S&DS 265 / 565 Introductory Machine Learning

Stochastic Gradient Descent

September 22

Goings on

- Assn 1 due next week visit us in OH!
- Assn 2 will be posted by same time
- Quiz 2 available on Canvas at 10:30am this morning
- Due in 48 hours; 20 mins once started

Outline for today

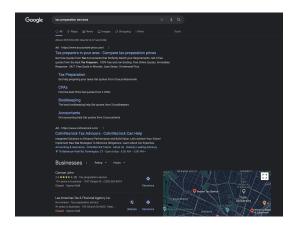
- Stochastic gradient descent
- Application to logistic regression
- Regularization
- Learning rate and scaling
- Jupyter notebook example

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?

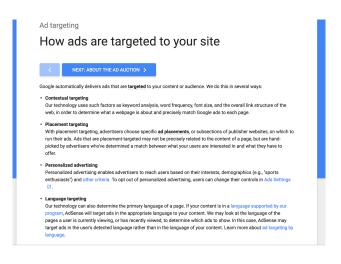
Recall:Classification tasks

 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: 1.1789641 e - 01 \quad 39: 6.0373064 e - 02 \quad 45: 1.3163488 e - 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 β 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 β so \hat{y} is closer to y

Here's the idea:

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

Change β_i by a little bit:

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

What happens to the squared error?

$$(y - \widehat{y})^{2} \to (y - \widehat{y} - \varepsilon x_{j})^{2}$$

$$\approx (y - \widehat{y})^{2} - 2(y - \widehat{y})x_{j} \varepsilon$$

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

1:

We then change the parameter as follows:

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

$$= \beta_{j} - \eta (\underbrace{-2(y - \widehat{y})x_{j}}_{g})$$

$$= \beta_{j} + \eta 2(y - \widehat{y})x_{j}$$

with η a small number. So, we taking

$$\varepsilon = \eta 2(y - \widehat{y})x_j = -\eta g$$

1:

Why is this a good idea? With this choice of ε the squared error decreases:

$$(y - \widehat{y})^{2} \rightarrow (y - \widehat{y} - \varepsilon x_{j})^{2}$$

$$\approx (y - \widehat{y})^{2} - 2(y - \widehat{y})\varepsilon x_{j}$$

$$= (y - \widehat{y})^{2} - 4\eta(y - \widehat{y})^{2}x_{j}^{2}$$

$$= (y - \widehat{y})^{2} - \eta g^{2}$$

$$< (y - \widehat{y})^{2}$$

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:

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

- η 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:

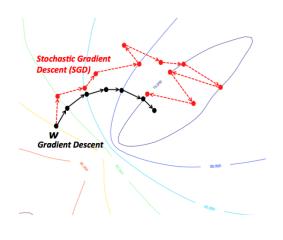
$$L(\beta + \eta \mathbf{v}) \approx L(\beta) + \eta \mathbf{v}^{\mathsf{T}} \nabla L(\beta)$$
$$L(\beta - \eta \nabla L(\beta)) \approx L(\beta) - \eta \|\nabla L(\beta)\|^{2}$$

This is why gradient descent is going downhill — if η 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:

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

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

- 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 learning rate

A conservative choice of learning rate is

$$\eta_t = \frac{1}{t}$$

A more agressive choice is

$$\eta_t = \frac{1}{\sqrt{t}}$$

In practice: Try learning rates C/\sqrt{t} for different choices of C, and monitor the error

$$\frac{1}{T}\sum_{t=1}^{T}(Y_t-\widehat{Y}_t)^2$$

Demo

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

SGD: choice of learning rate

Learning rate should scale as

$$\eta_t = \frac{1}{\sqrt{t}}$$

Problem: Some of the updates may be on different scales.

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SGD: choice of learning rate

Learning rate should scale as

$$\eta_t = \frac{1}{\sqrt{t}}$$

Problem: Some of the updates may be on different scales.

Solution: Let
$$g_{tj} = \frac{\partial L(y_t, \beta^T x_t)}{\partial \beta_j}$$

Scale gradients to get update rule

$$\beta_j \longleftarrow \beta_j - \eta \frac{g_{tj}}{\sqrt{\sum_{s=1}^t g_{sj}^2}}$$

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SGD: scaling issues

For a linear model, the SGD update is

$$\beta_j \longleftarrow \beta_j - C_t x_j$$

If x_j increases by a factor of two, the parameter β_j should decrease by a factor of two.

This update doesn't respect that scaling

SGD: scaling issues

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

SGD: Regularization

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

Gradient changes by an additive term $2\lambda\beta$. Update becomes

$$\beta_j \leftarrow \beta_j + \eta \{ (y - p(x))x_j - 2\lambda \beta_j \}$$

$$= (1 - 2\eta \lambda)\beta_j + \eta (y - p(x))x_j$$

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

• The penalty shrinks β_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