

## UiO : Department of Informatics

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INF 5860 Machine learning for image classification
Repetition of Annes lectures

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## The linear regression problem, summary

Hypothesis: $\quad h(\theta)=\hat{y}=\theta^{T} x$
Parameters: $\quad \theta^{j}, j=0 . . n$
Cost function: $J\left(\theta^{0}\right)=\frac{1}{2 m} \sum_{i=1}^{m}\left(\hat{y}_{i}-y_{i}\right)^{2}$
Goal: minimize $J(\theta)$
Gradient descent solution: repeat until convergence
for $\mathrm{j}=0$ : n

$$
\theta^{j}=\theta^{j}-\varepsilon \frac{\partial}{\partial \theta^{j}} J\left(\theta_{1}, \theta_{2}\right)
$$

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## Logistic regression model

- Want $0 \leq h_{\theta}(x) \leq 1$
- Let

$$
\begin{aligned}
& h_{\theta}(X)=g\left(\theta^{T} x\right) \\
& g(z)=\frac{1}{1+e^{-z}} \\
& h_{\theta}(X)=\frac{1}{1+e^{-\theta^{T} x}}
\end{aligned}
$$



- This is called the sigmoid function


## Decisions for logistic regression

- Decide $y=1$ if $h_{\theta}(x)>$ 0.5 , and $\mathrm{y}=0$ otherwise

$$
\begin{aligned}
& h_{\theta}(X)=g\left(\theta^{T} x\right) \\
& g(z)=\frac{1}{1+e^{-z}} \\
& h_{\theta}(X)=\frac{1}{1+e^{-\theta^{T} x}}
\end{aligned}
$$

- $g(z)>0.5$ if $z>0$

$$
\begin{gathered}
-\quad \theta^{\top} x>0 \\
g(z)<0.5 \text { if } z<0 \\
\theta^{\top} x<0
\end{gathered}
$$

$\theta^{\top} x=0$ gives the decision boundary

## Logistic regression cost

Minimize

$$
J(\theta)=\frac{1}{2 m} \sum_{i=1}^{m}\left(\operatorname{Cost}\left(h_{\theta}\left(x_{i}\right), y_{i}\right)\right)
$$

Due to the sigmoid function $g(z)$, this is a non-quadratic function, and non-convex.
Set

$$
\operatorname{Cost}\left(h_{\theta}(x), y\right)=\left\{\begin{array}{c}
-\log \left(h_{\theta}(x)\right) \text { if } \mathrm{y}=1 \\
-\log \left(1-h_{\theta}(x)\right) \text { if } \mathrm{y}=0
\end{array}\right.
$$

$$
\begin{array}{ll}
\text { Cost }=0 \text { if } \mathrm{y}=1 \text { and } h_{\theta}(x)=1 & \text { We skip deriving this cost, } \\
\text { If } \mathrm{y}=1 \text { and } h_{\theta}(x) \rightarrow 0: \text { Cost } \rightarrow \infty & \text { it is derived by maximizing the } \\
\text { log-likelihood that } \theta \text { fits the data }
\end{array}
$$

Cost $=0$ if $\mathrm{y}=0$ and $h_{\theta}(x)=0$
If $y=0$ and $h_{\theta}(x) \rightarrow 1$ : Cost $\rightarrow \infty$
Mimick a probability

## From 2 to multiple classes: Softmax

- The common generalization to multiple clasess is the softmax classifier.
- We want to predict the class label $y_{i}=\{1, \ldots C\}$ for sample $X(i,:), y$ can take one of $C$ discrete values, so it follow a multinomial distribution.
- This is derived from an assumption that the probability of class $y=k$ is

$$
h_{\theta}(x)=p(y=k \mid x, \theta)=\frac{e^{\theta_{k}^{T} x}}{\sum_{j=1}^{C} e^{\theta_{j}^{T} x}}
$$

- The score or loss function for class $i$ is

This is called the cross-entropy loss $\quad L_{i}=-\log \left(\frac{e^{\theta_{i}^{T} X(i .)}}{\sum_{j=1}^{k} e^{\theta_{j}^{T} X\left(i_{i}\right)}}\right)$

## Introduction to backpropagation and computational graphs

- We now have a network architecture and a cost function.
- A learning algorithm for the net should give us a way to change the weights in such a manner that the output is closer to the correct class labels.
- The activation function should assure that a small change in weights results in
small change in any weight (ior bias)
 a small change in ouputs.
- Backpropagation use partial derivatives to compute the derivative of the cost function $J$ with respect to all the weights.


## Gradients and partial derivatives

$$
\begin{aligned}
& f(x, y)=x y \rightarrow \frac{\partial f}{\partial x}=y \frac{\partial f}{\partial y}=x \\
& f(x, y)=x+y \rightarrow \frac{\partial f}{\partial x}=1 \frac{\partial f}{\partial y}=1 \\
& f(x, y)=\max (x, y) \rightarrow \frac{\partial f}{\partial x}=1(x \geq y) \frac{\partial f}{\partial y}=1(y \geq x)
\end{aligned}
$$

$f(x, y, z)=(x+y) z$ Let $\mathrm{q}=\mathrm{x}+\mathrm{y}$ and $f=q z$ and use the chain rule :
$\frac{\partial f}{\partial x}=\frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$

## Backwards propagation of gradients



Green numbers: forward propagation
Red numbers: backwards propagation

## Backwards propagation of gradients



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Red numbers: backwards propagation

## Backwards propagation of gradients



Green numbers: forward propagation
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## Backwards propagation of gradients



Green numbers: forward propagation
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Green numbers: forward propagation
Red numbers: backwards propagation

## Activation functions

- Reading material:
- cs231n.github.io/neural-networks-1
- Deep Learning: 6.2.2 and 6.3
- Active area of research, new functions are published annually. We will consider:
- Sigmoid activation
- Tanh activation
- ReLU activation
- And mention recent alternatives like:
- Leaky ReLU
- Maxout
- ELU


## Data preprocessing

- Scaling of the features matters:
- If we have the samples

> xi: yi

101, 101: 2
101, 99: 0
Original

> xi: yi

1, 1: 2
1, -1: 0


Error surface


Error surface

## Data preprocessing

- Scaling of the features matters:
- If we have the samples
xi: yi
0.2, 10: 2
$0.2,-10$ : 0
Original
xi: yi
1, 1: 2
1, -1: 0

Normalize
to unit variance


Error surface


Error surface

## Weight initialization

- Avoid all zero initialization!
- If all weights are equal, they will produce the same gradients and same outputs, and undergo exactly the same parameter updates.
- They will learn the same thing.
- We break symmetry by initializing the weights to have small random numbers.
- Initialization is more complicated for deep networks


## Batch normalization

- So far, we noticed that normalizing the inputs and the initial weights to zero mean, unit variance help convergence.
- As training progresses, the mean and variance of the weights will change, and at a certain point they make converenge slow again.
- This is called a covariance shift.
- Batch normalization (loffe and Szegedy) https://arxiv.org/abs/1502.03167 countereffects this.
- After fully connected layers (or convolutional layers), and before the nonlinearity, a batch normalization layer is inserted.
- This layer makes the input gaussian with zero mean and unit variance by applying

$$
\hat{x}_{k}=\frac{x_{k}-\mu_{k}}{\sqrt{\operatorname{Var}\left(x_{k}\right)}}
$$

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## Dropout

- Presented in http://jmlr.org/papers/volume15/srivastava14a/srivastava14a.pdf
- Achieves a similar effect as bagging by randomly setting the output of a node to zero (by multipying with a random vector of zeros with probability p).

(a) Standard Neural Net

(b) After applying dropout.

Example: cat class with nodes detecting

- Eyes
- Ears
- Tail
- Fur
- Legs
- Mouth

Figure 1: Dropout Neural Net Model. Left: A standard neural net with 2 hidden layers. Right: An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

## Dropout - training

- Choose a dropout probability p
- We can drop both inputs and nodes in hidden layers.
- Create a binary mask for all nodes with probability of zero=p.
- Consider a 3-layer network with dropout in the hidden layers

```
# Forward pass of 3-layer net
H1 = np. maximum(0,np.dot(W1,X)+b1)
U1 = np.random.rand(*H1.shape)<p # first dropout
H1 *= U1
H2 = np.maximum(0,np.dot(W2,H1)+b2)
U2 = np.random.rand(*H2.shape) <p # Second dropout
H2 *= U2
out = np.dot(W3,H2) +b3
```

- Backpropagate as usual, but take into account the drop.


## Dropout - predict : naive implementation

- A drop rate of $p$ will scale the outputs during training with a factor $p<1$.
- When we predict new data, without considering this scaling, the outputs will be larger.
- We have to scale the outputs during predict by p :

```
# predict
H1 = np.maximum(0,np.dot(W1,X)+b1)*p
H2 = np.macimum(0,np.dot(W2,H1)+b2)*p
out = np.dot(W3,H2)+b3
```

- Since test-time performance is critical, we normally apply «inverted dropout» and scale at training time.


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## Inverted dropout

```
p=0.5
#train
H1 = np.maximum(0,np.dot(W1,X)+b1)
U1 = (np.random.rand(*H1.shape)<p)/p #Scale now
H1 *= U1
H2 = np.maximum(0,np.dot(W2,H1)+b2)
U2 = (np.random.rand(*H2.shape) < p) / p # Second scaled dropout
H2 * = U2
out = np.dot(W3,H2)+b3
# predict
H1 = np.maximum(0,np.dot(W1,X)+b1) #No scaling necessary
H2 = np.macimum(0,np.dot(W2,H1)+b2)
out = np.dot(W3,H2)+b3
```


## Learning with minibatch gradient descent

- Setting the learning $\eta$ rate is difficult, and the performance is sensitive to it.
- Too low: slow convergence
- Too high: oscillating performance
- In practise when using minibatch gradient descent: decay the learning rate linearly until iteration $\tau$, then leave $\eta_{\tau}$ constan $n_{t}$ :
$-\eta_{k}=(1-\alpha) \eta_{0}+\alpha \eta_{\tau}$, where $\alpha=k / \tau$,


## Gradient descent oscillations



$$
\eta=0.19
$$


$\eta=0.20$

This is how gradient descent moves

## Gradient descent with momentum

```
v=mu*v - learning_rate*df # Integrate velocity
f+= v #Integrate position
```

- Physical interpretation: ball rolling downhill
- mu: friction coefficient
- mu normally between 0.5 and 0.99
- Can gradually decrease from 0.5 to 0.99 e.g.
- Allows velocity to build up in shallow directions, but is dampened in steep directions because of the sign changes.


## Nesterov momentum

- Idea: if we are at point $x$, with momentum the next estimate is $x+m u^{*} v$ due to velocity from previous iterations.
- Momentum update has two parts: $\mathrm{v}=\mathrm{mu} \mathrm{*}^{*}$ - learning_rate*df
- One due to velocity, and one due to current gradient
- Since velocity is pushing us to $x+m u^{*} v$, why not compute the gradient at point $x+m u^{*} v$, not point $x$ ? (Look ahead)

$$
\begin{aligned}
& x \text { x_ahead }=x+m u^{*} v \text { \#Only the velocity part } \\
& \text { \# Evaluate the gradient at } x \text { ahead } \\
& v=m u^{*} v-\text { learning_rate* } d x\left(x \_a h e a d\right) \\
& x+=v
\end{aligned}
$$

## AdaGrad updates (DL 8.5.1)

- From http://www.jmlr.org/papers/volume12/duchi11a/duchi11a.pdf
- Keep a cache of elementwise squared gradients $g=d x$

```
# Adagrad update
cache += dx**2
x += -learning_rate * dx/(np.sqrt(cache)+1e-7)
```

- Note that $\mathrm{x}, \mathrm{dx}$ and cache are vectors.
- cache builds of the accumulated gradients in each direction.
- If one direction has large gradient, we will take a smaller step in that direction.
- A problem with AdaGrad is that cache builds up larger and larger, and the step size can be smaller and smaller.
- Use RMSprop or ADAM instead


## RMSprop update

- DL 8.5.2 and
http://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides lec6.pdf

$$
\begin{array}{|l}
\hline \text { \# RMSprop update } \\
\text { decay }=0.9 \\
\text { cache }=\text { decay*cache }+(1-\text { decay })^{*} d x^{* *} 2 \\
\text { x += -learning_rate * dx/(np.sqrt(cache)+1e-7) } \\
\hline
\end{array}
$$

- Here cache is a moving average of the gradients for each weight
- Works better than AdaGrad.


## ADAM update

- DL 8.5.3 and https://arxiv.org/abs/1412.6980
- Like RMSprop but with momentum

```
# ADAM update, all variables are vectors
rho1 = 0.9, rho2 = 0.999, eps=0.001
# initialize first and second moment variables
s=0, r=0
tau = t+1
s = rho1*s + (1-rho1)*dx
r = rho2*r + (1-rho2)*dx.*dx #elementwise
sb=s/(1-rho1**tau)
rb =r/(1-rho2**tau)
x = x - eps*sb/(sqrt(rb) +1e-8)
```

