Machine Learning 2 DS 4420 - Spring 2020

Neural Networks & backprop Byron C Wallace



• In 2020, neural networks are the dominant technology in machine learning (for better or worse)!

- In 2020, neural networks are the dominant technology in machine learning (for better or worse)!
- Today, we'll go over some of the fundamentals of NNs and modern libraries (we saw a preview last week, with auto-diff)!

- In 2020, neural networks are the dominant technology in machine learning (for better or worse)!
- Today, we'll go over some of the fundamentals of NNs and modern libraries (we saw a preview last week, with auto-diff)!
- This will also serve as a refresher on gradient descent

Gradient Descent in Linear Models

Last time we thought in **probabilistic terms** and discussed **maximum likelihood estimation** for "generative" models

Gradient Descent in Linear Models

Last time we thought in **probabilistic terms** and discussed **maximum likelihood estimation** for "generative" models

Today we'll take the view of learning as **search/ optimization**

Gradient Descent in Linear Models

Last time we thought in **probabilistic terms** and discussed **maximum likelihood estimation** for "generative" models

Today we'll take the view of learning as **search/ optimization**

We'll start with linear models, review **gradient descent**, and then talk about **neural nets** + **backprop**



The simplest loss is probably 0/1 loss: 0 if we're correct 1 if we're wrong

What's an algo that minimizes this?

The **Perceptron**!

Consider a simple linear model with parameters w

$$\hat{y}_i = \begin{cases} 1 & \text{if } |w \cdot x_i| > 0 \\ -1 & \text{otherwise} \end{cases}$$

Consider a simple linear model with parameters w

$$\hat{y}_i = \begin{cases} 1 & \text{if } | w \cdot x_i > 0 \\ -1 & \text{otherwise} \end{cases}$$
 (assumes bias term moved into x or omitted)

Consider a simple linear model with parameters w

$$\hat{g}_i = \begin{cases} 1 & \text{if } [w \cdot x_i > o] \\ -1 & \text{otherwise} \end{cases}$$
 (assumes bias term moved into x or omitted)

The learning problem is to estimate w

Consider a simple linear model with parameters w

$$\hat{y}_i = \begin{cases} 1 & \text{if } (w \cdot x_i > 0) \\ -1 & \text{otherwise} \end{cases}$$
 (assumes bias term moved into x or omitted)

The learning problem is to estimate *w* What is our criterion for a good *w*? Minimal **loss**



Perceptron!



Algorithm 5 PERCEPTRONTRAIN(D, MaxIter)	
$w_d \leftarrow o, \text{ for all } d = 1 \dots D$	// initialize weights
$_{2:} b \leftarrow o$	// initialize bias
$_{3:}$ for iter = 1 MaxIter do	
4: for all $(x,y) \in \mathbf{D}$ do	
$_{5:} \qquad a \leftarrow \sum_{d=1}^{D} w_d x_d + b$	// compute activation for this example
6: if $ya \le o$ then	
$w_d \leftarrow w_d + yx_d$, for all $d = 1$. D // update weights
$b \leftarrow b + y$	// update bias
9: end if	
10: end for	
III: end for	
12: return w_0, w_1, \ldots, w_D, b	

Fig and Alg from CIML [Daume]



Problems with 0/1 loss

- If we're wrong by .0001 it is "as bad" as being wrong by .9999
- Because it is discrete, optimization is hard if the instances are not linearly separable



Smooth loss

Idea: Introduce a "smooth" loss function to make optimization easier Example: Hinge loss





Zero/one: Hinge: Logistic:

Exponential:

Squared:

 $\ell^{(\mathsf{hin})}(y,\hat{y}) = \max\{0, 1 - y\hat{y}\}$ $\ell^{(\log)}(y,\hat{y}) = \frac{1}{\log 2}\log\left(1 + \exp[-y\hat{y}]\right)$ $\ell^{(\exp)}(y,\hat{y}) = \exp[-y\hat{y}]$

Fig and Eq's from CIML [Daume]

Regularization

 $\min_{w,b} \sum_{n} \ell(y_n, w \cdot x_n + b)$

Regularization

$$\min_{w,b} \sum_{n} \ell(y_n, w \cdot x_n + b) + \lambda R(w, b)$$
Prevent *w* from "getting to crazy"

Gradient descent



By Gradient_descent.png: The original uploader was Olegalexandrov at English Wikipedia.derivative work: Zerodamage - This file was derived from: Gradient descent.png:, Public Domain, https://commons.wikimedia.org/w/index.php?curid=20569355

Algorithm 21 GradientDescent($\mathcal{F}, K, \eta_1, ...$)

- 1: $z^{(0)} \leftarrow \langle 0, 0, \ldots, 0 \rangle$
- 2: for $k = 1 \dots K$ do
- 3: $g^{(k)} \leftarrow \nabla_z \mathcal{F}|_{z^{(k-1)}}$ 4: $z^{(k)} \leftarrow z^{(k-1)} - \eta^{(k)} g^{(k)}$
- 5: end for
- 6: return $z^{(K)}$

// initialize variable we are optimizing

// compute gradient at current location
// take a step down the gradient

Alg from CIML [Daume]

$$\nabla_{w}\mathcal{L} = \nabla_{w}\sum_{n} \exp\left[-y_{n}(w \cdot x_{n}+b)\right] + \nabla_{w}\frac{\lambda}{2}||w||^{2}$$

$$\nabla_{\boldsymbol{w}} \mathcal{L} = \nabla_{\boldsymbol{w}} \sum_{n} \exp\left[-y_{n}(\boldsymbol{w} \cdot \boldsymbol{x}_{n} + b)\right] + \nabla_{\boldsymbol{w}} \frac{\lambda}{2} ||\boldsymbol{w}||^{2}$$
$$= \sum_{n} \left(\nabla_{\boldsymbol{w}} - y_{n}(\boldsymbol{w} \cdot \boldsymbol{x}_{n} + b)\right) \exp\left[-y_{n}(\boldsymbol{w} \cdot \boldsymbol{x}_{n} + b)\right] + \lambda \boldsymbol{w}$$

$$\nabla_{\boldsymbol{w}} \mathcal{L} = \nabla_{\boldsymbol{w}} \sum_{n} \exp\left[-y_{n}(\boldsymbol{w} \cdot \boldsymbol{x}_{n} + b)\right] + \nabla_{\boldsymbol{w}} \frac{\lambda}{2} ||\boldsymbol{w}||^{2}$$
$$= \sum_{n} \left(\nabla_{\boldsymbol{w}} - y_{n}(\boldsymbol{w} \cdot \boldsymbol{x}_{n} + b)\right) \exp\left[-y_{n}(\boldsymbol{w} \cdot \boldsymbol{x}_{n} + b)\right] + \lambda \boldsymbol{w}$$

$$= -\sum_{n} y_{n} x_{n} \exp\left[-y_{n}(\boldsymbol{w} \cdot \boldsymbol{x}_{n} + b)\right] + \lambda \boldsymbol{w}$$

Limitations of linear models

Idea: Basically stack together a bunch of linear models.

This introduces *hidden units* which are neither observations (x) nor outputs (y)



Idea: Basically stack together a bunch of linear models.

This introduces *hidden units* which are neither observations (x) nor outputs (y)



Idea: Basically stack together a bunch of linear models.

This introduces *hidden units* which are neither observations (x) nor outputs (y)



The challenge: How do we update weights associated with each node in this *multi-layer* regime?

back-propagation = gradient descent + chain rule

Algorithm 27 FORWARD**PROPAGATION**(x)

- 1: for all input nodes *u* do
- 2: $h_u \leftarrow$ corresponding feature of x
- 3: end for
- $_{4:}$ for all nodes v in the network whose parent's are computed **do**

5:
$$a_v \leftarrow \sum_{u \in par(v)} w_{(u,v)} h_u$$

- 6: $h_v \leftarrow \tanh(a_v)$
- $_{7:}$ end for
- 8: return a_y

Tanh is another common activation function







Algorithm 28 BACKPROPAGATION(x, y)

- ¹: run ForwardPropagation(*x*) to compute activations
- 2: $e_y \leftarrow y a_y$ // compute overall network error
- $_{3:}$ for all nodes v in the network whose error e_v is computed **do**
- 4: for all $u \in par(v)$ do
- 5: $g_{u,v} \leftarrow -e_v h_u$

- // compute gradient of this edge
- 6: $e_u \leftarrow e_u + e_v w_{u,v} (1 \tanh^2(a_u))$ // compute the "error" of the parent node
- 7: end for
- 8: end for
- 9: **return** all gradients g_e





What are we doing with these gradients again?

Gradient descent



By Gradient_descent.png: The original uploader was Olegalexandrov at English Wikipedia.derivative work: Zerodamage - This file was derived from: Gradient descent.png:, Public Domain, https://commons.wikimedia.org/w/index.php?curid=20569355

If you're interested in learning more...

DS4440 // practical neural networks // spring 2019