Lecture Two
Supervised Learning: Regression

Adapted from
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Stanford ML

Supervised Learning and Linear Regression

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

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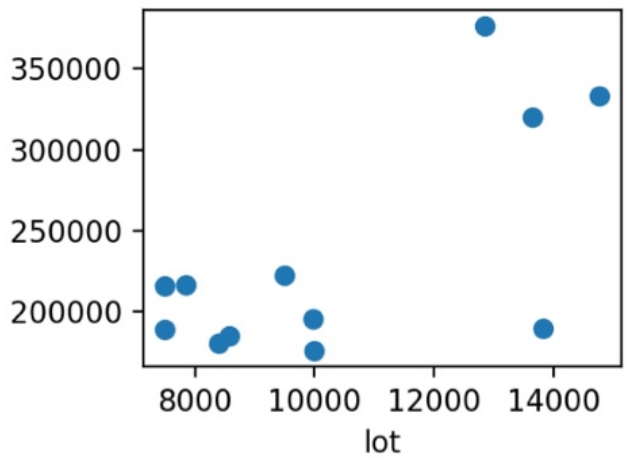
- If $\mathcal{Y}$ is continuous, then called a *regression problem*.
- If $\mathcal{Y}$ is discrete, then called a *classification problem*.

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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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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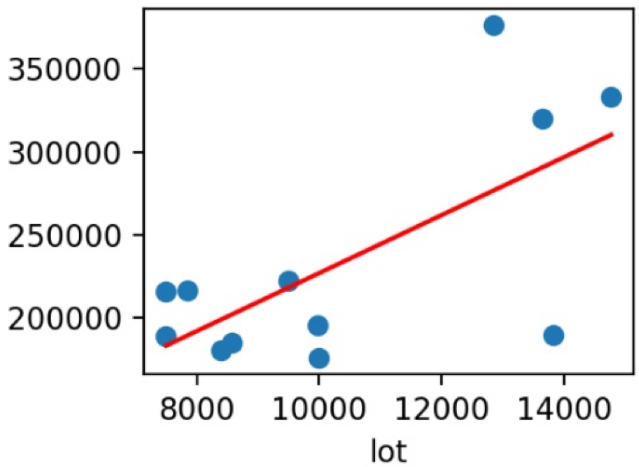

Slightly More Interesting Data

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

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

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

Vector Notation for Prediction

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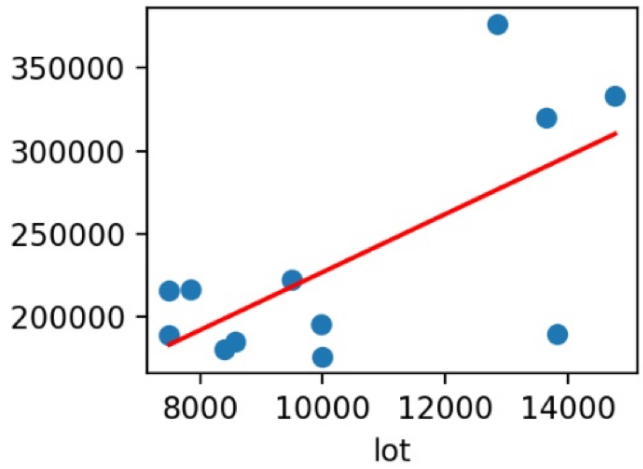
We have n examples (i.e., $i = 1, \ldots, n$). There are d features so $x^{(i)}$ and θ are $d + 1$ dimensional (since $x_0 = 1$)

Visual version of linear regression



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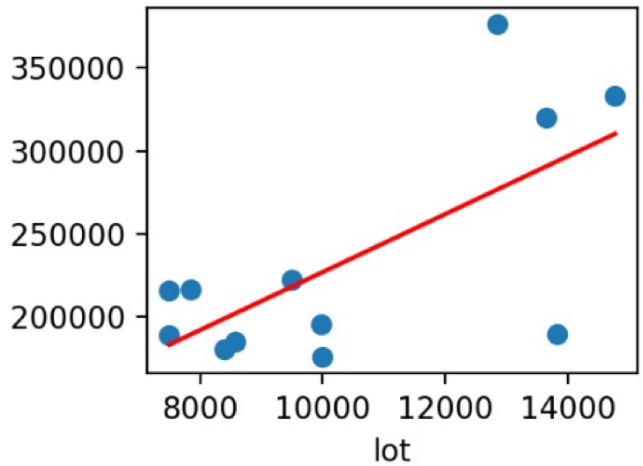

Let $h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j$ want to choose θ so that $h_\theta(x) \approx y$. One popular idea called **least squares**

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

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

$$h_\theta(x) = \theta_0 x_0 + \theta_1 x_1 + \cdots + \theta_d x_d \text{ so } \frac{\partial}{\partial \theta_j} h_\theta(x) = x_j$$

Gradient Descent Computation

Thus, our update rule for component j can be written:

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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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  - 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:

All minibatches are used for each iteration, or epoch and then start the next one

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

- 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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- 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.

Summary from Today

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