## 2-INF-150: Machine Learning – Neural Nets

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October 24, 2018

## (preliminary) plan

- 3. 10. Python / Numpy
- 17. 10. Regression / Learning Theory
- 24. 10. Neural Networks
- 14. 11. Support Vector Machines / Decision Trees / Forests
- 5. 12. PCA / Clustering

## Today

- (Almost) no coding necessary
- (Artificial) Neural Networks
- Convolutional Neural Networks
- Special Bonus

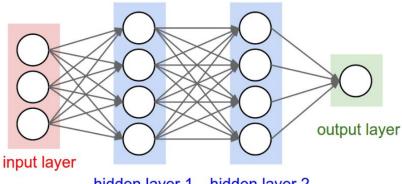
## Setup

- Start Linux
- Open command line
- pip3 install sklearn
- pip3 install tensorflow
- pip3 install keras

## Setup II.

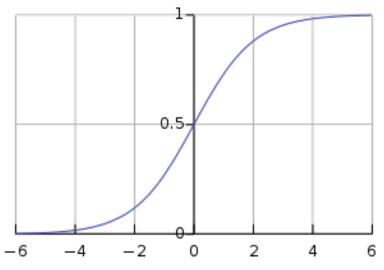
- mkdir ml\_exercise3
- cd ml\_exercise3
- git clone https://github.com/NaiveNeuron/ml\_exercises.git
- or download directly https://github.com/NaiveNeuron/ml\_exercises/archive/master.zip
- cd assignment2
- Run jupyter-notebook (Please, do not run on shared disk)

## MLP

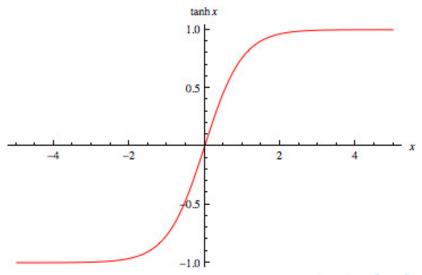


hidden layer 1 hidden layer 2

# sigmoid

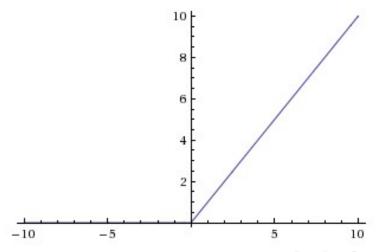


## tanh



ReLU

#### Rectified Linear Unit

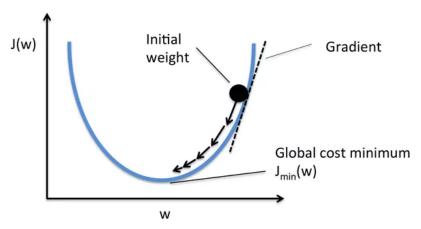


#### Gradient Descent Variants

#### Core idea of gradient descent

Minimize  $J(\theta)$  parametrized by  $\theta \in \mathbb{R}^d$  by updating  $\theta$  in the opposite direction of the gradient  $\nabla_{\theta}J(\theta)$ .

# Gradient Descent Variants Core idea of gradient descent



#### Batch Gradient Descent

aka Vanilla Gradient Descent

$$\theta_{t+1} = \theta_t - \eta \cdot \nabla_{\theta_t} J(\theta_t)$$

- Might be very slow
- No-go for big datasets
- Impossible to update "online" (new examples on-the-fly)
- Guaranteed to converge to the global minimum for convex error surfaces and to a local minimum for non-convex surfaces

```
for i in range(nb_epochs):
   params_grad = evaluate_gradient(loss_function, data, params)
   params = params - learning_rate * params_grad
```

#### Stochastic Gradient Descent

$$\theta_{t+1} = \theta_t - \eta \cdot \nabla_{\theta_t} J(\theta_t; x^{(i)}; y^{(i)})$$

- Usually faster convergence
- Where batch gradient descent does redundant computation,
   SGD updates frequently and creates fluctuations.
- When slowly decreasing the learning rate, SGD shows the same convergence behaviour as batch gradient descent

```
for i in range(nb_epochs):
    np.random.shuffle(data)
    for example in data:
        params_grad = evaluate_gradient(loss_function, example, params)
        params = params - learning_rate * params_grad
```

#### Mini-batch Gradient Descent

$$\theta = \theta - \eta \cdot \nabla_{\theta} J(\theta; \mathbf{x}^{(i:i+n)}; \mathbf{y}^{(i:i+n)})$$

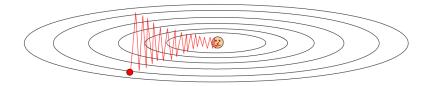
- Best of both worlds
- Reduced variance of parameter updates more stable convergence
- SGD and Mini-batch Gradient Descent are used interchangeably

```
for i in range(nb_epochs):
    np.random.shuffle(data)
    for batch in get_batches(data, batch_size=50):
        params_grad = evaluate_gradient(loss_function, batch, params)
        params = params - learning_rate * params_grad
```

## Gradient Descent - Challenges

- Choosing a proper learning rate is difficult (too small, too large, too steady...)
- Learning rate schedules help, but still need to be pre-defined in advance
- Same learning rate for all parameter updates (larger updates to more infrequent features might be more desirable)
- Ending up trapped in suboptimal local optima

## Stochastic Gradient Descent



#### Momentum

$$v_t = \gamma v_{t-1} + \eta \nabla_{\theta} J(\theta)$$
$$\theta_{t+1} = \theta_t - v_t$$

- Helps navigate SGD when one dimension curves more steeply than than the other (common around local optima)
- Basically fights against oscillations
- ullet Momentum term  $\gamma$  is usually set to 0.9
- "Pushing a ball down a hill" metaphor

#### Nesteroy Momentum





#### Nesterov Accelerated Gradient

Let's not blindly trust gravity

$$v_{t} = \gamma v_{t-1} + \eta \nabla_{\theta} J(\theta - \gamma v_{t-1})$$
$$\theta_{t+1} = \theta_{t} - v_{t}$$

- Give the moving ball some notion of where it is going
- $\theta \gamma v_{t-1}$  approximates (gives a rough idea of) the next position of the parameters
- "Update with anticipation" prevents the ball from going too fast
- Is able to adapt updates to the slope we'd like to also adapt updates to "parameter importance"



## Parameter space



#### AdaGrad

$$\begin{aligned} g_{t,i} &= \nabla_{\theta} J(\theta_i) \\ \theta_{t+1,i} &= \theta_{t,i} - \eta \cdot g_{t,i} \\ \theta_{t+1,i} &= \theta_{t,i} - \frac{\eta}{\sqrt{G_{t,ii} + \epsilon}} \cdot g_{t,i} \end{aligned}$$

- $G_t \in \mathbb{R}^{d \times d}$  diagonal matrix where  $G_{t,ii}$  is the sum of the squares of the gradients w.r.t  $\theta_i$  up to time t.
- $\epsilon$  helps to avoid division-by-zero issues (usually on the order of 1e-8)
- Main benefit: no need for manually decaying/tuning the learning rate
- Main weakness: accumulation of squared gradients in the denominator
- Learning rate will shrink (sometimes way too much)

## **RMSProp**

## RMSProp update

[Tieleman and Hinton, 2012]

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

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

## **RMSProp**

#### rmsprop: A mini-batch version of rprop

- rprop is equivalent to using the gradient but also dividing by the size of the gradient.
  - The problem with mini-batch rprop is that we divide by a different number for each mini-batch. So why not force the number we divide by to be very similar for adjacent mini-batches?
- rmsprop: Keep a moving average of the squared gradient for each weight  $MeanSquare(w, t) = 0.9 \ MeanSquare(w, t-1) + 0.1 \left(\frac{\partial E}{\partial w}(t)\right)^2$
- Dividing the gradient by \( \sqrt{MeanSquare(w, t)} \) makes the learning work much better (Tilmen Tieleman, unpublished).

Introduced in a slide in Geoff Hinton's Coursera class, lecture 6

Cited by several papers as:

[52] T. Tieleman and G. E. Hinton. Lecture 6.5-rmsprop: Divide the gradient by a running average of its recent magnitude., 2012



#### Adam

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$
$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$

Both  $m_t$  and  $v_t$  are initialized as 0s, so they need to be bias-corrected.

$$\hat{m}_t = rac{m_t}{1-eta_1^t}$$
  $\hat{v}_t = rac{v_t}{1-eta_2^t}$   $heta_{t+1} = heta_t - rac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t$ 

#### Adam

## Adam update

[Kingma and Ba, 2014]

```
# Adam
m,v = #... initialize caches to zeros
for t in xrange(1, big_number):
    dx = #... evaluate gradient
    m = betal*m + (1-betal)*dx # update first moment
    v = beta2*v + (1-beta2)*(dx**2) # update second moment
    mb = m/(1-beta1**t) # correct bias
    vb = v/(1-beta2**t) # correct bias
    x += - learning rate * mb / (np.sqrt(vb) + 1e-7)

RMSProp-like
```

The bias correction compensates for the fact that m,v are initialized at zero and need some time to "warm up".

## Visual Demo

#### So what should one use?

- RMSProp and Adam are very similar
- Bias-correction in Adam has been shown to outpreform RMSProp slightly towards the end
- Adam is usually a good default choice for CNNs, RMSProp might be worth considering for big RNNs

## ConvNets

#### ConvNets

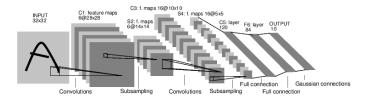
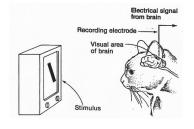
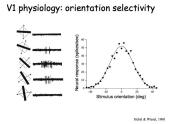


Figure: LeNet [LeCun et al., 1998]

#### Hubel & Wiesel

1959 - Receptive fields of single neurones in the cat's striate cortex 1962 - Receptive fields, binocular interaction and functional architecture in the cat's visual cortex





#### AlexNet.

#### ImageNet Classification with Deep Convolutional Neural Networks

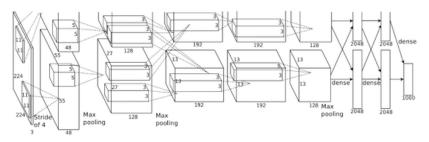


Figure: AlexNet [Krizhevsky, Sutskever, Hinton, 2012]

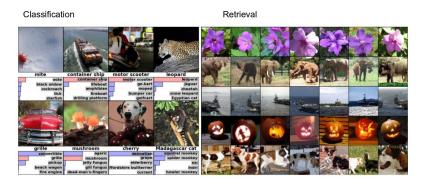


Figure: [Krizhevsky 2012]

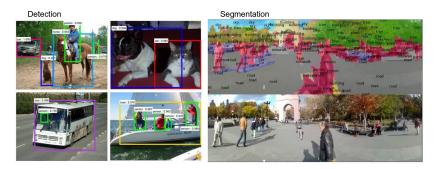


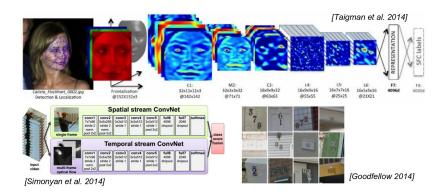
Figure: [Faster R-CNN: Ren, He, Girshick, Sun 2015] Detection Segmentation & [Farabet et al., 2012]





NVIDIA Tegra X1

Figure: Self driving cars

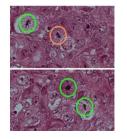




[Toshev, Szegedy 2014]



[Mnih 2013]

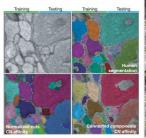




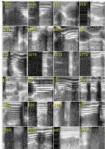
[Ciresan et al. 2013]



[Sermanet et al. 2011] [Ciresan et al.]

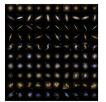


[Turaga et al., 2010]



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[Denil et al. 2014]





Whale recognition, Kaggle Challenge



Mnih and Hinton, 2010



Image Captioning

[Vinyals et al., 2015]



reddit.com/r/deepdream

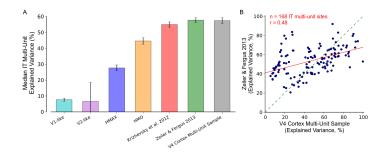
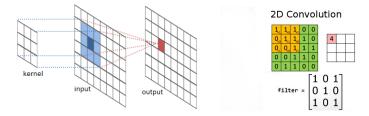
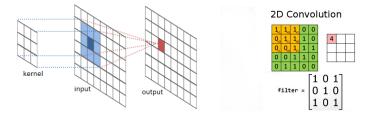


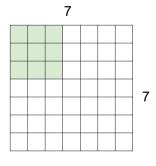
Figure: Deep Neural Networks Rival the Representation of Primate IT Cortex for Core Visual Object Recognition [Cadieu et al., 2014]



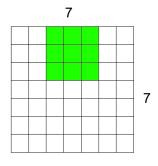


We don't have to go with stride 1

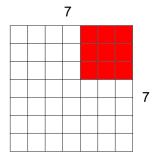
We don't have to go with stride 1



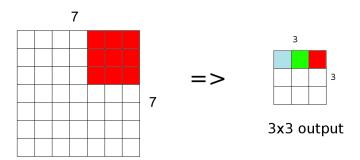
7x7 input (spatially) assume 3x3 filter applied with stride 2

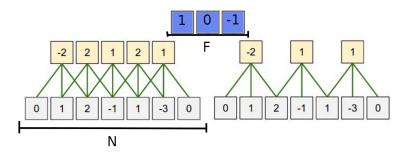


7x7 input (spatially) assume 3x3 filter applied with stride 2



7x7 input (spatially) assume 3x3 filter applied with stride 2



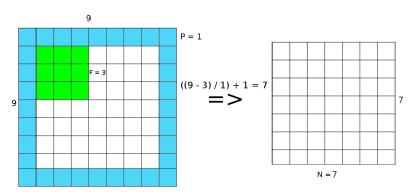


Output size:  $\frac{N-F}{stride} + 1$ 



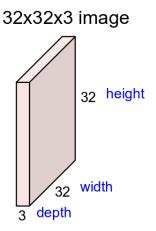
What if I want to keep spatial dimension?

What if I want to keep spatial dimension? Pad the input!

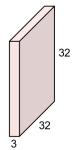


Output size: 
$$\frac{N-F+2P}{stride} + 1$$





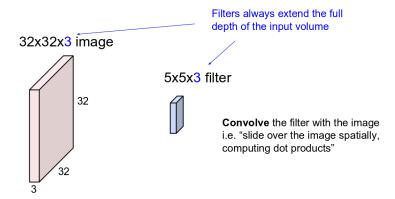
### 32x32x3 image

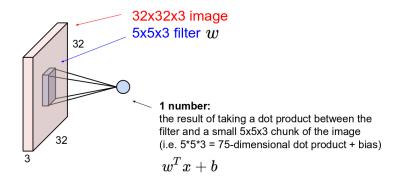


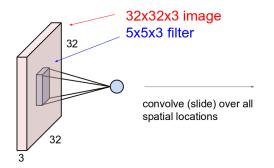
#### 5x5x3 filter



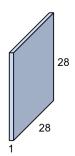
**Convolve** the filter with the image i.e. "slide over the image spatially, computing dot products"



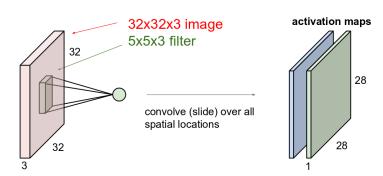




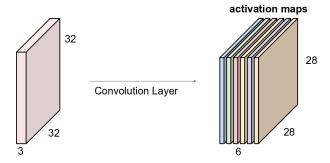
#### activation map



#### consider a second, green filter

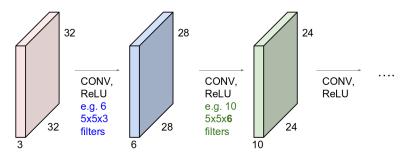


For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:



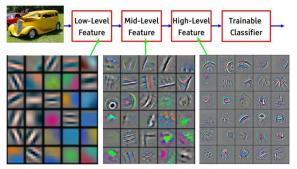
We stack these up to get a "new image" of size 28x28x6!

**Preview:** ConvNet is a sequence of Convolutional Layers, interspersed with activation functions

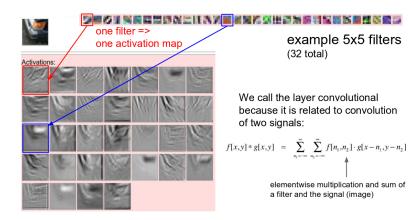


#### Preview

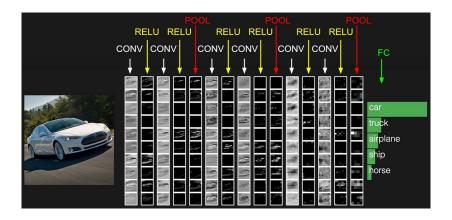
[From recent Yann LeCun slides]



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

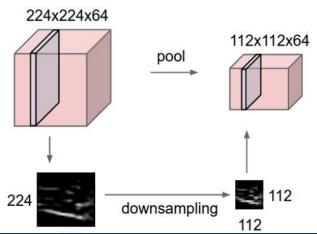


#### Convolutional Neural Network

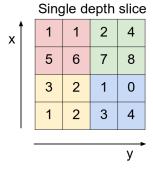


## Pooling layer

- makes the representations smaller and more manageable
- operates over each activation map independently:



# Max pool

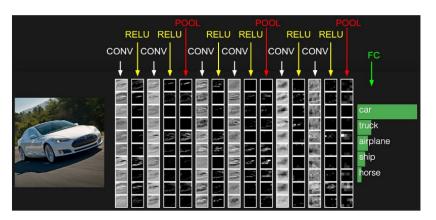


max pool with 2x2 filters and stride 2

6	8
3	4

## Fully Connected layers

Contains neurons that connect to the entire input volume, as in ordinary  ${\sf NN}$ 



## Quite a lot for one short presentation

Do not worry, we realize that as well.

## Quite a lot for one short presentation

Do not worry, we realize that as well.

But it's so cool we could not resist...

#### Data



