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6.390 Intro to Machine Learning

Lecture 2: Linear regression and regularization

Shen Shen

Feb 9, 2024

(many slides adapted from Tamara Broderick)

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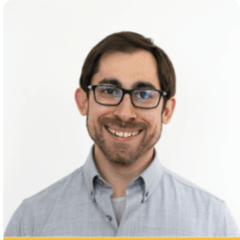
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Logistical issues? Personal concerns? We'd love to help out at **6.390-personal@mit.edu**

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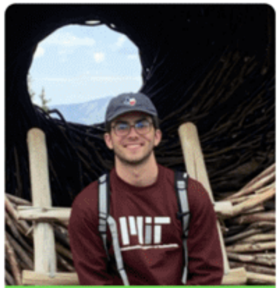

Andi Spiride


Lucian Covarrubias

and ~40 awesome LAs

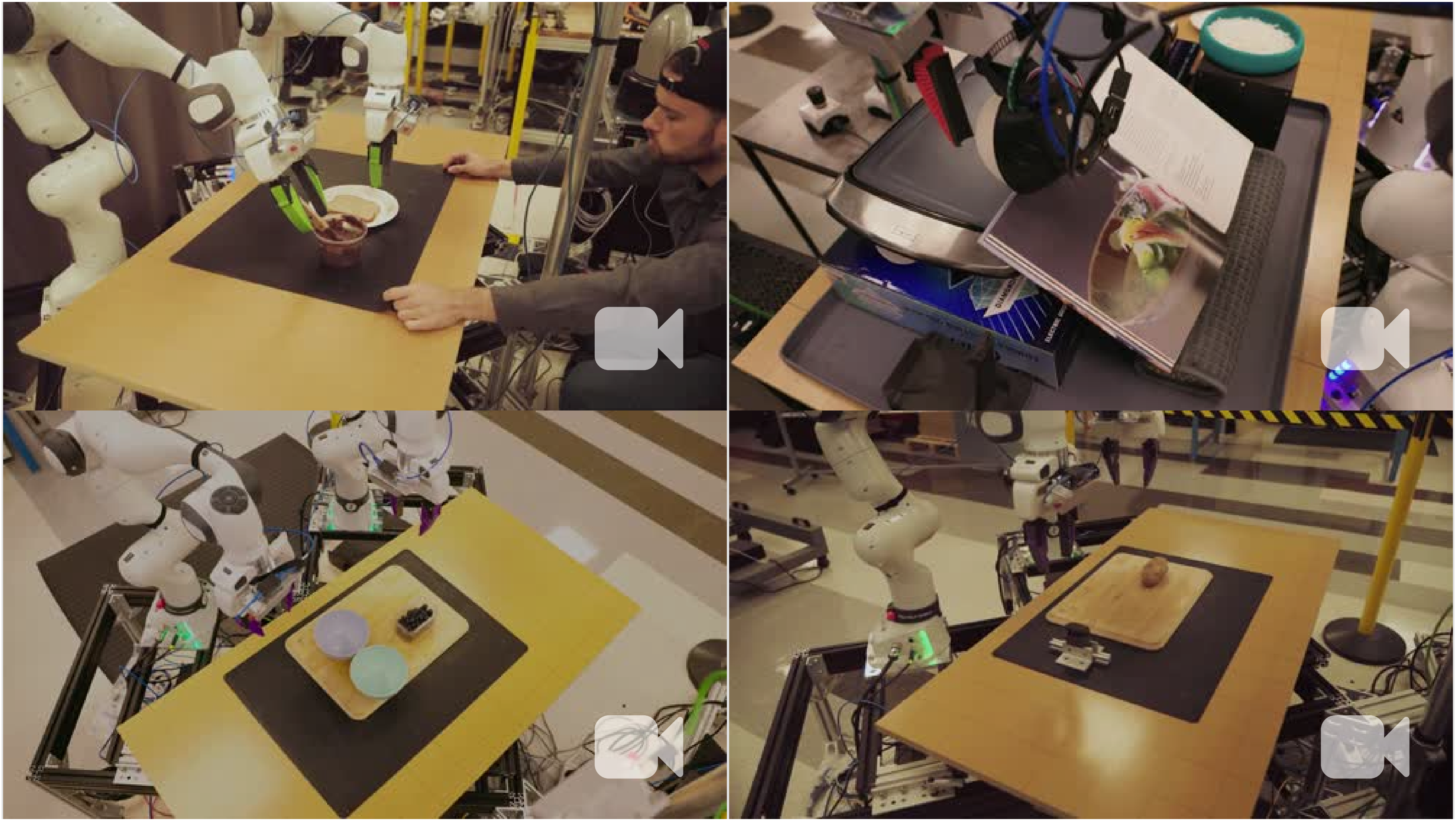
Logistics

- 11am Section 3 and 4 are completely full and we have many requests to switch. Physical space packed.
- If at all possible, please help us by signup/switch to other slots.

- OHs start this Sunday, please also join our Piazza
- Thanks for all the assignments feedback. We are adapting on-the-go but these certainly benefit future semesters.
- Start to get assignments due now. (first up, exercises 2, keep an eye on the "due")

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

Optimization + first-principle physics



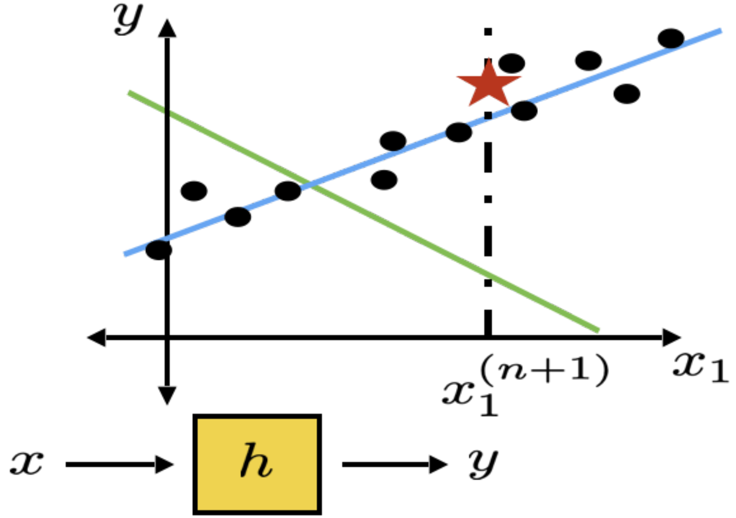
https://www.youtube.com/embed/fn3KWM1kuAw?enablejsapi=1

Outline

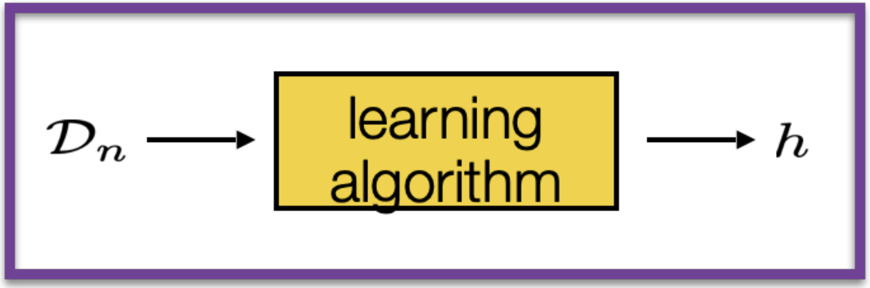
- Recap of last (content) week.
- Ordinary least-square regression
  - Analytical solution (when exists)
  - Cases when analytical solutions don't exist
    - Practically, visually, mathamtically
- Regularization
- Hyperparameter, cross-validation

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!)

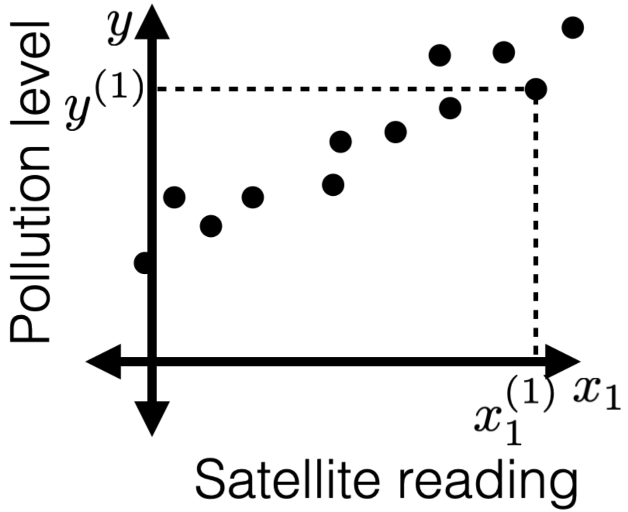


Example: predict pollution level

(Training) data

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

- Training data $\mathcal{D}_n = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$



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

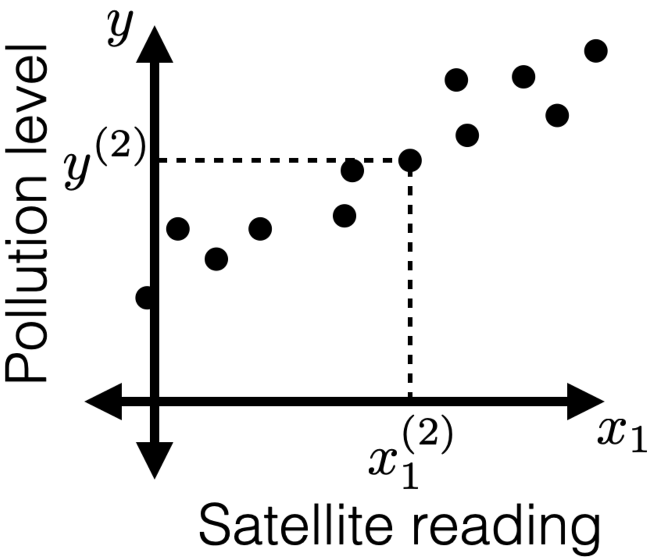
How to label? Hypothesis $h : \mathbb{R}^d \to \mathbb{R}$

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

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

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

Linear regressors

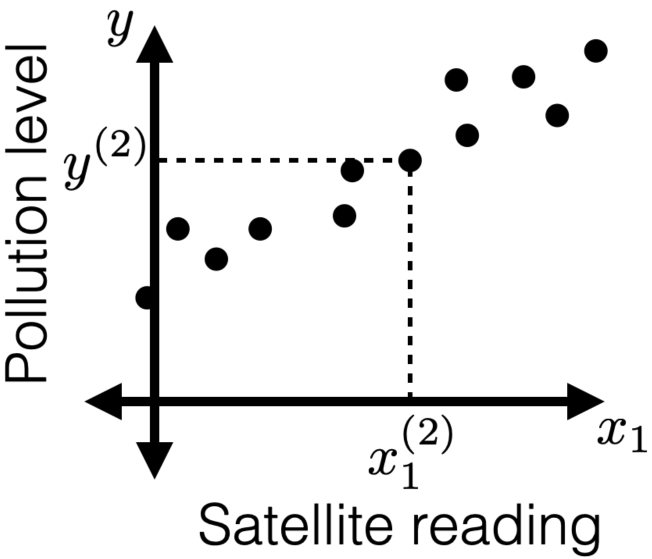


Linear regressors

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

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

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



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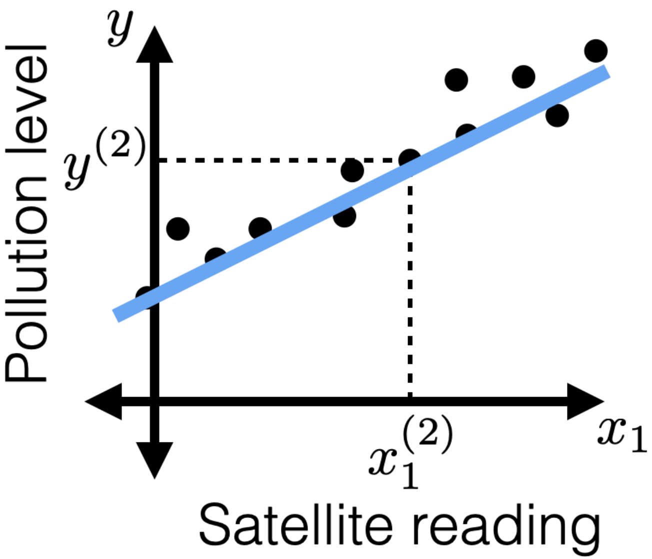

Linear regressors

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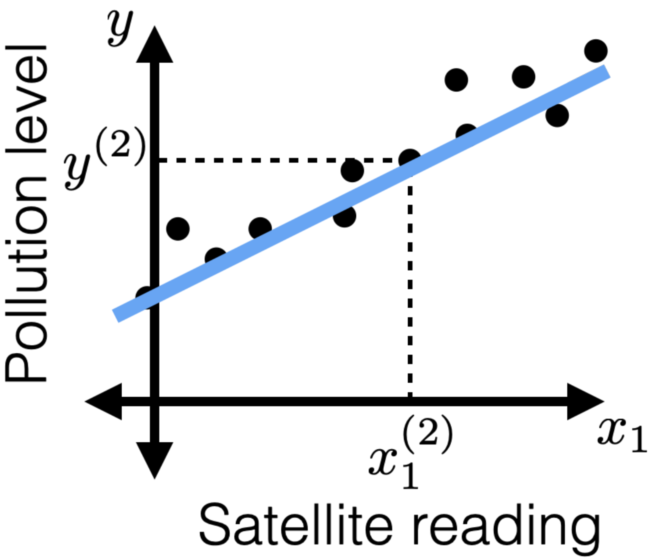
$$h(x; \theta, \theta_0) = \theta x + \theta_0$$

parameters



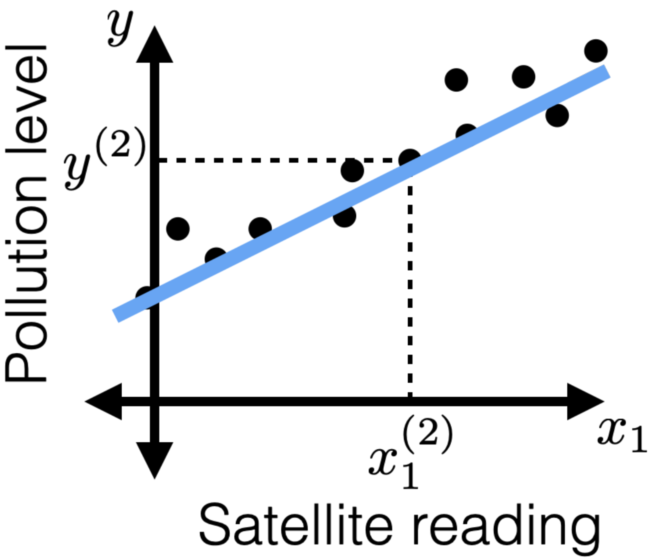
Linear regressors

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

- A linear regression hypothesis when d=1:

  parameters

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



- A linear reg. hypothesis when d≥1:

$$\begin{aligned} h(x; \theta, \theta_0) &= \theta_1 x_1 + \cdots + \theta_d x_d + \theta_0 \\ &= \theta^\top x + \theta_0 \end{aligned}$$

OR

$$\begin{aligned} h(x) &= \theta_1 x_1 + \cdots + \theta_d x_d + (\theta_0)(1) \\ &= \theta^\top x \end{aligned}$$

Linear regressors

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

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

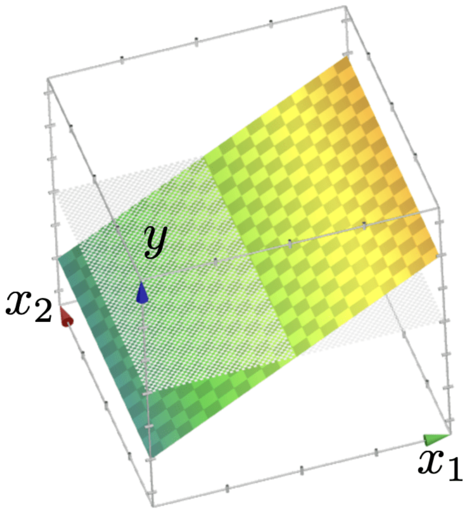
1x2,2x1

OR

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

1x3,3x1

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

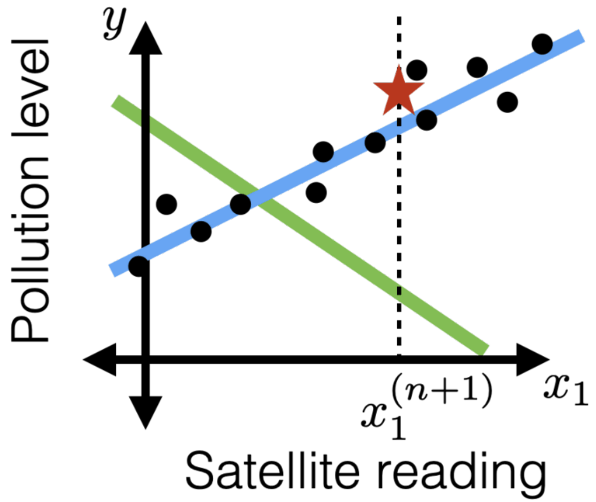


- Our hypothesis class in linear regression will be the set of all such *h*

Hypothesis is a "hyperplane"

How good is a regression hypothesis?

- Should predict well on future data
- How good is a regressor at one point? Loss $L(g, a)$ g: guess, a: actual
  - Ex: squared loss
    $$L(g, a) = (g - a)^2$$
  - Example: asymmetric loss
    $$L(g, a) = \begin{cases} (g-a)^2 \text{ if } g > a \\ 2(g-a)^2 \text{ if } g \leq a \end{cases}$$

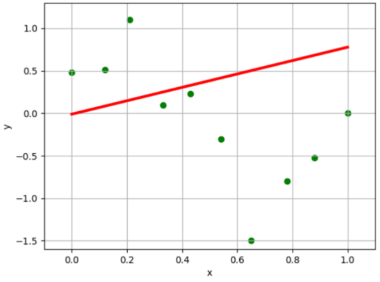


- Test error (n' new points): $\mathcal{E}(h) = \frac{1}{n'} \sum_{i=n+1}^{n+n'} L(h(x^{(i)}), y^{(i)})$
- Training error: $\mathcal{E}_n(h) = \frac{1}{n} \sum_{i=1}^{n} L(h(x^{(i)}), y^{(i)})$
- One idea: prefer h to $\tilde{h}$ if $\mathcal{E}_n(h) < \mathcal{E}_n(\tilde{h})$

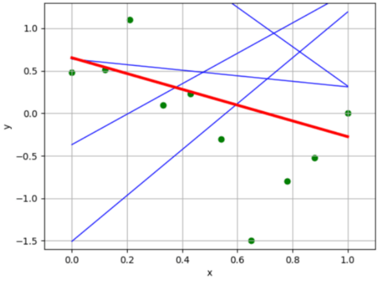
1.3)

Now, here are some executions for different values of k (shown in red is the hypothesis with the lowest MSE, among the k tested).

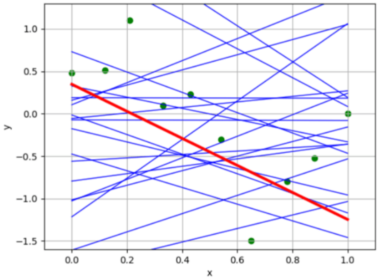
(A) k=1



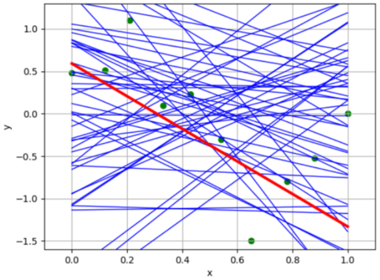
(B) k=5



(C) k=20



(D) k=50



- What happens as we increase `k`? Compare the four “best” linear regressors found by the random regression algorithm with different values of `k` chosen, which one does your group think is "best of the best"?
- How does it match your initial guess about the best hypothesis?
- 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: Another way

- How about we just consider all hypotheses in our class and choose the one with lowest training error?
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- Recall: training error: $\mathcal{E}_n(h) = \frac{1}{n}\sum_{i=1}^{n} L(h(x^{(i)}), y^{(i)})$
- Training error: square loss, linear regr., extra “1” feature

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

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Define

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

nxd

nx1

Linear regression: Another way

- Training error: square loss, linear regr., extra “1” feature

$$J(\theta) = \frac{1}{n}\sum_{i=1}^{n}(\theta^\top x^{(i)} - y^{(i)})^2 \quad \boxed{= \frac{1}{n}(\tilde{X}\theta - \tilde{Y})^\top(\tilde{X}\theta - \tilde{Y})}$$

Define

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nxd

nx1

Linear regression: A Direct Solution

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

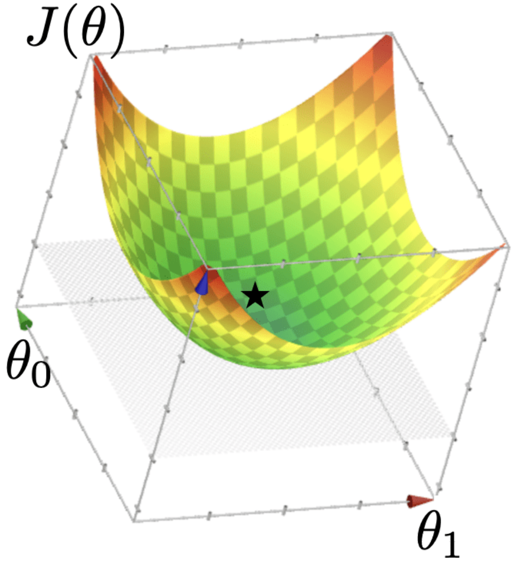
- Q: what kind of function is $J(\theta)$

- Q: how does $J(\theta)$ look like?

- A: $J(\theta)$ quadratic function;

  typically look like a "bowl" (but

  there're exceptions)



Linear regression: A Direct Solution

- Goal: minimize $J(\theta) = \frac{1}{n}(\tilde{X}\theta - \tilde{Y})^\top(\tilde{X}\theta - \tilde{Y})$
- Uniquely minimized at a point if gradient at that point is zero and function "curves up" [see linear algebra]
- Gradient $\nabla_\theta J(\theta) \overset{\text{set}}{=} 0$

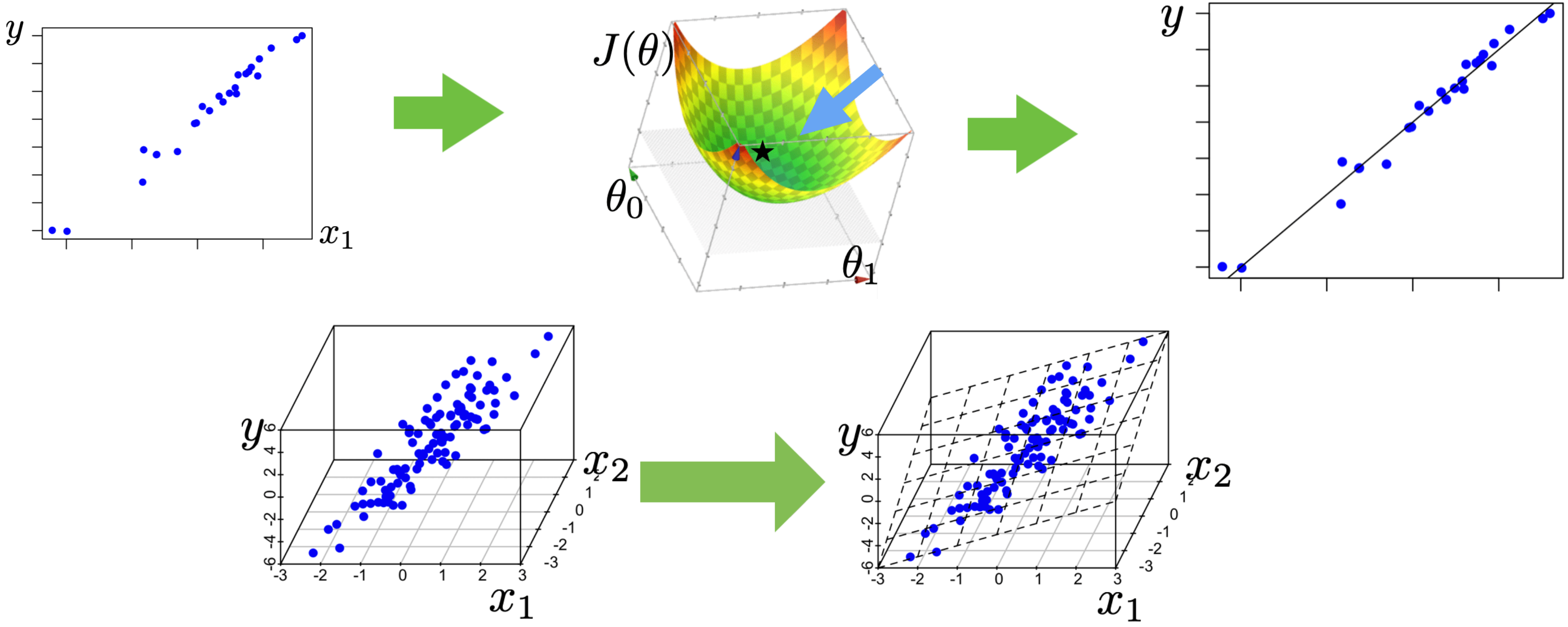
dx1

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

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

- When θ^* exists, guaranteed to be unique minimizer of

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

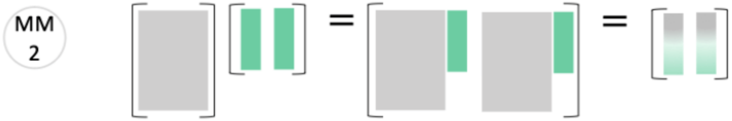


Now, the catch: $\theta^* = \left(\tilde{X}^\top \tilde{X}\right)^{-1} \tilde{X}^\top \tilde{Y}$ may not be well-defined

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

- Indeed, it's possible that $\left(\tilde{X}^\top \tilde{X}\right)$ is not invertible.

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



$\boldsymbol{Ax}$ and $\boldsymbol{Ay}$ are linear combinations of columns of A.

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

Now, the catch: $\theta^* = \left(\tilde{X}^\top \tilde{X}\right)^{-1} \tilde{X}^\top \tilde{Y}$ is not well-defined

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

Recall

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

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

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

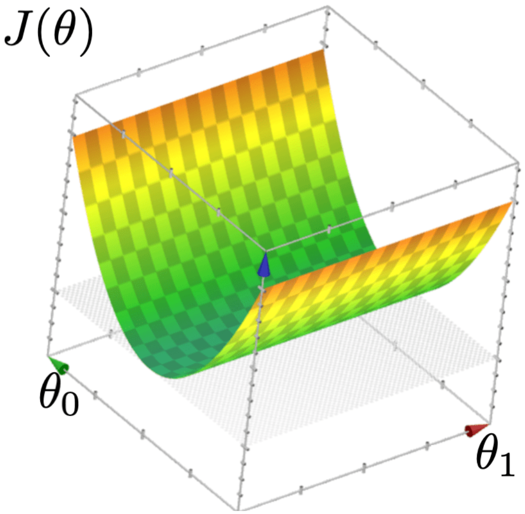
Recap:

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

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

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

- Both cases do happen in practice
- In both cases, loss function is a "half-pipe"
- In both cases, infinitily-many optimal hypotheses
- Side-note: sometimes noise can resolve invertabiliy issue, but undesirable



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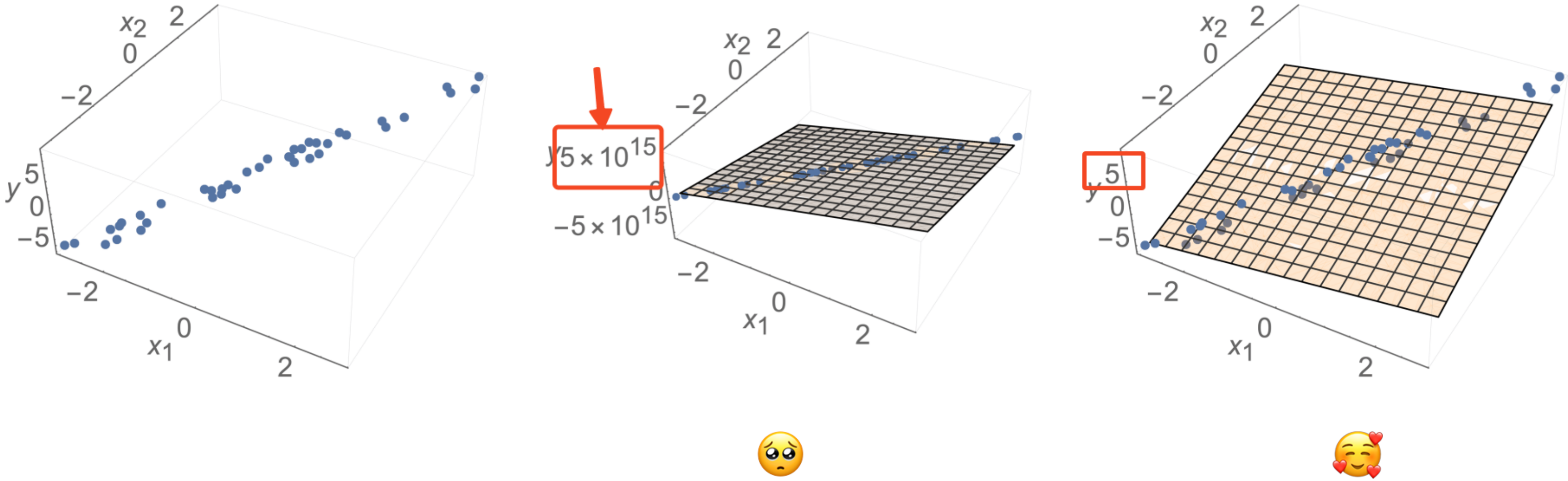
Regularization



- How to choose among hyperplanes? Preference for θ components being near zero

Ridge Regression Regularization

- Linear regression with square penalty: ridge regression

$$J_{\text{ridge}}(\theta, \theta_0) = \frac{1}{n} \sum_{i=1}^{n} (\theta^\top x^{(i)} + \theta_0 - y^{(i)})^2 + \lambda \|\theta\|^2$$

Ridge Regression Regularization

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Ridge Regression Regularization

- Linear regression with square penalty: ridge regression

$$J_{\text{ridge}}(\theta, \theta_0) = \frac{1}{n}\sum_{i=1}^{n}(\theta^\top x^{(i)} + \theta_0 - y^{(i)})^2 + \boxed{\lambda\|\theta\|^2} \qquad \boxed{(\lambda > 0)}$$

- Special case: ridge regression with no offset

$$J_{\text{ridge}}(\theta) = \frac{1}{n}(\tilde{X}\theta - \tilde{Y})^\top(\tilde{X}\theta - \tilde{Y}) + \lambda\|\theta\|^2$$

- Min at: $\nabla_\theta J_{\text{ridge}}(\theta) = 0$

$$\Rightarrow \theta = (\underbrace{\tilde{X}^\top \tilde{X}}_{\text{dxn,nxd}} + n\lambda \underbrace{\boxed{I}}_{\text{dxd}})^{-1}\tilde{X}^\top \tilde{Y}$$

- When $\lambda > 0$, always “curves up” & can invert
- Can also solve with an offset

λ is a hyper-parameter

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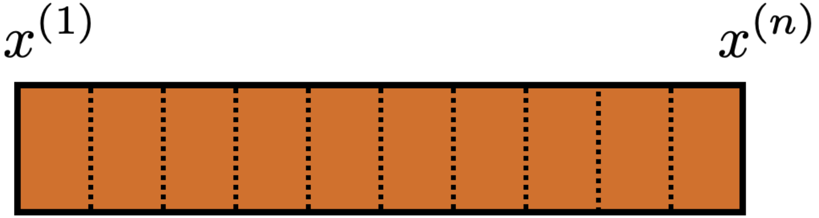
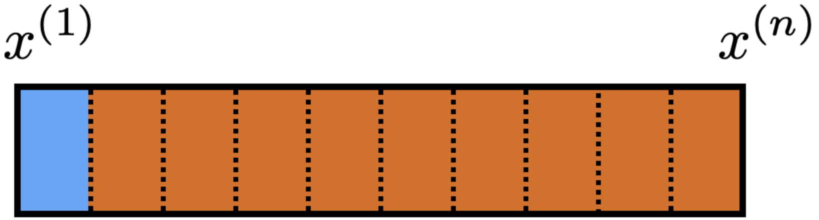
Cross-validation




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

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
```
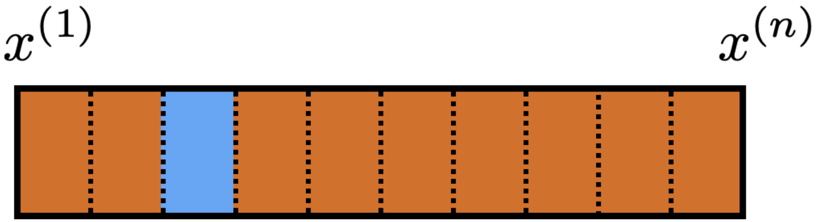

Cross-validation



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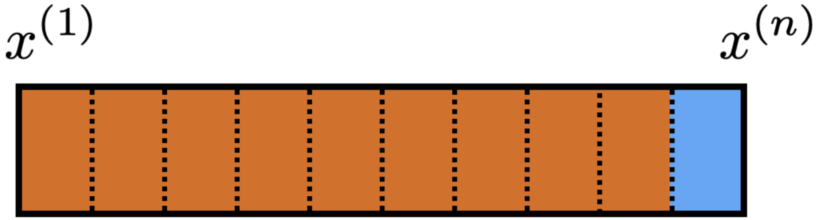
  for i = 1 to k

...

Cross-validation



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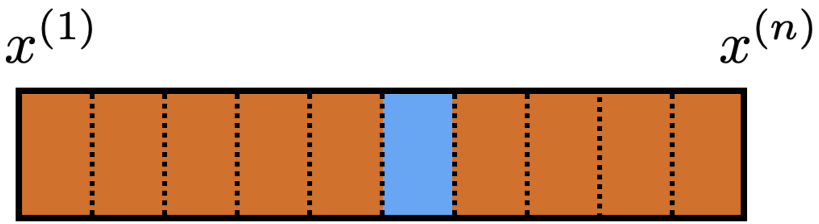


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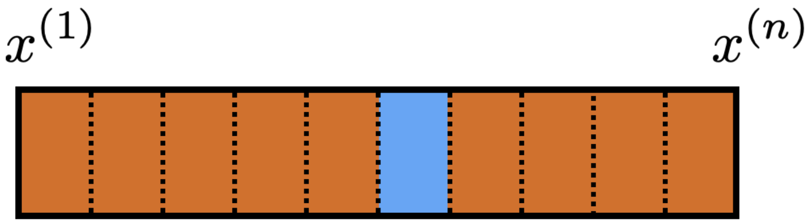
Cross-validation



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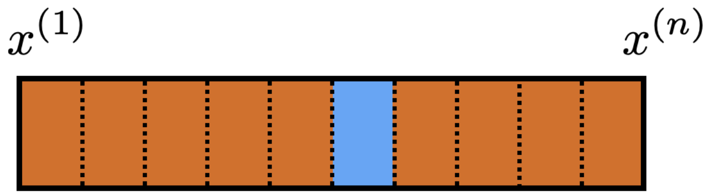
    compute "test" error $\mathcal{E}(h_i, \mathcal{D}_{n,i})$ of h_i on $\mathcal{D}_{n,i}$

Cross-validation



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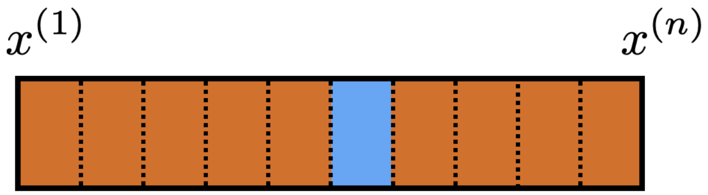
Return $\frac{1}{k} \sum_{i=1}^{k} \mathcal{E}(h_i, \mathcal{D}_{n,i})$

Cross-validation



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    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 about cross-validation

- good idea to shuffle data first
- a way to "reuse" data
- not evaluating a hypothesis, but rather
- evaluating learning algorithm. (e.g. hypothesis class, hyper-parameter)
- Could e.g. have an outer loop for picking good hyper-parameter/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 to 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!
- Hyper-parameters and how to pick them. Cross-validation

We'd love it for you to share some lecture feedback.

Thanks!