香港科技大學
THE HONG KONG
UNIVERSITY OF SCIENCE
AND TECHNOLOGY

COMP 5212
Machine Learning
Lecture 2

Supervised Learning: Regression

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Sep 10, 2024

Announcement

Lecture on Sep 17 (Mid-Autumn Festival) is rescheduled to Sep 23 (Monday) from 130pm - 250pm at LG3009.

Supervised Learning

- A hypothesis or a prediction function is function $h : \mathcal{X} \to \mathcal{Y}$

Supervised Learning

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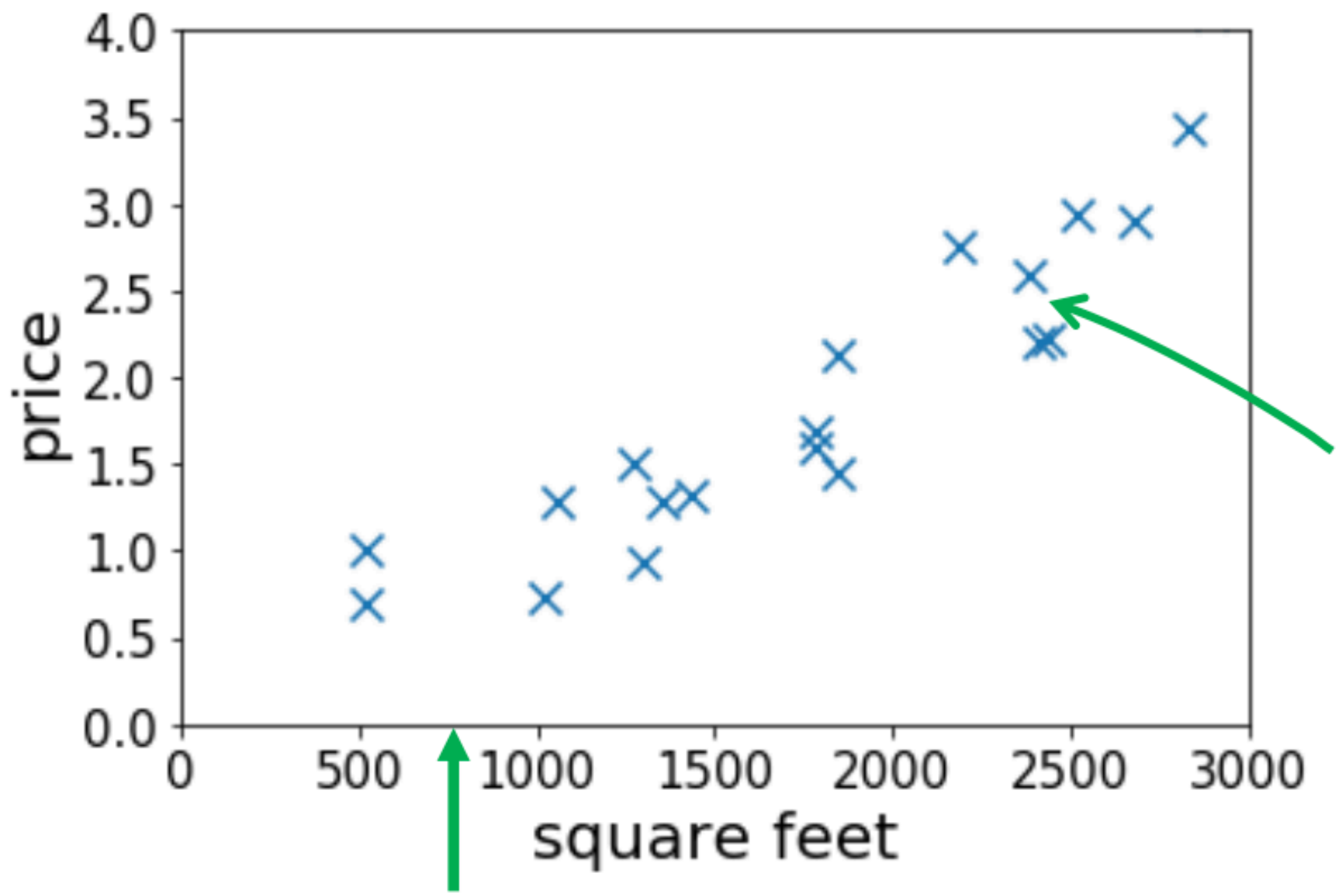

15th sample
$(x^{(15)}, y^{(15)})$

$x = 800$
$y = ?$

Supervised Learning

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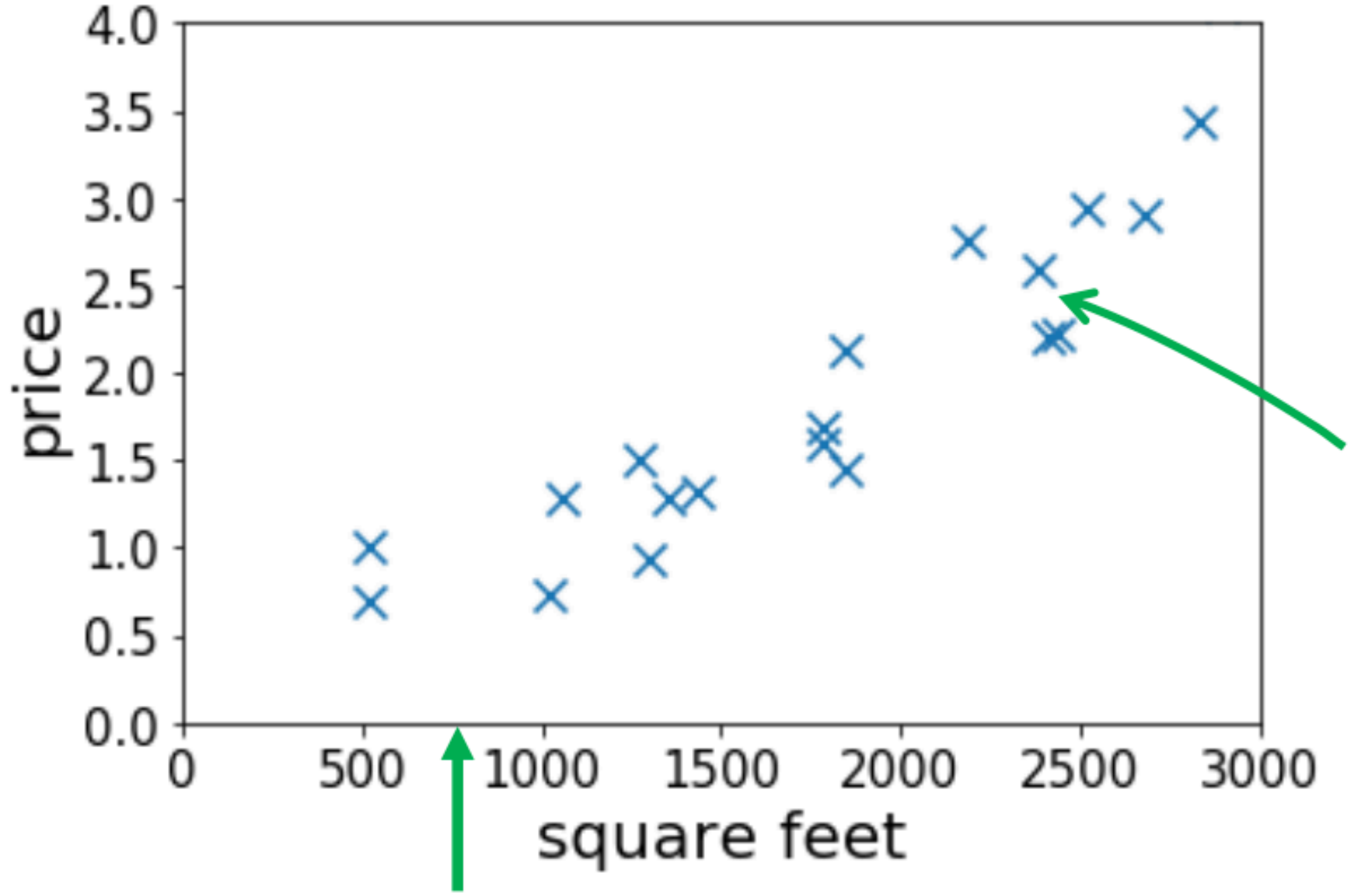

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CAT

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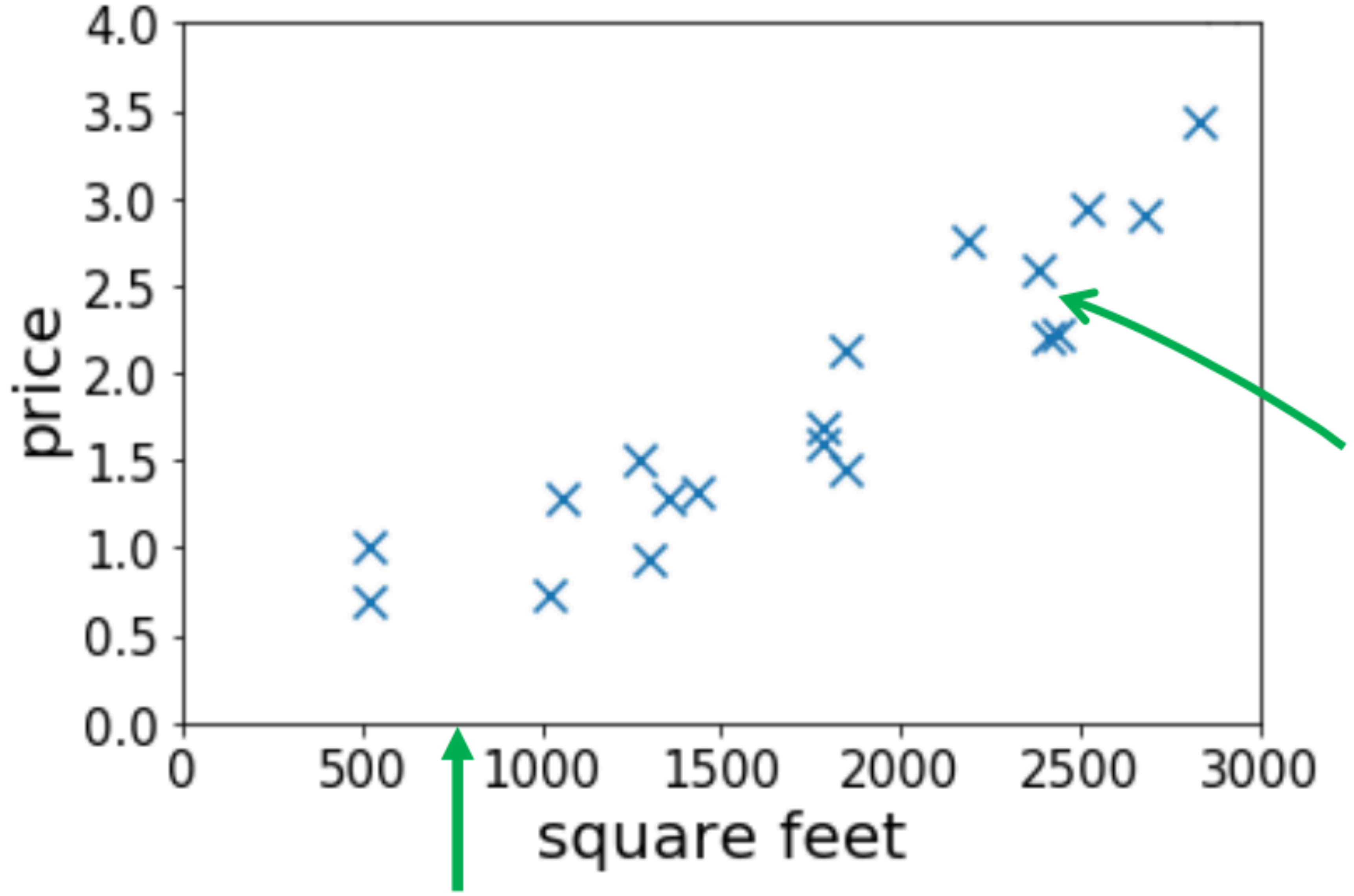

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- A training set is set of pairs $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$

  s.t. $x^{(i)} \in \mathcal{X}$ and $y^{(i)} \in \mathcal{Y}$ for $i = 1, \ldots, n$.

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- Given a training set our goal is to produce a good prediction function h

- If $\mathcal{Y}$ is continuous, then called a regression problem
- If $\mathcal{Y}$ is discrete, then called a classification problem

Supervised Learning

- How to define "good" for a prediction function?
  - Metrics / performance
  - Good on unseen data

Validation dataset is another set of pairs $\{(\hat{x}^{(1)}, \hat{y}^{(1)}), \cdots, (\hat{x}^{(m)}, \hat{y}^{(m)})\}$

Does not overlap with training dataset

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Does not overlap with training dataset

Test dataset is another set of pairs $\{(\tilde{x}^{(1)}, \tilde{y}^{(1)}), \cdots, (\tilde{x}^{(L)}, \tilde{y}^{(L)})\}$

Does not overlap with training and validation dataset

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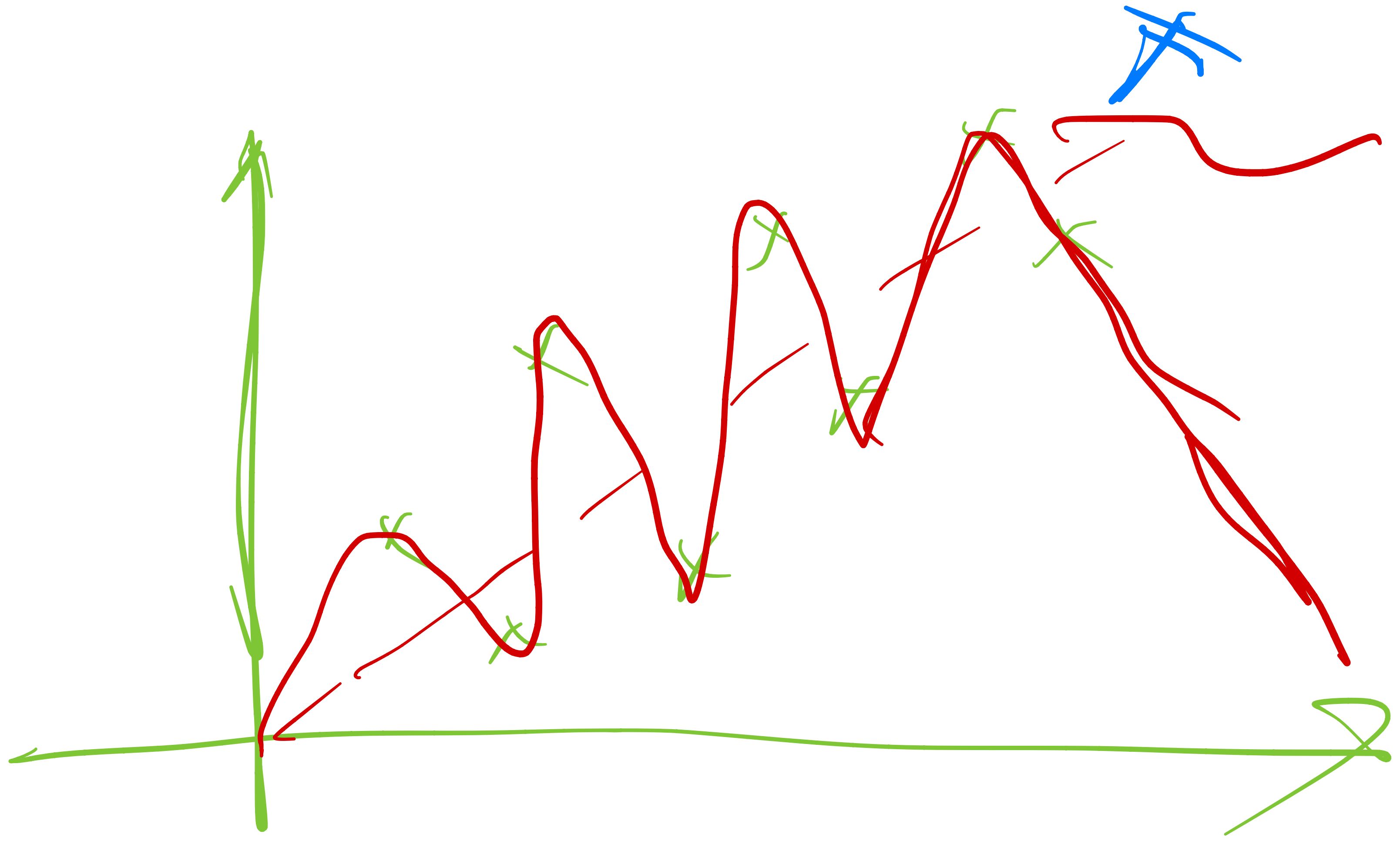
Completely unseen before deployment

Realistic setting

Supervised Learning



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100K   90K → training   10K → validation

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Realistic setting

Hyperparameter tuning is a form of training

Supervised Training

Train

Validation

Test

unsupervised

$M \leftarrow x$

labeled validation (x, y)

x

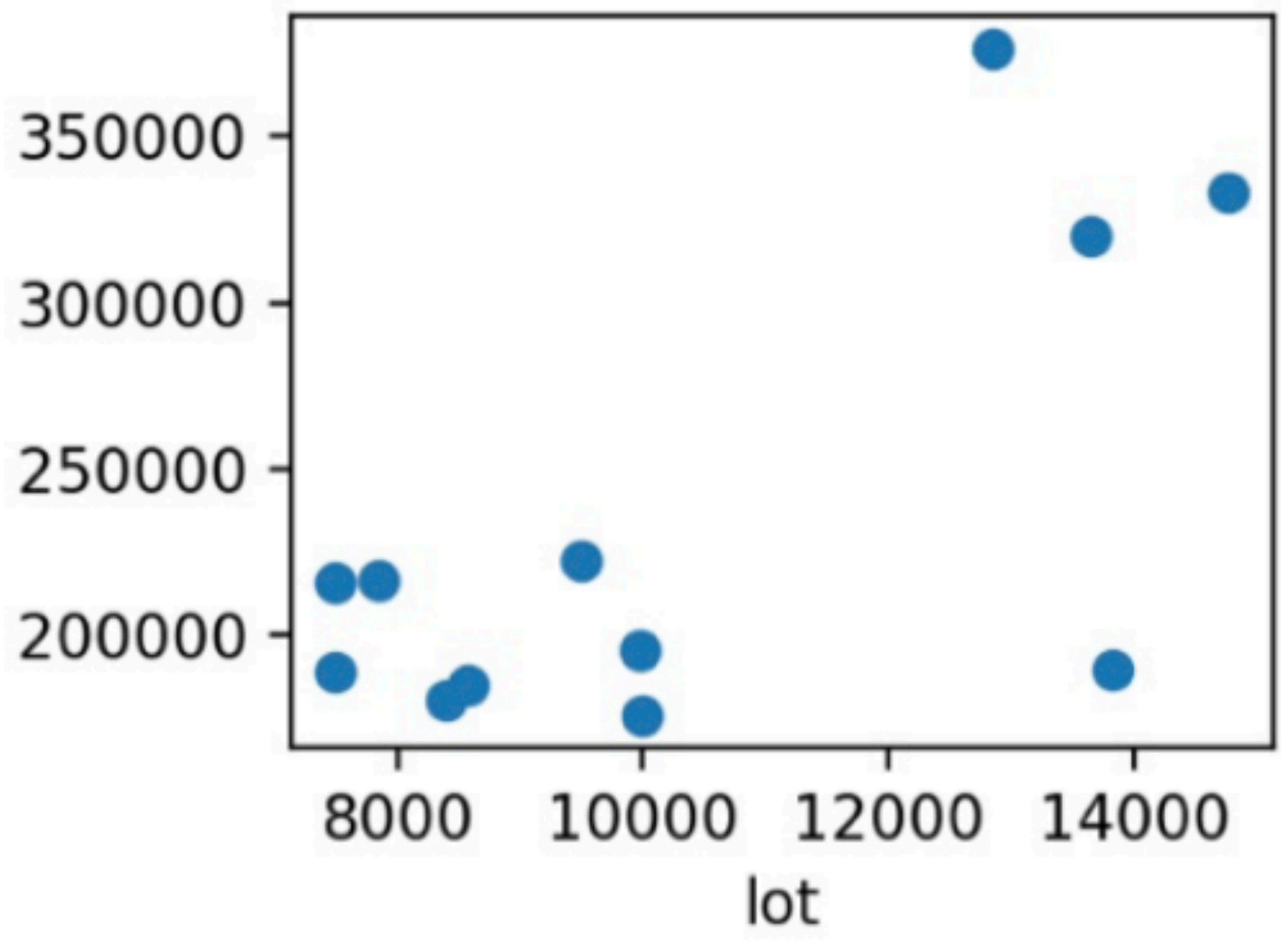
Not only for supervised learning

Example: Regression using Housing Data

Example from Stanford CS229

Example Housing Data

	SalePrice	Lot.Area
4	189900	13830
5	195500	9978
9	189000	7500
10	175900	10000
12	180400	8402
22	216000	7500
36	376162	12858
47	320000	13650
55	216500	7851
56	185088	8577



Represent h as a Linear Function

$h(x) = \theta_0 + \theta_1 x_1$ is an *affine function*

Popular choice

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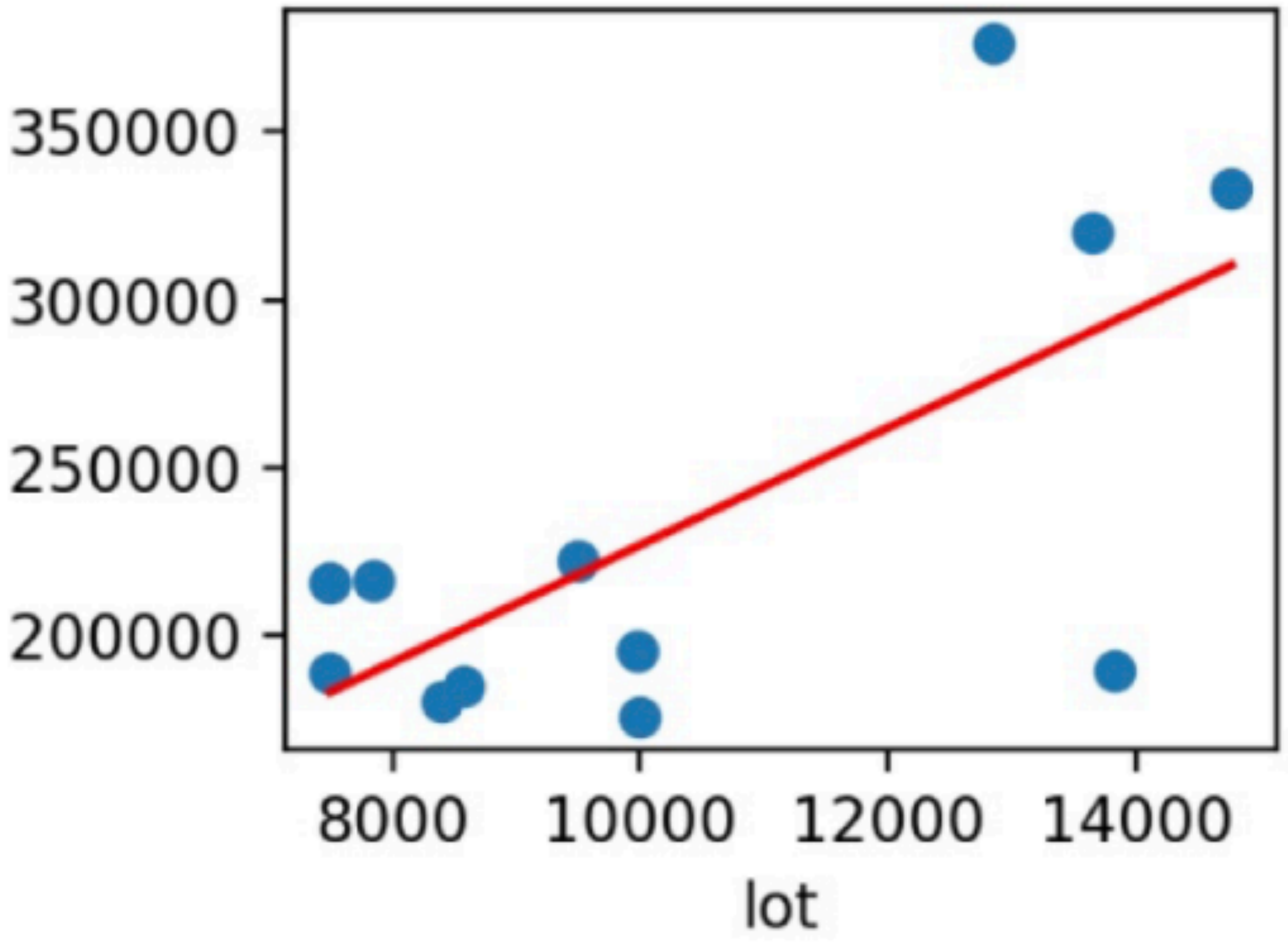
Popular choice

2

The function is defined by **parameters** θ_0 and θ_1, the function space is greatly reduced

Simple Line Fit



More Features

	size	bedrooms	lot size
$x^{(1)}$	2104	4	45k
$x^{(2)}$	2500	3	30k

	Price
$y^{(1)}$	400
$y^{(2)}$	900

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What's a prediction here?

$$h(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3.$$

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What's a prediction here?

$$h(x) = \theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3.$$

$x_0 = 1$

3 x

With the convention that $x_0 = 1$ we can write:

$$h(x) = \sum_{j=0}^{3} \theta_j x_j$$

4 terms

Vector Notations

Vector Notations

	size	bedrooms	lot size		Price
$x^{(1)}$	2104	4	45k	$y^{(1)}$	400
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We write the vectors as (important notation)

$$\theta = \begin{pmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{pmatrix} \text{ and } x^{(1)} = \begin{pmatrix} x_0^{(1)} \\ x_1^{(1)} \\ x_2^{(1)} \\ x_3^{(1)} \end{pmatrix} = \begin{pmatrix} 1 \\ 2104 \\ 4 \\ 45 \end{pmatrix} \text{ and } y^{(1)} = 400$$

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We call θ **parameters**, $x^{(i)}$ is the input or the **features**, and the output or **target** is $y^{(i)}$. To be clear,

(x, y) is a training example and $(x^{(i)}, y^{(i)})$ is the i^{th} example.

Vector Notations

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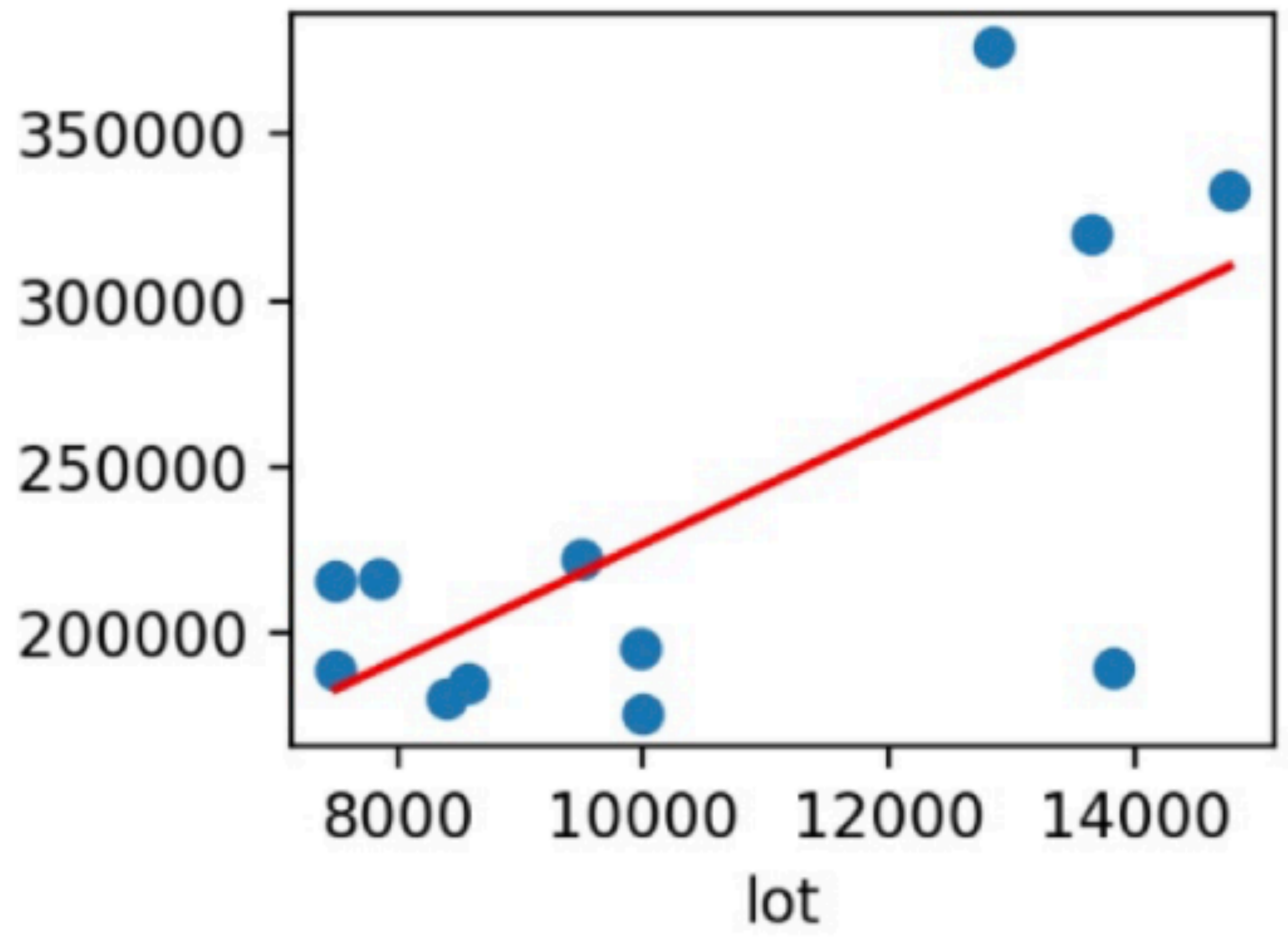
We have n examples. There are d features. $x^{(i)}$ and θ are d+1 dimensional (since $x_0^{(i)} = 1$)

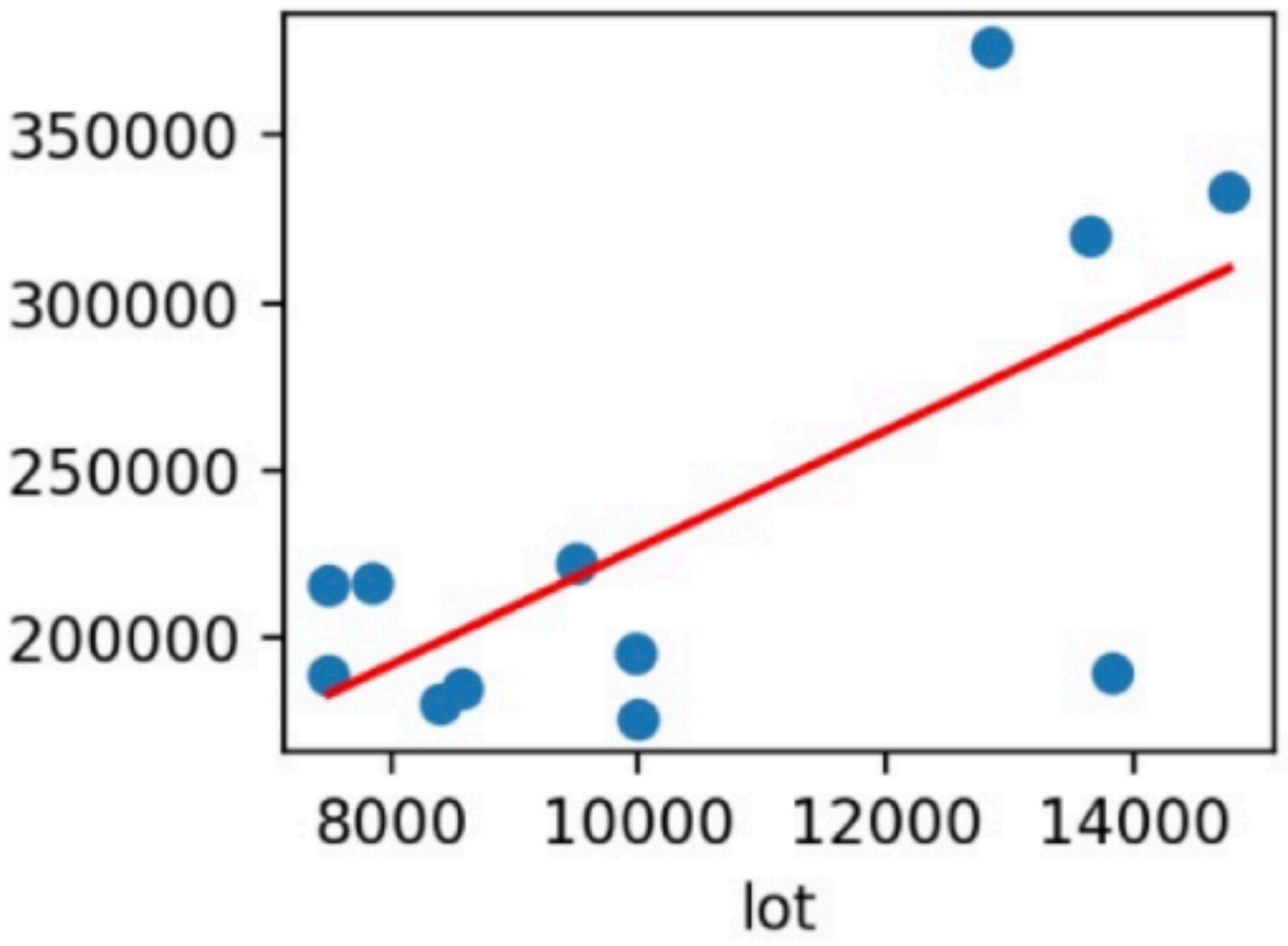
Vector Notation of Prediction



Kernel methods

$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T\theta$$

Vector Notation of Prediction



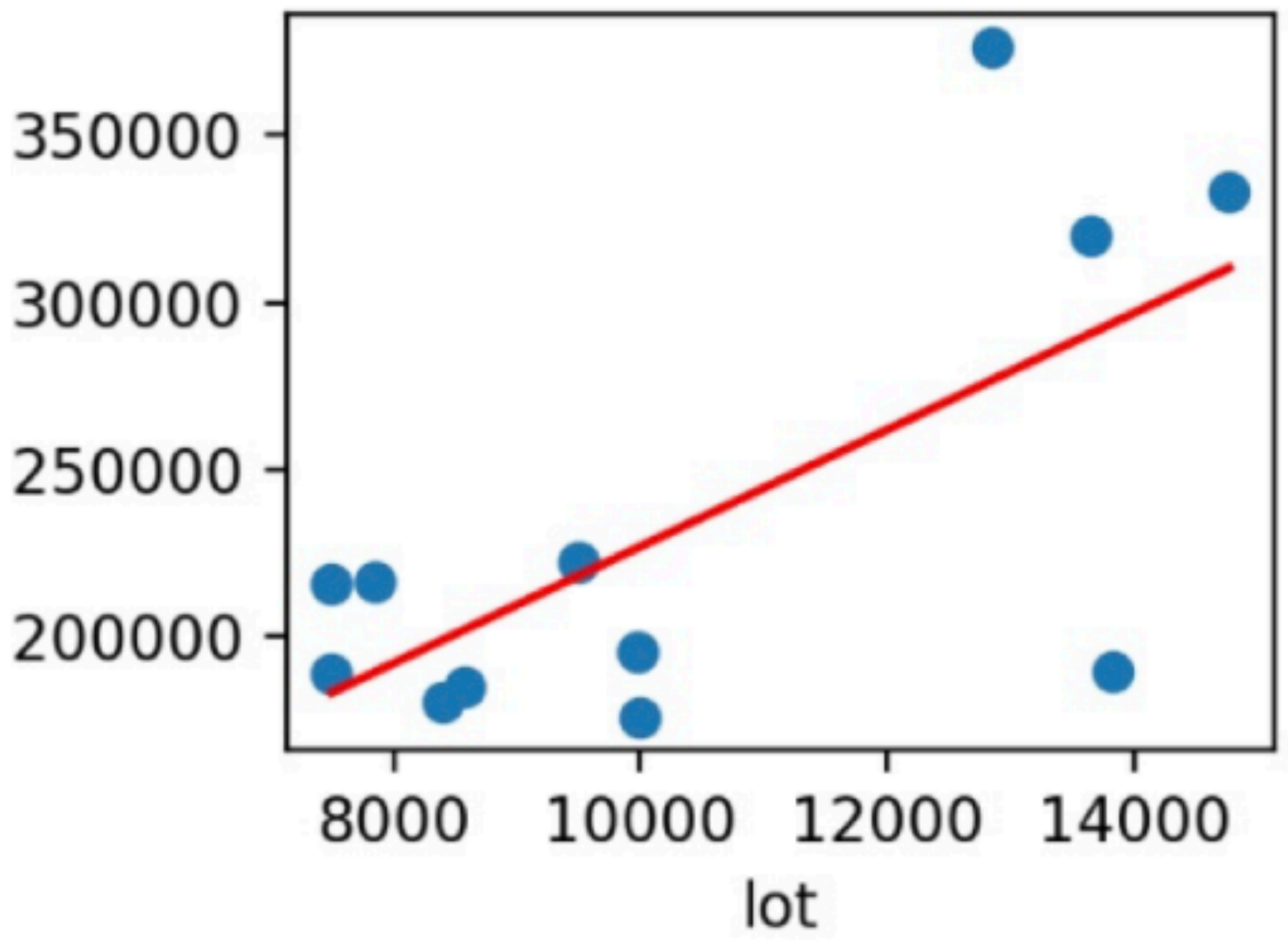
$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T \theta$$

how to define metric

We want to choose θ so that $h_\theta(x) \approx y$

similarity

Loss Function

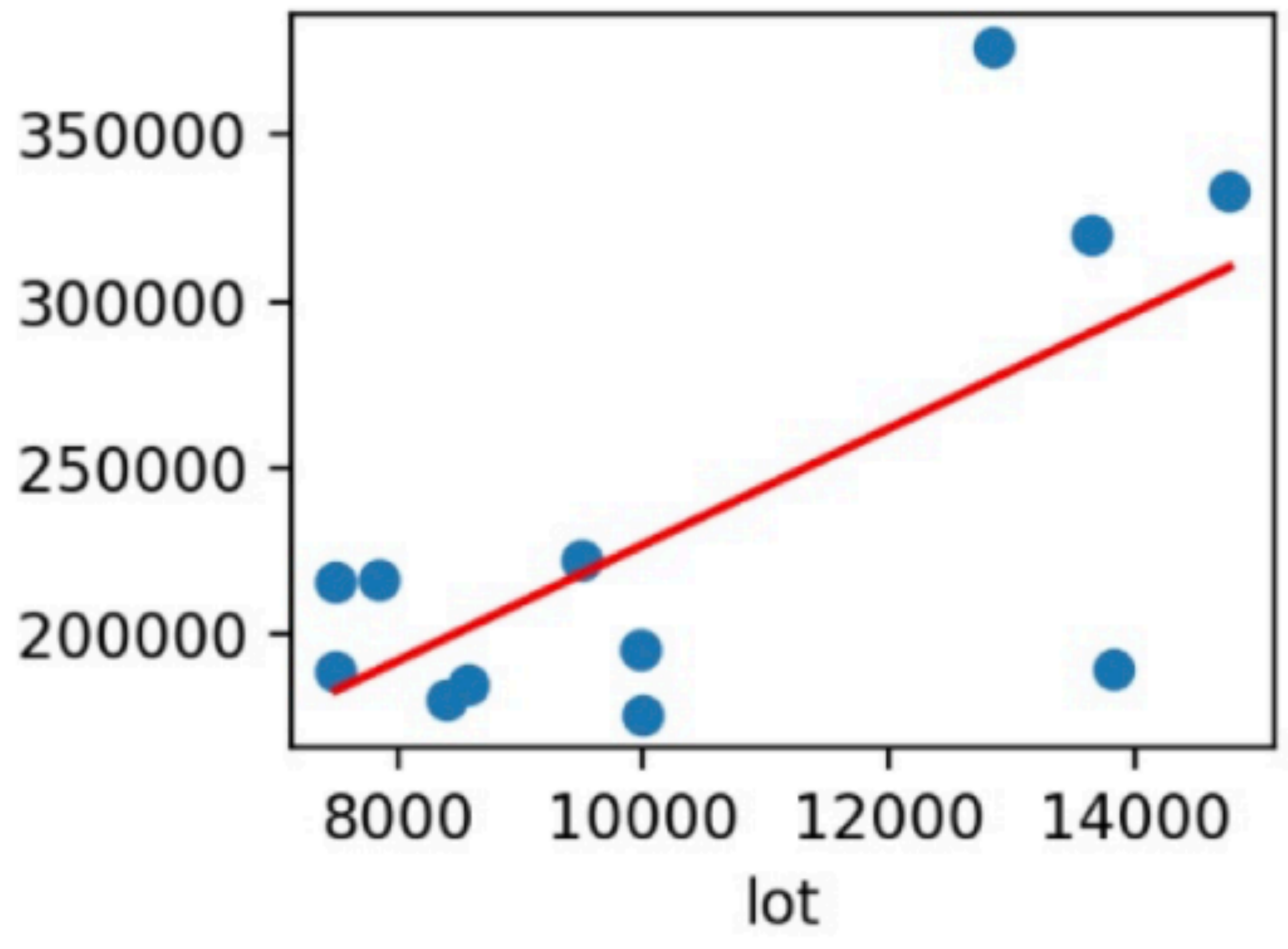


$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T\theta$$

We want to choose θ so that $h_\theta(x) \approx y$

How to quantify the deviation of $h_\theta(x)$ from y

Least Squares



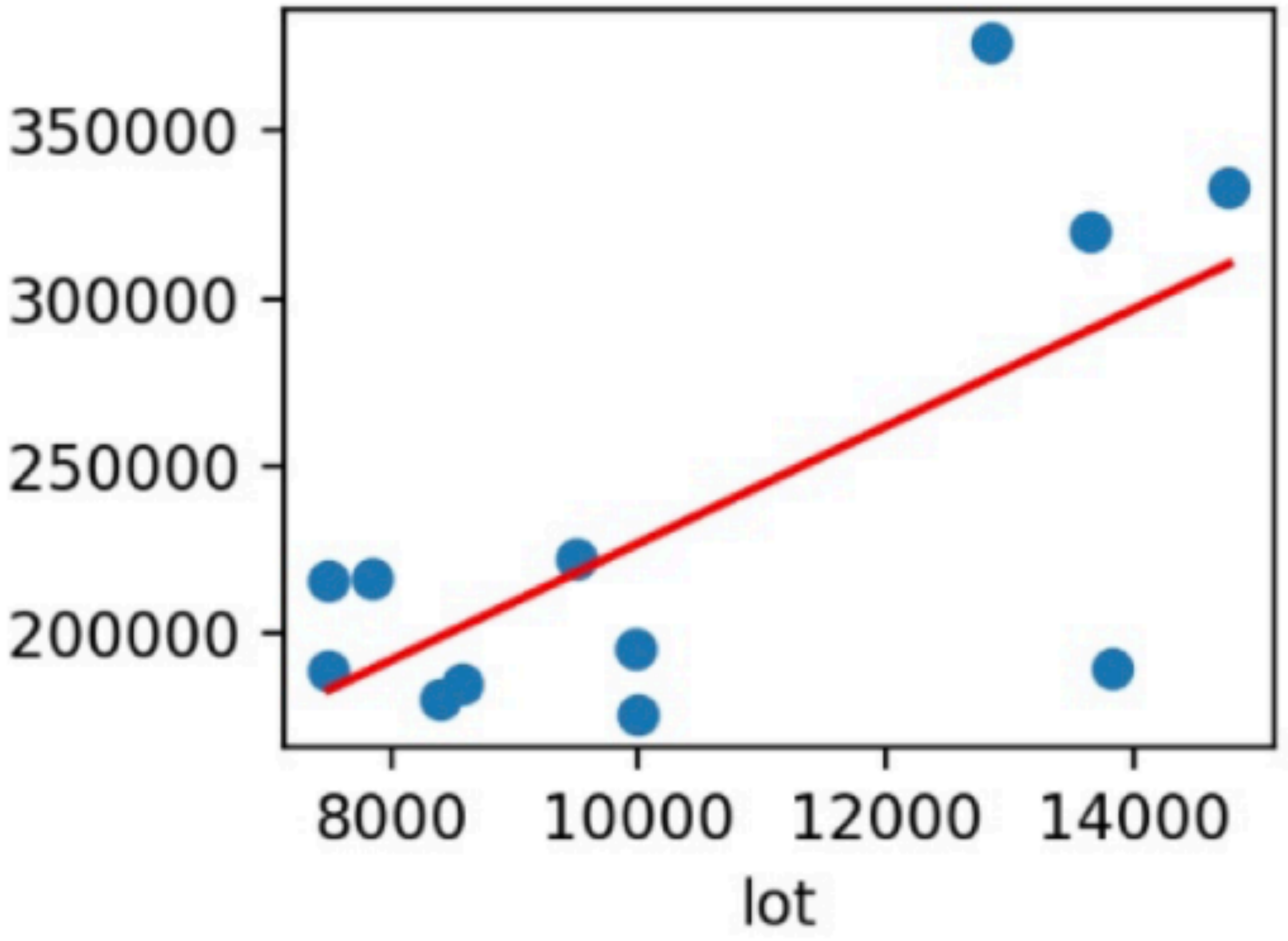
$\| \vec{h_\theta(x)} - \vec{y} \|$

$\| \vec{h_\theta(x)} - \vec{y} \|^2$

$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T \theta$$

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

Least Squares



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

Choose

$$\theta = \underset{\theta}{\operatorname{argmin}}\, J(\theta).$$

Solving Least Square Problem

Direct Minimization

$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T\theta \qquad J(\theta) = \frac{1}{2}\sum_{i=1}^{n}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

Choose

$$\theta = \underset{\theta}{\operatorname{argmin}}\, J(\theta).$$

Solving Least Square Problem

rank(X) < d

N data samples

d feature size

$X \in R^{N \times d}$

$X^T X \in R^{d \times N} \times R^{N \times d}$

$\in R^{d \times d}$

$$
\begin{aligned}
\nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(X\theta - \vec{y})^T(X\theta - \vec{y}) \\
&= \frac{1}{2}\nabla_\theta \left((X\theta)^T X\theta - (X\theta)^T\vec{y} - \vec{y}^T(X\theta) + \vec{y}^T\vec{y}\right) \\
&= \frac{1}{2}\nabla_\theta \left(\theta^T(X^T X)\theta - \vec{y}^T(X\theta) - \vec{y}^T(X\theta)\right) \\
&= \frac{1}{2}\nabla_\theta \left(\theta^T(X^T X)\theta - 2(X^T\vec{y})^T\theta\right) \\
&= \frac{1}{2}\left(2X^T X\theta - 2X^T\vec{y}\right) \\
&= X^T X\theta - X^T\vec{y}
\end{aligned}
$$

$= 0$

N < d

$\Downarrow$

rank(X) ≤ min(N, d)

rank(X) < d

$\boxed{N > d}$

$$X^T X\theta = X^T\vec{y} \qquad \theta = (X^T X)^{-1} X^T\vec{y}.$$

rank(AB) ≤ min(rank(A), rank(B))

whether $(X^T X)^{-1}$ exists

$$X \;\; n \left[\begin{array}{cc} v_2 & v_5 \\ 2 & 5 \\ 1 & 2 \\ 2 & 4 \\ 5 & 10 \\ 6 & 12 \\ 12 & 24 \end{array} \right] \quad d$$

$\underbrace{n < d}$ $\rightarrow$ not fullrank

$n > d$

$$v_5 = 2 \cdot v_2$$

$$\text{rank}(X) < d$$

Solving Least Square Problem

$$\begin{aligned}
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&= \frac{1}{2}\left(2X^TX\theta - 2X^T\vec{y}\right) \\
&= X^TX\theta - X^T\vec{y}
\end{aligned}$$

Normal equations $X^TX\theta = X^T\vec{y}$ $\qquad$ $\theta = (X^TX)^{-1}X^T\vec{y}.$

Solving Least Square Problem

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Normal equations $X^TX\theta = X^T\vec{y}$ $\qquad\qquad$ $\theta = (X^TX)^{-1}X^T\vec{y}.$

When is X^TX invertible? What if it is not invertible?

Why Least-Square Loss Function?

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

Why Least-Square Loss Function?

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

maximum likelihood

Assume

$$y^{(i)} = \theta^T x^{(i)} + \epsilon^{(i)}$$

noise

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x, y: random variable

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random noise

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ϵ: deviation of prediction from the truth, Gaussian random variable

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$\varepsilon^{(i)}$ $\varepsilon^{(i+1)}$

x, y: random variable

ϵ: deviation of prediction from the truth, Gaussian random variable

$x^{(i)}, y^{(i)}$: observations, or the data

$\epsilon^{(i)}$: the actual prediction error of the i_{th} example, sampled from the Gaussian distribution, IID (independently and identically distributed)

Why Least-Square Loss Function?

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$$p(\epsilon^{(i)}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\epsilon^{(i)})^2}{2\sigma^2}\right)$$

P(y)

Σ

Why Least-Square Loss Function?

$$p(\epsilon^{(i)}) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(\epsilon^{(i)})^2}{2\sigma^2}\right)$$

$\epsilon \sim N(0, 1)$

$$\boxed{p(y^{(i)}|x^{(i)};\theta) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(y^{(i)}-\theta^T x^{(i)})^2}{2\sigma^2}\right)}$$

$x \sim N(\mu, \sigma^2)$

$\epsilon = y - \theta^T x$

$ax+b \sim N(a\mu+b, a^2)$

Why Least-Square Loss Function?

$P(A_1, A_2 \cdots A_n) = P(A_1) P(A_2 | A_1) P(A_3 | A_1 A_2) \cdots$

$$p(\epsilon^{(i)}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(\epsilon^{(i)})^2}{2\sigma^2}\right)$$

one data example

$$p(y^{(i)}|x^{(i)};\theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right)$$

$$\begin{aligned} p(\vec{y}|X;\theta) &= \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)};\theta) \\ &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right) \end{aligned}$$

Why Least-Square Loss Function?

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$$p(\vec{y}|X;\theta) = \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)};\theta)$$

Function of θ

$$= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right)$$

Why Least-Square Loss Function?

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L(\theta) &= \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta) \\
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Likelihood Function

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Likelihood Function

What is a reasonable guess of θ?

Why Least-Square Loss Function?

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Likelihood Function

What is a reasonable guess of θ?

Maximize the probability of Y's happening!

$$\arg\max_{\theta} L(\theta) = \arg\max_{\theta} \log L(\theta)$$

Maximum Likelihood Estimation (MLE)

$$
\begin{aligned}
\ell(\theta) &= \log L(\theta) \\
&= \log \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right) \\
&= \sum_{i=1}^{n} \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right) \\
&= \underbrace{n \log \frac{1}{\sqrt{2\pi}\sigma}}_{\text{constant}} - \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)})^2.
\end{aligned}
$$

$$
\arg\max_{\theta} l(\theta) = \arg\max_{\theta} - \underbrace{\frac{1}{\sigma^2} \frac{1}{2} \sum_{i=1}^{n} (y^{(i)} - \theta^T x^{(i)})^2}_{\text{least square}}
$$

Why MLE?

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Likelihood Function

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Maximize the probability of Y's happening?

Maximizing likelihood estimation -> $\hat{\theta}$

Why MLE?

$$\begin{aligned} L(\theta) &= \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta) \\ &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y^{(i)} - \theta^T x^{(i)})^2}{2\sigma^2}\right) \end{aligned}$$

Likelihood Function

What is a reasonable guess of θ?

Maximize the probability of Y's happening?

Maximizing likelihood estimation -> $\hat{\theta}$ $\hat{\theta}$

Ground-truth θ^* θ^*

$\hat{\theta} \rightarrow \theta^*$

$$\underbrace{\boxed{E_{x \sim p_{data}}[\hat{\theta}] = \theta^*}}_{\neq}$$ unbiased estimator

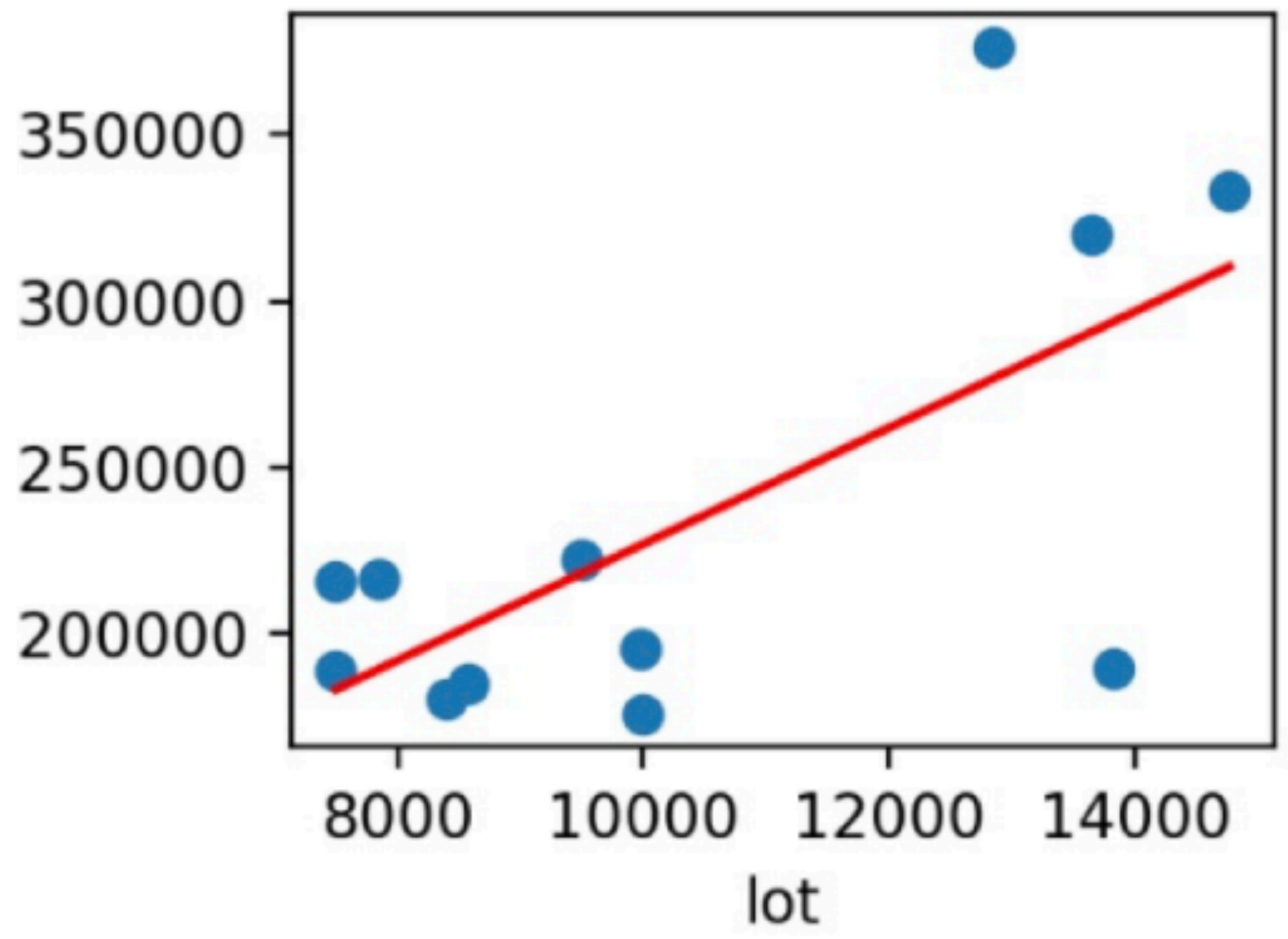
biased estimator

$x_1 \cdots x_n \sim D$ mean μ, σ^2

$$E\left[\hat{\mu} = \underbrace{\frac{x_1 + \cdots x_n}{n}}\right] = \mu \qquad \mathrm{Var}\,\theta = \underbrace{E[(x-\mu)^2]}$$

$$E\left[\underbrace{\sigma^2} = \frac{\sum_i (x_i - \hat{\mu})^2}{n}\right] = \sigma^2 \cdot \frac{n-1}{n} \qquad \frac{\sum_i (x_i - \hat{\mu})^2}{n-1} \rightarrow \sigma^2$$

Another Solution — Gradient Descent



$$h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j = x^T\theta \qquad J(\theta) = \frac{1}{2}\sum_{i=1}^{n}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$$

Choose

$$\theta = \operatorname*{argmin}_{\theta} J(\theta).$$

Gradient Descent

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

Gradient Descent

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

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

Gradient Descent

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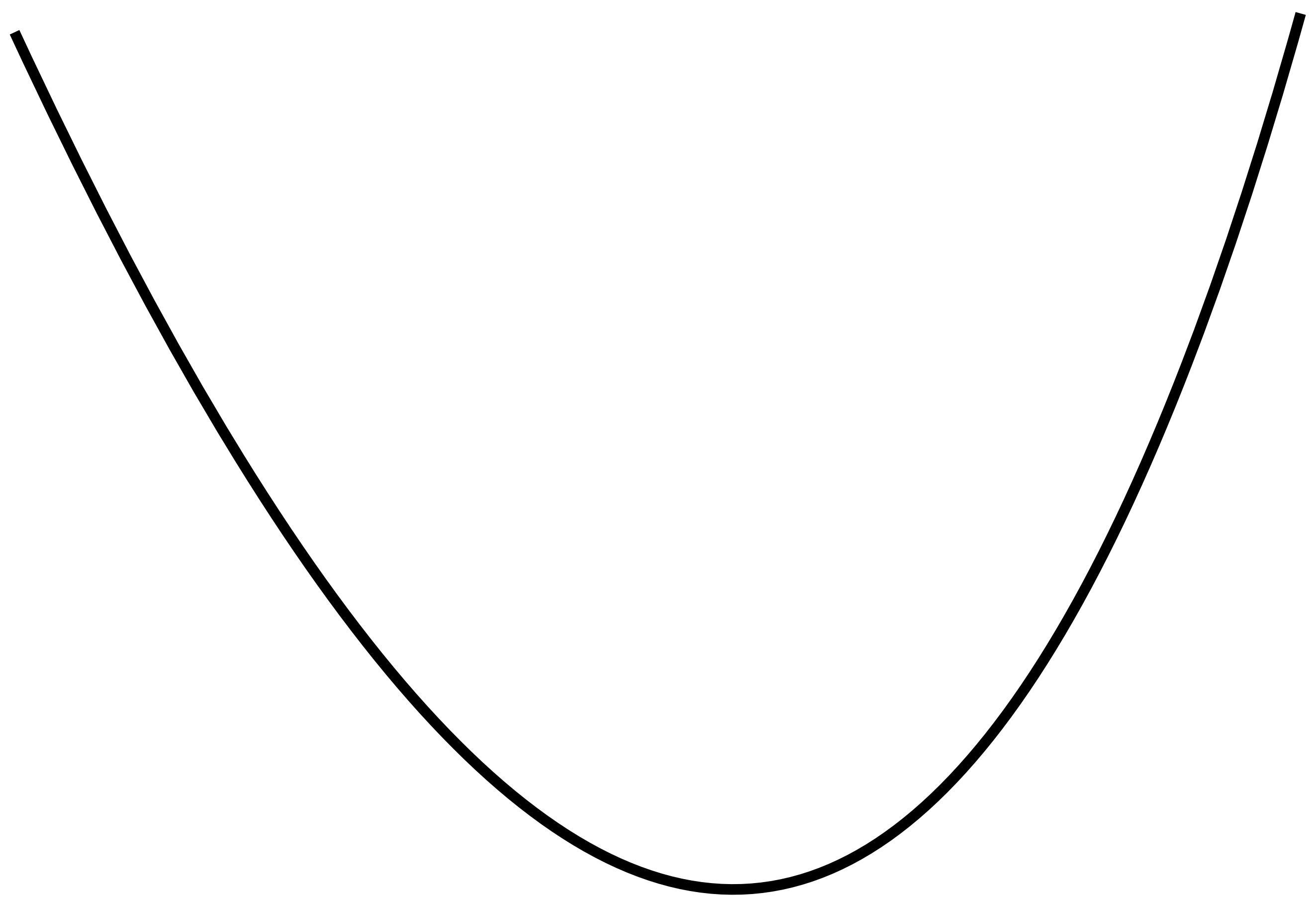

Gradient Descent

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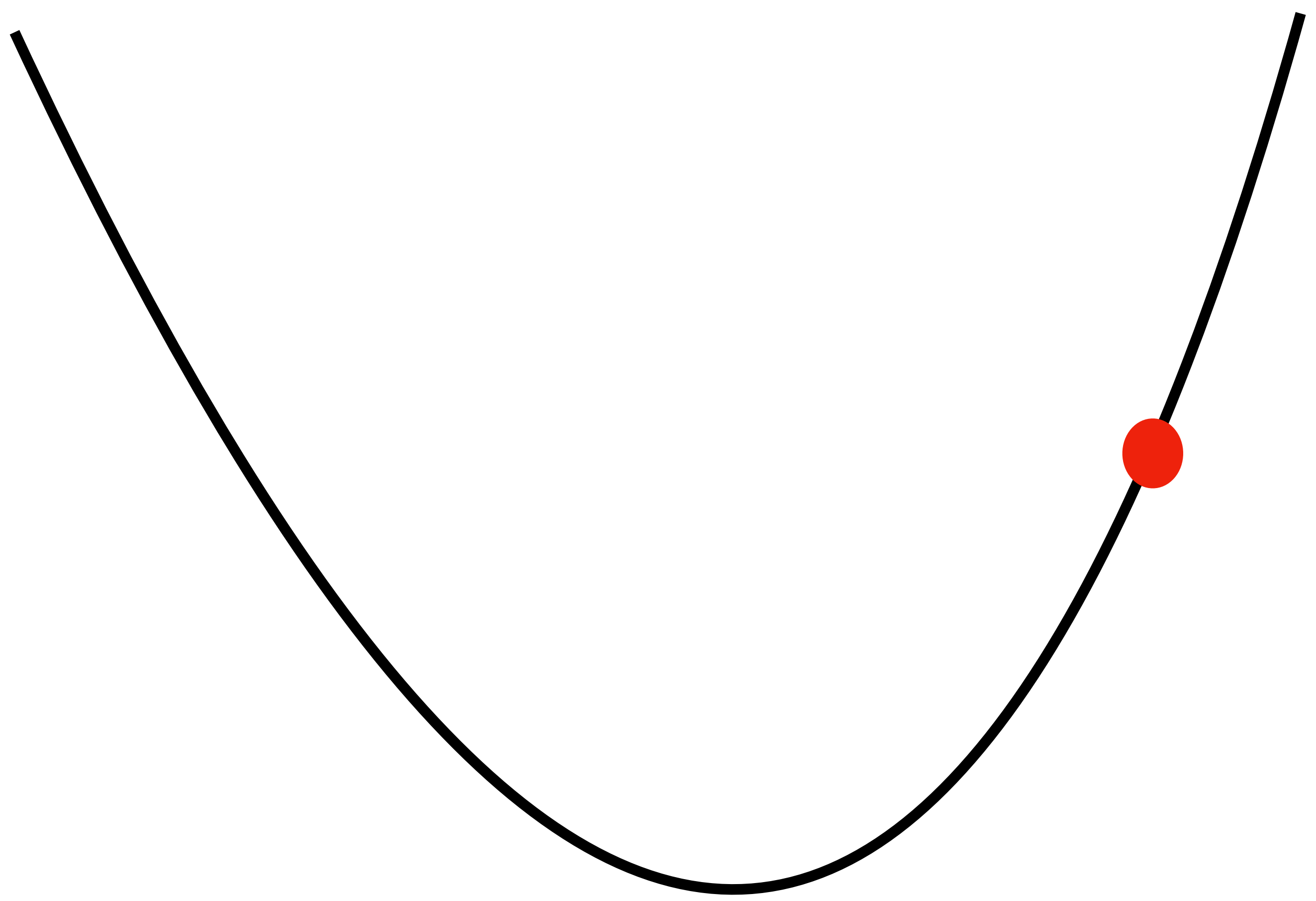

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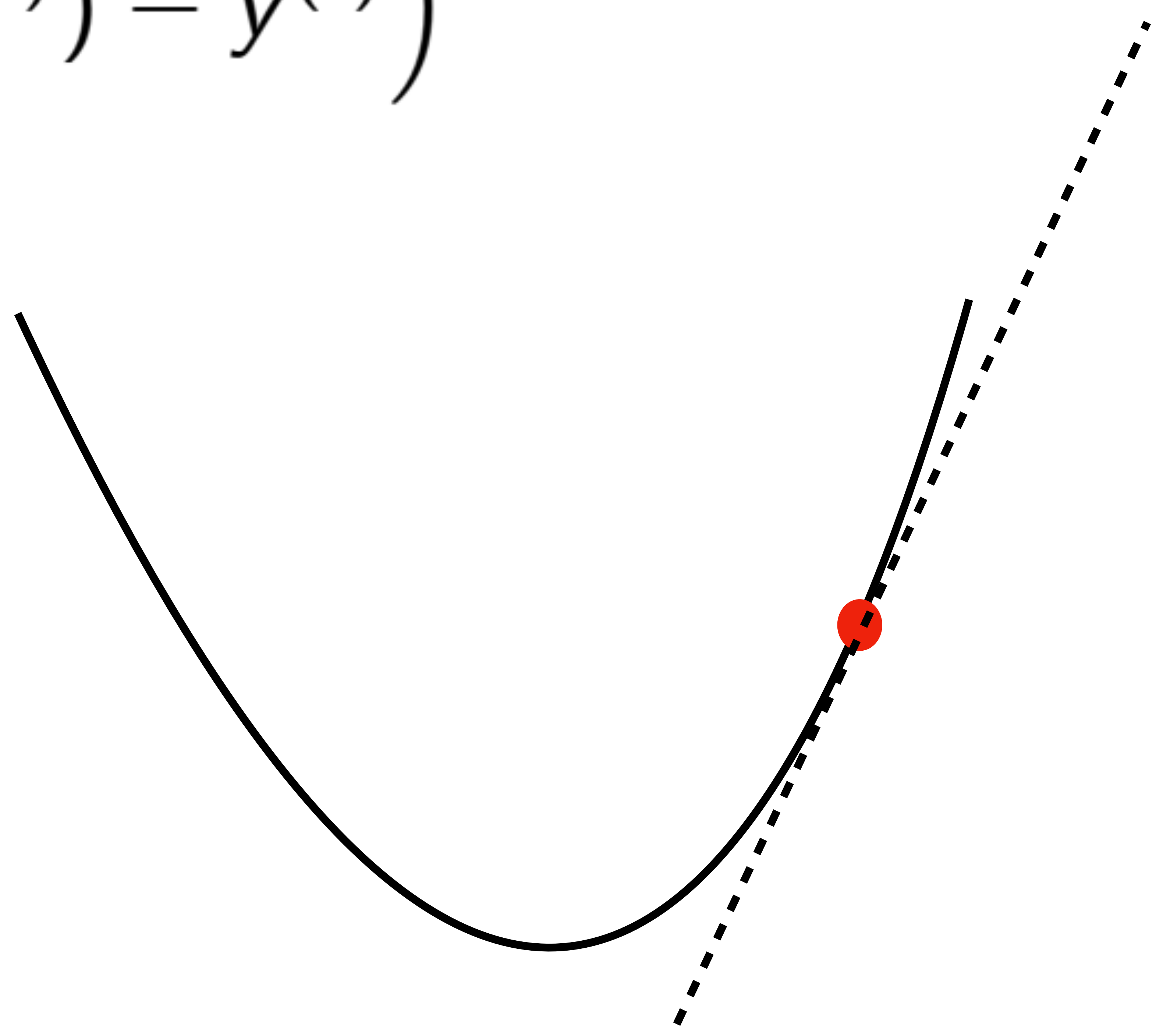

Gradient Descent

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

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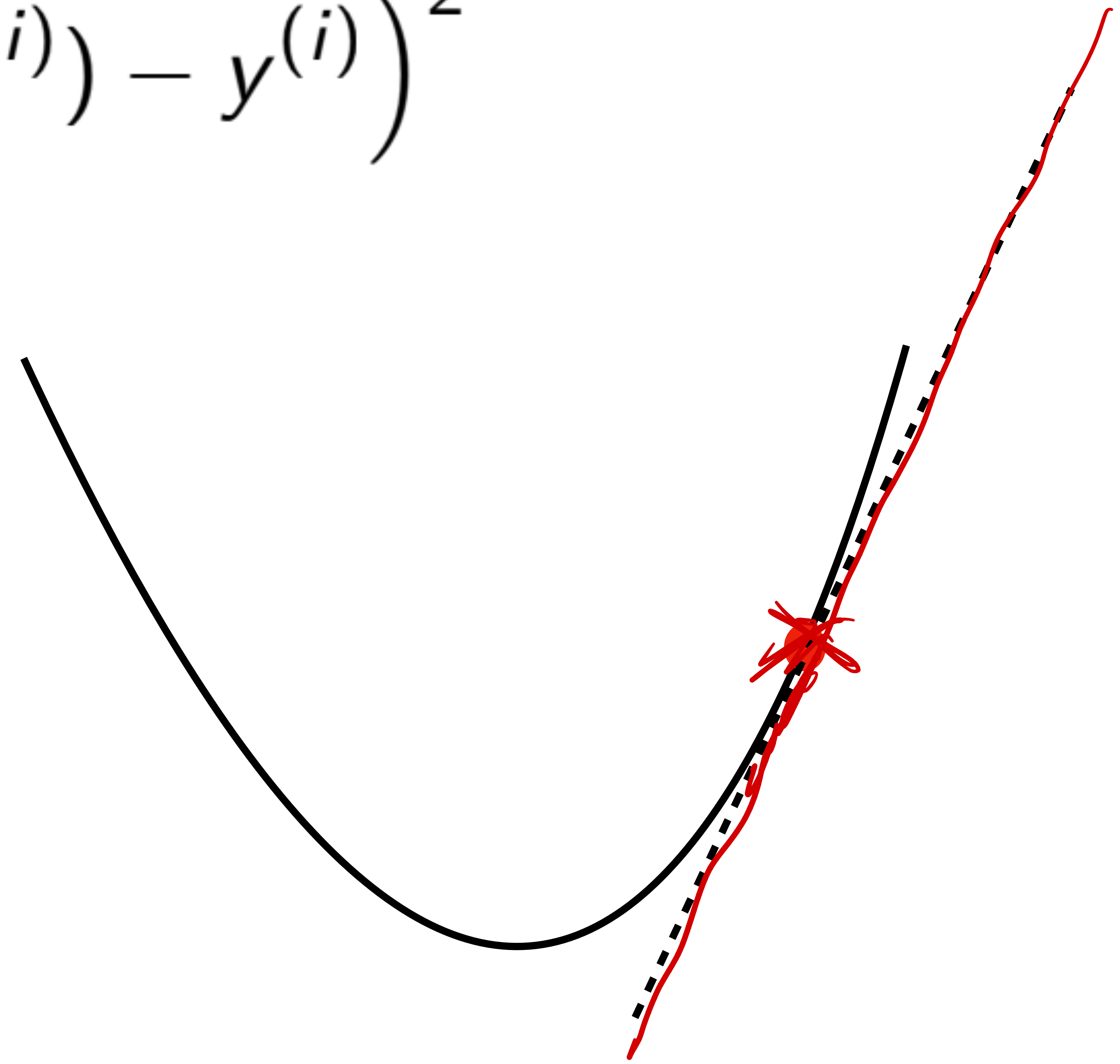


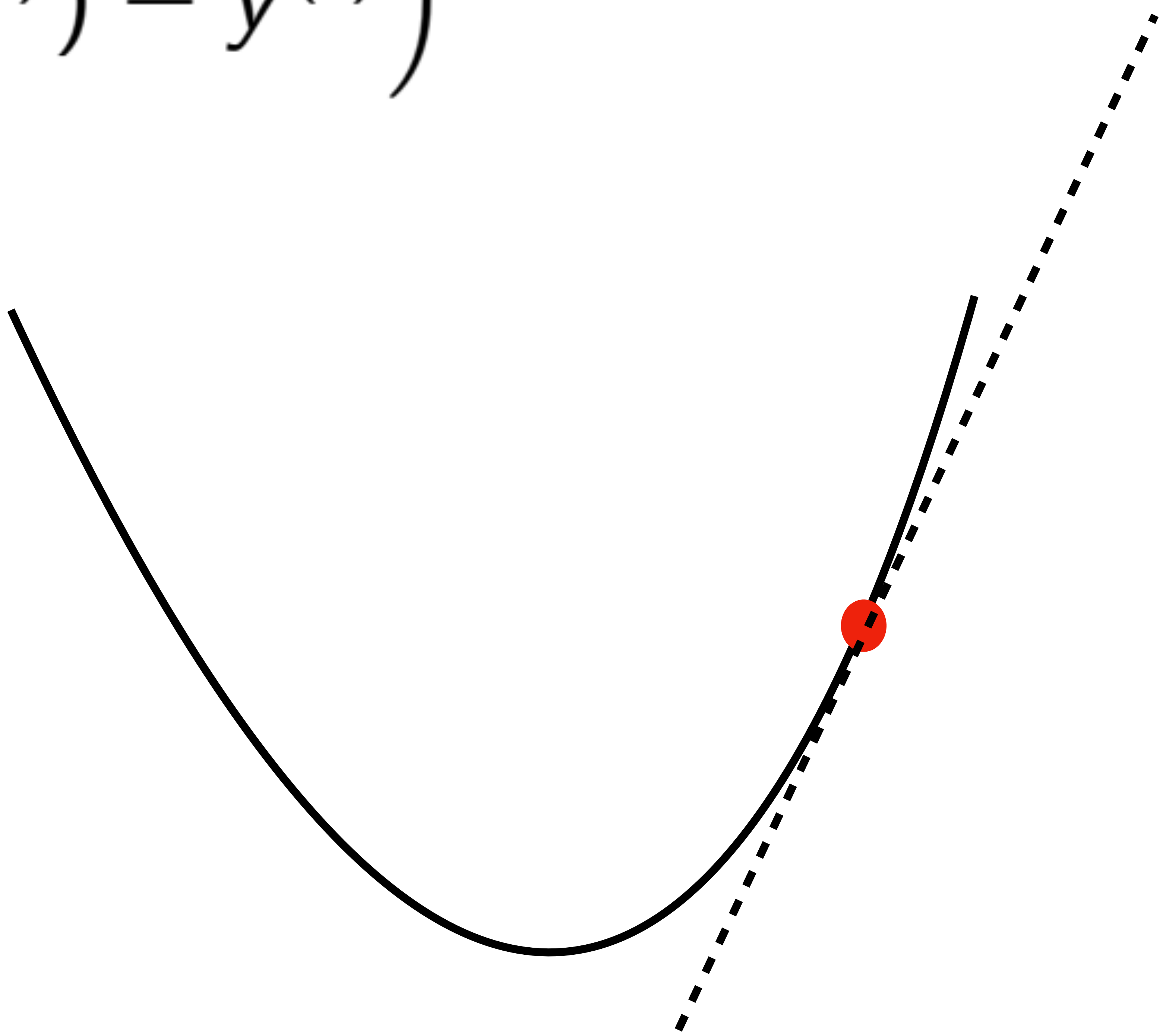
The direction of the steepest descrease of J

Gradient Descent

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

Learning Rate

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$



The direction of the steepest descrease of J

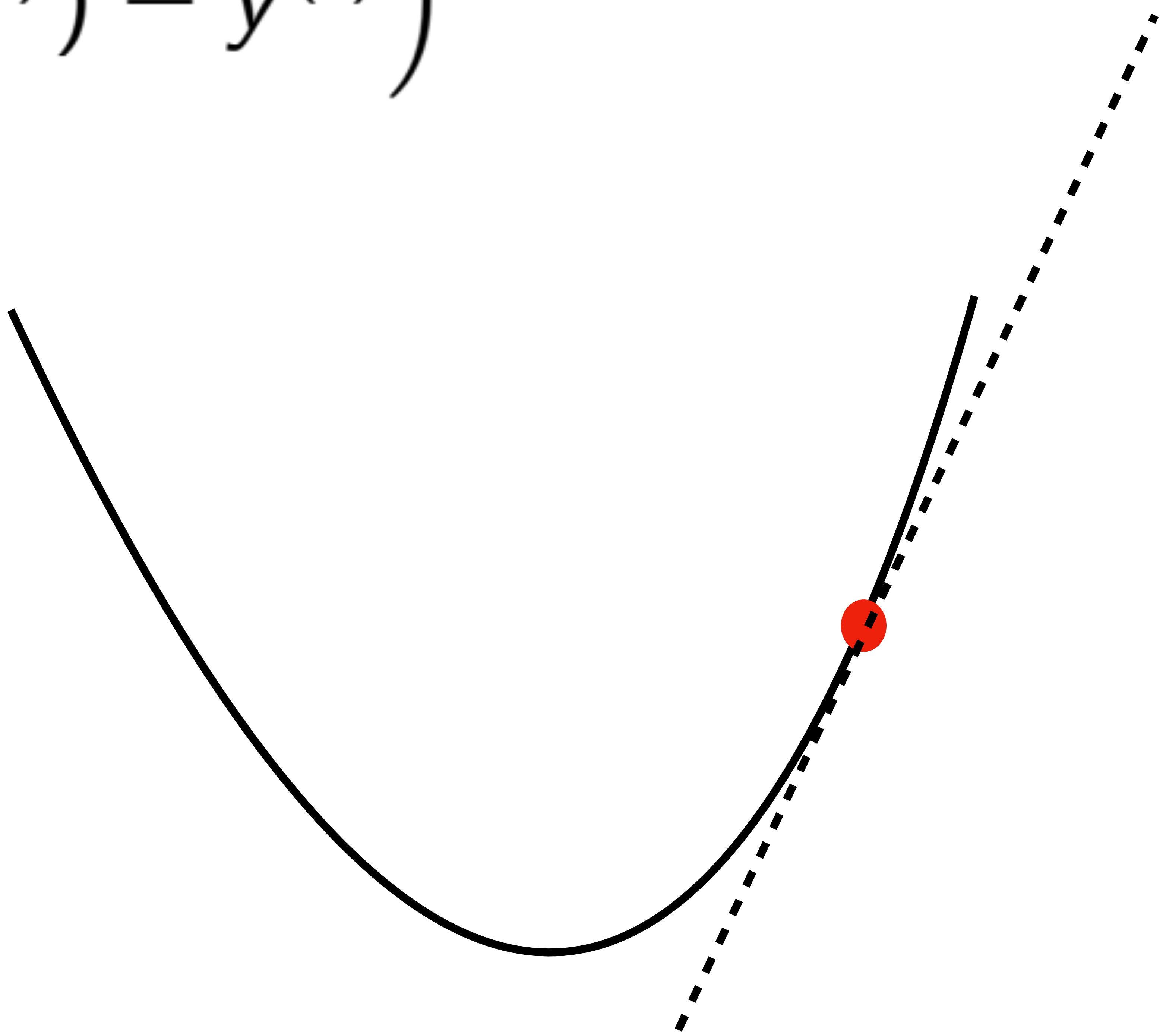
Gradient Descent

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

Learning Rate

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

This update is simultaneously performed for all values of j = 0,...,d.



The direction of the steepest descrease of J

Gradient Descent

For a single training example:

$$
\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} \left(h_\theta(x) - y\right)^2 \\
&= 2 \cdot \frac{1}{2} \left(h_\theta(x) - y\right) \cdot \frac{\partial}{\partial \theta_j} \left(h_\theta(x) - y\right) \\
&= \left(h_\theta(x) - y\right) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{d} \theta_i x_i - y \right) \\
&= \boxed{\left(h_\theta(x) - y\right) x_j}
\end{aligned}
$$

linear

Gradient Descent

For a single training example:

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} \left(h_\theta(x) - y\right)^2 \\
&= 2 \cdot \frac{1}{2} \left(h_\theta(x) - y\right) \cdot \frac{\partial}{\partial \theta_j} \left(h_\theta(x) - y\right) \\
&= \left(h_\theta(x) - y\right) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{d} \theta_i x_i - y \right) \\
&= \left(h_\theta(x) - y\right) x_j
\end{aligned}$$

LMS (Least Mean Square) Update Rule

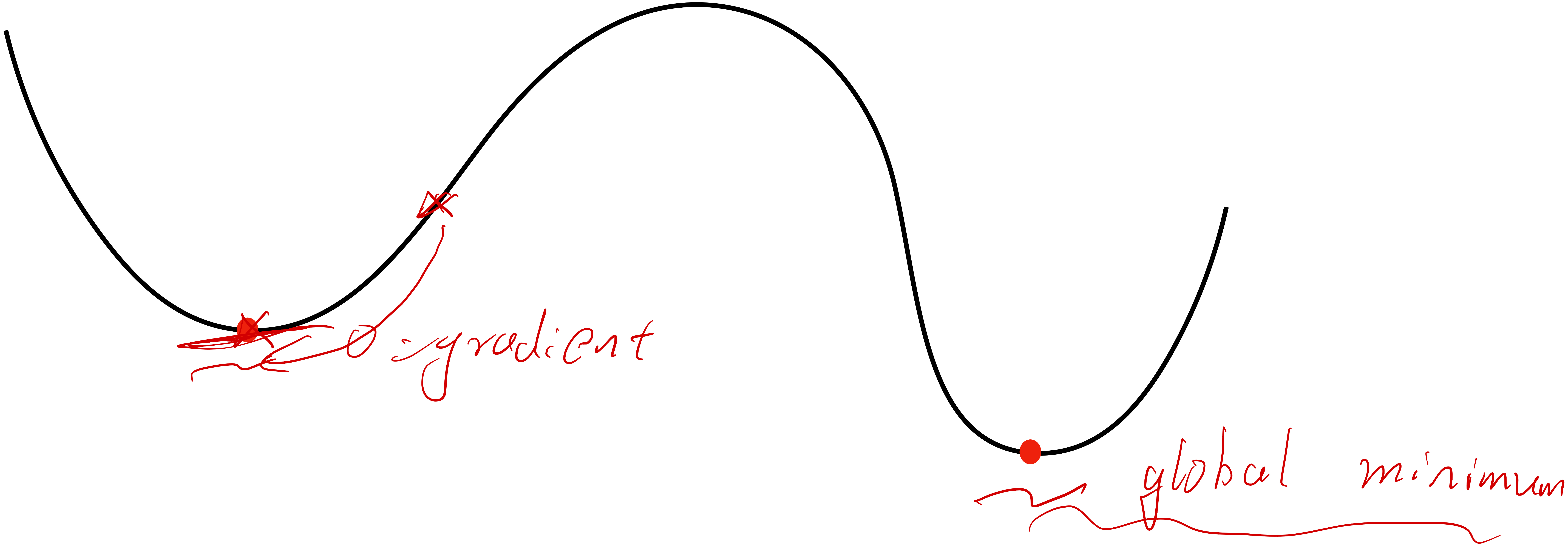
Batch Gradient Descent

For a multiple training examples:

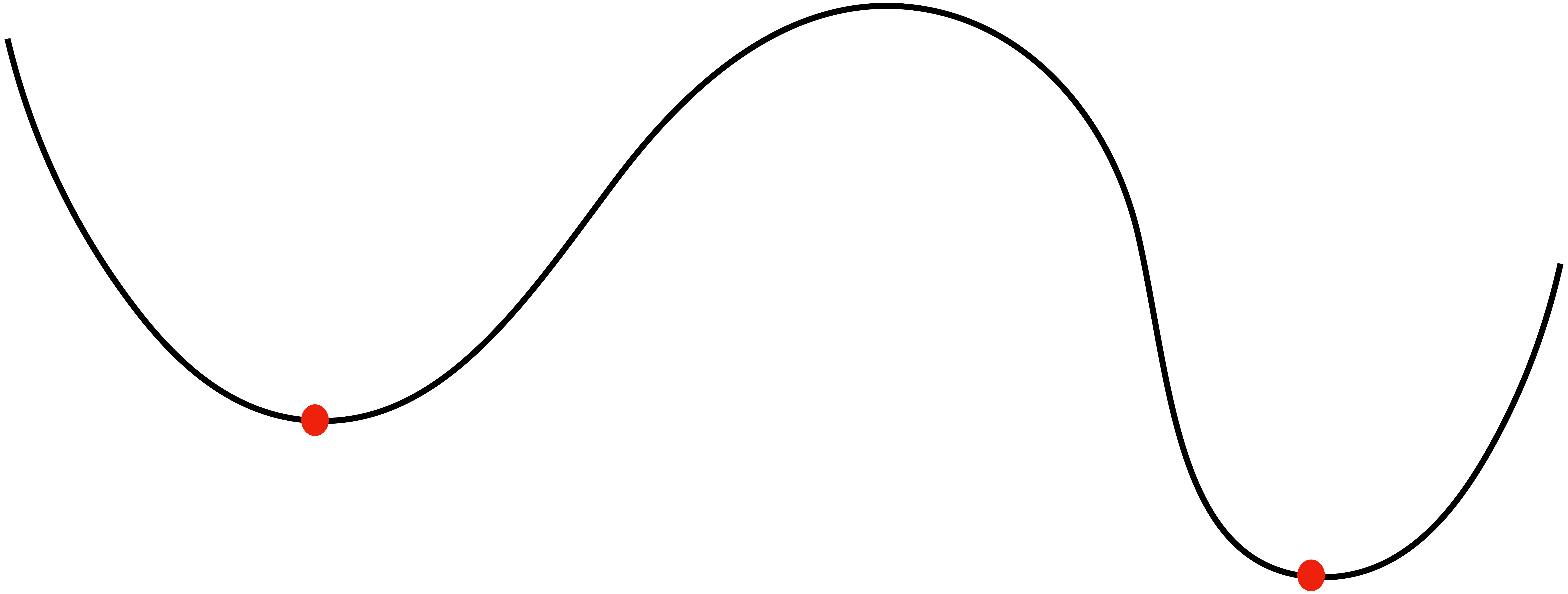
$$\theta_j := \theta_j + \alpha \sum_{i=1}^{n} \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)}$$

Repeat until convergence

Local Minimum



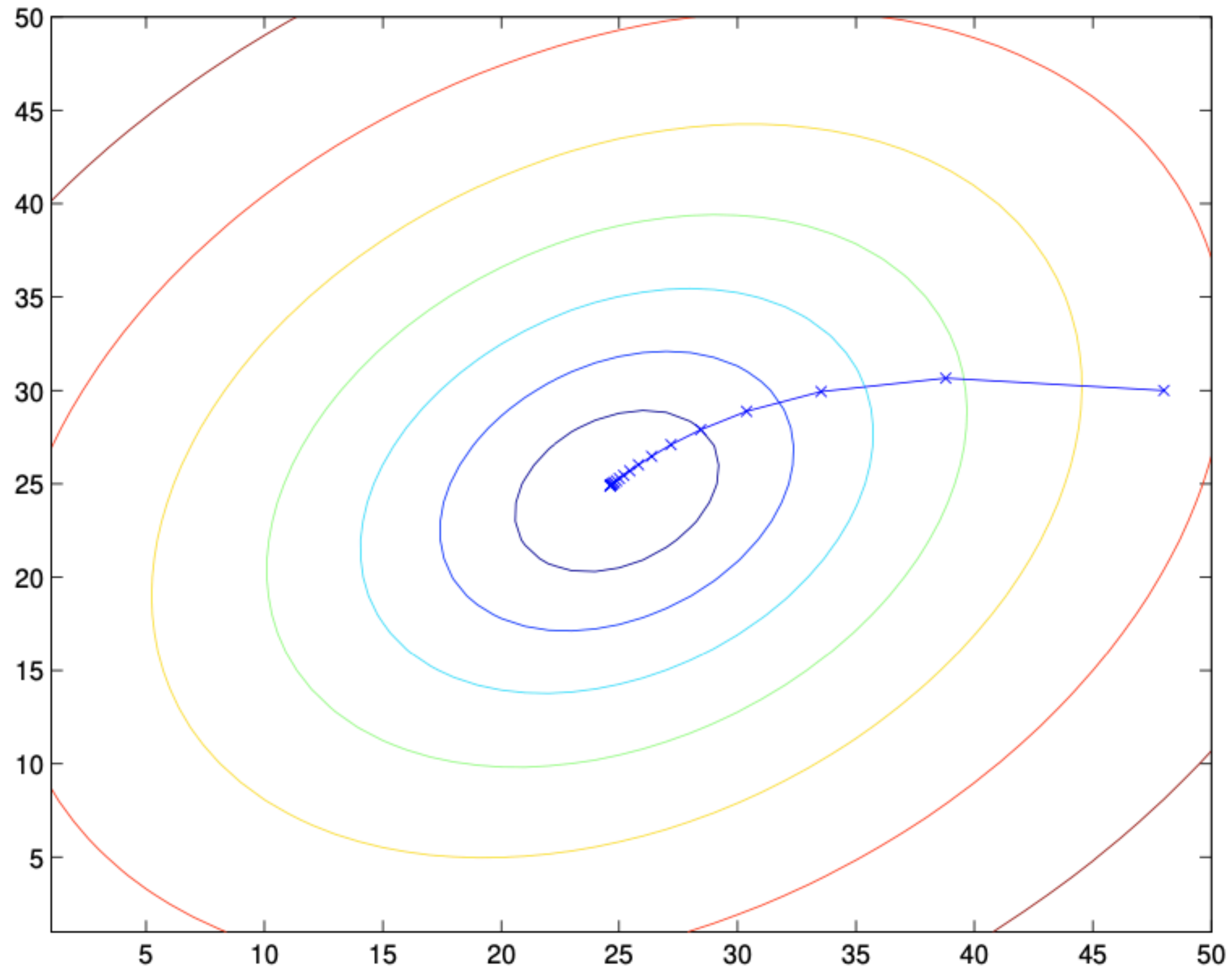
Local Minimum



For least square optimization, are we likely to get local minima rather than the global minima through gradient descent?

J is a convex quadratic function

There is only one local minima for J



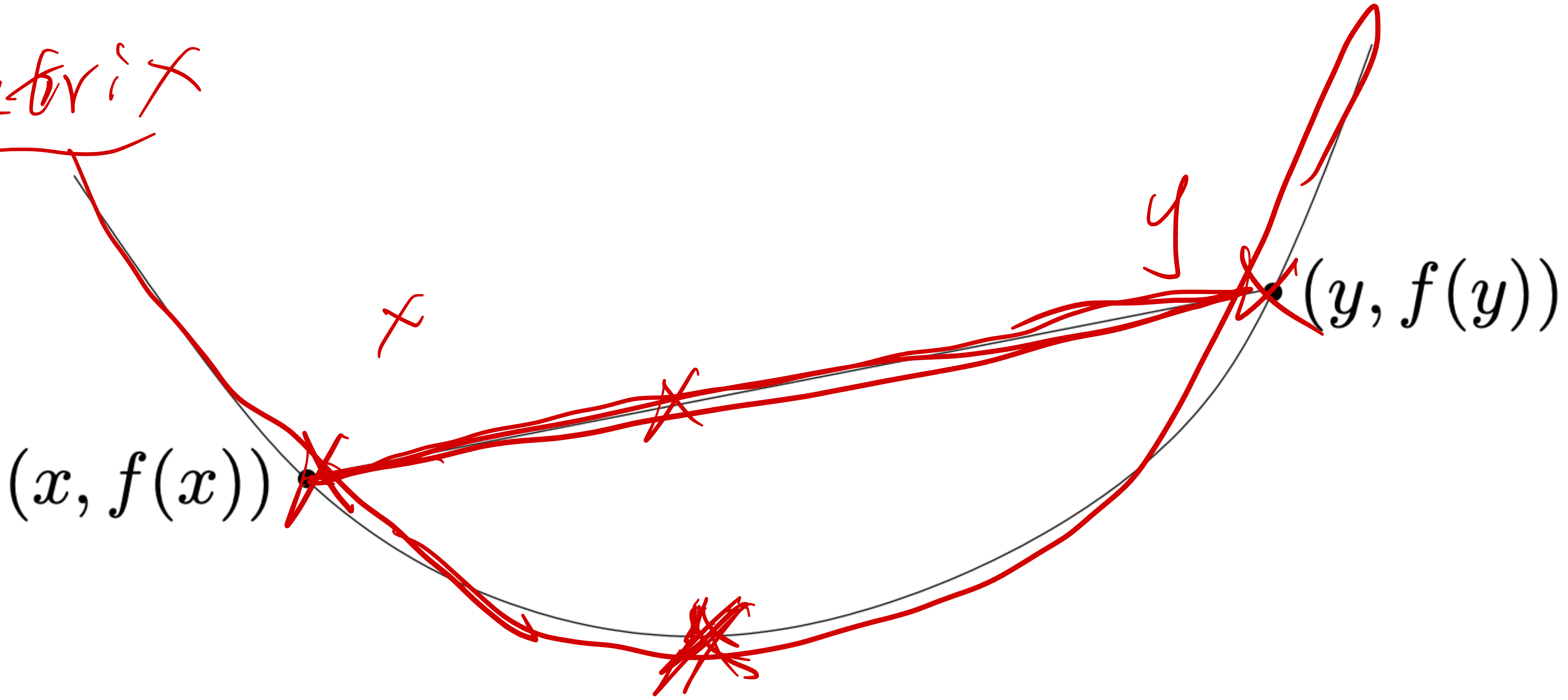
Evidence lower bound (ELBO)

Convex Function

Jensen inequality

$$f(tx + (1-t)y) \le tf(x) + (1-t)f(y) \quad \text{for } 0 \le t \le 1$$

Hessian matrix



$tx + (1-t)y$

$f(t_1 x_1 + t_3 x_3 + (1 - t_1 - \cdots - t_3) x_4) \le$

Thank You!
Q & A

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