

6.036: Introduction to Machine Learning

Lecture start: Tuesdays 9:35am

Lecture team: Prof. Tamara Broderick & TA Elizabeth Zou

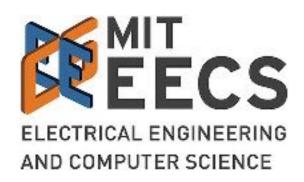
Questions? Ask on Piazza

Materials: slides, video will all be available on Canvas

Live Zoom feed: https://mit.zoom.us/j/94238622313

Today's Plan

- Meet the team
- II. Machine learning setup
- III. Linear regression
- IV. Regularization



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Elizabeth

Broderick Zou

Learning

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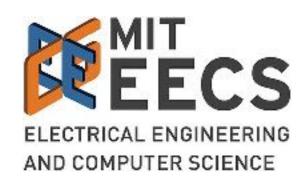
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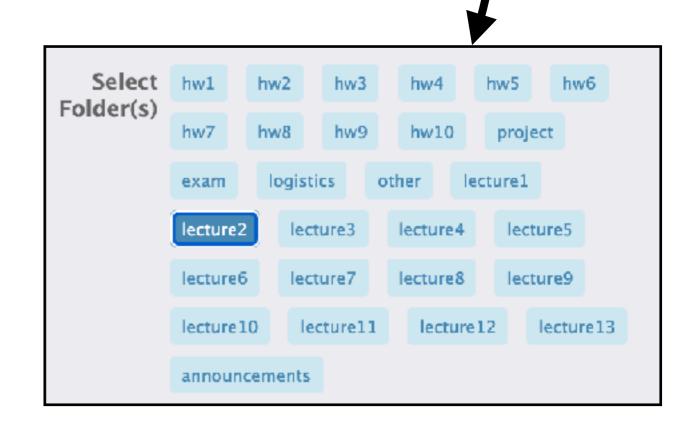
Questions? Ask on Piazza: "lecture (week) 2" folder

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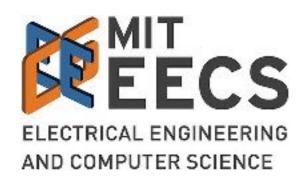
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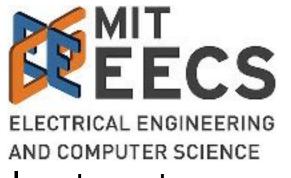


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Instructors:



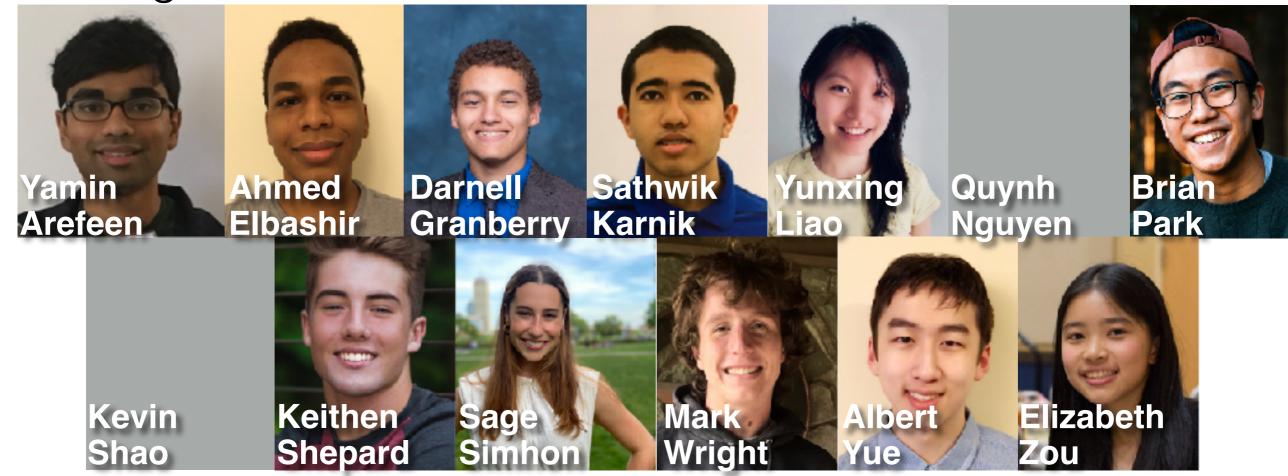
ELECTRICAL ENGINEERING AND COMPUTER SCIENCE

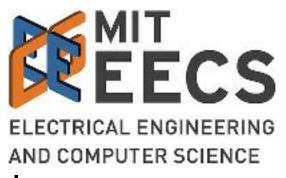
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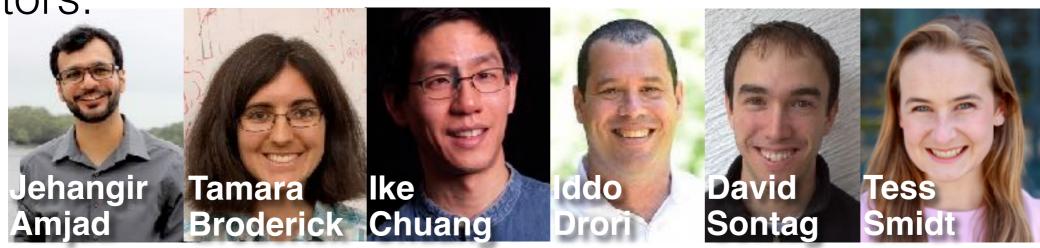
Teaching Assistants:



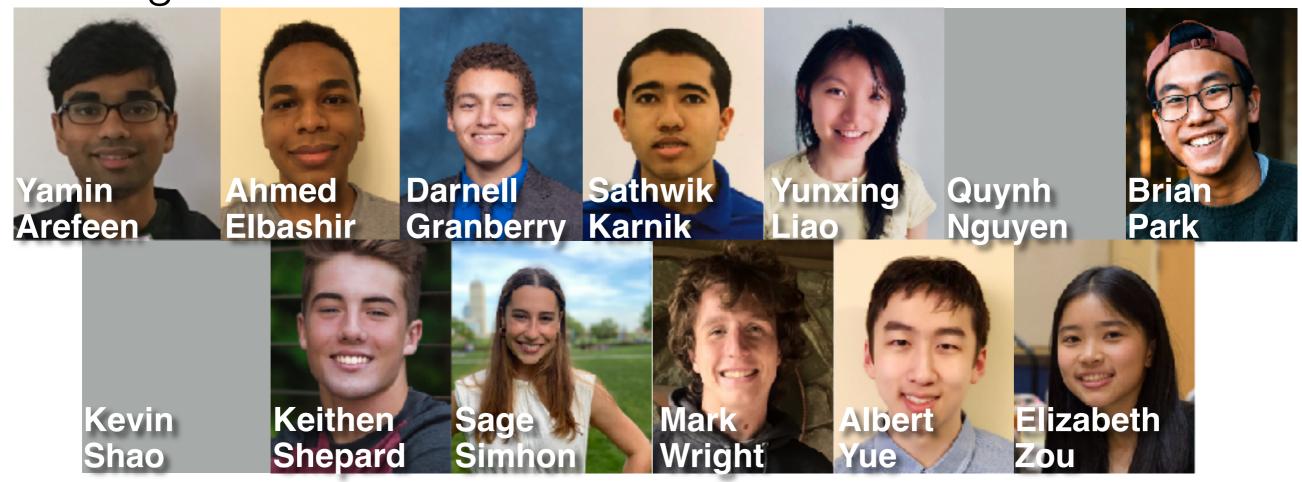


6.036: Introduction to Machine Learning, Staff

Instructors:



Teaching Assistants:



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NEWS 22 July 2021

DeepMind's AI predicts structures for a vast trove of proteins

AlphaFold neural network produced a 'totally transformative' database of more than 350,000 structures from *Homo* sapiens and 20 model organisms.

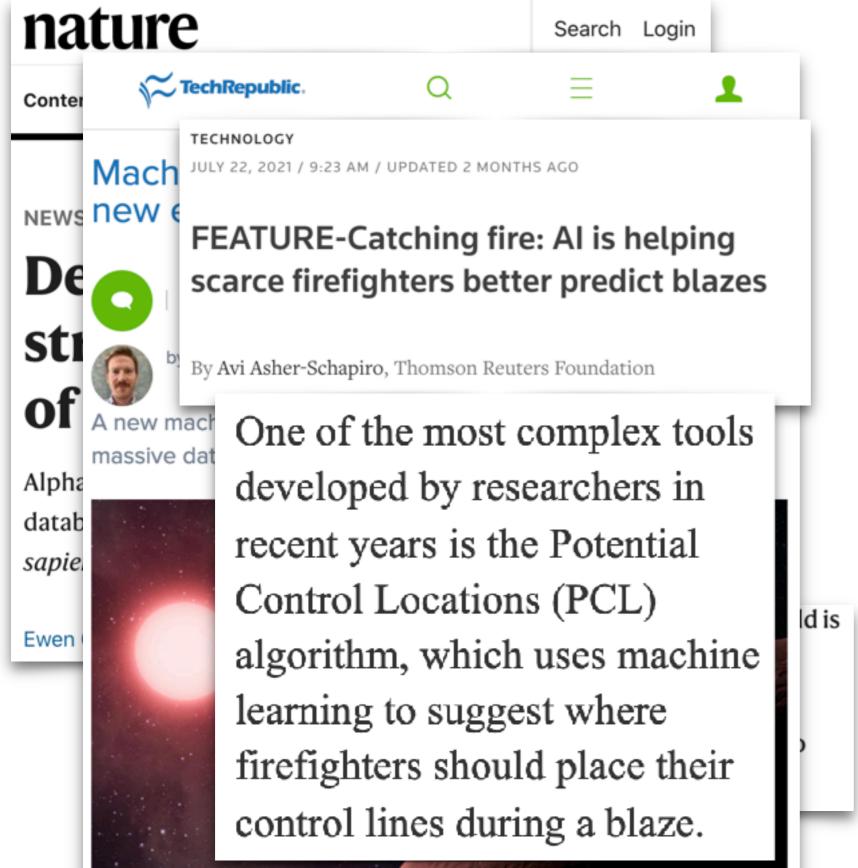
Ewen Callaway

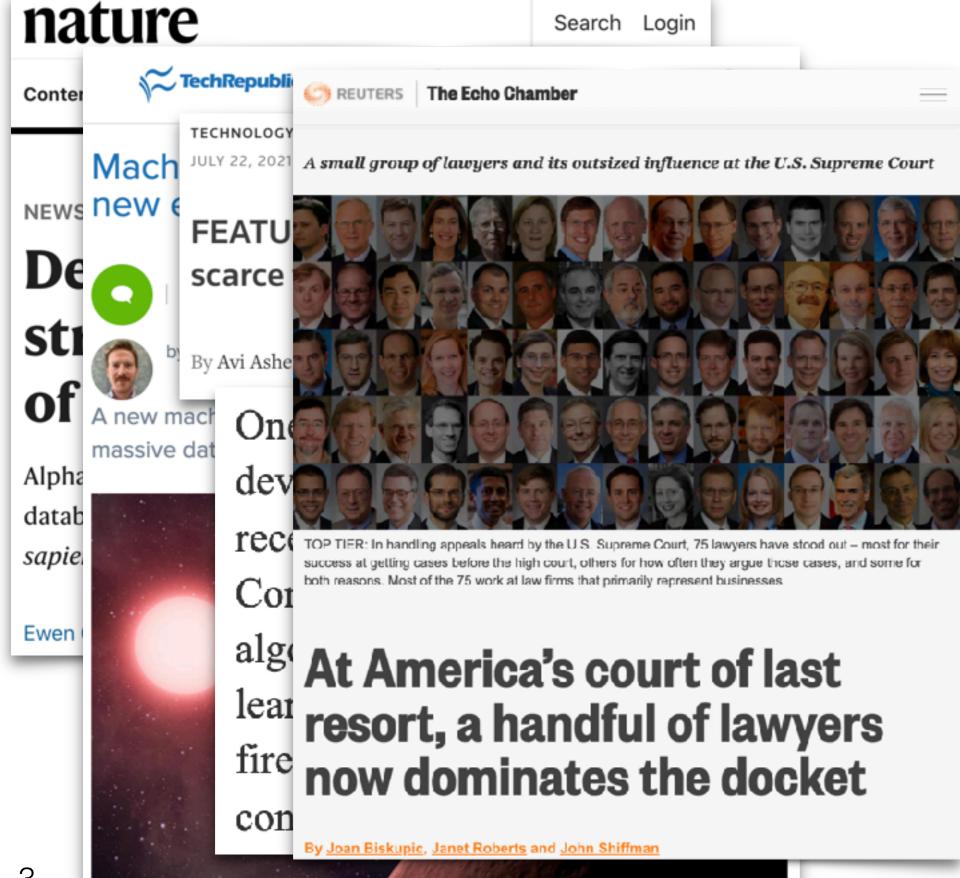
Underpinning the latest version of AlphaFold is a novel machine learning approach that incorporates physical and biological knowledge about protein structure, leveraging multi-sequence alignments, into the design of the deep learning algorithm.

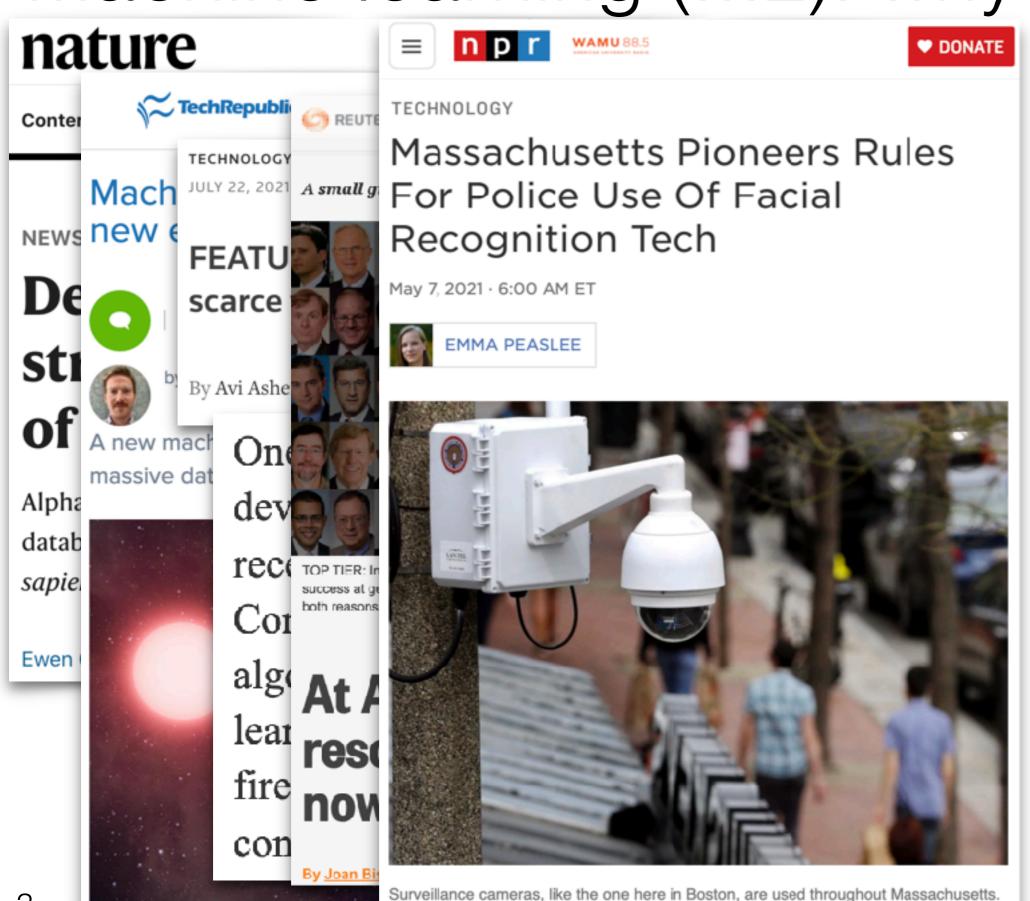
[https://www.techrepublic.com/article/machine-learning-algorithm-confirms-50-new-exoplanets-in-historic-first/]



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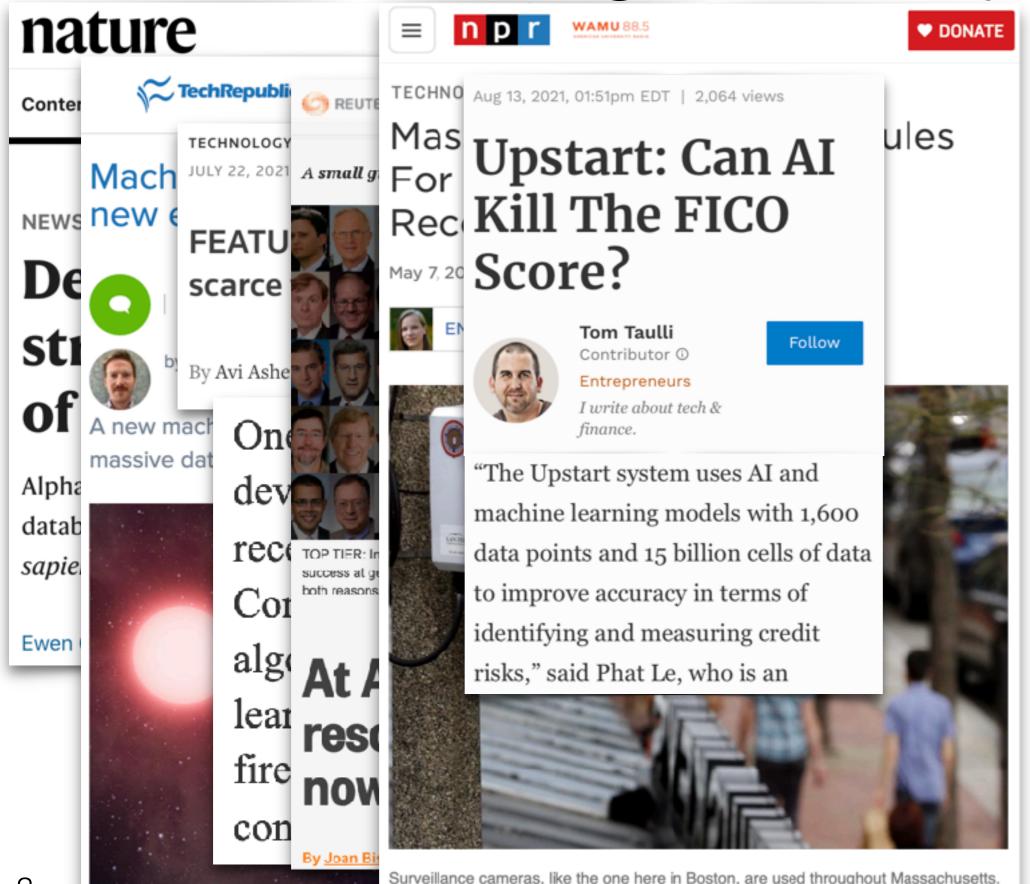




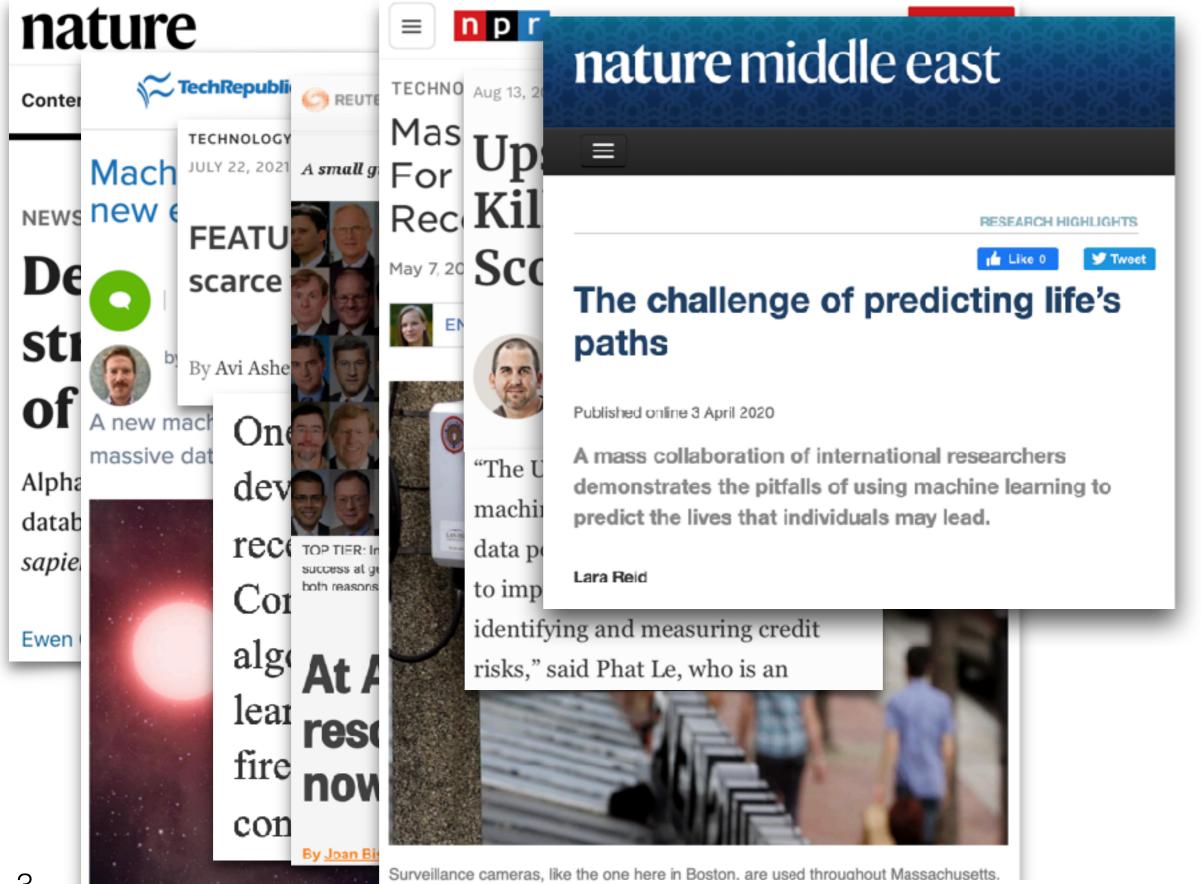


The state now regulates how police use facial recognition technology.

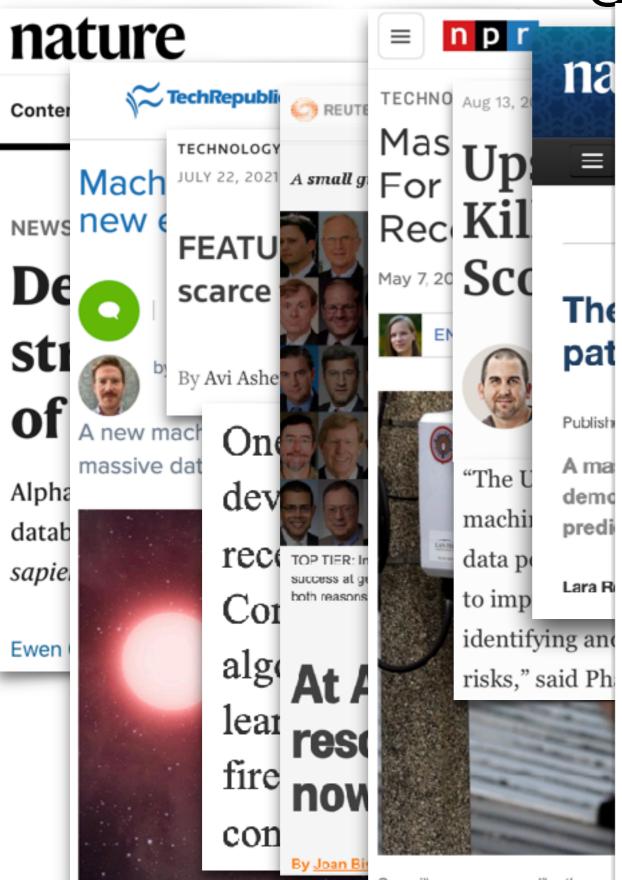
[https://www.npr.org/ 2021/05/07/982709480/ massachusetts-pioneers-rulesfor-police-use-of-facialrecognition-tech]



The state now regulates how p [https://www.forbes.com/sites/tomtaulli/2021/08/13/upstart-can-ai-kill-the-fico-score/]



The state now regulates how poll [https://www.natureasia.com/en/nmiddleeast/article/10.1038/nmiddleeast.2020.46]



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Artificial intelligence / Machine learning

Hundreds of AI tools have been built to catch covid. None of them helped.

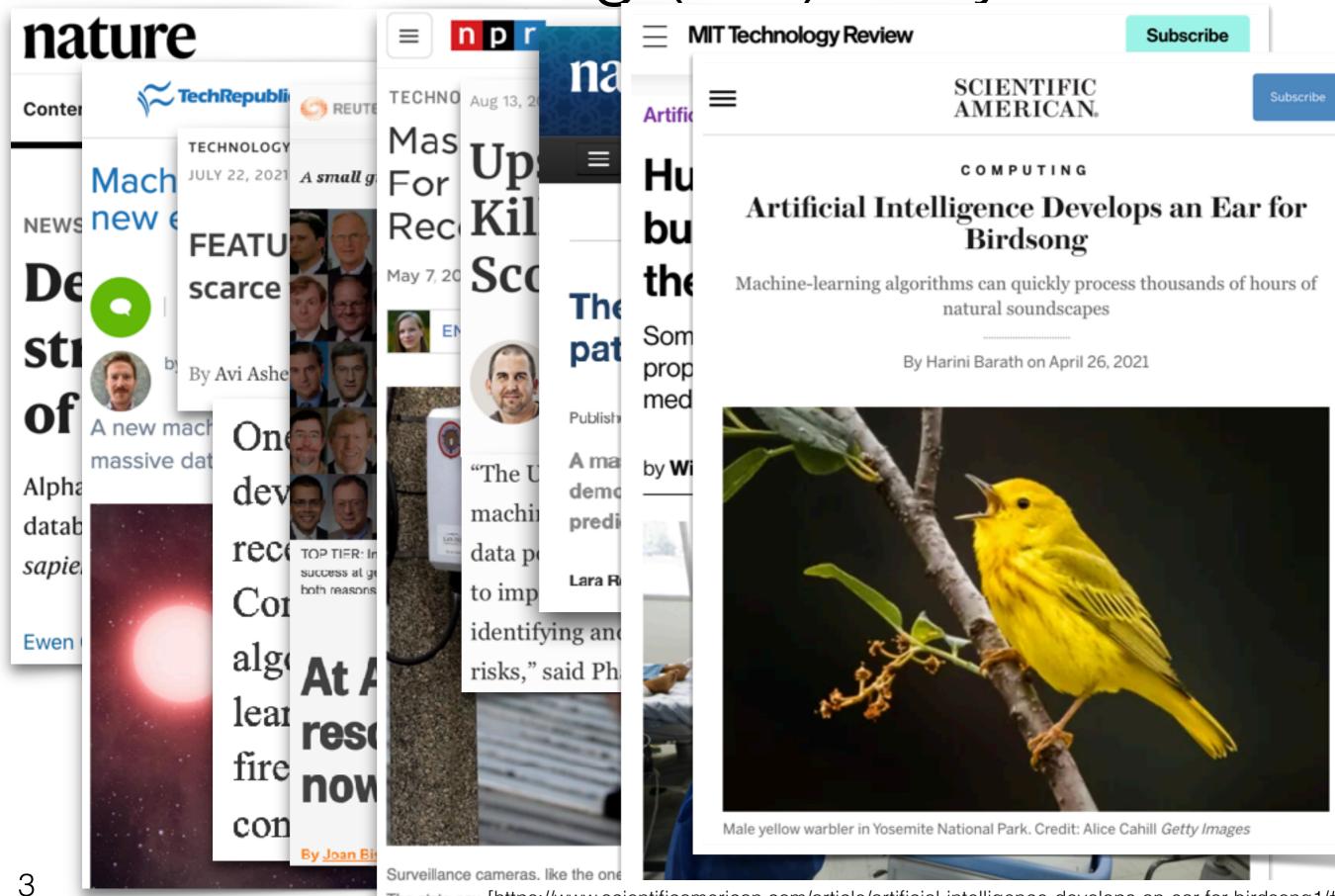
Some have been used in hospitals, despite not being properly tested. But the pandemic could help make medical AI better.

by Will Douglas Heaven

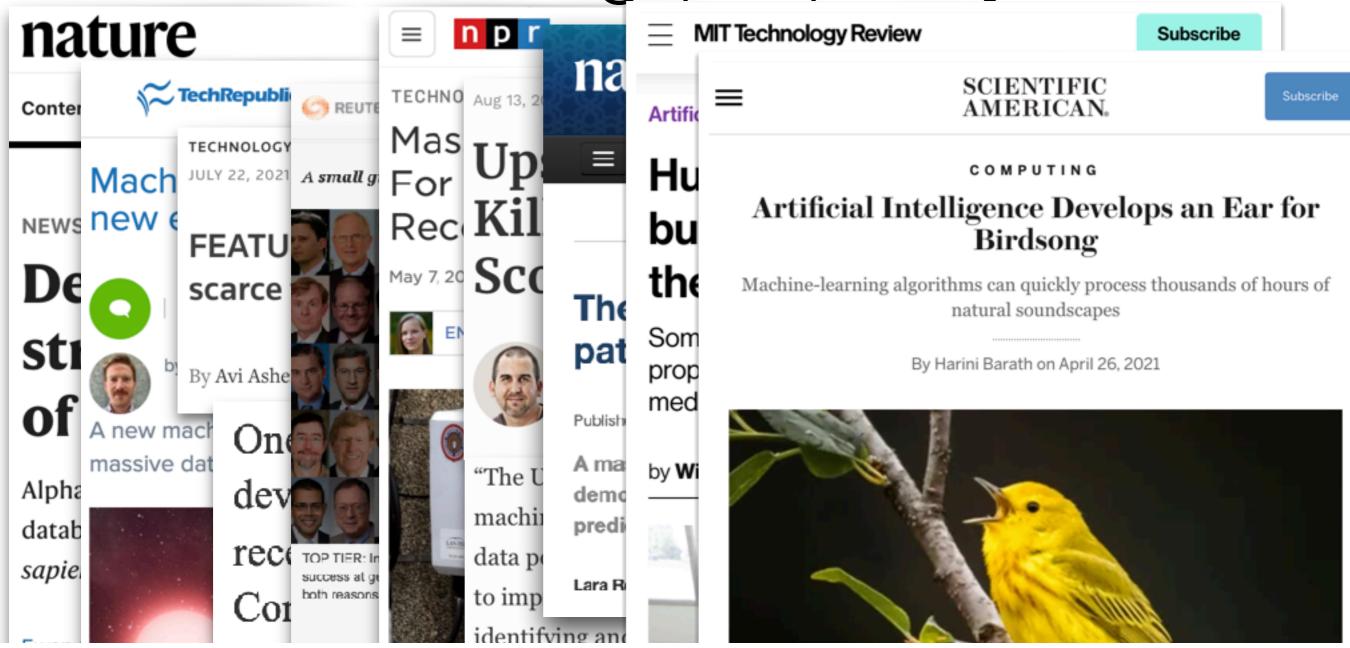
July 30, 2021



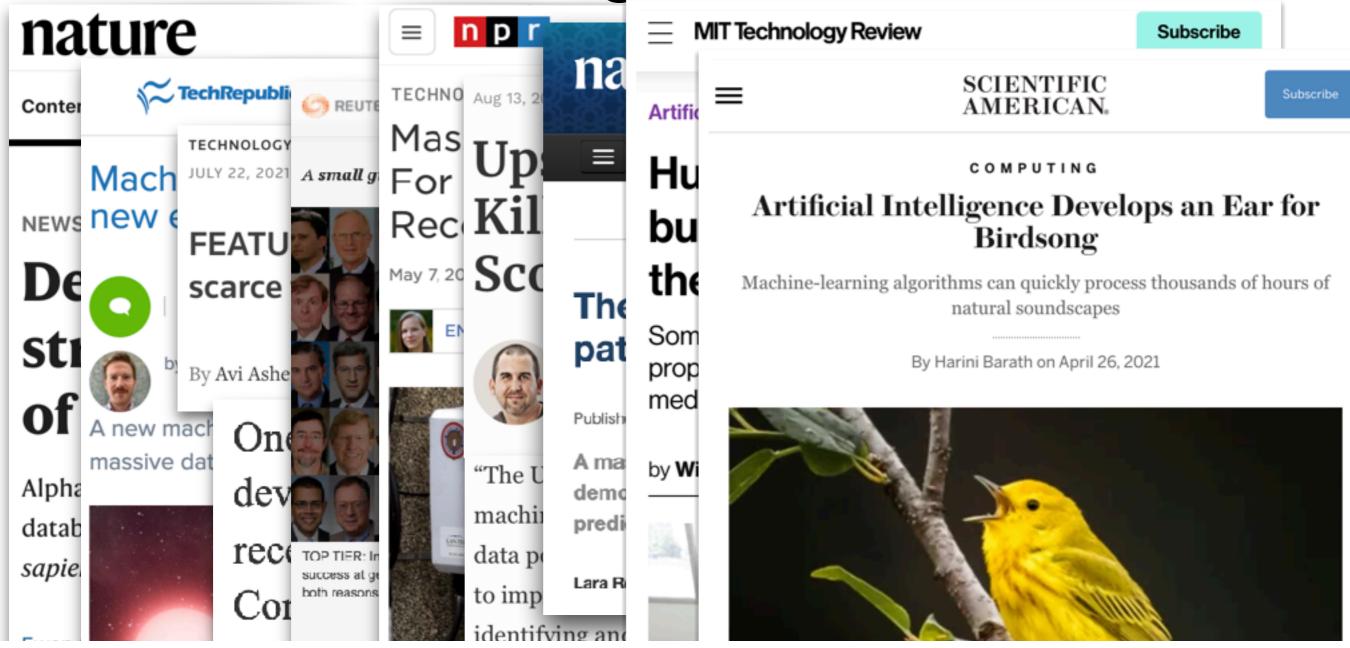
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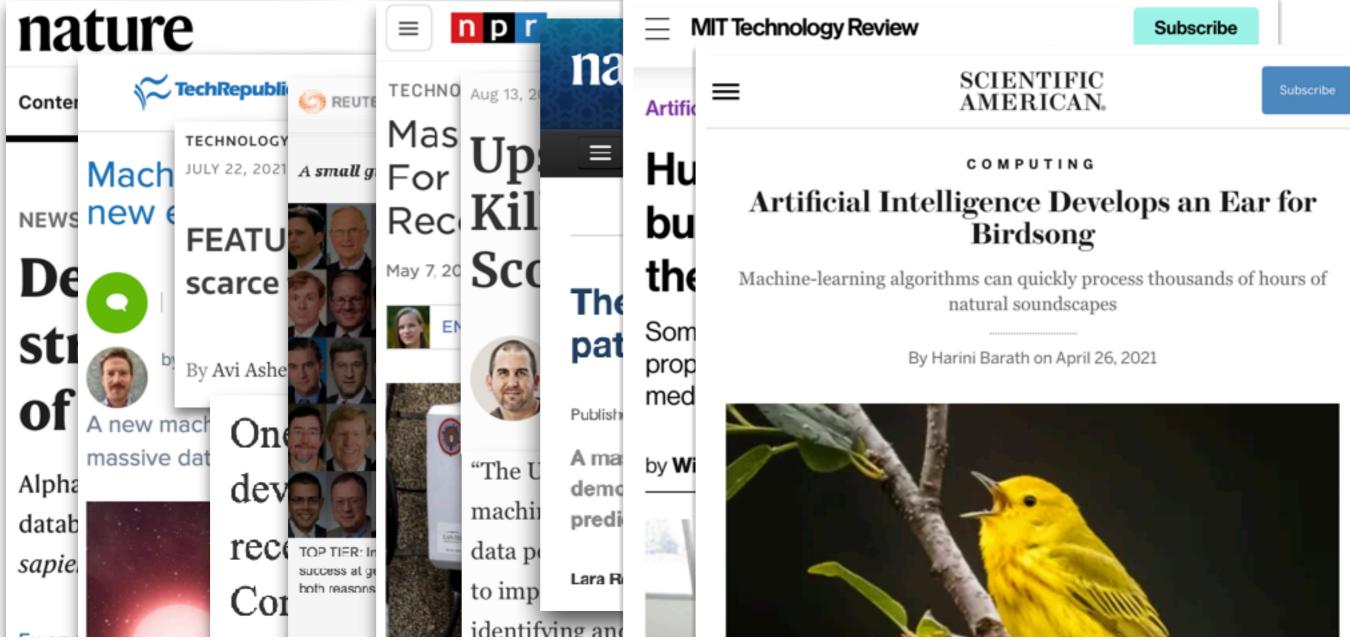
The state now [https://www.scientificamerican.com/article/artificial-intelligence-develops-an-ear-for-birdsong1/#]



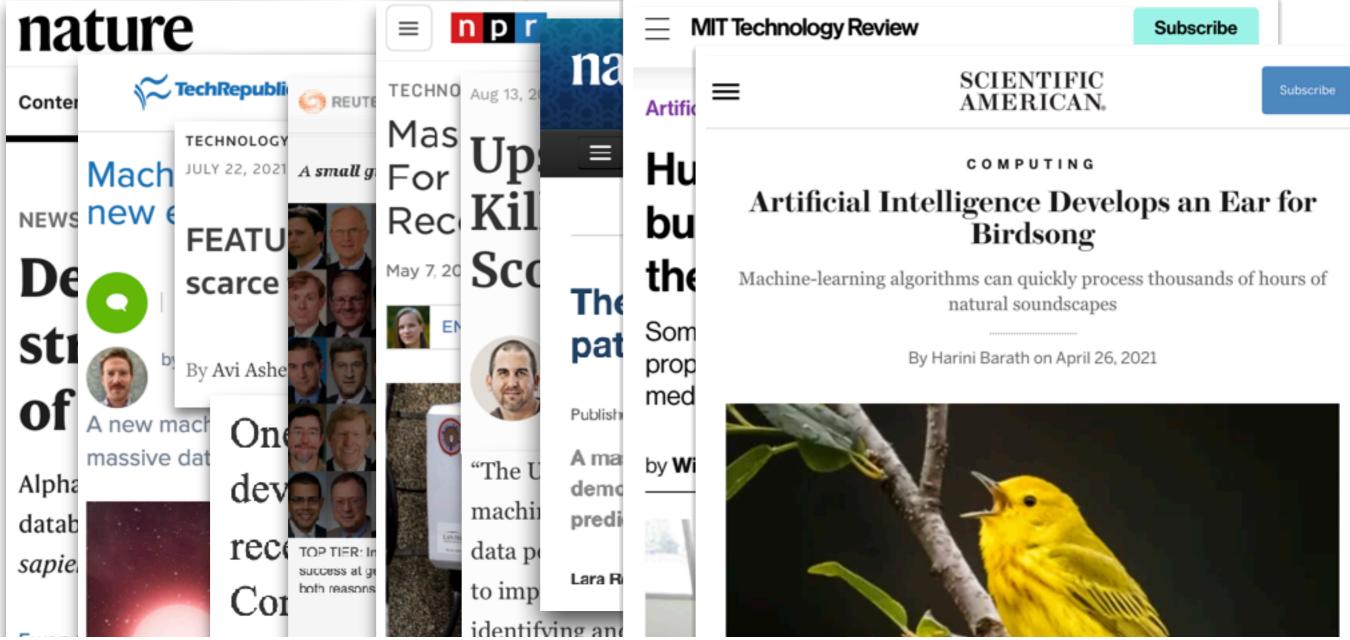
What is ML?



• What is ML? A set of methods for making decisions from data. (See the rest of the course!)



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- Why study ML? To apply; to understand; to evaluate



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- Why study ML? To apply; to understand; to evaluate
- Notes: ML is a tool with pros & cons. ML is built on math

Example: predict pollution level

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What do we have?

Example: predict pollution level

What do we have? (Training) data

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• *n* training data points

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$$x^{(i)} = (x_1^{(i)}, \dots, x_d^{(i)})^{\top} \in \mathbb{R}^d$$

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Satellite reading

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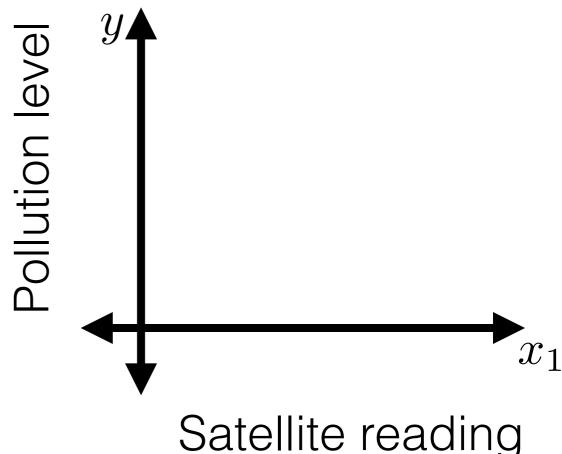
• Label $y^{(i)} \in \mathbb{R}$



Satellite reading

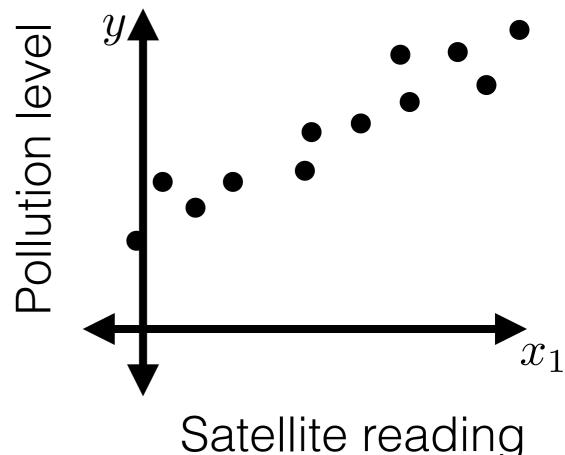
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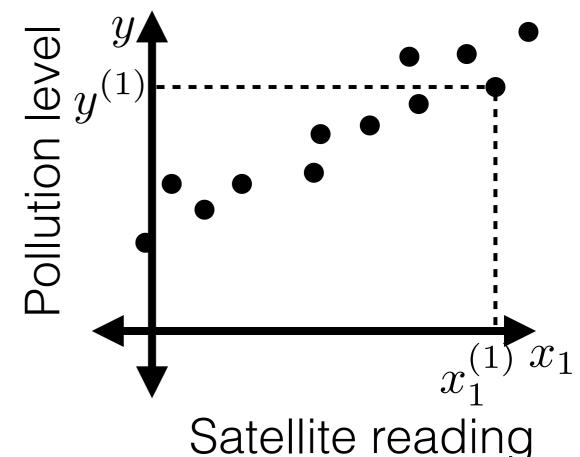
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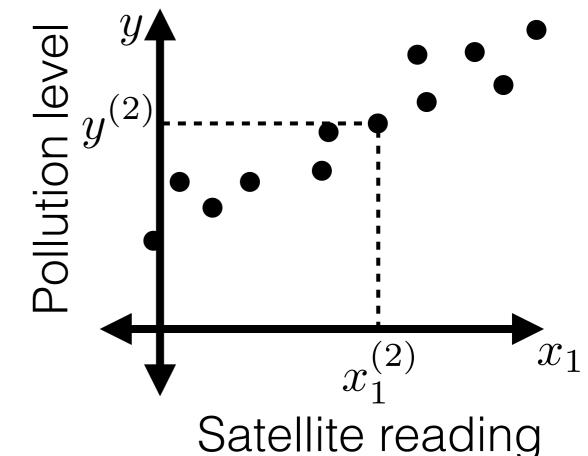
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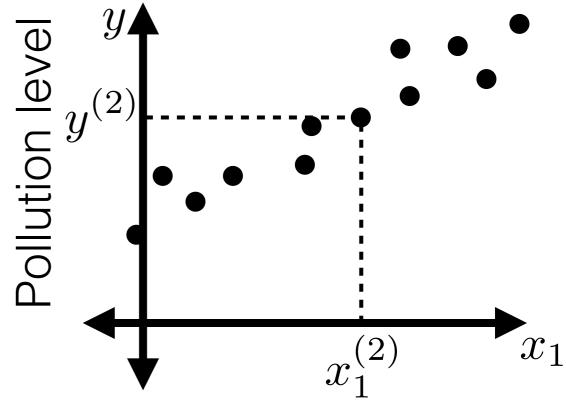
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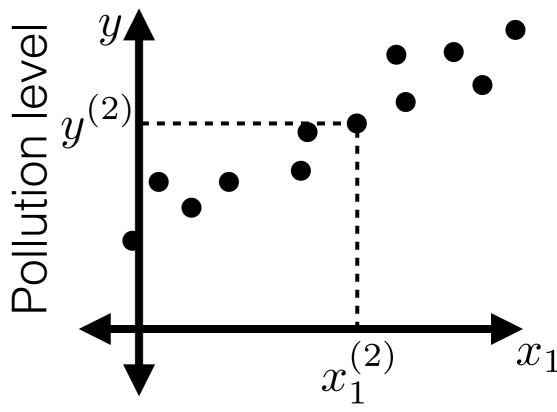
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What do we want?



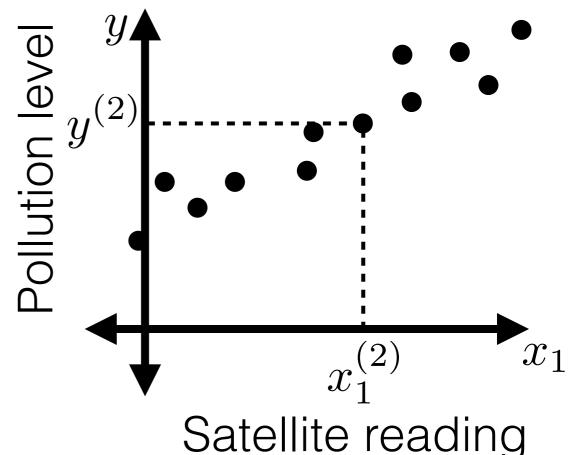
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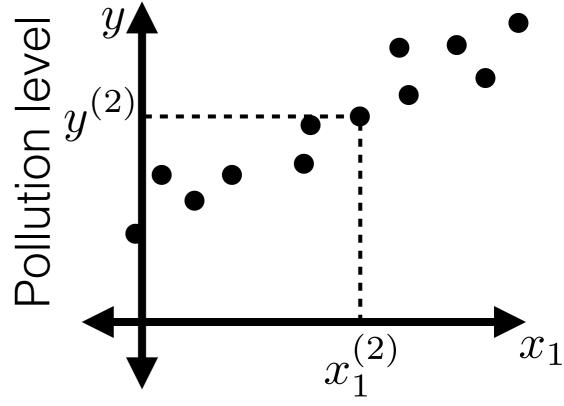
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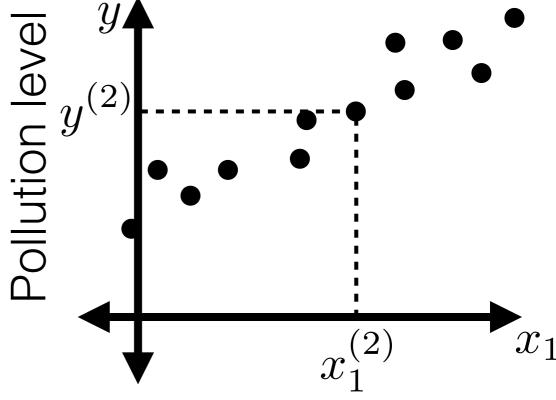
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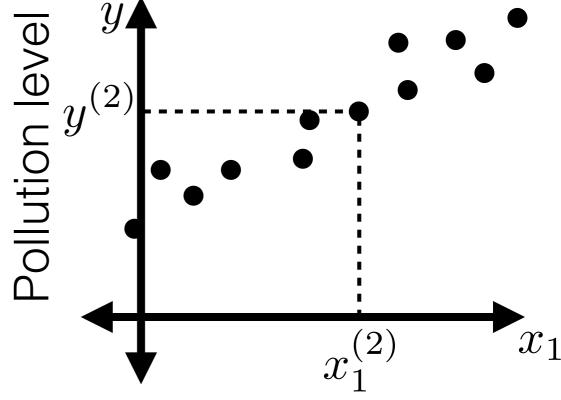
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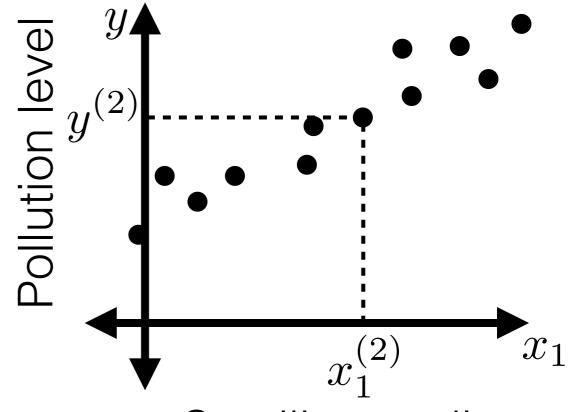
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Is this a hypothesis?

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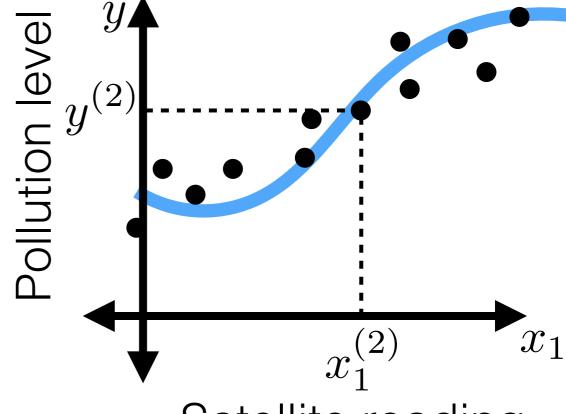
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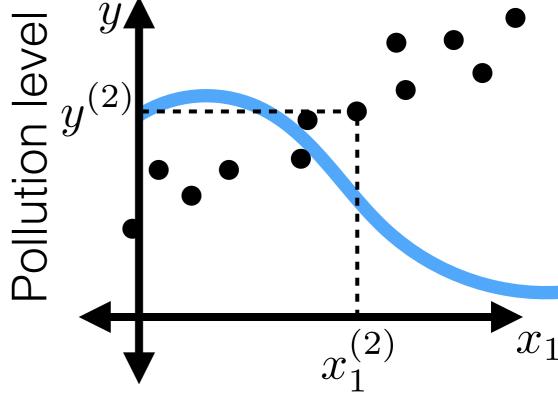
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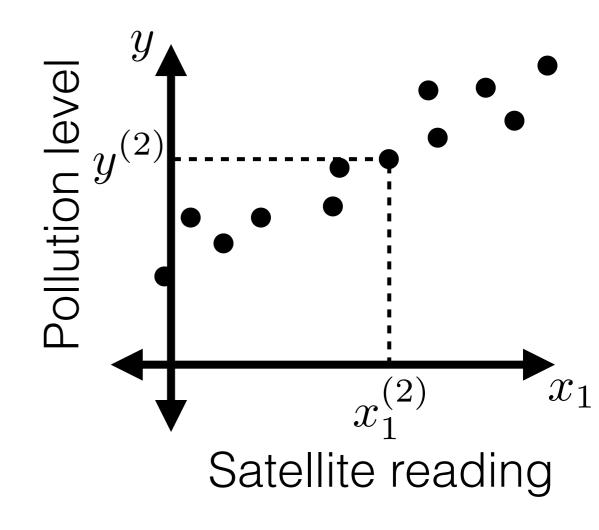
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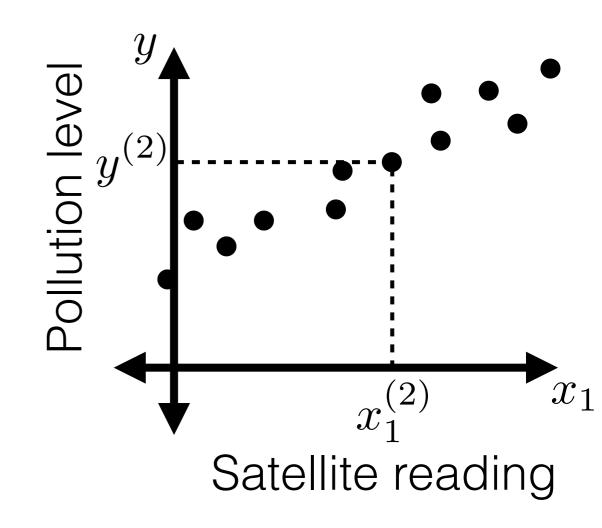
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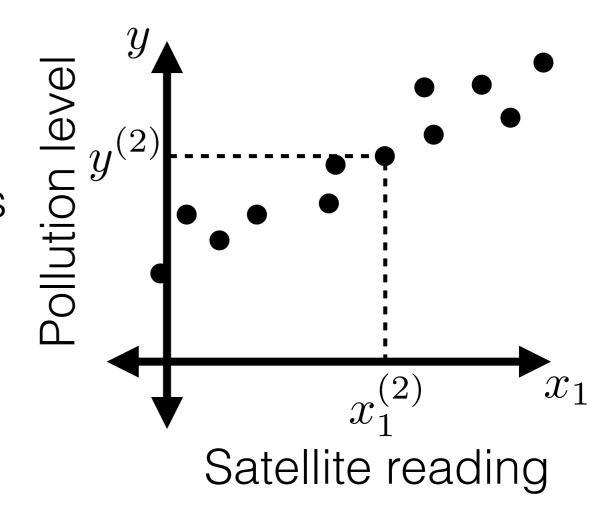
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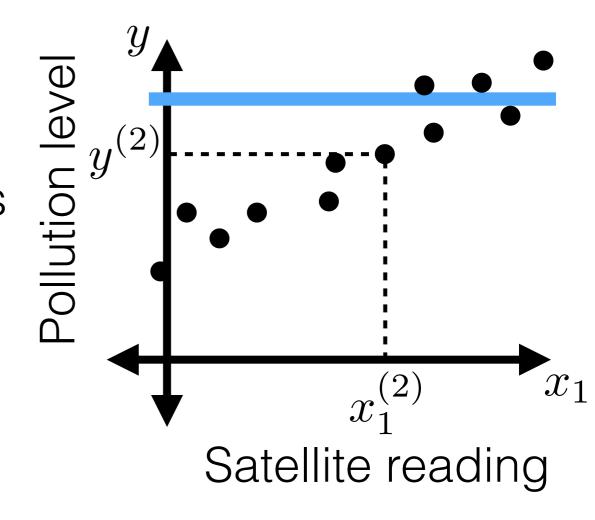
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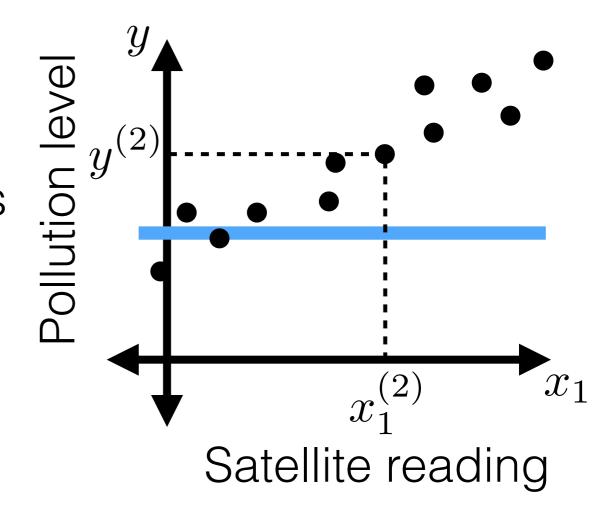
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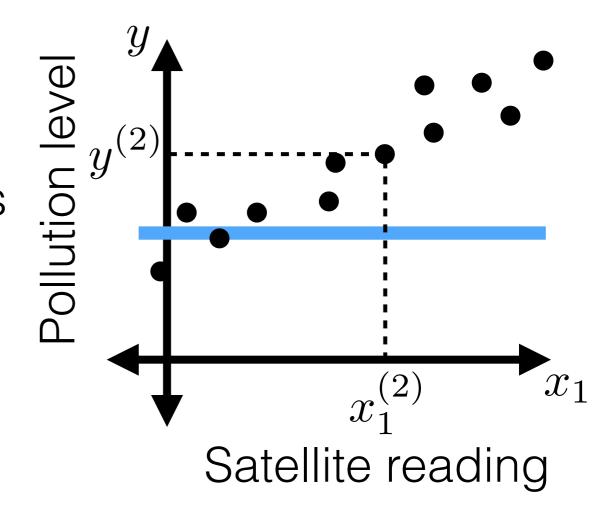
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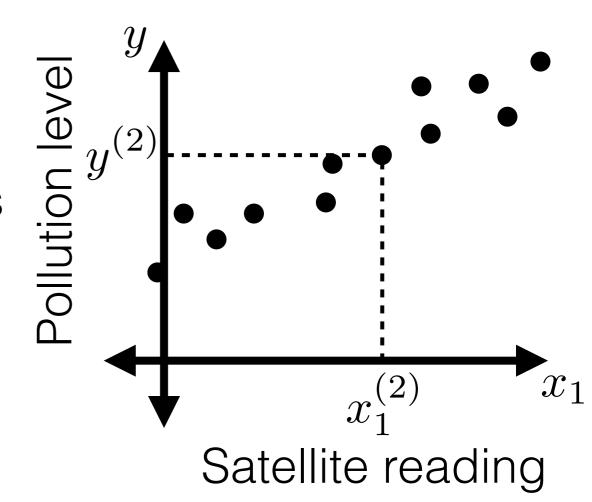


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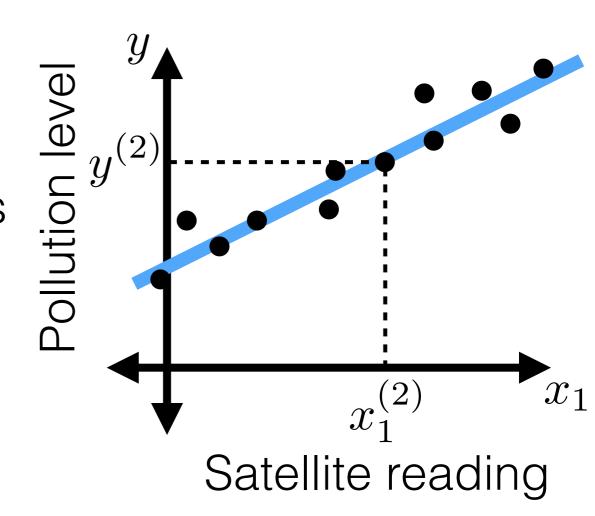
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- A linear regression hypothesis when d=1:

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



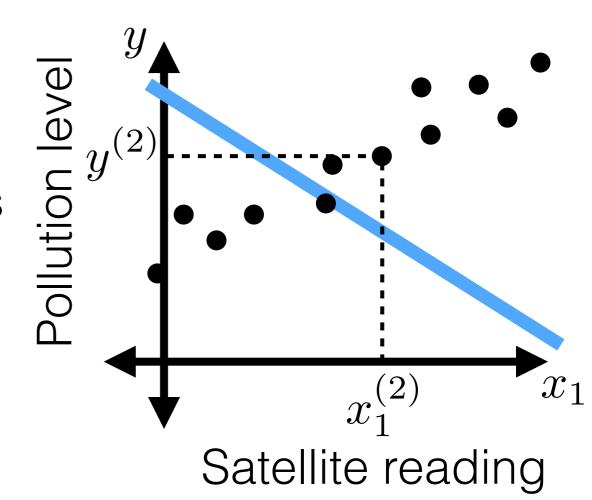
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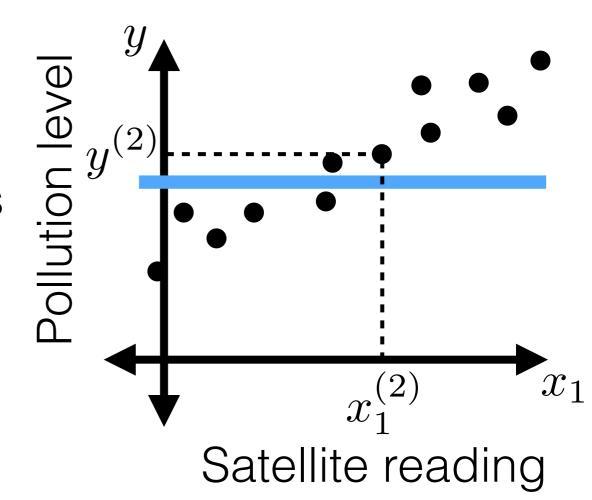
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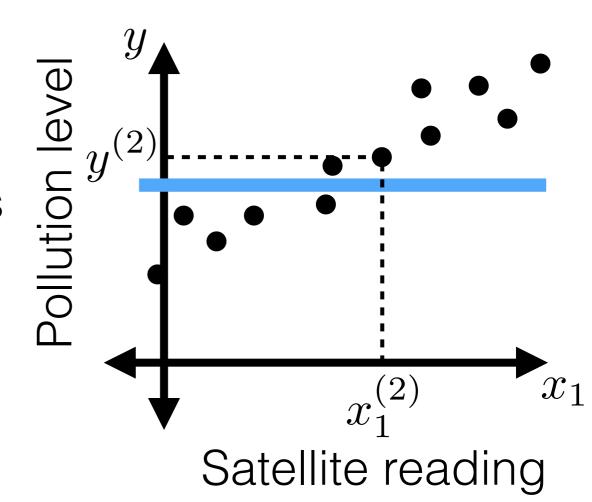
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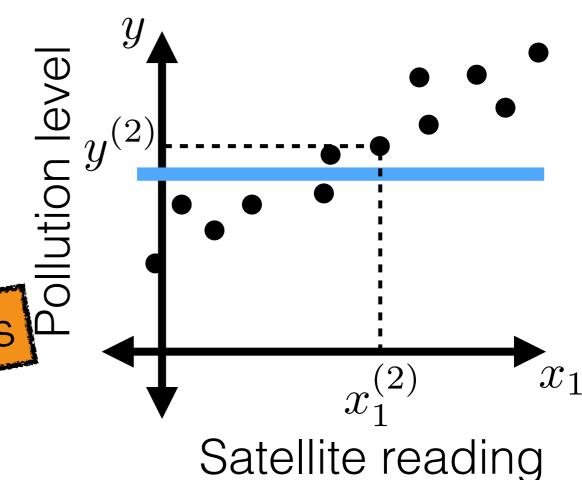
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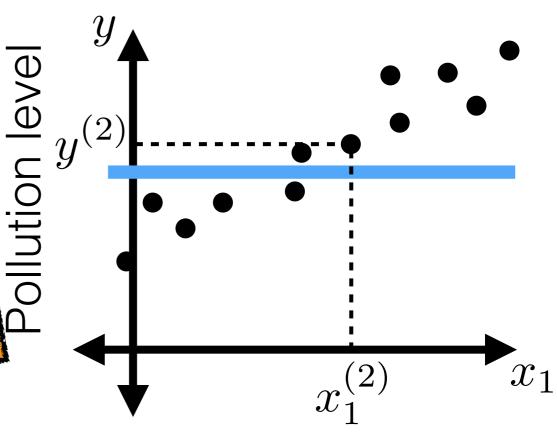


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$$h(x; \theta, \overline{\theta_0}) = \theta x + \theta_0$$

A linear reg. hypothesis when d≥1:

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



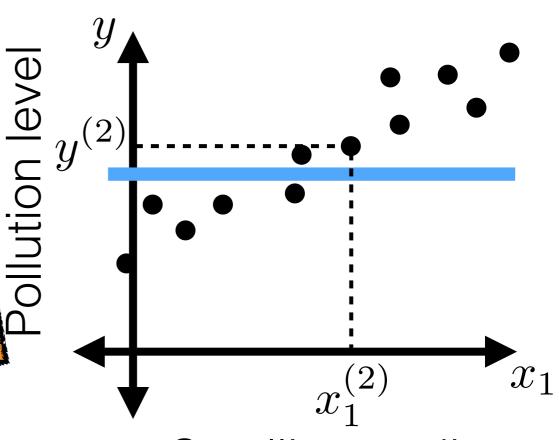
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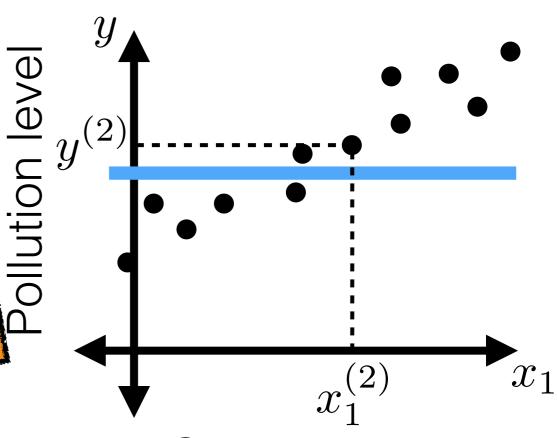
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1xd,dx1



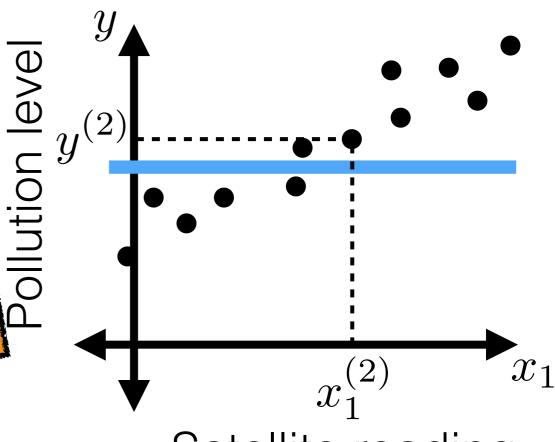
- Hypothesis class \mathcal{H} : set of h
 - Example: all constant functions
- A linear regression hypothesis parameters when d=1

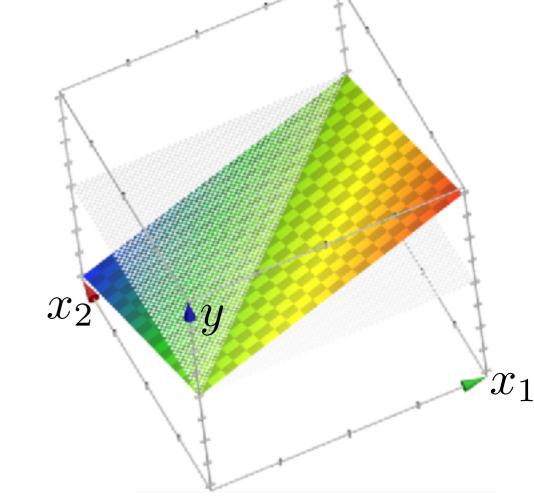
$$h(x; \theta, \overline{\theta_0}) = \theta x + \theta_0$$

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

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

= $\theta^{\mathsf{T}} x + \theta_0$
1xd,dx1



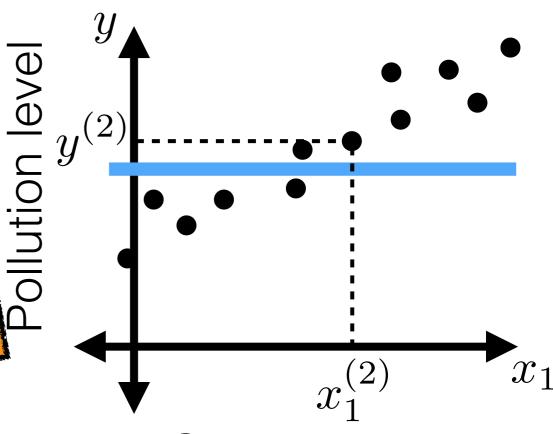


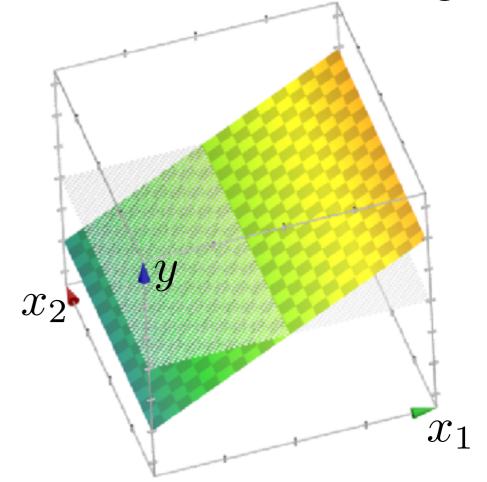
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$$= \theta_1^\top x + \theta_0$$
$$= \theta_1 x_1 + \dots + \theta_0$$
$$= \theta_1 x_1 + \dots + \theta_0$$
$$= \theta_1 x_1 + \dots + \theta_0$$





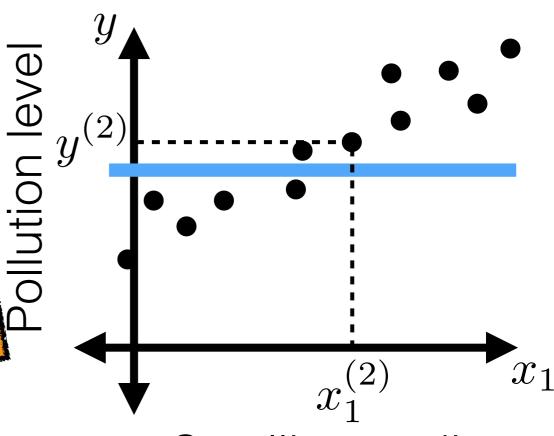
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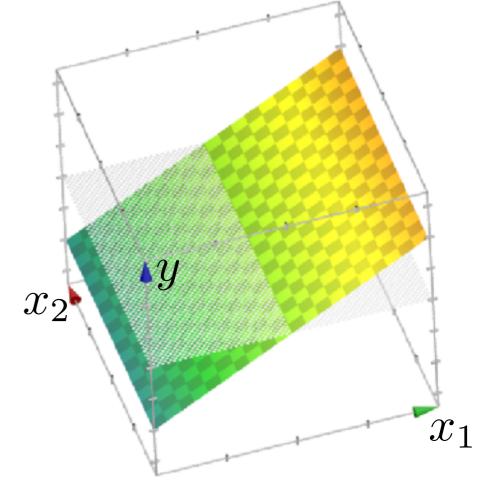
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$$= \theta^\top x + \theta_0$$
1xd,dx1





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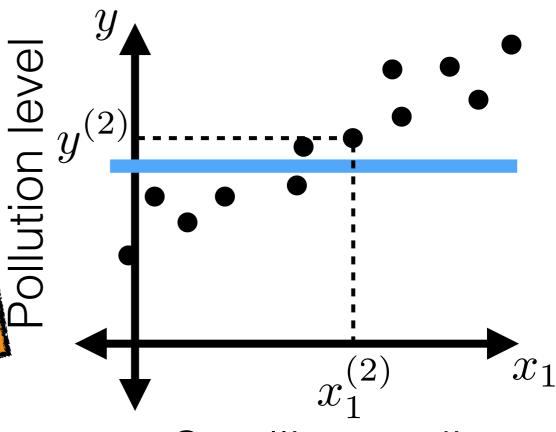
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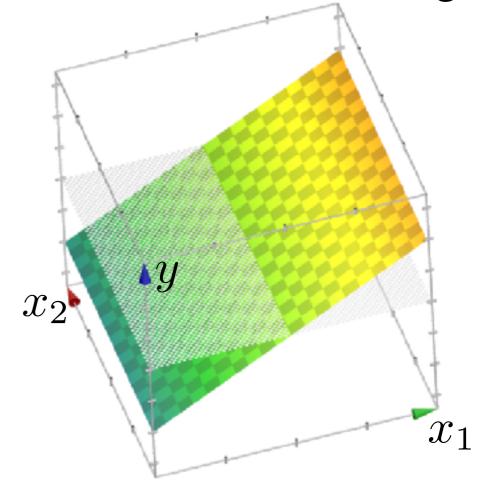
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1xd,dx1

$$h(x) = \theta_1 x_1 + \dots + \theta_d x_d + (\theta_0)(1)$$





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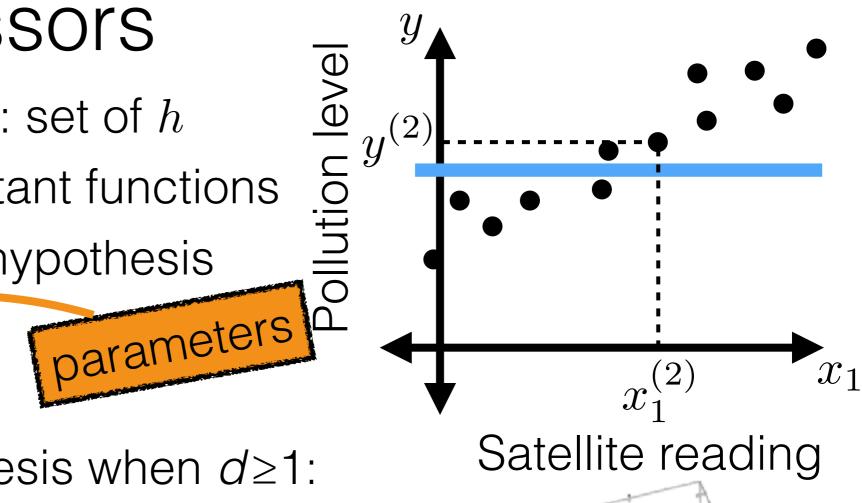
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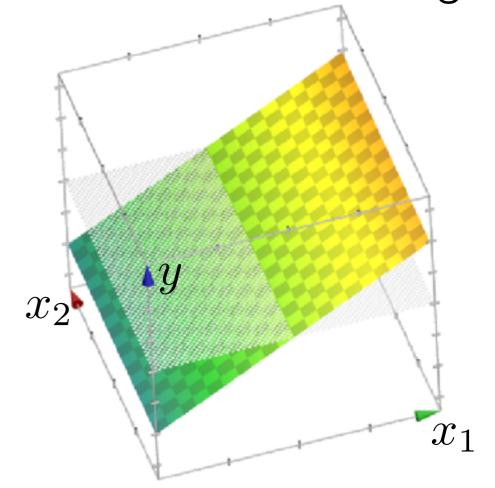
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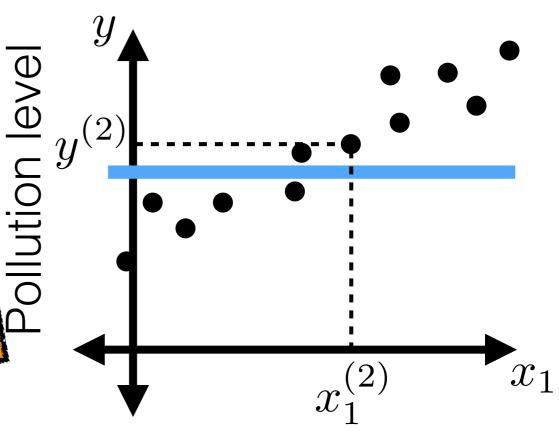
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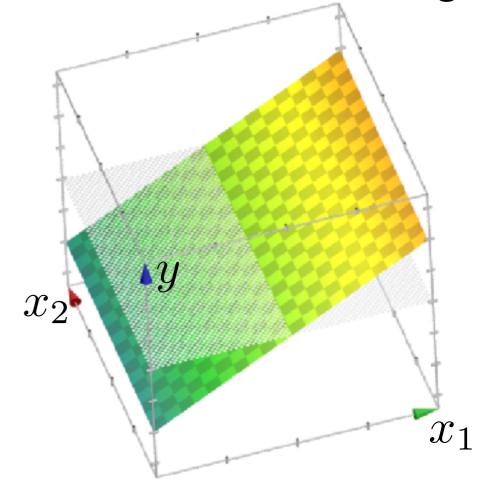
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$$= \theta^\top x + \theta_0$$
1xd,dx1

OR
$$h(x; \theta) = \theta_1 x_1 + \dots + \theta_d x_d + (\theta_0)(1)$$
$$= \theta^{\top} x$$





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

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

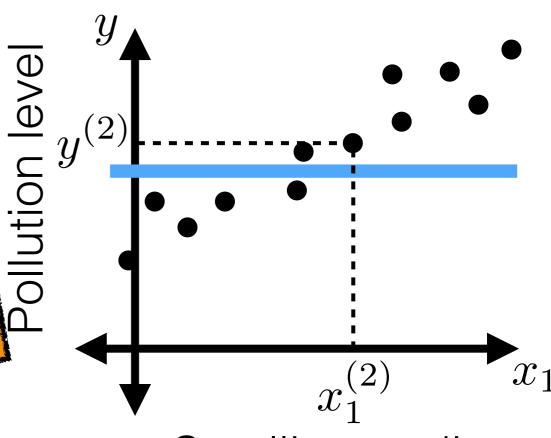
• A linear reg. hypothesis when *d*≥1:

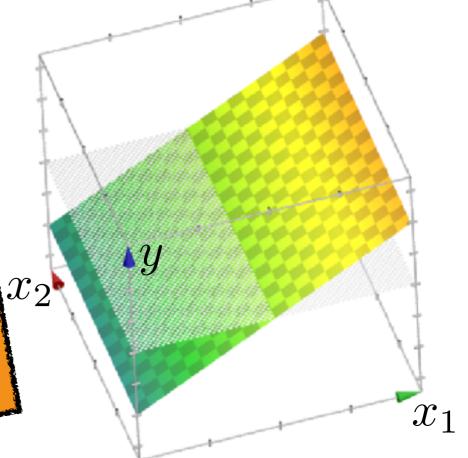
$$h(x; \theta, \theta_0) = \theta_1 x_1 + \dots + \theta_d x_d + \theta_0$$

$$= \theta^\top x + \theta_0$$
1xd,dx1

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

Notational trick: not the same $\theta \& x!$





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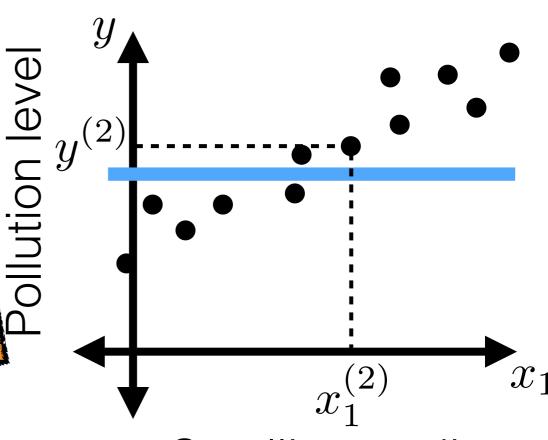
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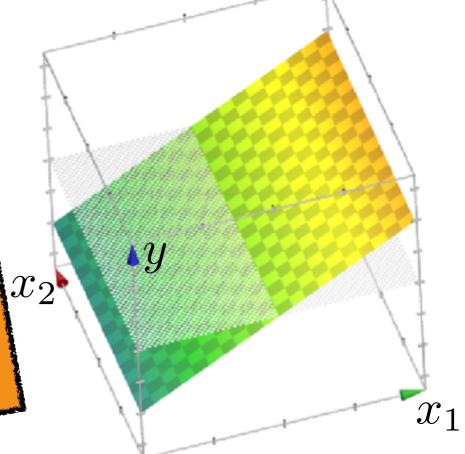
$$= \theta^\top x + \theta_0$$
1x2,2x1

OR
$$h(x;\theta) = \theta_1 x_1 + \dots + \theta_d x_d + (\theta_0)(1)$$

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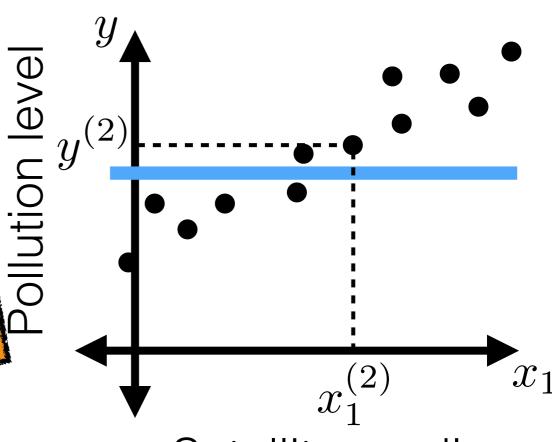
• A linear reg. hypothesis when *d*≥1:

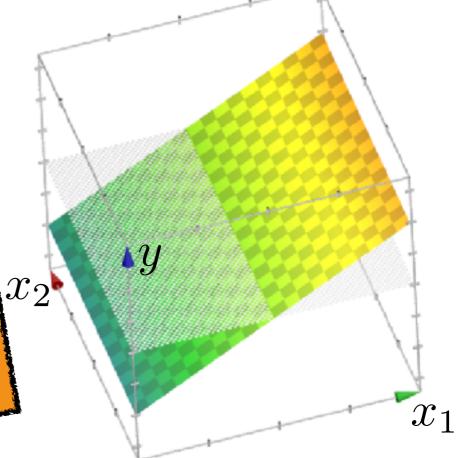
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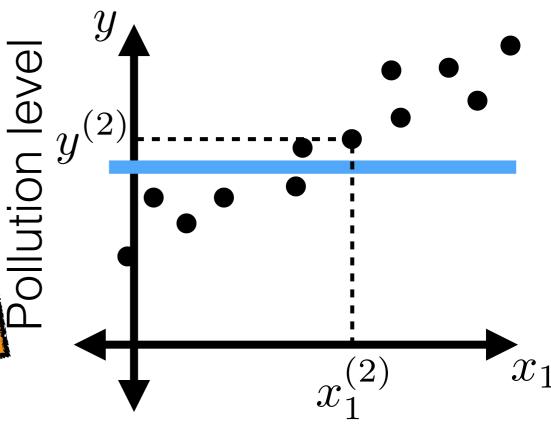


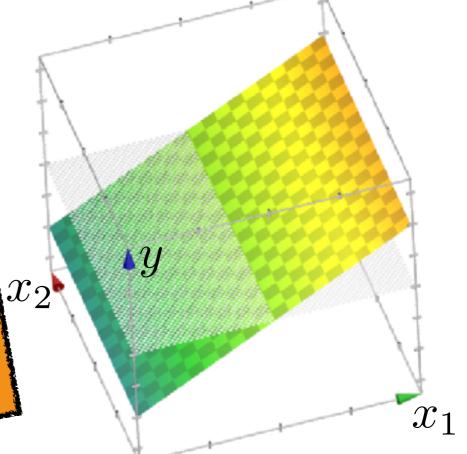
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 $h(x;\theta) = \theta_1 x_1 + \dots + \theta_d x_d + (\theta_0)(1)$ $=\theta^{\top}x$ 1x3,3x1

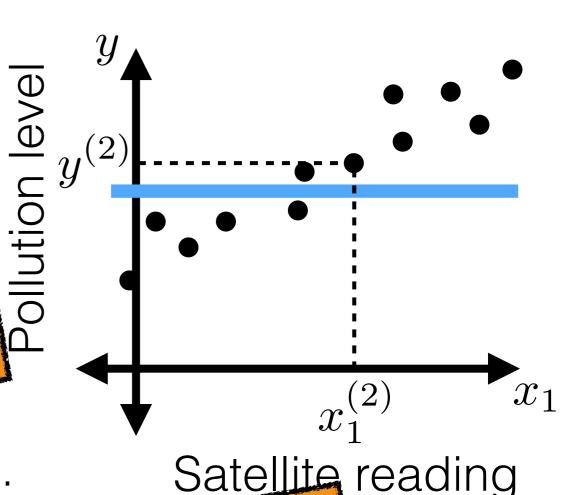
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A linear reg. hypothesis when d≥1:

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

 $h(x;\theta) = \theta_1 x_1 + \dots + \theta_d x_d + (\theta_0)(1)$ $=\theta^{+}x$ 1x3,3x1

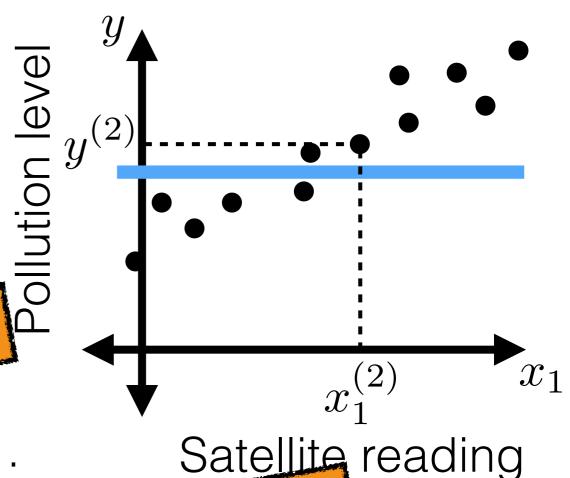
"hyperplane"

Notational trick: not the same 0 & x!

 x_1

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• A linear reg. hypothesis when $d \ge 1$:

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

$$= \theta^\top x$$
1x3,3x1
Notational

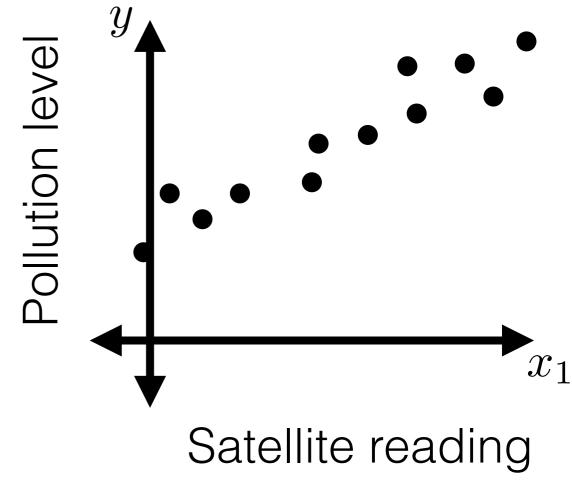
Our hypothesis class in linear regression will be

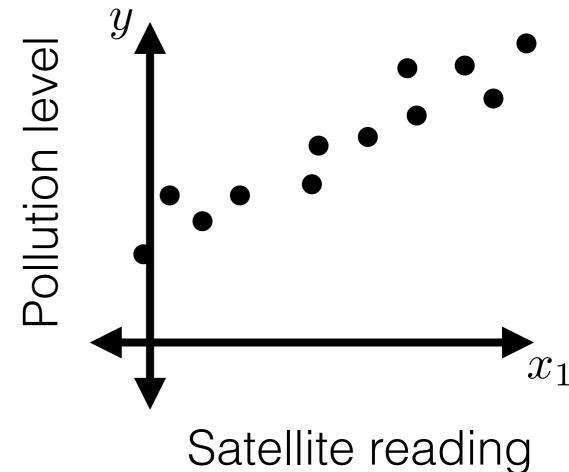
the set of all such h

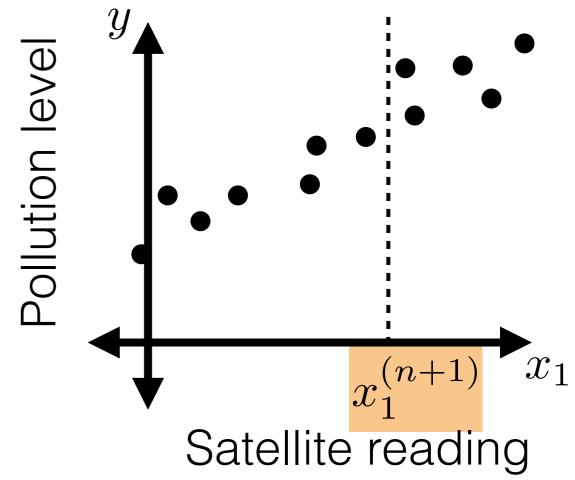
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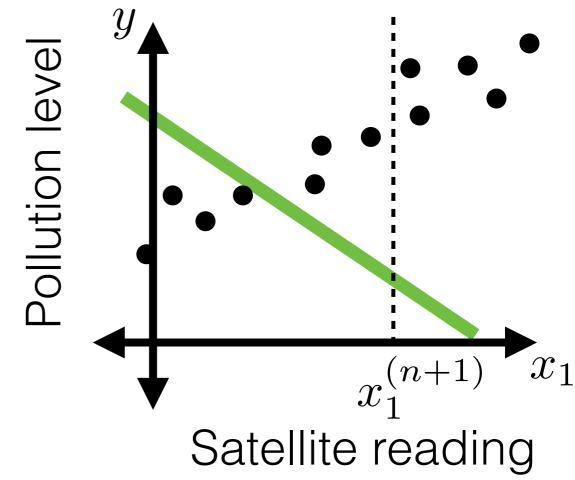
Hypothesis is a "hyperplane"

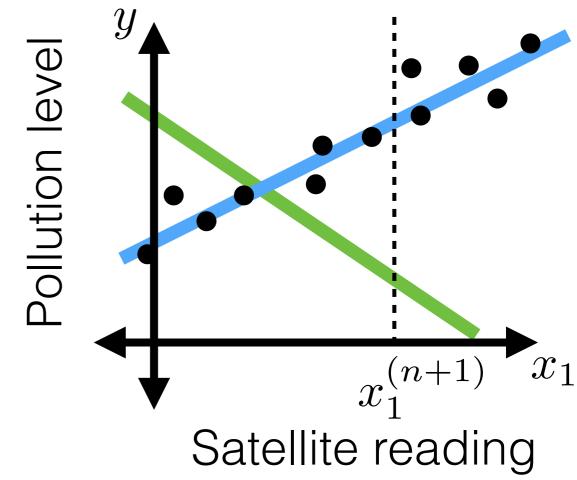
 x_1

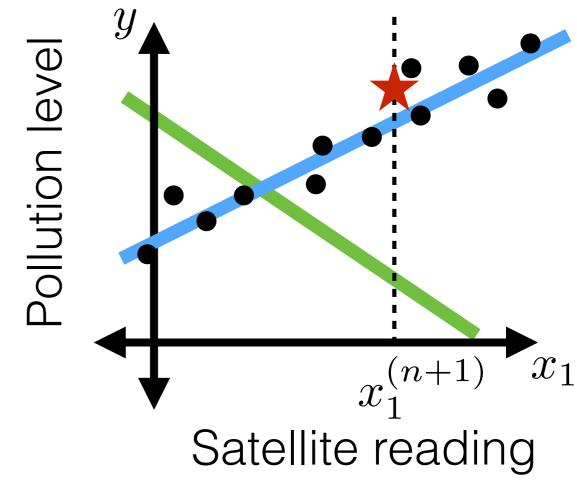




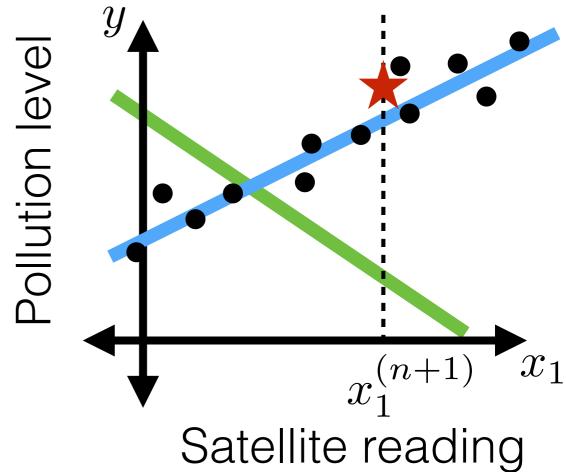






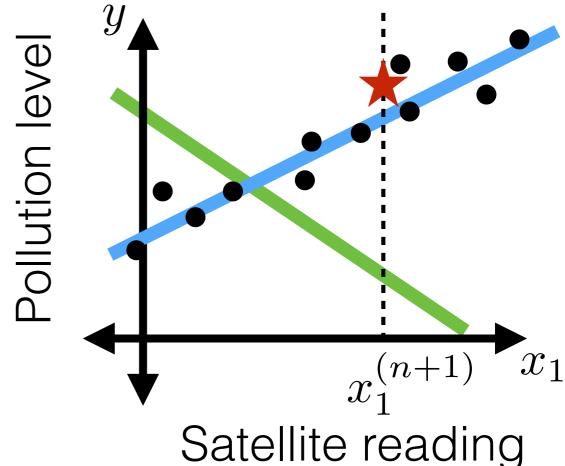


- Should predict well on future data
- How good is a regressor at one point? Loss ${\cal L}(g,a)$



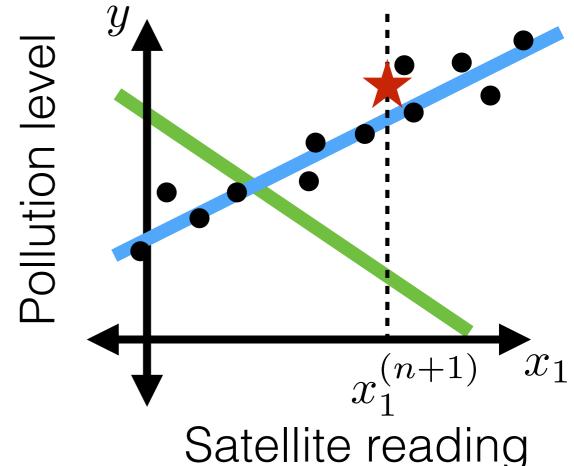
a: actual

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

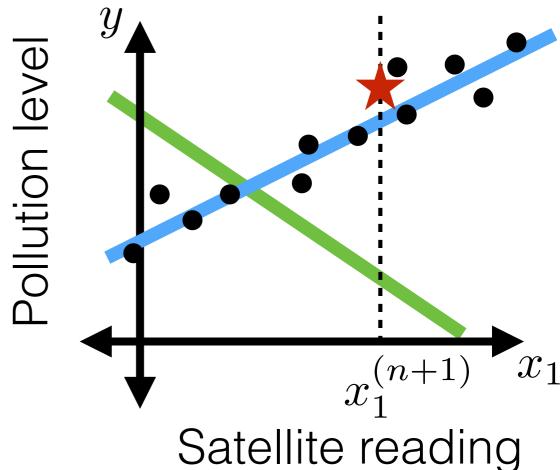
$$L(g,a) = (g-a)^2$$



- Should predict well on future data
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Example: asymmetric loss

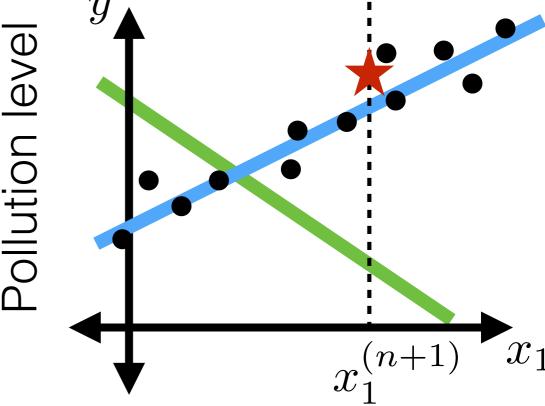


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Example: asymmetric loss

$$L(g, a) = \begin{cases} (g - a)^2 & \text{if } g > a \\ 2(g - a)^2 & \text{if } g \le a \end{cases}$$



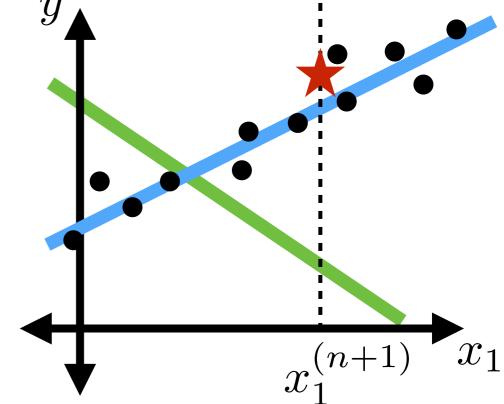
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Pollution level



• Test error (n' new points):
$$\mathcal{E}(h) = \frac{1}{n'} \sum_{i=n+1}^{n+n'} L(h(x^{(i)}), y^{(i)})$$

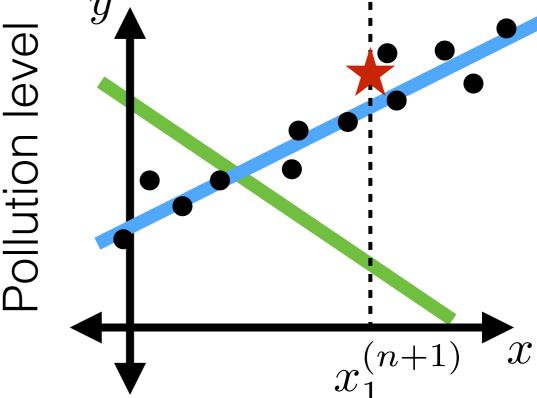
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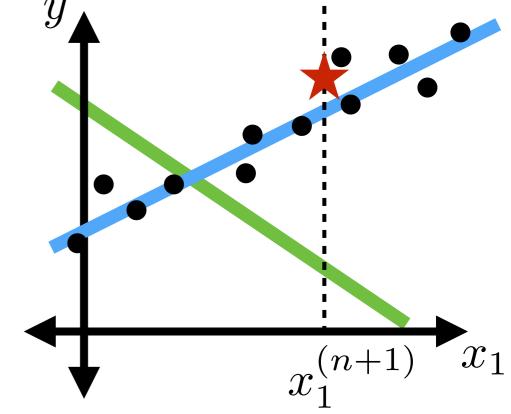
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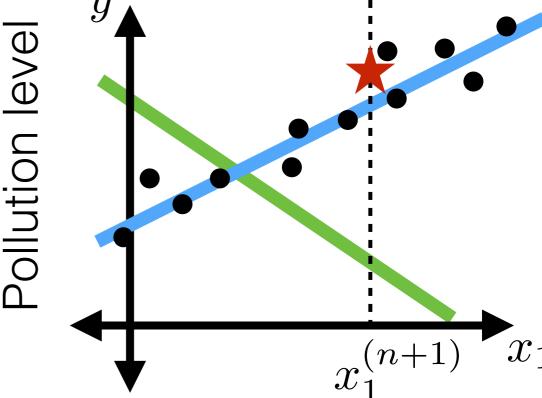
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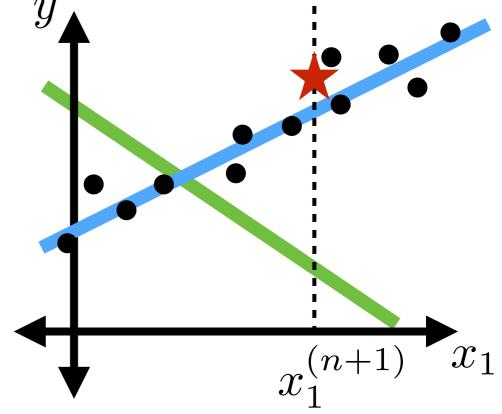
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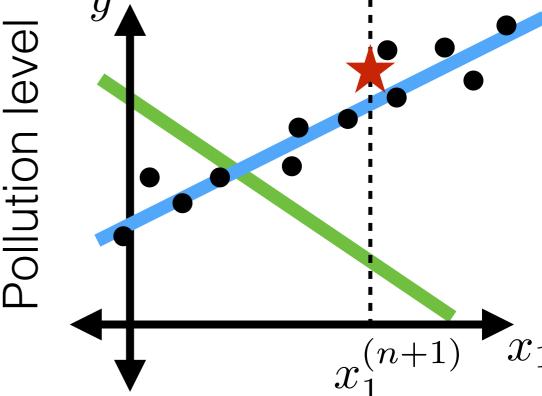
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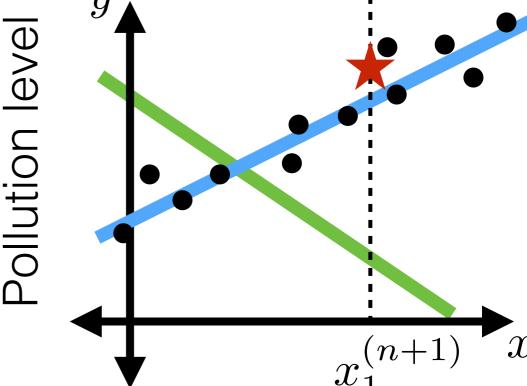


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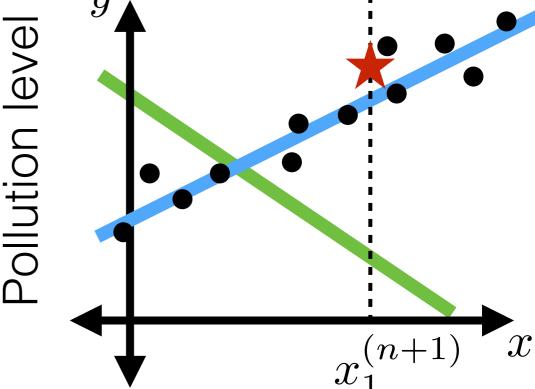
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$$\mathcal{E}_n(h) = \frac{1}{n} \sum_{i=1}^n L(h(x^{(i)}), y^{(i)})$$

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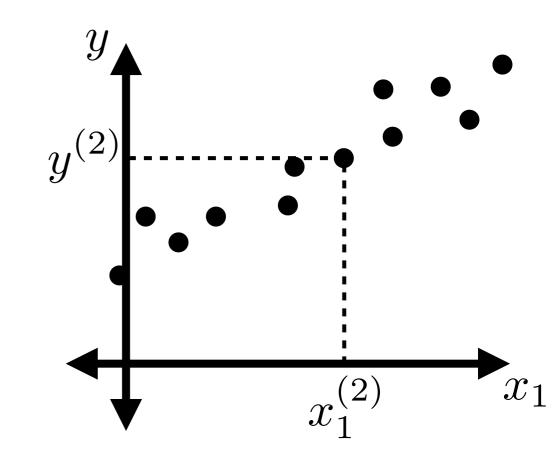
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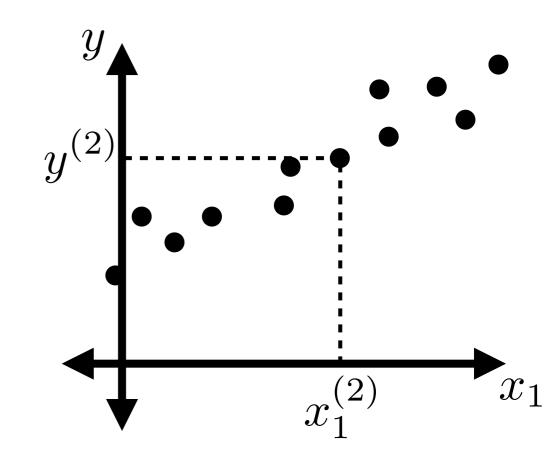


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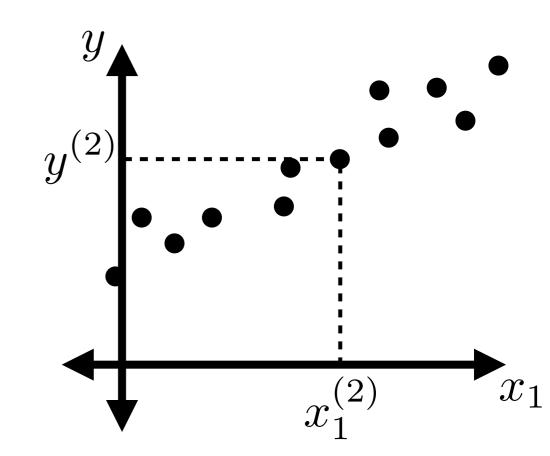
- Training error: $\mathcal{E}_n(h) = \frac{1}{n} \sum_{i=1}^n L(h(x^{(i)}), y^{(i)})$
- One idea: prefer h to \tilde{h} if $\mathcal{E}_n(h) < \mathcal{E}_n(\tilde{h})$



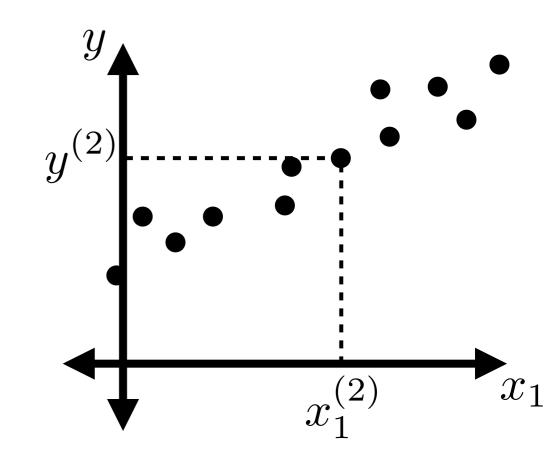
• Have data; have hypothesis class



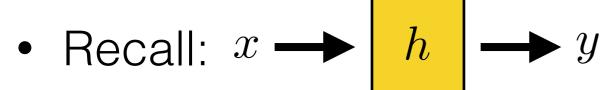
- Have data; have hypothesis class
- Want to choose a good regressor

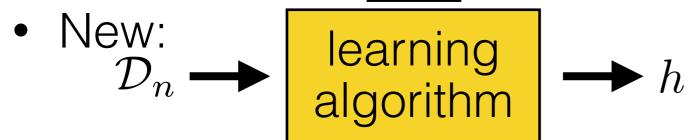


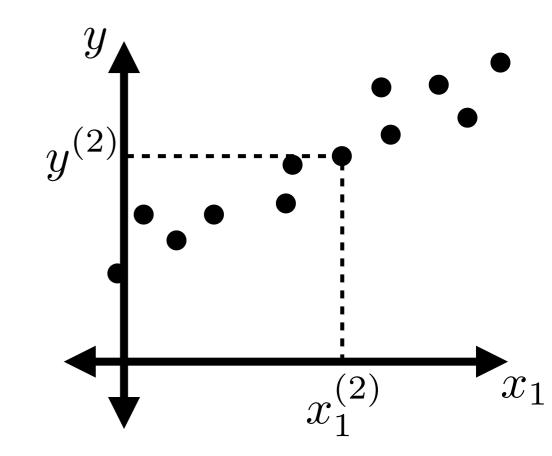
- Have data; have hypothesis class
- Want to choose a good regressor
 - Recall: $x \longrightarrow h \longrightarrow y$



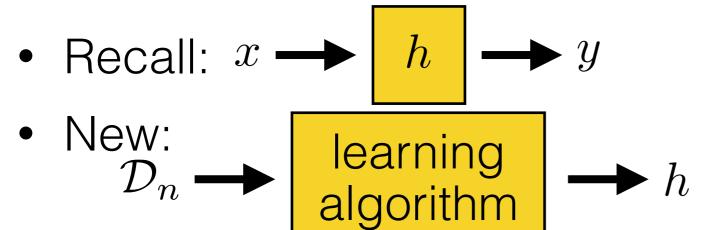
- Have data; have hypothesis class
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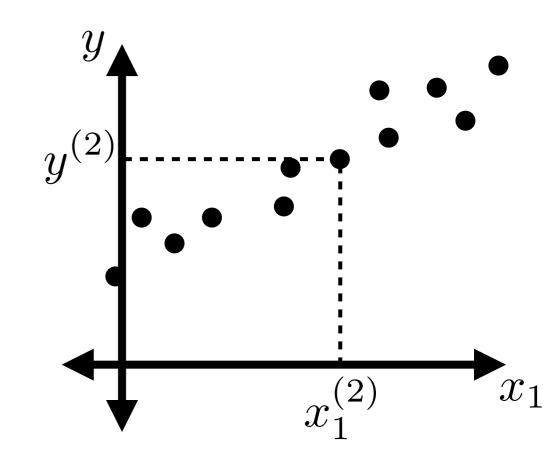




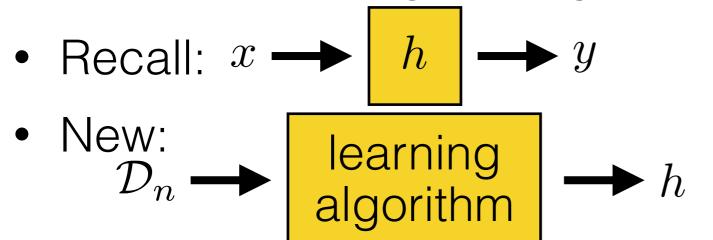
- Have data; have hypothesis class
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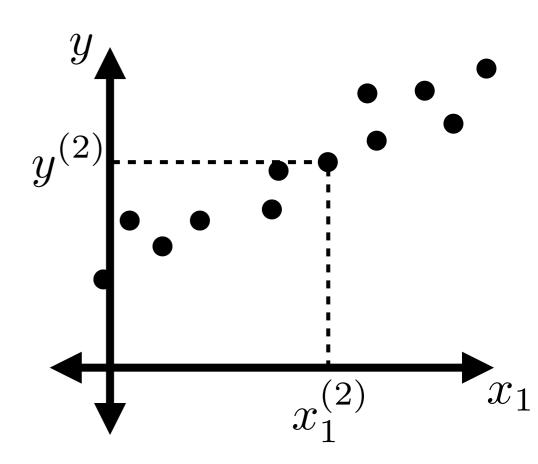


• Example:



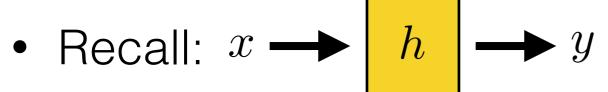
- Have data; have hypothesis class
- Want to choose a good regressor

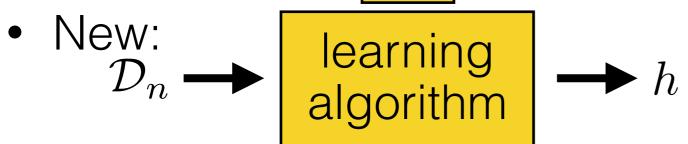


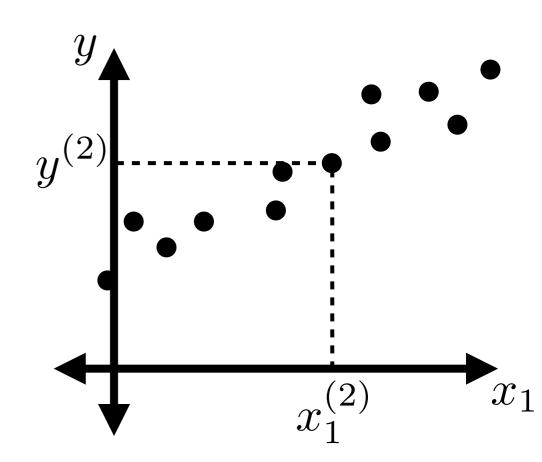


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 - Suppose someone already generated 1 trillion hypotheses, e.g. at random, indexed by j:

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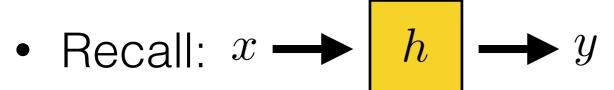


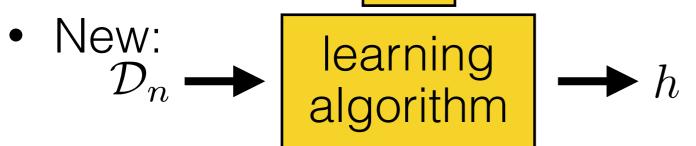


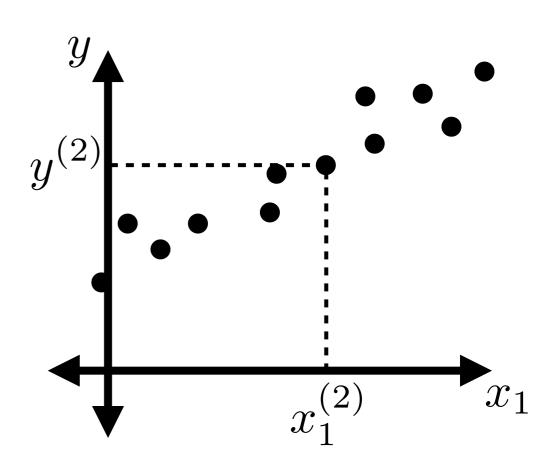
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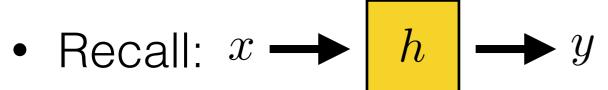


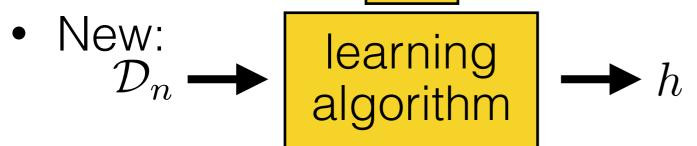


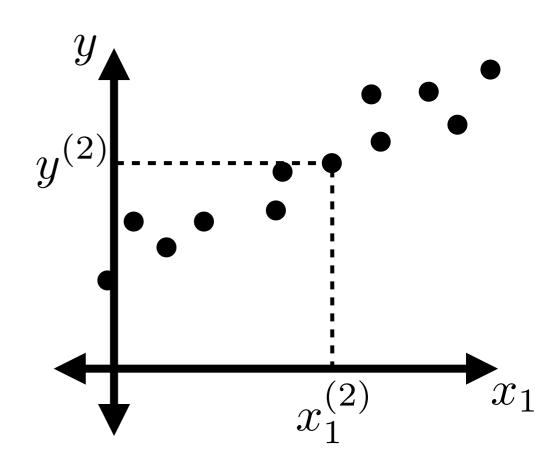
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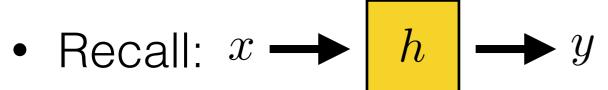


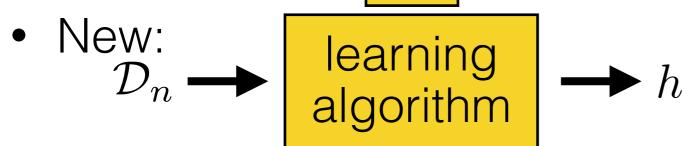
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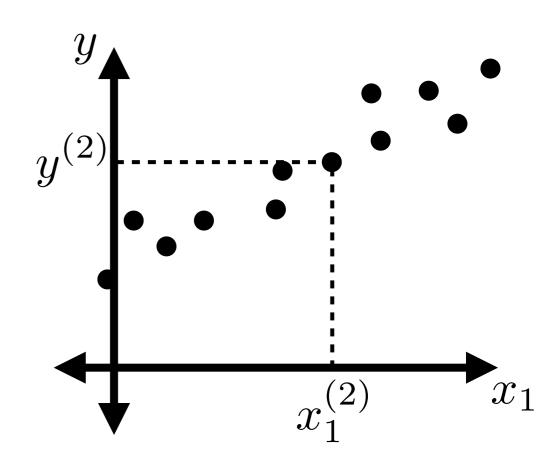
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Ex_learning_alg(\mathcal{D}_n ; k)

- Have data; have hypothesis class
- Want to choose a good regressor





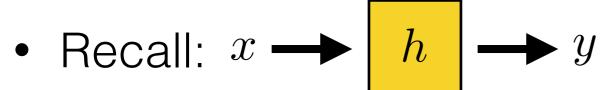


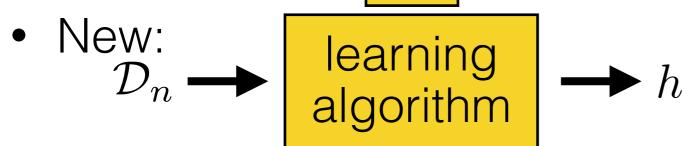
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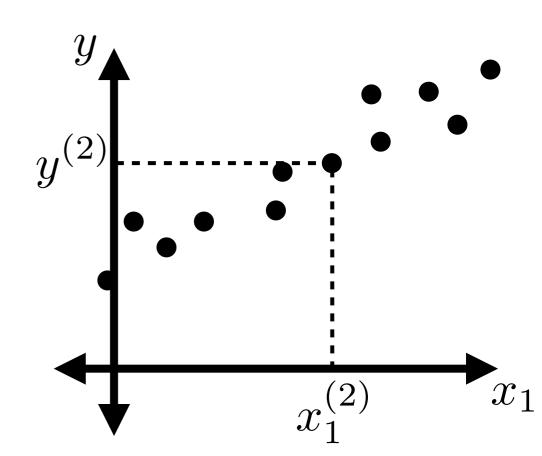
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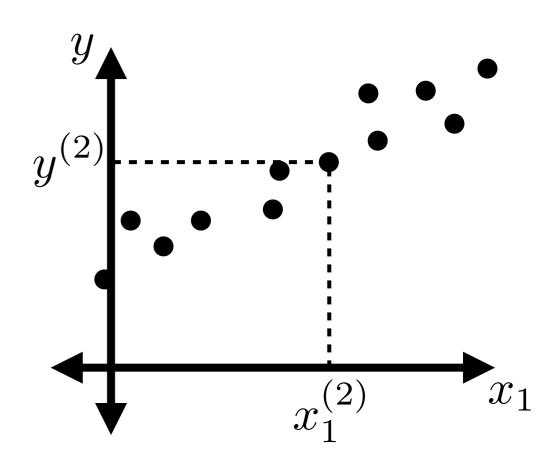


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 - Recall: $x \longrightarrow h \longrightarrow y$
 - New: D_n \longrightarrow learning algorithm $\longrightarrow h$



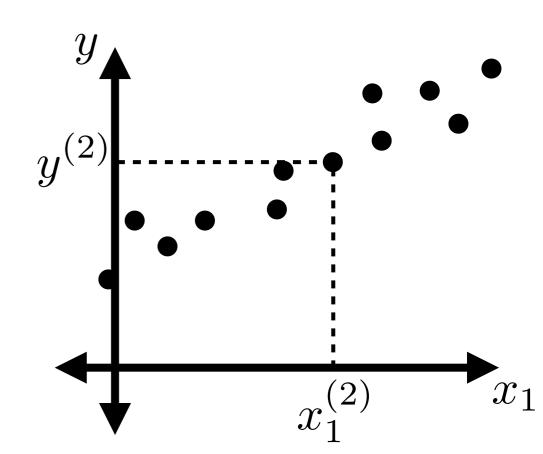
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• How does training error of Ex_learning_alg(\mathcal{D}_n ;1) compare to the training error of Ex_learning_alg(\mathcal{D}_n ;2)?

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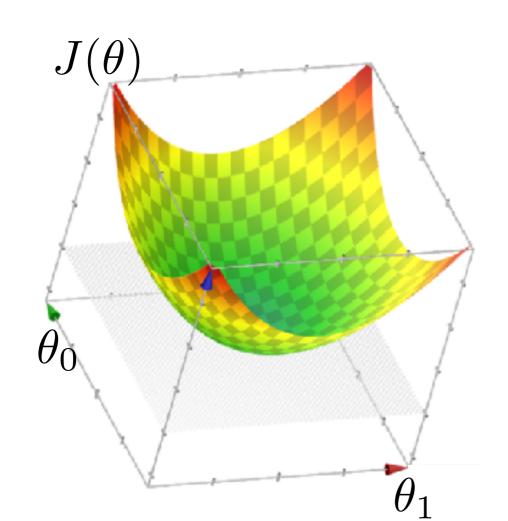
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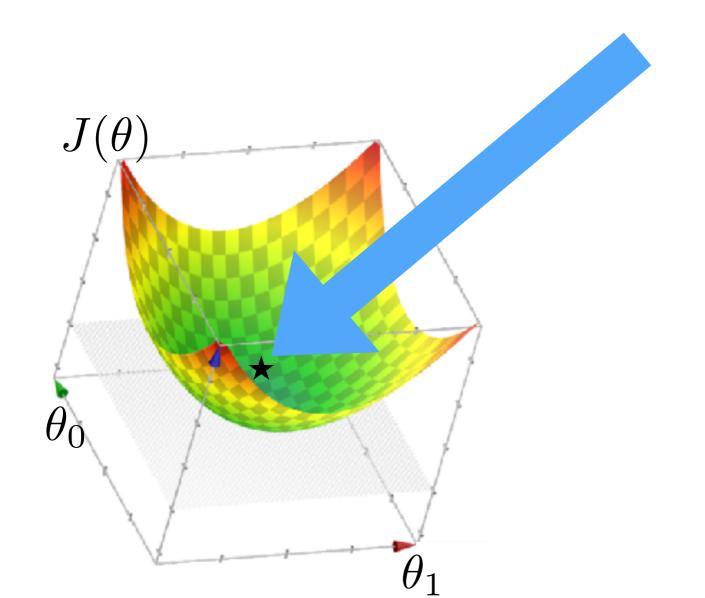
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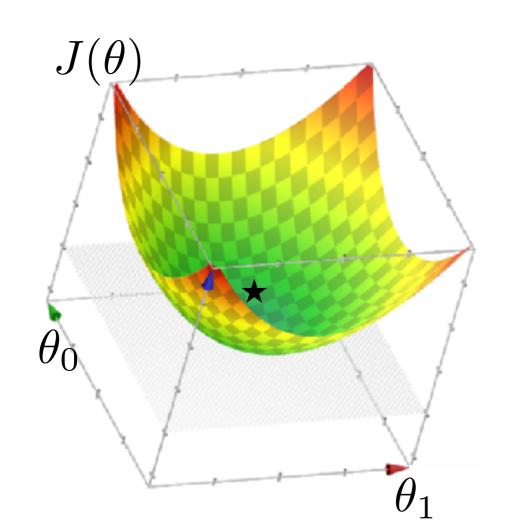
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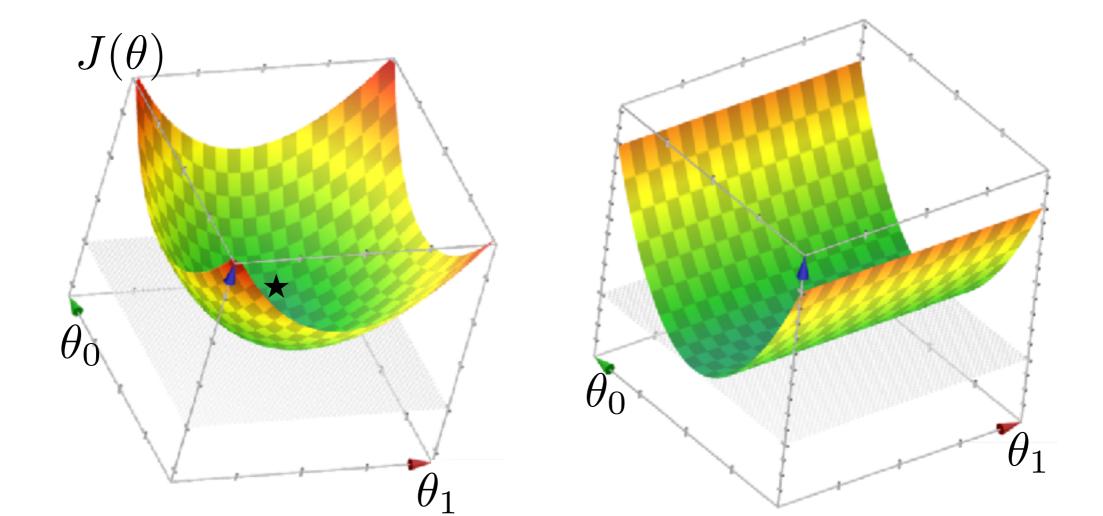
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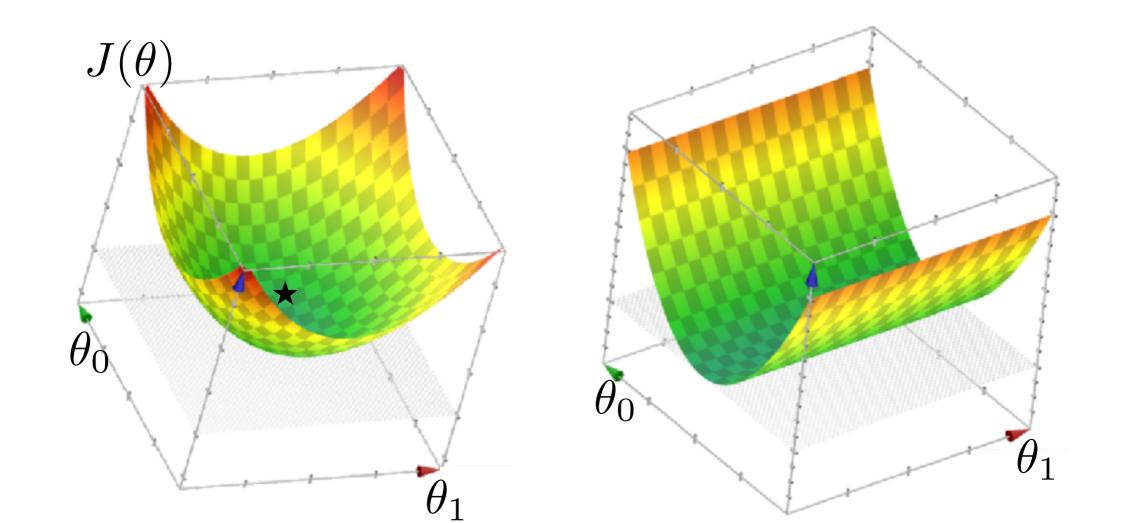








- Goal: minimize $J(\theta) = \frac{1}{n} (\tilde{X}\theta \tilde{Y})^{\top} (\tilde{X}\theta \tilde{Y})$
- Uniquely minimized at a point if gradient at that point is zero and function "curves up" [see linear algebra]



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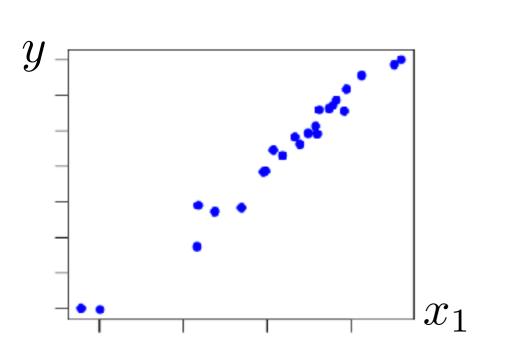
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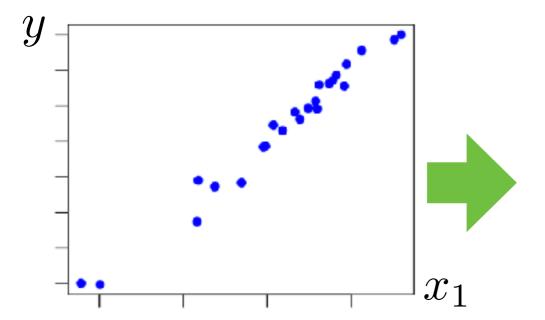
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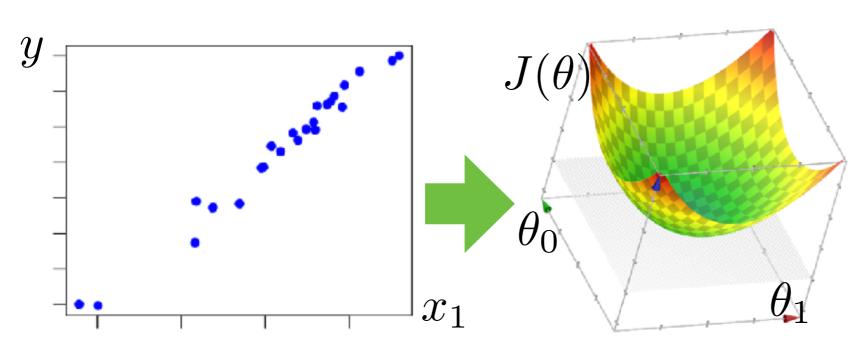
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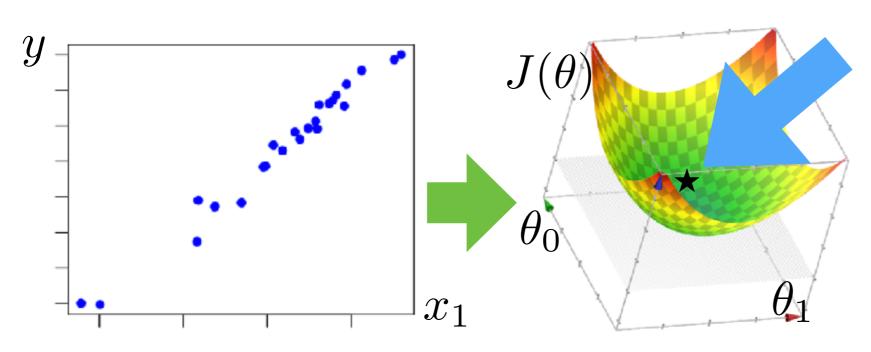
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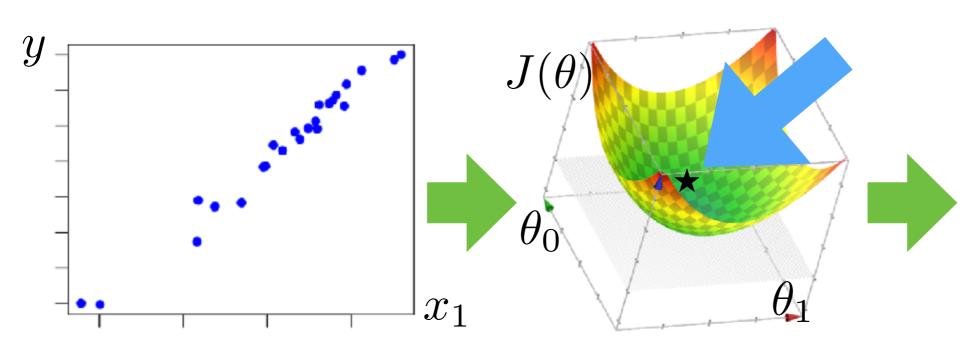
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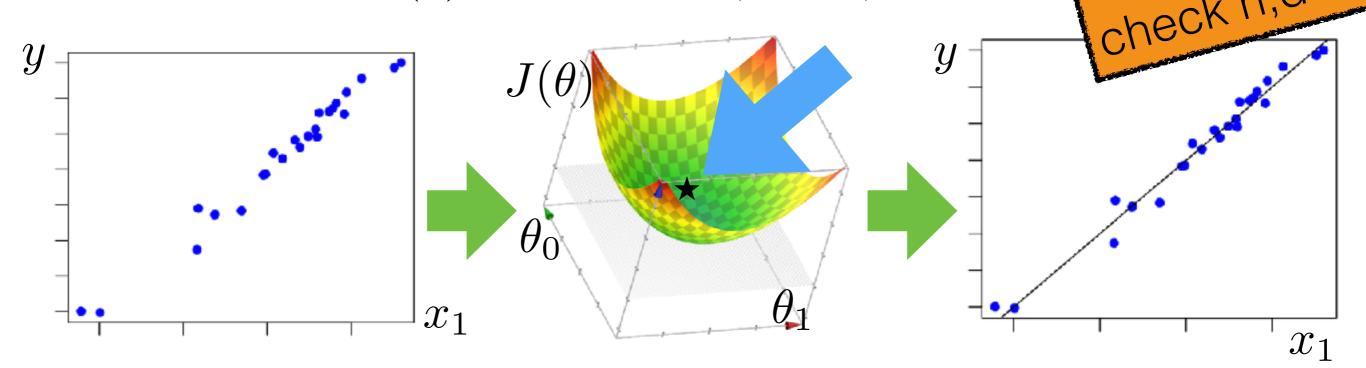
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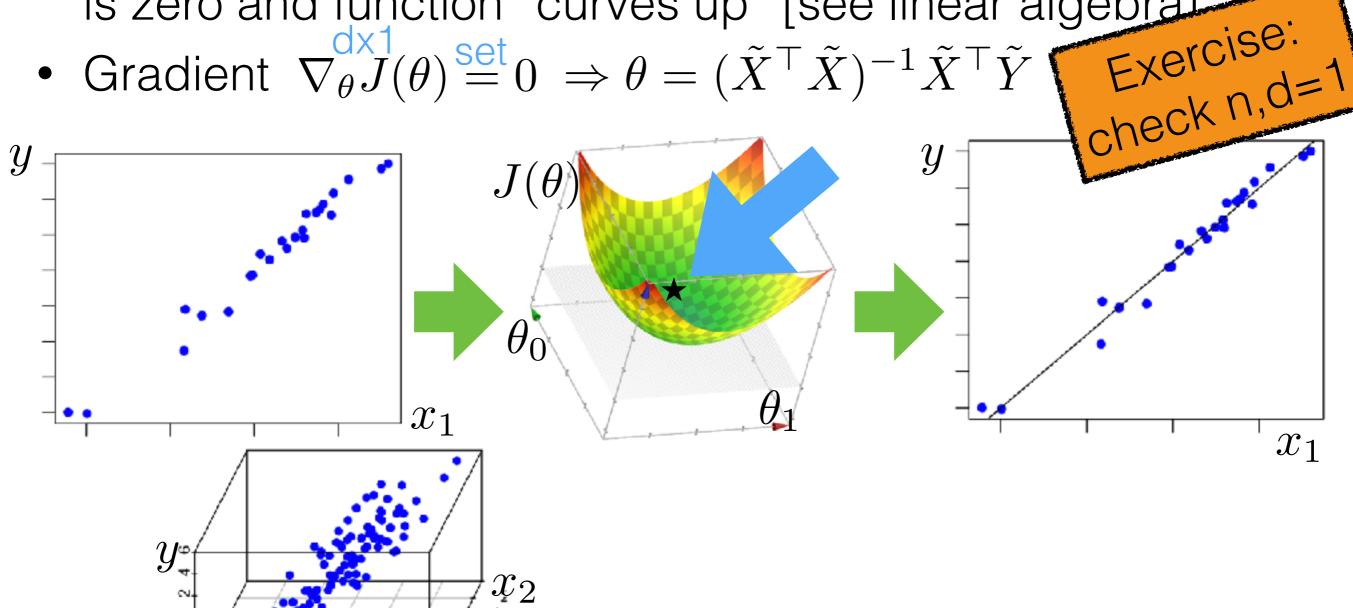
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- Goal: minimize $J(\theta) = \frac{1}{2} (\tilde{X}\theta \tilde{Y})^{\top} (\tilde{X}\theta \tilde{Y})$
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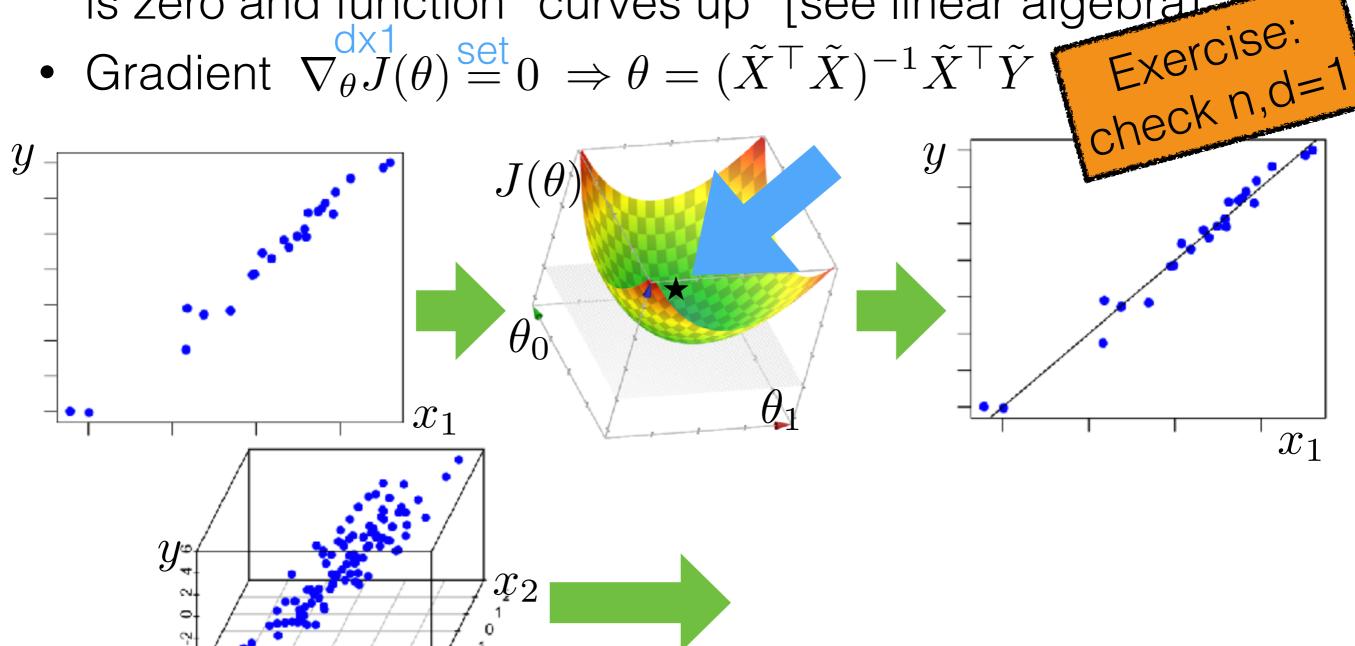
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Linear regression: A Direct Solution

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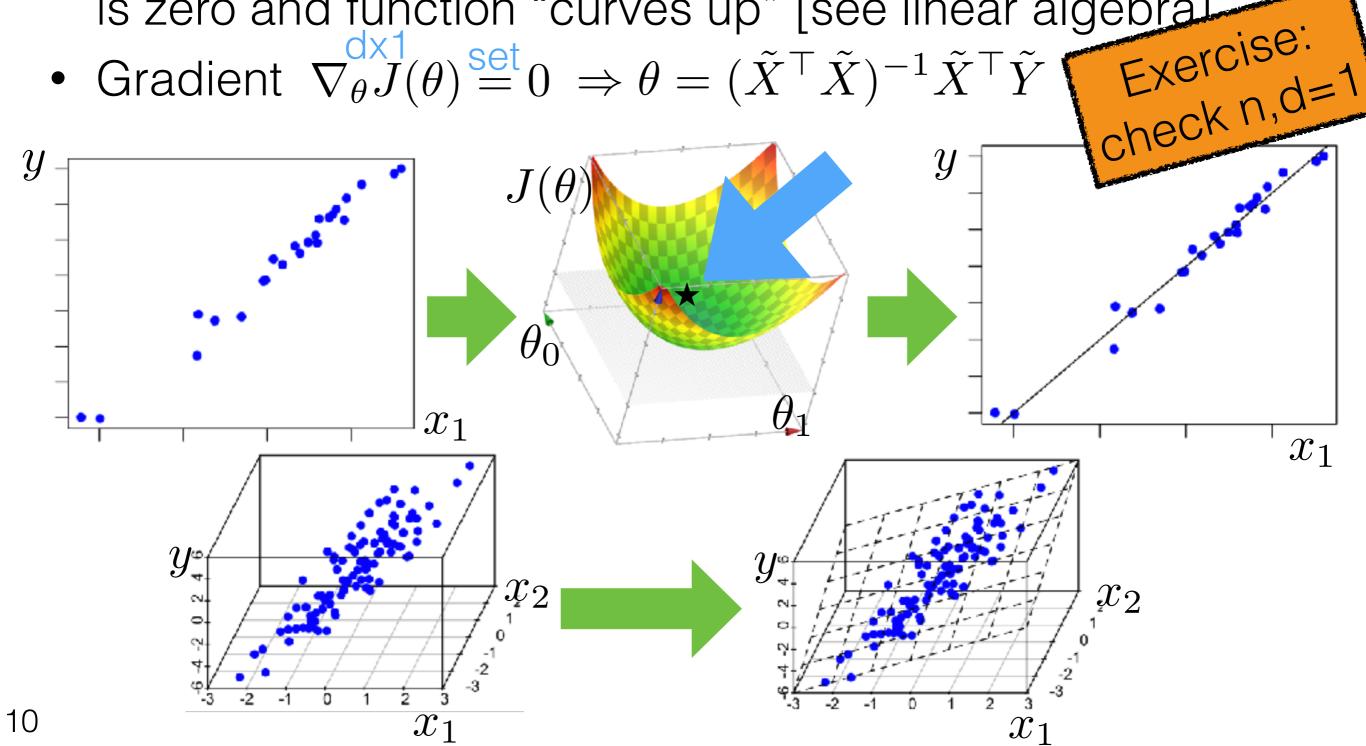
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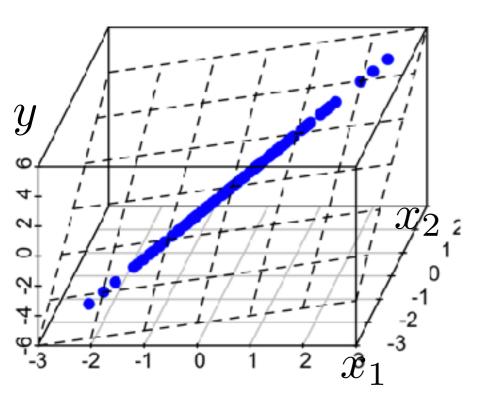
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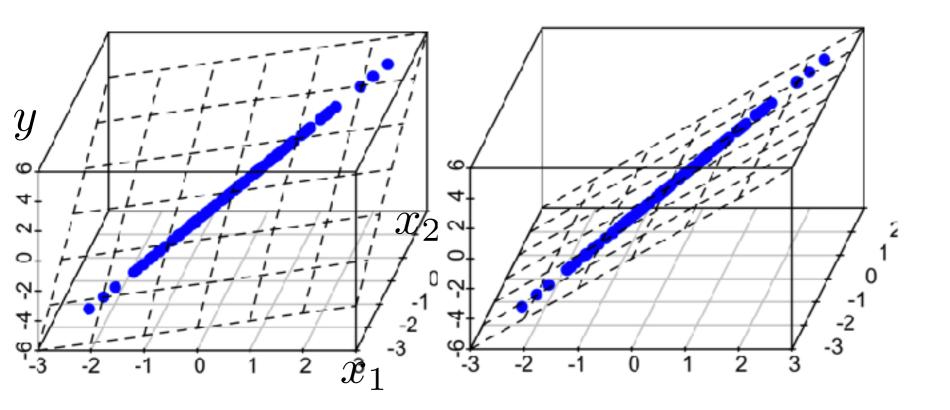
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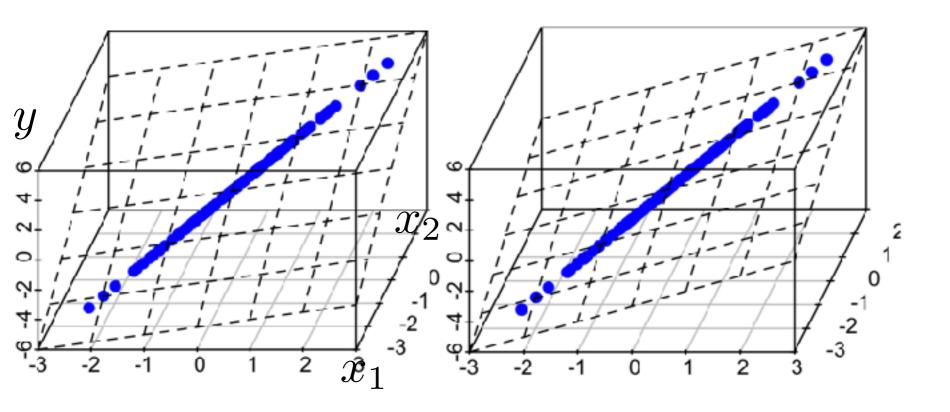
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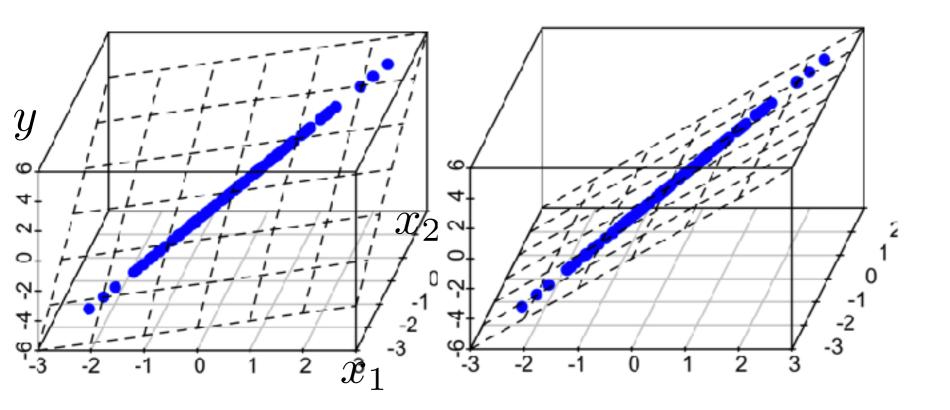
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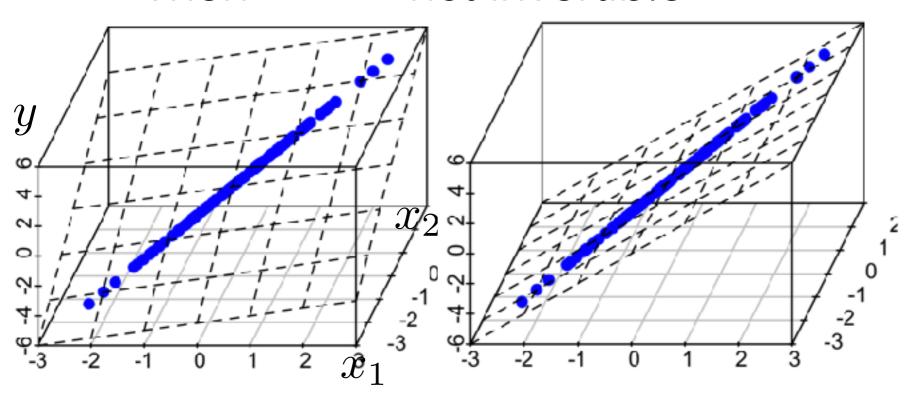
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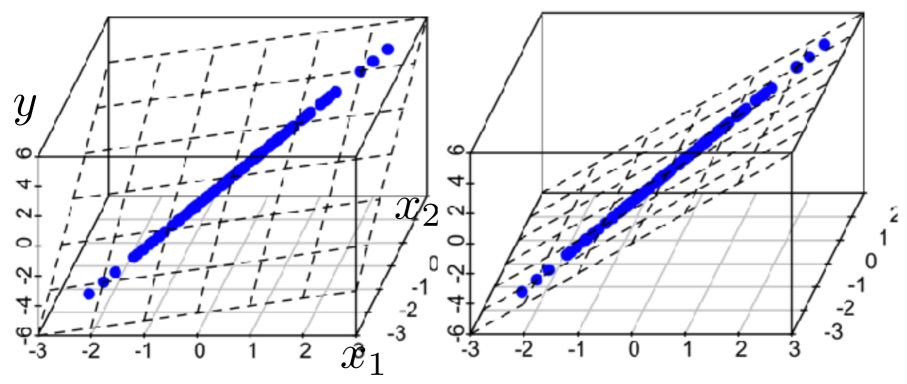
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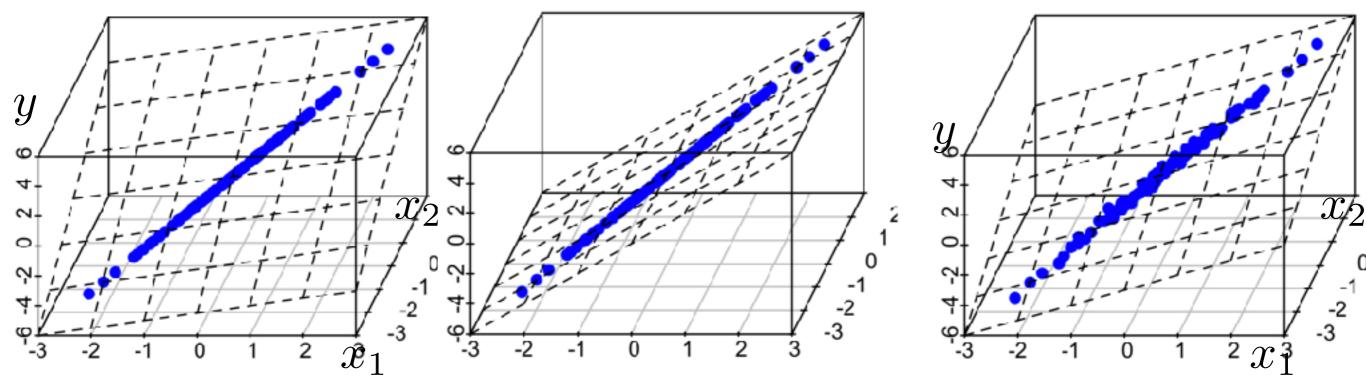


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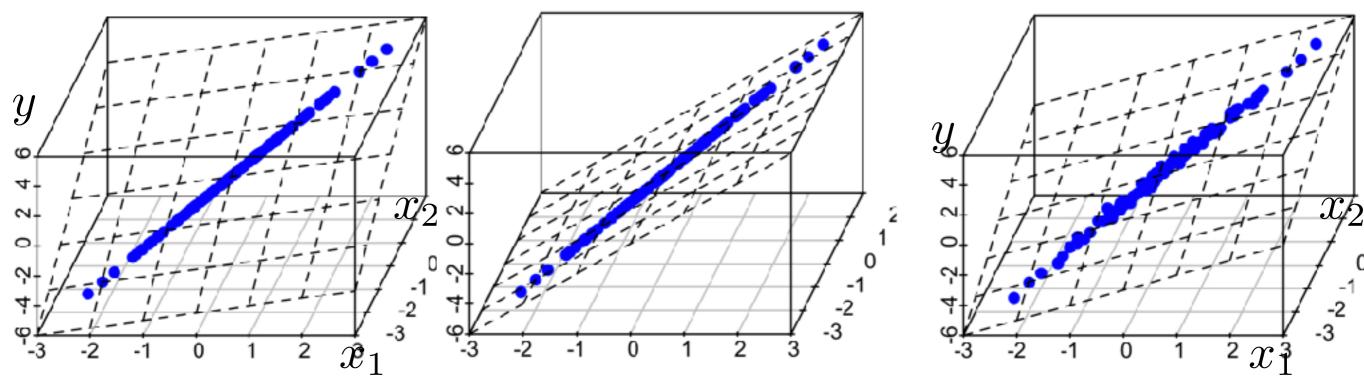
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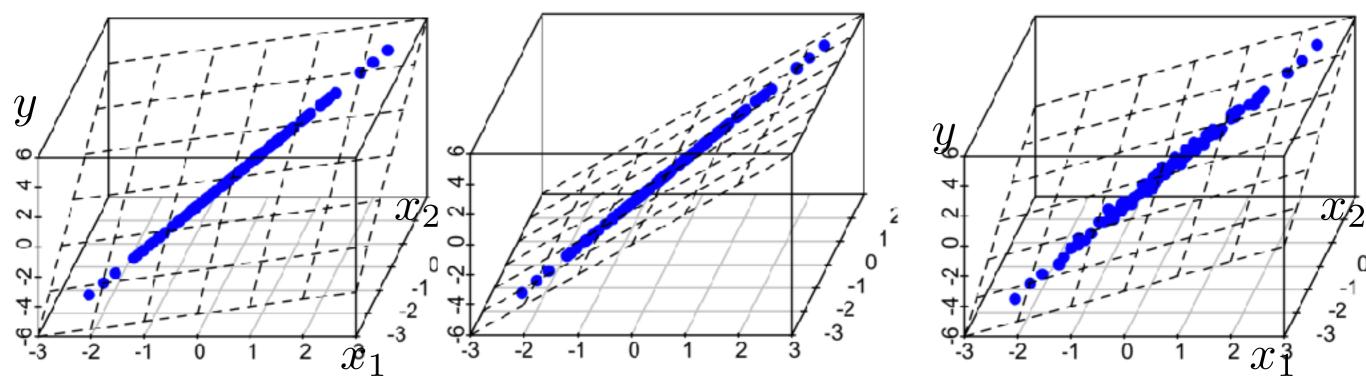
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- Sometimes there's technically a unique best hyperplane, but just because of noise
- Practical: real-life features often have this issue
- How to choose among hyperplanes? Preference for θ components being near zero

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What happens if $\lambda < 0$?

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- How to choose λ ? One option: cross validation (see HW!)

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