S&DS 265 / 565 Introductory Machine Learning

# **Stochastic Gradient Descent**

September 19

## Goings on

- Assn 1 due today at midnight
- Assn 2 will be posted this evening
- Quiz 2 next Thursday

# **Outline for today**

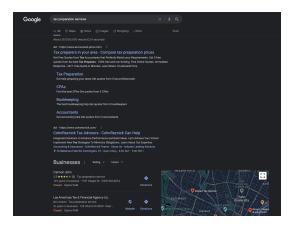
- Continue discussion of generative/discriminative
- Stochastic gradient descent
- Application to logistic regression
- Regularization
- Learning rate and scaling
- Jupyter notebook example

# Stochastic gradient descent

- Suppose that we want to fit a really big model, where the number of samples n and number of variables p are very large
- The classical algorithms in standard software packages will fail
- How can we train such models?

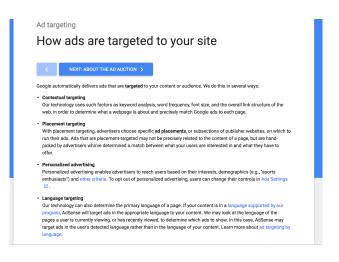
#### **Recall:Classification tasks**

 Ad click-through prediction. Predict whether or not a user will click on an ad presented. Used for ranking ads and setting prices.



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### **Example**

- We want to classify ads according to whether or not they will be clicked on by a user
- We have a very large collection of training data
- Ads are represented in terms of a sparse list of features

```
1 \mid 5 : 1.1789641e - 01 39 : 6.0373064e - 02 45 : 1.3163488e - 01
```

- The dataset is too large to load into memory, and the number of features is also very large
- New data are continually arriving
- How can we efficiently train a classifier?

## Online learning

#### We will introduce a method that

- Reads in the data points one (or a few) at a time
- Updates the model for each sample
- Exploits sparsity of the features
- Uses little memory, never reads in the entire dataset

# Stochastic gradient descent

Initialize all parameters to zero:  $\beta_j = 0, j = 1, ..., p$ .

Read through the data one record at a time, and update the model.

- Read data item x
- ② Make a prediction  $\hat{y}(x)$
- Observe the true response/label y
- **4** Update the parameters  $\beta$  so  $\hat{y}$  is closer to y

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# Stochastic gradient descent

To begin, suppose we are doing *linear regression*. We initialize all parameters to zero:  $\beta_j = 0, j = 1, ..., p$ .

We read through the data one record at a time, and update the model.

- Read data item x
- ② Make a prediction  $\hat{y}(x) = \sum_{j=1}^{p} \beta_j x_j$
- Observe the true response/label y
- **4** Update the parameters  $\beta$  so  $\hat{y}$  is closer to y

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#### Here's the idea:

- For each parameter  $\beta_j$ , see what happens to the loss if that parameter is increased a little bit.
- If the loss goes down (up), then increase (decrease)  $\beta_j$  proportionately
- Do this simultaneously for all of the parameters
- Rinse and repeat

Change  $\beta_i$  by a little bit:

$$\beta_j \to \beta_j + \varepsilon$$

What happens to the squared error?

$$\frac{1}{2}(y-\widehat{y})^{2} \to \frac{1}{2}(y-\widehat{y}-\varepsilon x_{j})^{2} 
\approx \frac{1}{2}(y-\widehat{y})^{2}-(y-\widehat{y})x_{j} \varepsilon 
= \frac{1}{2}(y-\widehat{y})^{2}+\underbrace{(\widehat{y}-y)x_{j}}_{q} \varepsilon$$

1:

We then change the parameter as follows:

$$\beta_{j} \to \beta_{j} - \eta g$$

$$= \beta_{j} - \eta \underbrace{(\widehat{y} - y)x_{j}}_{g}$$

$$= \beta_{j} + \eta (y - \widehat{y})x_{j}$$

with  $\eta > 0$  a small positive "step size".

1:

Why is this a good idea? With this choice of  $\varepsilon = -\eta g$  the squared error decreases:

$$\begin{aligned} \frac{1}{2}(y-\widehat{y})^2 &\to \frac{1}{2}(y-\widehat{y}-\varepsilon x_j)^2 \\ &\approx \frac{1}{2}(y-\widehat{y})^2 + \varepsilon g \\ &= \frac{1}{2}(y-\widehat{y})^2 - \eta g^2 \\ &< \frac{1}{2}(y-\widehat{y})^2 \end{aligned}$$

so we're moving "downhill"!

1:

# SGD for general loss

Suppose  $L(y, \beta^T x)$  is the loss for an input (x, y), e.g.,  $(y - \beta^T x)^2$ 

SGD update:

$$\beta_{j} \longleftarrow \beta_{j} - \eta \frac{\partial L(y, \boldsymbol{\beta}^{T} \boldsymbol{x})}{\partial \beta_{j}}$$
$$\boldsymbol{\beta} \longleftarrow \boldsymbol{\beta} - \eta \nabla_{\boldsymbol{\beta}} L(y, \boldsymbol{\beta}^{T} \boldsymbol{x}) \quad \text{(vector notation)}$$

- $\eta$  is the *learning rate* or "step size"
- Needs to be chosen carefully, getting smaller over time

# **Gradient descent for general loss**

If  $L(\beta)$  is the loss function over subset of training set:

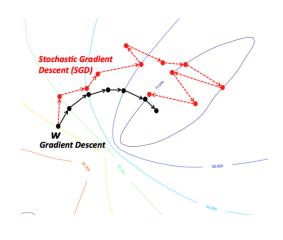
$$L(\beta + \eta \mathbf{v}) \approx L(\beta) + \eta \mathbf{v}^{\mathsf{T}} \nabla L(\beta)$$
$$L(\beta - \eta \nabla L(\beta)) \approx L(\beta) - \eta \|\nabla L(\beta)\|^{2}$$

This is why gradient descent is going downhill — if  $\eta$  is small enough.

"Batch" gradient descent uses the entire training set in each step of gradient descent.

Stochastic gradient descent computes a quick approximation to this gradient, using only a single or a small "mini-batch" of data points

# Batch vs. stochastic gradient descent



https://wikidocs.net/3413

SGD Update:

$$\beta_j \longleftarrow \beta_j + \eta(y - p(x))x_j$$

$$\beta_j x_j \longleftarrow \beta_j x_j + \eta (y - p(x)) x_j^2$$

$$p(x) = \frac{1}{1 + \exp(-\beta^T x)}$$

Case checking:

• Suppose y = 1 and probability p(x) is high?

SGD Update:

$$\beta_j \longleftarrow \beta_j + \eta(y - p(x))x_j$$

$$\beta_j x_j \longleftarrow \beta_j x_j + \eta (y - p(x)) x_j^2$$

$$p(x) = \frac{1}{1 + \exp(-\beta^T x)}$$

- Suppose y = 1 and probability p(x) is high? *small change*
- Suppose y = 1 and probability p(x) is small?

SGD Update:

$$\beta_j \longleftarrow \beta_j + \eta(y - p(x))x_j$$

$$\beta_j x_j \longleftarrow \beta_j x_j + \eta (y - p(x)) x_j^2$$

$$p(x) = \frac{1}{1 + \exp(-\beta^T x)}$$

- Suppose y = 1 and probability p(x) is high? *small change*
- Suppose y = 1 and probability p(x) is small? big change  $\uparrow$
- Suppose y = 0 and probability p(x) is small?

SGD Update:

$$\beta_j \longleftarrow \beta_j + \eta(y - p(x))x_j$$

$$\beta_j x_j \longleftarrow \beta_j x_j + \eta (y - p(x)) x_j^2$$

$$p(x) = \frac{1}{1 + \exp(-\beta^T x)}$$

- Suppose y = 1 and probability p(x) is high? *small change*
- Suppose y = 1 and probability p(x) is small? big change  $\uparrow$
- Suppose y = 0 and probability p(x) is small? *small change*
- Suppose y = 0 and probability p(x) is big?

#### SGD Update:

$$\beta_j \longleftarrow \beta_j + \eta(y - p(x))x_j$$

$$\beta_j x_j \longleftarrow \beta_j x_j + \eta (y - p(x)) x_j^2$$

$$p(x) = \frac{1}{1 + \exp(-\beta^T x)}$$

- Suppose y = 1 and probability p(x) is high? small change
- Suppose y = 1 and probability p(x) is small? big change  $\uparrow$
- Suppose y = 0 and probability p(x) is small? *small change*
- Suppose y = 0 and probability p(x) is big? big change  $\downarrow$

### SGD: choice of step size

In theory, we need to let the step size  $\eta$  decrease as the algorithm progresses.

This prevents the estimates from oscillating back and forth without converging.

### **Demo**

Open the demo notebook sgd.ipynb and follow along...

### SGD: Scaling

We generally want to "standardize" each variable — subtract out the mean and divide by the standard deviation

$$x_j \leftarrow \frac{x_j - \mathsf{mean}(x_j)}{\sqrt{\mathsf{var}(x_j)}}$$

But this involves "looking ahead" to compute the mean and variance, and destroys the online property of the algorithm

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### **SGD: Scaling**

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But this involves "looking ahead" to compute the mean and variance, and destroys the online property of the algorithm

Solution: The mean and variance can be updated in an online manner, in constant time, by storing auxiliary variables for each component j.

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### **SGD: Regularization**

A "ridge" penalty  $\frac{1}{2}\lambda \sum_{i=1}^{p} \beta_i^2$  is easily handled.

Gradient changes by an additive term  $\lambda\beta$ . Update becomes

$$\beta_j \leftarrow \beta_j + \eta \{ (y - p(x))x_j - \lambda \beta_j \}$$

$$= (1 - \eta \lambda)\beta_j + \eta (y - p(x))x_j$$

Observe that this "does the right thing" whether  $\beta_j$  wants to be large positive or negative.

• The penalty shrinks  $\beta_i$  toward zero

### What did we learn today?

- Stochastic gradient descent is a simple algorithm that can be applied to large classification and regression problems
- A parameter is updated according to how much the loss changes when that parameter is changed by a little bit
- This is the "go to" algorithm for fitting large or complex machine learning models
- Choosing the learning rate is a little tricky