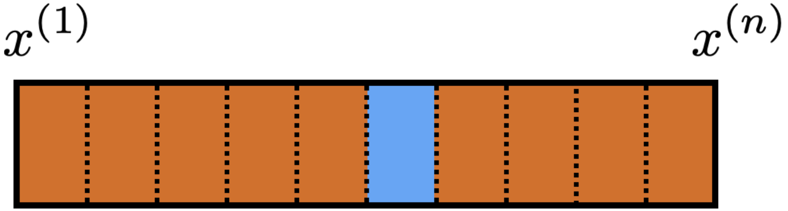

Cross-validation




```
Cross-validate(𝒟_n , k )
  Divide 𝒟_n into k chunks 𝒟_{n,1},...,𝒟_{n,k} (of
  roughly equal size)
  for i = 1 to k
    train h_i on 𝒟_n\𝒟_{n,i} (i.e. except chunk i)
    compute "test" error ℰ(h_i, 𝒟_{n,i}) of h_i on 𝒟_{n,i}
```

Cross-validation



```
Cross-validate( D_n , k )
  Divide D_n into k chunks D_{n,1},...,D_{n,k} (of
  roughly equal size)
  for i = 1 to k
    train h_i on D_n\D_{n,i} (i.e. except chunk i)
    compute "test" error E(h_i, D_{n,i}) of h_i on D_{n,i}
  Return (1/k) sum_{i=1}^{k} E(h_i, D_{n,i})
```

Cross-validate($\mathcal{D}_n$, k)

Divide $\mathcal{D}_n$ into k chunks $\mathcal{D}_{n,1},\ldots,\mathcal{D}_{n,k}$ (of roughly equal size)

for i = 1 to k

train h_i on $\mathcal{D}_n \backslash \mathcal{D}_{n,i}$ (i.e. except chunk i)

compute "test" error $\mathcal{E}(h_i, \mathcal{D}_{n,i})$ of h_i on $\mathcal{D}_{n,i}$

Return $\frac{1}{k}\sum_{i=1}^{k}\mathcal{E}(h_i, \mathcal{D}_{n,i})$

Comments on (cross)-validation

- good idea to shuffle data first
- a way to "reuse" data
- it's not to evaluate a hypothesis
- rather, it's to evaluate learning algorithm (e.g. hypothesis class choice, hyperparameters)
- Could e.g. have an outer loop for picking good hyperparameter or hypothesis class

Summary

- One strategy for finding ML algorithms is to reduce the ML problem to an optimization problem.
- For the ordinary least squares (OLS), we can find the optimizer analytically, using basic calculus! Take the gradient and set it to zero. (Generally need more than gradient info; suffices in OLS)
- Two ways to approach the calculus problem: write out in terms of explicit sums or keep in vector-matrix form. Vector-matrix form is easier to manage as things get complicated (and they will!)
- There are some good discussions in the lecture notes.

Summary

- What does it mean for linear regression to be well posed.
- When there are many possible solutions, we need to indicate our preference somehow.
- Regularization is a way to construct a new optimization problem.
- Least-squares regularization leads to the ridge-regression formulation. Good news: we can still solve it analytically!
- Hyperparameters and how to pick them; cross-validation.

https://docs.google.com/forms/d/e/1FAIpQLSftMB5hSccgAbIAFmP_LuZt95w6KFx0x_R3uuzBP8WwjSzZeQ/viewform?embedded=true

We'd love to hear your thoughts.

Thanks!