CS 229 Lecture Two
Supervised Learning: Regression

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Disclaimers

- I'm trying a new format with slides (vs. whiteboard).
- The course notes maintained by Tengyu are your *best source*, the lecture is to give you the overall sense and highlight issues.
- The slides are new (copied from old hand-written notes), so apologies for any bugs. Please flag them!
- I'm worried that the lecture pacing will be too fast. Please slow me down with questions.
- I talk fast, please watch on slower speed.

Supervised Learning and Linear Regression

- Definitions
- Linear Regression
- Batch and Stochastic Gradient
- Normal Equations

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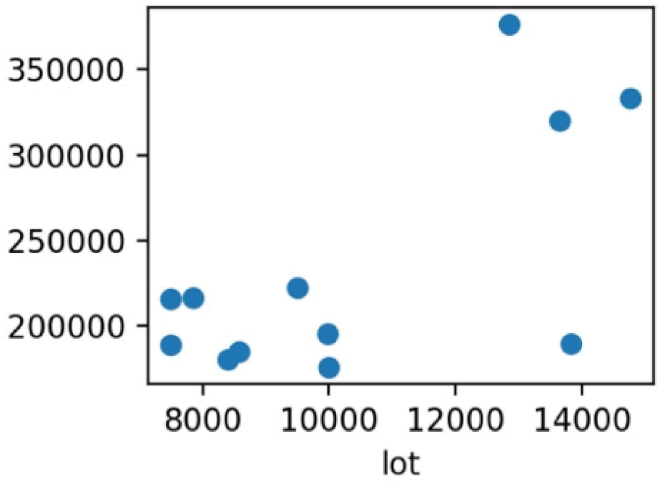
- If $\mathcal{Y}$ is continuous, then called a *regression problem*.
- If $\mathcal{Y}$ is discrete, then called a *classification problem*.

Our first example: Regression using Housing Data.

Example Data (Housing Prices from Ames Dataset from Kaggle)

	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



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An example prediction?

Notice the prediction is defined by the *parameters* θ_0 and θ_1. This is a huge reduction in the space of functions!

Simple Line Fit

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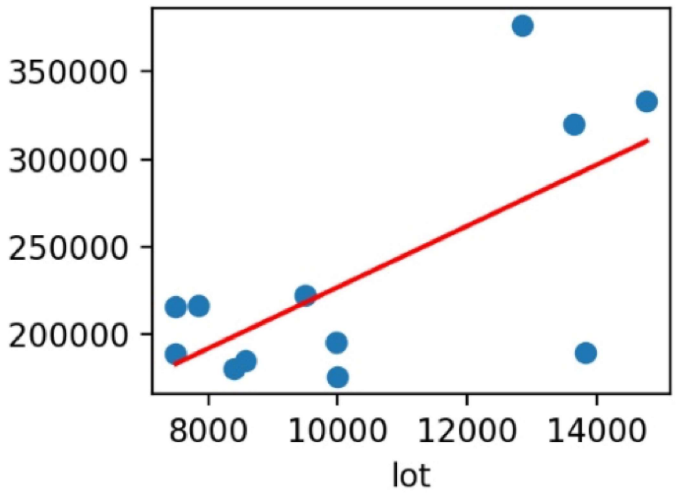

Slightly More Interesting Data

We add *features* (bedrooms and lot size) to incorporate more information about houses.

	size	bedrooms	lot size		Price
$x^{(1)}$	2104	4	45k	$y^{(1)}$	400
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$$h(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3.$$

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

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

Vector Notation for Prediction

	size	bedrooms	lot size		Price
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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.

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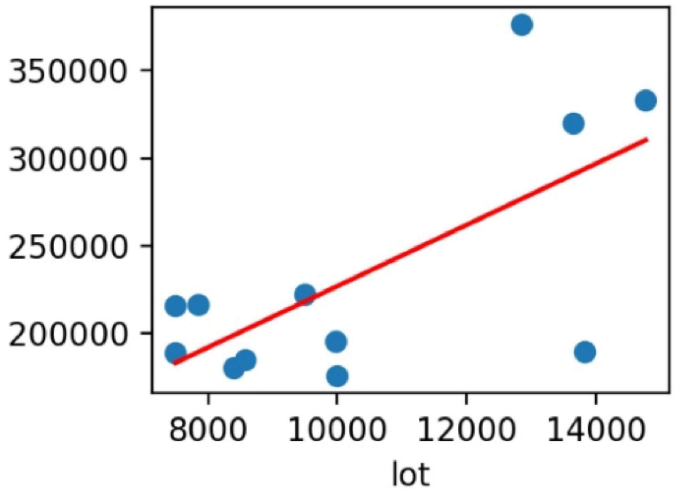
We have n examples (i.e., $i = 1, \ldots, n$). There are d features so $x^{(i)}$ and θ are $d + 1$ dimensional (since $x_0 = 1$)

Visual version of linear regression



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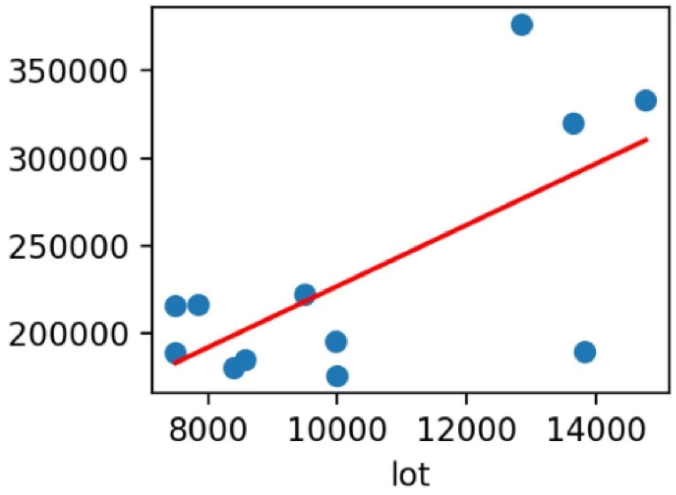

Let $h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j$ want to choose θ so that $h_\theta(x) \approx y$. One popular idea called **least squares**

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

Choose

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

Linear Regression Summary

- We saw our first hypothesis class *affine* or *linear* functions.
- We refreshed ourselves on notation and introduced terminology like **parameters**, **features**, etc.
- We saw this paradigm that a "good" hypothesis is some how one that *is close to* the data (objective function J).

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- Next, we'll see how to solve these equations.

Solving the least squares optimization problem.

Gradient Descent

$$\theta^{(0)} = 0$$

$$\theta_j^{(t+1)} = \theta_j^{(t)} - \alpha \frac{\partial}{\partial \theta_j} J(\theta^{(t)}) \qquad \text{for } j = 0, \ldots, d.$$

Gradient Descent Computation

$$\theta_j^{(t+1)} = \theta_j^{(t)} - \alpha \frac{\partial}{\partial \theta_j} J(\theta^{(t)}) \text{ for } j = 0, \ldots, d.$$

Note that α is called the **learning rate** or **step size**.

Let's compute the derivatives...

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta^{(t)}) &= \sum_{i=1}^{n} \frac{1}{2} \frac{\partial}{\partial \theta_j} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2 \\
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For our *particular* h_θ we have:

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We write this in *vector notation* for $j = 0, \ldots, d$ as:

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

Saves us a lot of writing! And easier to understand . . . eventually.

Batch Versus Stochastic Minibatch: Motivation

Consider our update rule:

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- In some modern applications (more later) n may be in the billions or trillions!
  - E.g., we try to "predict" every word on the web.
- **Idea** Sample a few points (maybe even just one!) to *approximate* the gradient called **Stochastic Gradient** (SGD).
  - SGD is the workhorse of modern ML, e.g., pytorch and tensorflow.

Stochastic Minibatch

- We randomly select a **batch** of $B \subseteq \{1, \ldots, n\}$ where $|B| < n$.
- We approximate the gradient using just those B points as follows (vs. gradient descent)

$$\frac{1}{|B|} \sum_{j \in B} \left(h_\theta(x^{(j)}) - y^{(j)} \right) x^{(j)} \text{ v.s. } \frac{1}{n} \sum_{j=1}^{n} \left(h_\theta(x^{(j)}) - y^{(j)} \right) x^{(j)}.$$

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- So our update rule for SGD is:

$$\theta^{(t+1)} = \theta^{(t)} - \alpha_B \sum_{j \in B} \left(h_\theta(x^{(j)}) - y^{(j)} \right) x^{(j)}.$$

- NB: scaling of $|B|$ versus n is "hidden" inside choice of α_B.

Stochastic Minibatch vs. Gradient Descent

- Recall our rule B points as follows:

$$\theta^{(t+1)} = \theta^{(t)} - \alpha_B \sum_{j \in B} \left(h_\theta(x^{(j)}) - y^{(j)} \right) x^{(j)}.$$

- If $|B| = \{1, \ldots, n\}$ (the whole set), then they coincide.
- Smaller B implies a lower quality approximation of the gradient (higher variance).
- Nevertheless, it may actually converge faster! (Case where the dataset has many copies of the same point–extreme, but lots of redundancy)

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- Smaller B implies a lower quality approximation of the gradient (higher variance).
- Nevertheless, it may actually converge faster! (Case where the dataset has many copies of the same point–extreme, but lots of redundancy)
- In practice, choose B proportional to what works well on modern parallel hardware (GPUs).

Summary of this Subsection of Optimization

- Our goal was to optimize a loss function to find a good predictor.
- We learned about gradient descent and the workhorse algorithm for ML, **Stochastic Gradient Descent** (SGD).
- We touched on the tradeoffs of choosing the right batch size.

Normal Equations

- Least squares with linear hypothesis is *really* special, we can solve it exactly (algebraically)!
  - We'll derive the *Normal Equations* for least squares.

Notation for Least Squares with Linear h_θ

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

Let's get some convenient notation

$$X = \begin{pmatrix} x^{(1)} \\ x^{(2)} \\ \vdots \\ x^{(n)} \end{pmatrix} \in \mathbb{R}^{n\times(d+1)} \text{ and } y = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{pmatrix} \in \mathbb{R}^n$$

We may call X the **Design Matrix**.

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With this notation for linear $h_\theta(x)$, matrix multiplication is evaluation of h_θ, that is

$$X\theta = \begin{pmatrix} h(x^{(1)}) \\ h(x^{(2)}) \\ \vdots \\ h(x^{(n)}) \end{pmatrix} \text{ and so } J(\theta) = \frac{1}{2}(X\theta - y)^T(X\theta - y)$$

Vector Derivatives

Recall that for a real-valued matrix function $f : \mathbb{R}^{n \times d} \to \mathbb{R}$, we mean

$$\nabla_A f(A) = \begin{pmatrix} \frac{\partial}{\partial_{a_{11}}} f(A) & \frac{\partial}{\partial_{a_{12}}} f(A) & \dots & \frac{\partial}{\partial_{a_{1d}}} f(A) \\ \frac{\partial}{\partial_{a_{21}}} f(A) & \frac{\partial}{\partial_{a_{22}}} f(A) & \dots & \frac{\partial}{\partial_{a_{2d}}} f(A) \\ \vdots & \vdots & & \vdots \\ \frac{\partial}{\partial_{a_{n1}}} f(A) & \frac{\partial}{\partial_{a_{n2}}} f(A) & \dots & \frac{\partial}{\partial_{a_{nd}}} f(A) \end{pmatrix}$$

Here $A \in \mathbb{R}^{n \times d}$.

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Here $A \in \mathbb{R}^{n \times d}$.

- With this notation, to find the minimum of $J(\theta)$ we compute $\nabla_\theta J(\theta) = 0$.
- Note that $\nabla_\theta J(\theta) \in \mathbb{R}^{d+1}$ since $\theta \in \mathbb{R}^{d+1}$.

The normal equation

From our previous derivation,

$$\nabla_\theta J(\theta) = \nabla_\theta \frac{1}{2}(X\theta - y)^T(X\theta - y).$$

multiplying out we have:

$$\nabla_\theta J(\theta) = X^T X\theta - X^T y.$$

Setting $\nabla_\theta J(\theta) = 0$, solving for θ assuming $(X^T X)^{-1}$ exists, we obtain:

$$\theta = \left(X^T X\right)^{-1} X^T y.$$

We have the optimal solution for θ!

Some slight cheating...

$$\theta = \left(X^T X\right)^{-1} X^T y.$$

- We've assumed $(X^T X)^{-1}$ exists. What happens if not? Is θ uniquely defined? Up to what?
- Why was $\nabla_\theta J(\theta) = 0$ a minimum? Notice that

$$\nabla_\theta^2 J(\theta) = \nabla_\theta \left(X^T X\theta - X^T y\right) = X^T X \succeq 0$$

  that is, it's second derivative is positive (semi)definite.
- We did some quick vector calculus, if this isn't familiar practice on Friday!

Summary from Today

- We saw a *lot of notation*
  - The TAs can help you practice on Friday!
- We learned about linear regression: the model, how to solve, and more.
- We learned the workhorse algorithm for ML called **SGD**.
- Next time: Classification!