CMSC 478

KMA Solaiman

Supervised Learning: Linear Regression, Learning Algorithm and Gradient Descent

Slides are slightly adapted from Chris Re´, Stanford ML

Supervised Learning and Linear Regression

- Definitions
- Linear Regression
    - Learning Algorithm
    - Cost / Loss Function
    - Gradient Descent
- Batch and Stochastic Gradient

Supervised Learning

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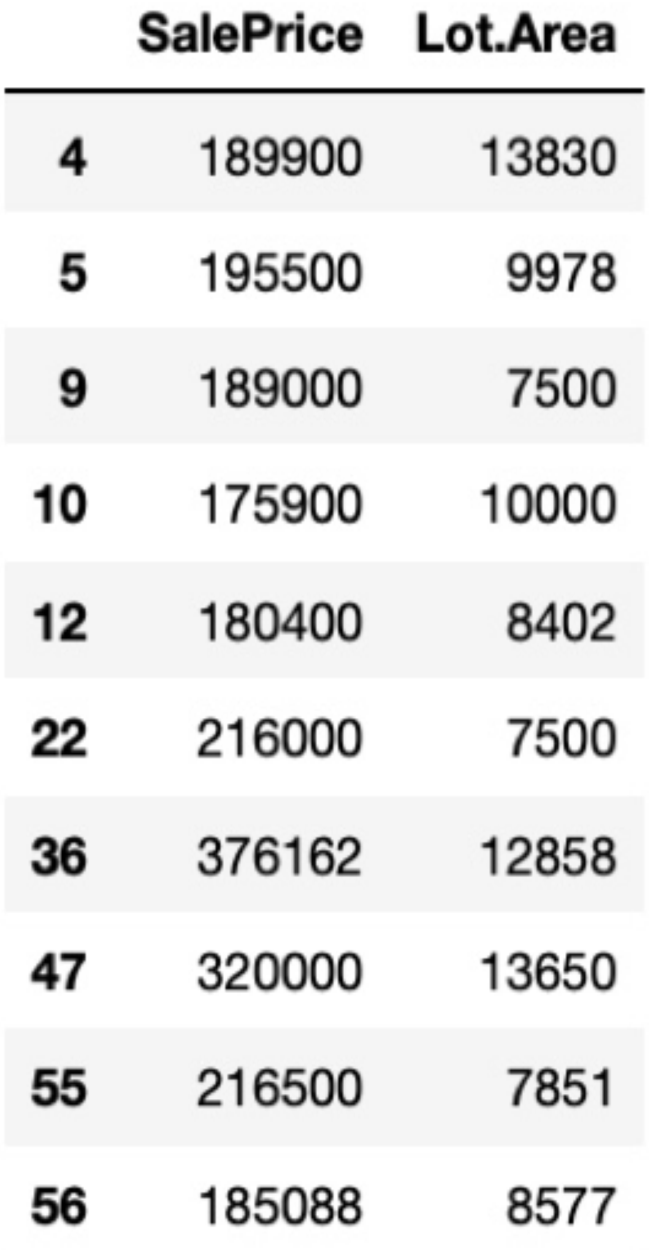
- If $\mathcal{Y}$ is continuous, then called a *regression problem*.
- If $\mathcal{Y}$ is discrete, then called a *classification problem*.

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
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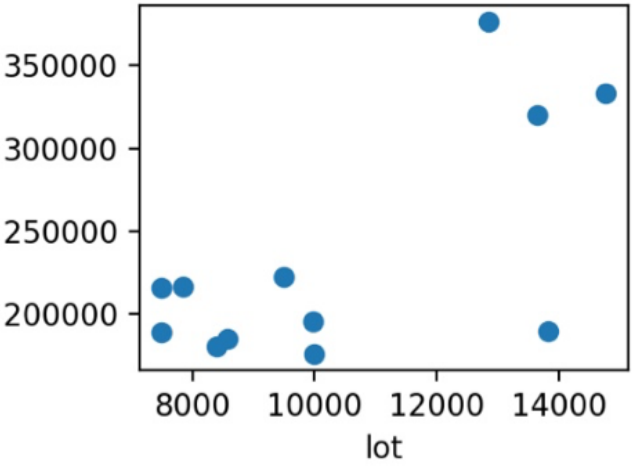

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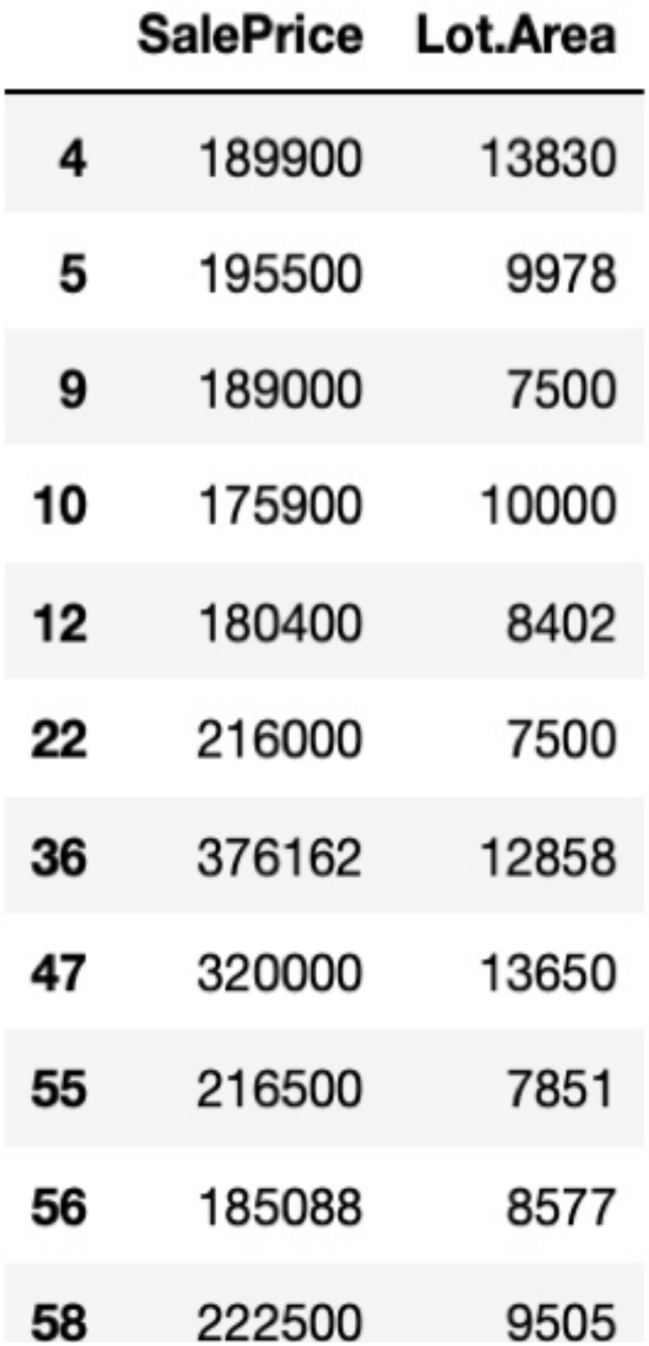
Notice the prediction is defined by the *parameters* θ_0 and θ_1. This is a huge reduction in the space of functions!

Simple Line Fit



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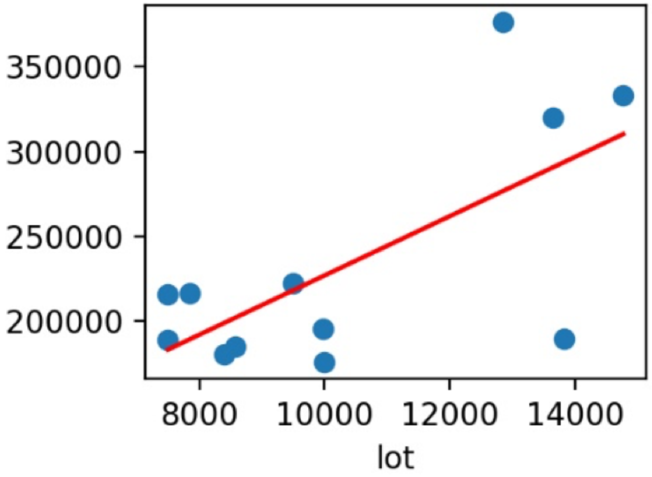

Slightly More Interesting Data

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

	size	bedrooms	lot size
$x^{(1)}$	2104	4	45k
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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

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

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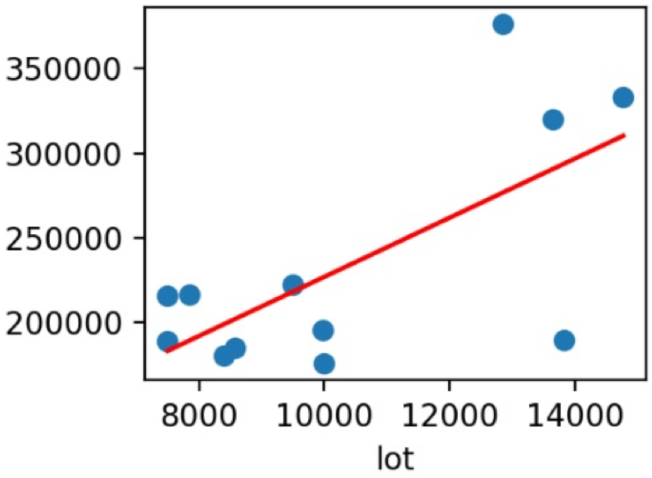
We have n examples (i.e., $i = 1, \ldots, n$). There are d features so $x^{(i)}$ and θ are $d + 1$ dimensional (since $x_0 = 1$)

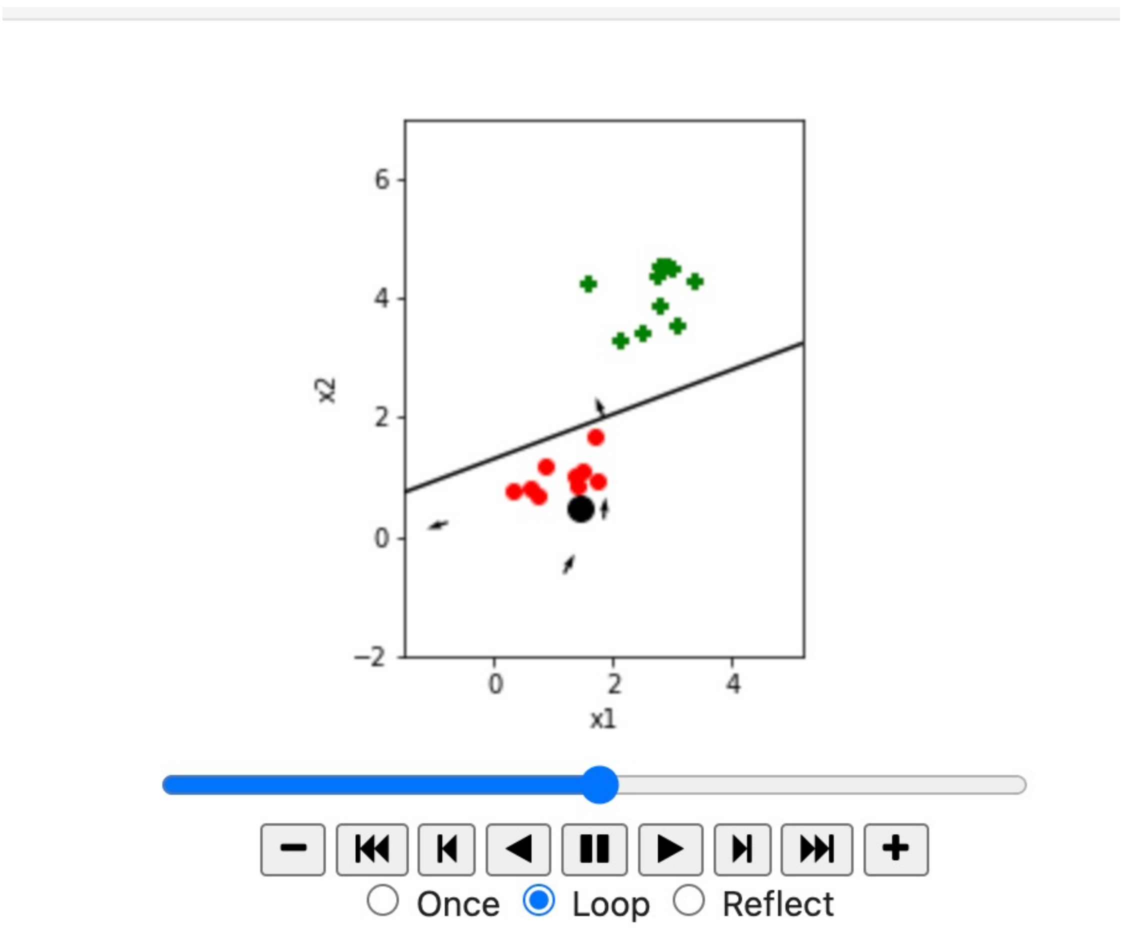
Visual version of linear regression



Let $h_\theta(x) = \sum_{j=0}^{d} \theta_j x_j$ want to choose θ so that $h_\theta(x) \approx y$.

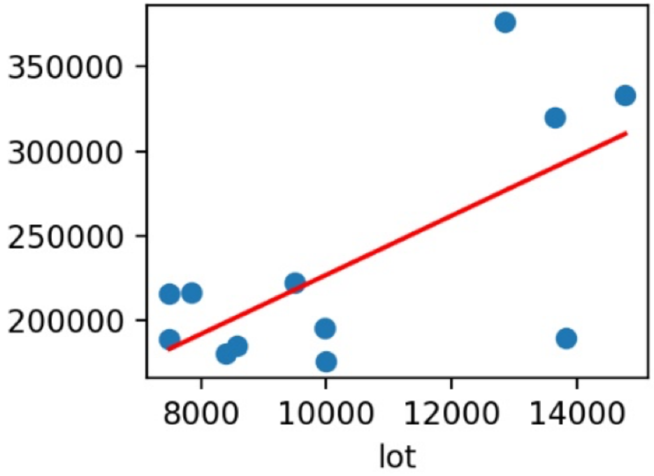
Fitting a good line

Animation



○ Once ● Loop ○ Reflect

Visual version of linear regression: Learning



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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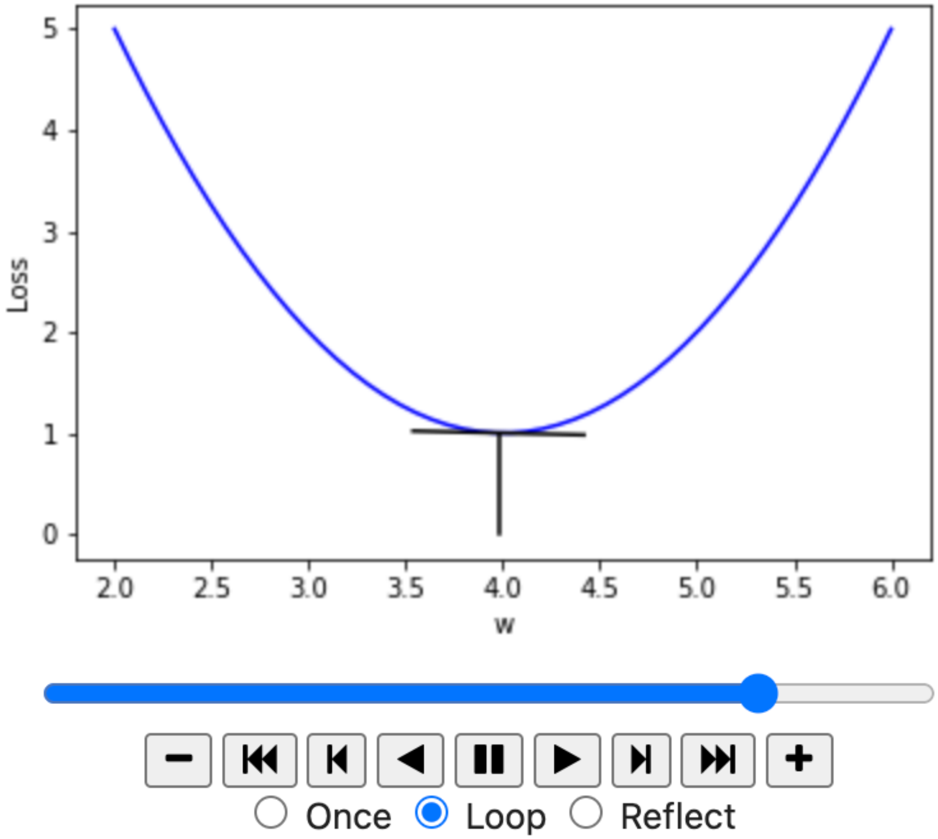
- We saw this paradigm that a “good” hypothesis is some how one that *is close to* the data (objective function J).
- Next, we’ll see how to solve these equations.

Solving the least squares optimization problem.

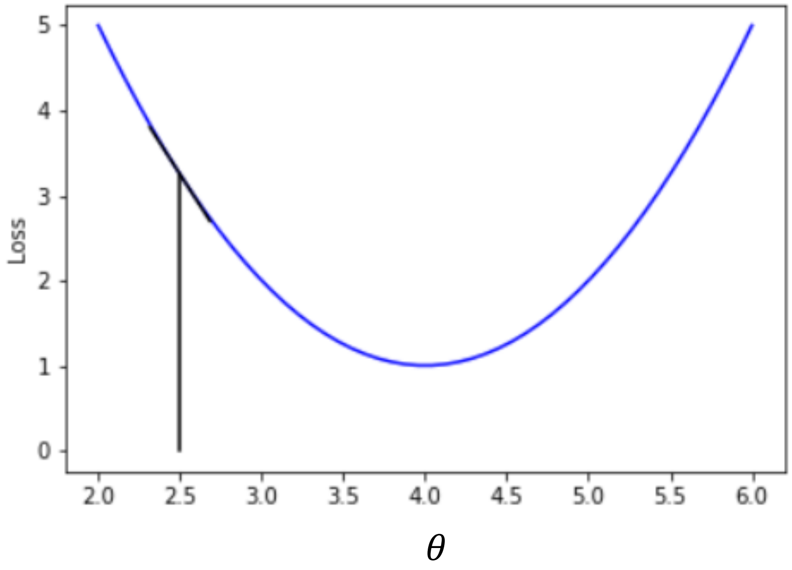
Gradient Descent

Animation



Gradient Descent

- $\mathcal{J}(\theta) = (\theta - 4)^2 + 1$
- Find the weight (value of θ) that minimizes the loss $\mathcal{J}$
- $\mathcal{J}'(\theta) = ?$
- θ = 2.5
- given the current value of w, adjusting θ by an amount that has the negative of the sign of $\mathcal{J}'(\theta)$ leads to a smaller value of $\mathcal{J}$.



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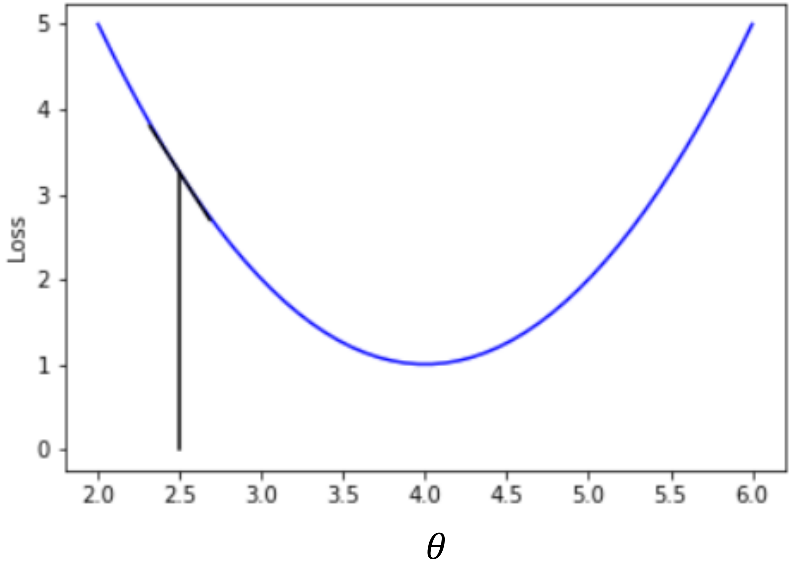

$\theta = \theta - \alpha * \mathcal{J}'(\theta)$

Gradient Descent

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

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...

$$\begin{aligned}\frac{\partial}{\partial \theta_j} J(\theta^{(t)}) &= \sum_{i=1}^{n} \frac{1}{2} \frac{\partial}{\partial \theta_j} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2 \\ &= \sum_{i=1}^{n} \left(h_\theta(x^{(i)}) - y^{(i)} \right) \frac{\partial}{\partial \theta_j} h_\theta(x^{(i)})\end{aligned}$$

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\end{aligned}$$

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:

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

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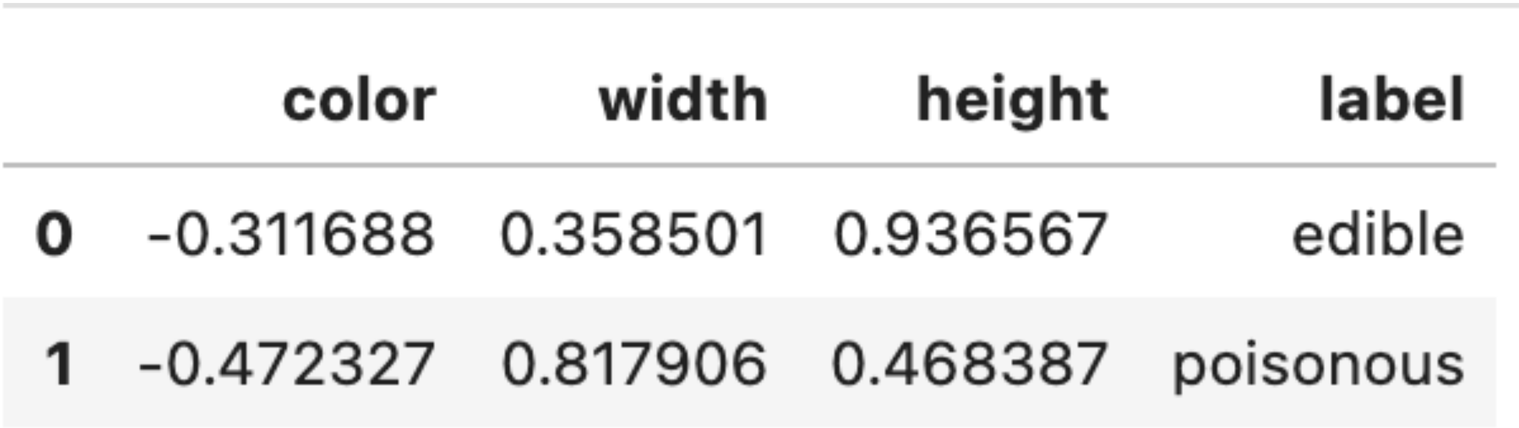
We write this in *vector notation* for $j = 0, \ldots, d$ as:

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

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

Linear Classification: Mushroom and Goats



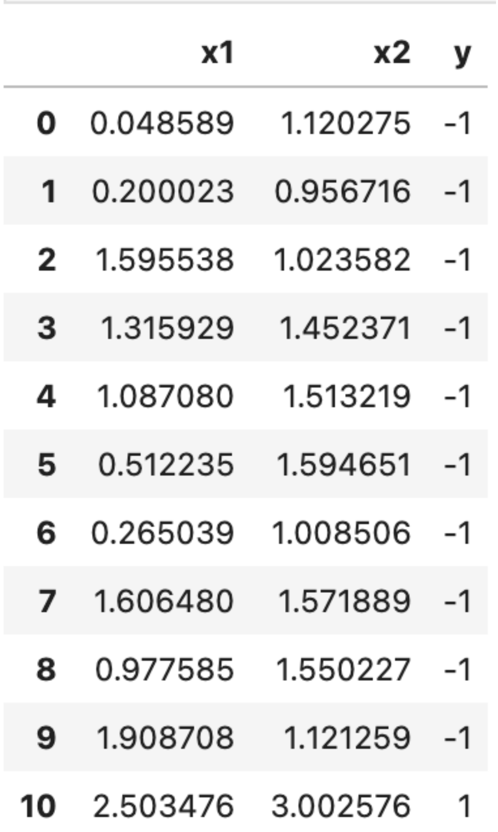
	color	width	height	label
0	-0.311688	0.358501	0.936567	edible
1	-0.472327	0.817906	0.468387	poisonous

$$\mathbf{sign}(w_c * \mathbf{color} + w_w * \mathbf{width} + w_h * \mathbf{height})$$

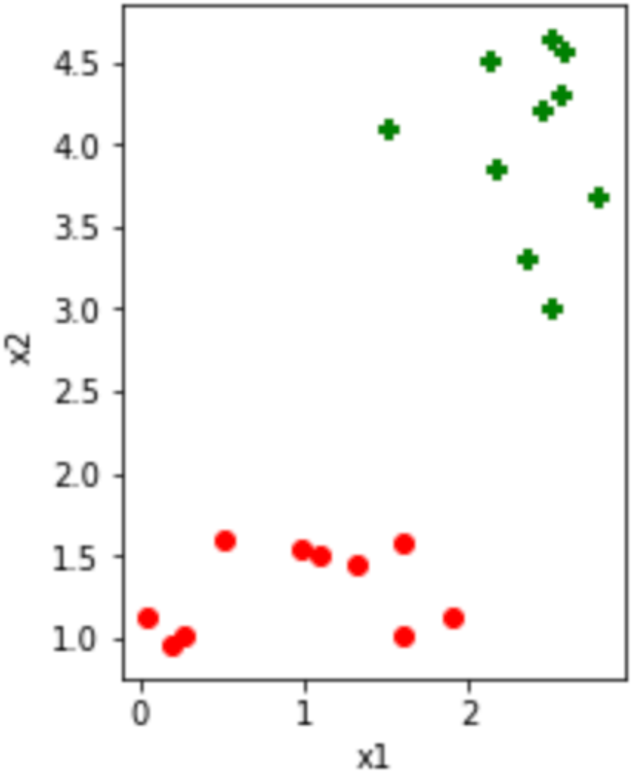
$$\mathbf{sign}(0 * -0.472327 + 1 * 0.817906 - 1 * 0.468387) = \mathbf{sign}(0.349519) = +1$$

$$\mathbf{sign}(0 * -0.311688 + 1 * 0.358501 - 1 * 0.936567) = \mathbf{sign}(-0.578066) = -1$$

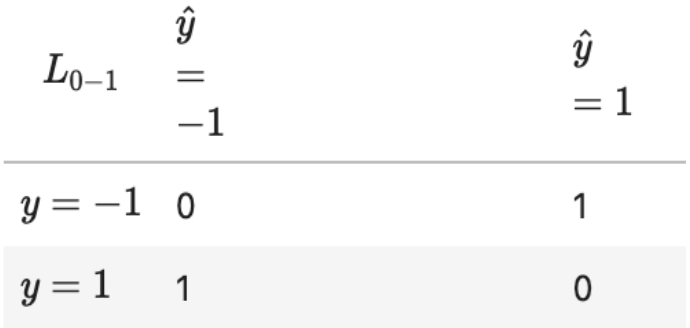
Linear Classification



	x1	x2	y
0	0.048589	1.120275	-1
1	0.200023	0.956716	-1
2	1.595538	1.023582	-1
3	1.315929	1.452371	-1
4	1.087080	1.513219	-1
5	0.512235	1.594651	-1
6	0.265039	1.008506	-1
7	1.606480	1.571889	-1
8	0.977585	1.550227	-1
9	1.908708	1.121259	-1
10	2.503476	3.002576	1



Loss Function for Classification: 0-1 Loss



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$y = -1$	0	1
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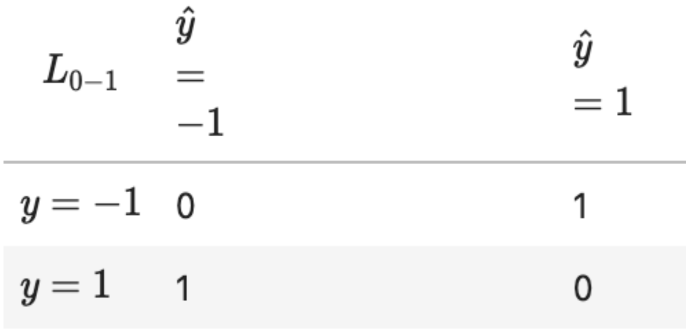

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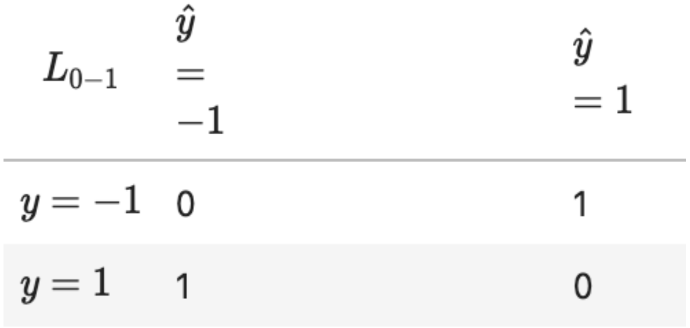

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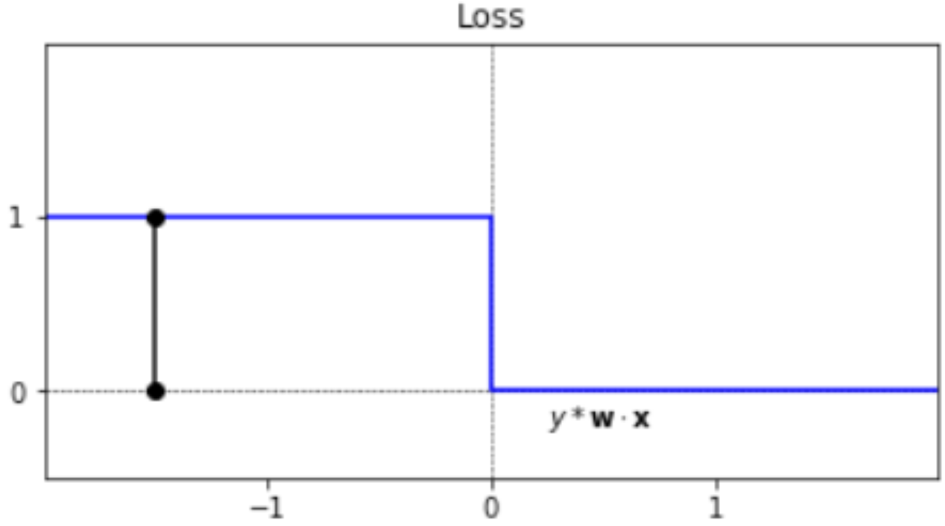

Batch Versus Stochastic Minibatch: Motivation

Consider our update rule:

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

- A single update, our rule examines *all* n data points.

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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 $B \subseteq \{1, \dots, n\}$ 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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- 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.

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!