## Summary

- We had covered so far
- Linear models (linear and logistic regression) - always a good start, simple yet powerful
- Model Assessment and Selection - basics for all methods
- Trees, Random Forests, and Boosting - good for high dim mixed-type features
- Support Vector Machines - good for small amount of data but high dim geometric features
- Next, neural networks for unstructured data (image, language etc.):
- Convolutional Neural Networks - image data
- Generative models and GANs - new unsupervised learning for image, etc.
- Recurrent Neural Networks, LSTM - sequence data
- Transformer, BERT - machine translation etc.
- Reinforcement Learning - Markov decision process, playing games, etc.


## Kaggle survey: Top ML Methods

https://www.kaggle.com/surveys/2017

## Academic

What data science methods are used at work?
Logistic regression is the most commonly reported data science method used at
work for all industries except Military and Security where Neural Networks are used
slightly more frequently.
Company Size $*$ Academic $\%$ Job Title


Industry
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Company Size $\ddagger$ Industry $\Rightarrow$ IobTtite


## What type of data is used at work?

https://www.kaggle.com/surveys/2017

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## What type of data is used at work?

Relational data is the most commonly reported type of data used at work for all industries except for Academia and the Military and Security industry where text data's used more.

Company Size $\hat{*}$ Academic $\Rightarrow$ Job Title $=$


## Industry

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Company Size $*$ Industry $\Rightarrow$ Job Title $\Rightarrow$


## Acknowledgement



A following-up course at HKUST: https://deeplearning-math.github.io/

## Some reference books

- Deep Learning with Python, Manning Publications 2017
- by François Chollet
- https://www.manning.com/books/deep-learning-withpython? a aid=keras\&a bid=76564dff
- Deep Learning, MIT Press 2016
- By Ian Goodfellow, Yoshua Bengio, and Aaron Courville,
- http://www.deeplearningbook.org/
- Many other public resources


## A Brief History of Neural Networks

## Perceptron: single-layer

- Invented by Frank Rosenblatt (1957)



## The Perceptron Algorithm

$$
\ell(w)=-\sum_{i \in \mathcal{M}_{w}} y_{i}\left\langle w, \mathbf{x}_{i}\right\rangle, \quad \mathcal{M}_{w}=\left\{i: y_{i}\left\langle\mathbf{x}_{i}, w\right\rangle<0, y_{i} \in\{-1,1\}\right\} .
$$

The Perceptron Algorithm is a Stochastic Gradient Descent method (Robbins-Monro 1950; Kiefer-Wolfowitz 1951) :

$$
\begin{aligned}
w_{t+1} & =w_{t}-\eta_{t} \nabla_{i} \ell(w) \\
& =\left\{\begin{array}{lr}
w_{t}-\eta_{t} y_{i} \mathbf{x}_{i}, & \text { if } y_{i} w_{t}^{T} \mathbf{x}_{i}<0 \\
w_{t}, & \text { otherwise }
\end{array}\right.
\end{aligned}
$$

## Finite Stop of Perceptron for Separable Data

The perceptron convergence theorem was proved by Block (1962) and Novikoff (1962). The following version is based on that in Cristianini and Shawe-Taylor (2000).

Theorem 1 (Block, Novikoff). Let the training set $S=\left\{\left(\mathbf{x}_{1}, t_{1}\right), \ldots,\left(\mathbf{x}_{n}, t_{n}\right)\right\}$ be contained in a sphere of radius $R$ about the origin. Assume the dataset to be linearly separable, and let $\mathbf{w}_{\mathrm{opt}},\left\|\mathbf{w}_{\mathrm{opt}}\right\|=1$, define the hyperplane separating the samples, having functional margin $\gamma>0$. We initialise the normal vector as $\mathbf{w}_{0}=0$. The number of updates, $k$, of the perceptron algorithms is then bounded by

$$
\begin{equation*}
k \leq\left(\frac{2 R}{\gamma}\right)^{2} \tag{10}
\end{equation*}
$$



Input ball: $\quad R=\max _{i}\left\|\mathbf{x}_{i}\right\|$.
Margin: $\quad \gamma:=\min _{i} y_{i} f\left(x_{i}\right)$

## Proof.

Proof. Though the proof can be done using the augmented normal vector and samples defined in the beginning, the notation will be a lot easier if we introduce a different augmentation: $\hat{\mathbf{w}}=\left(\mathbf{w}^{\top}, b / R\right)^{\top}=\left(w_{1}, \ldots, w_{D}, b / R\right)^{\top}$ and $\hat{\mathbf{x}}=\left(\mathbf{x}^{\top}, R\right)^{\top}=\left(x_{1}, \ldots, x_{D}, R\right)^{\top}$.

## Proof (continued, growth of $\left.\left|w_{k}\right|\right)$

We first derive an upper bound on how fast the normal vector grows. As the hyperplane is unchanged if we multiply $\hat{\mathbf{w}}$ by a constant, we can set $\eta=1$ without loss of generality. Let $\hat{\mathbf{w}}_{k+1}$ be the updated (augmented) normal vector after the $k$ th error has been observed.

$$
\begin{align*}
\left\|\hat{\mathbf{w}}_{k+1}\right\|^{2} & =\left(\hat{\mathbf{w}}_{k}+t_{i} \hat{\mathbf{x}}_{i}\right)^{\top}\left(\hat{\mathbf{w}}_{k}+t_{i} \hat{\mathbf{x}}_{i}\right)  \tag{11}\\
& =\hat{\mathbf{w}}_{k}^{\top} \hat{\mathbf{w}}_{k}+\hat{\mathbf{x}}^{\top} \hat{\mathbf{x}}_{i}+2 t_{i} \hat{\mathbf{w}}_{k}^{\top} \hat{\mathbf{x}}_{i}  \tag{12}\\
& =\left\|\hat{\mathbf{w}}_{k}\right\|^{2}+\left\|\hat{\mathbf{x}}_{i}\right\|^{2}+2 t_{i} \hat{\mathbf{w}}_{k}^{\top} \hat{\mathbf{x}}_{i} . \tag{13}
\end{align*}
$$

Since an update was triggered, we know that $t_{i} \hat{\mathbf{w}}_{k}^{\top} \hat{\mathbf{x}}_{i} \leq 0$, thus

$$
\begin{align*}
\left\|\hat{\mathbf{w}}_{k}\right\|^{2}+\left\|\hat{\mathbf{x}}_{i}\right\|^{2}+2 t_{i} \hat{\mathbf{w}}_{k}^{\top} \hat{\mathbf{x}}_{i} & \leq\left\|\hat{\mathbf{w}}_{k}\right\|^{2}+\left\|\hat{\mathbf{x}}_{i}\right\|^{2}  \tag{14}\\
& =\left\|\hat{\mathbf{w}}_{k}\right\|^{2}+\left(\left\|\mathbf{x}_{i}\right\|^{2}+R^{2}\right)  \tag{15}\\
& \leq\left\|\hat{\mathbf{w}}_{k}\right\|^{2}+2 R^{2} . \tag{16}
\end{align*}
$$

This implies that $\left\|\hat{\mathbf{w}}_{k}\right\|^{2} \leq 2 k R^{2}$, thus

$$
\begin{equation*}
\left\|\hat{\mathbf{w}}_{k+1}\right\|^{2} \leq 2(k+1) R^{2} . \tag{17}
\end{equation*}
$$

## Proof (continued, projection on $\mathrm{w}_{\text {opt }}$ )

We then proceed to show how the inner product between an update of the normal vector and $\hat{\mathbf{w}}_{\text {opt }}$ increase with each update:

$$
\begin{align*}
\hat{\mathbf{w}}_{\mathrm{opt}}^{\top} \hat{\mathbf{w}}_{k+1} & =\hat{\mathbf{w}}_{\mathrm{opt}}^{\top} \hat{\mathbf{w}}_{k}+t_{i} \hat{\mathbf{w}}_{\mathrm{opt}}^{\top} \hat{\mathbf{x}}_{i}  \tag{18}\\
& \geq \hat{\mathbf{w}}_{\mathrm{opt}}^{\top} \hat{\mathbf{w}}_{k}+\gamma  \tag{19}\\
& \geq(k+1) \gamma, \tag{20}
\end{align*}
$$

since $\hat{\mathbf{w}}_{\mathrm{opt}}^{\top} \hat{\mathbf{w}}_{k} \geq k \gamma$. We therefore have

$$
\begin{equation*}
k^{2} \gamma^{2} \leq\left(\hat{\mathbf{w}}_{\mathrm{opt}}^{\top} \hat{\mathbf{w}}_{k}\right)^{2} \leq\left\|\hat{\mathbf{w}}_{\mathrm{opt}}\right\|^{2}\left\|\hat{\mathbf{w}}_{k}\right\|^{2} \leq 2 k R^{2}\left\|\hat{\mathbf{w}}_{\mathrm{opt}}\right\|^{2} \tag{21}
\end{equation*}
$$

where we have made use of the Cauchy-Schwarz inequality. As $k^{2} \gamma^{2}$ grows faster than $2 k R^{2}$, Eq. (21) can hold if and only if

$$
\begin{equation*}
k \leq 2\left\|\hat{\mathbf{w}}_{\text {opt }}\right\|^{2^{2}} \frac{R^{2}}{\gamma^{2}} \tag{22}
\end{equation*}
$$

## Proof (continued, combined bounds)

As $b \leq R$, we can rewrite the norm of the normal vector:

$$
\begin{equation*}
\left\|\hat{\mathbf{w}}_{\mathrm{opt}}\right\|^{2}=\left\|\mathbf{w}_{\mathrm{opt}}\right\|^{2}+\frac{b^{2}}{R^{2}} \leq\left\|\mathbf{w}_{\mathrm{opt}}\right\|^{2}+1=2 \tag{23}
\end{equation*}
$$

The bound on $k$ now becomes

$$
\begin{equation*}
k \leq 4 \frac{R^{2}}{\gamma^{2}}=\left(\frac{2 R}{\gamma}\right)^{2} \tag{24}
\end{equation*}
$$

which therefore bounds the number of updates necessary to find the separating hyperplane.

## Locality or Sparsity of Computation

Minsky and Papert, 1969
Perceptron can't do XOR classification Perceptron needs infinite global information to compute connectivity


Locality or Sparsity is important:
Locality in time?
Locality in space?


## Convolutional Neural Networks: shift invariances and locality

- Can be traced to Neocognitron of Kunihiko Fukushima (1979)
- Yann LeCun combined convolutional neural networks with back propagation (1989)
- Imposes shift invariance and locality on the weights
- Forward pass remains similar
- Backpropagation slightly changes - need to sum over the gradients from all spatial positions



# Multilayer Perceptrons (MLP) and Back-Propagation (BP) Algorithms 

## Rumelhart, Hinton, Williams (1986)

Learning representations by back-propagating errors, Nature, 323(9): 533-536

BP algorithms as stochastic gradient descent algorithms (Robbins-Monro 1950; Kiefer-
Wolfowitz 1951) with Chain rules of Gradient maps

MLP classifies XOR, but the global hurdle on topology (connectivity) computation still exists

## BP Algorithm: Forward Pass

- Cascade of repeated [linear operation followed by coordinatewise nonlinearity]'s
- Nonlinearities: sigmoid, hyperbolic tangent, (recently) ReLU.

```
Algorithm 1 Forward pass
Input: \(x_{0}\)
Output: \(x_{L}\)
    1: for \(\ell=1\) to \(L\) do
    2: \(\quad x_{\ell}=f_{\ell}\left(W_{\ell} x_{\ell-1}+b_{\ell}\right)\)
    3: end for
```


## BP algorithm = Gradient Descent Method

- Training examples $\left\{x_{0}^{i}\right\}_{i=1}^{n}$ and labels $\left\{y^{i}\right\}_{i=1}^{n}$
- Output of the network $\left\{x_{L}^{i}\right\}_{i=1}^{m}$
- Objective

$$
\begin{equation*}
J\left(\left\{W_{l}\right\},\left\{b_{l}\right\}\right)=\frac{1}{n} \sum_{i=1}^{n} \frac{1}{2}\left\|y^{i}-x_{L}^{i}\right\|_{2}^{2} \tag{1}
\end{equation*}
$$

Other losses include cross-entropy, logistic loss, exponential loss, etc. - Gradient descent

$$
\begin{aligned}
W_{l} & =W_{l}-\eta \frac{\partial J}{\partial W_{l}} \\
b_{l} & =b_{l}-\eta \frac{\partial J}{\partial b_{l}}
\end{aligned}
$$

In practice: use Stochastic Gradient Descent (SGD)

## Derivation of BP: Lagrangian Multiplier

 LeCun et al. 1988Given $n$ training examples $\left(I_{i}, y_{i}\right) \equiv$ (input,target) and $L$ layers

- Constrained optimization

$$
\begin{array}{ll}
\min _{W, x} & \sum_{i=1}^{n}\left\|x_{i}(L)-y_{i}\right\|_{2} \\
\text { subject to } & x_{i}(\ell)=f_{\ell}\left[W_{\ell} x_{i}(\ell-1)\right], \\
& i=1, \ldots, n, \quad \ell=1, \ldots, L, x_{i}(0)=I_{i}
\end{array}
$$

- Lagrangian formulation (Unconstrained)

$$
\begin{aligned}
& \min _{W, x, B} \mathcal{L}(W, x, B) \\
\mathcal{L}(W, x, B)=\sum_{i=1}^{n} \quad & \left\{\left\|x_{i}(L)-y_{i}\right\|_{2}^{2}+\right. \\
& \left.\sum_{\ell=1}^{L} B_{i}(\ell)^{T}\left(x_{i}(\ell)-f_{\ell}\left[W_{\ell} x_{i}(\ell-1)\right]\right)\right\}
\end{aligned}
$$

## back-propagation - derivation

- $\frac{\partial \mathcal{L}}{\partial B}$

Forward pass

$$
x_{i}(\ell)=f_{\ell}[\underbrace{W_{\ell} x_{i}(\ell-1)}_{A_{i}(\ell)}] \quad \ell=1, \ldots, L, \quad i=1, \ldots, n
$$

$$
\text { - } \frac{\partial \mathcal{L}}{\partial x}, z_{\ell}=\left[\nabla f_{\ell}\right] B(\ell)
$$

Backward (adjoint) pass

$$
\begin{aligned}
& z(L)=2 \nabla f_{L}\left[A_{i}(L)\right]\left(y_{i}-x_{i}(L)\right) \\
& z_{i}(\ell)=\nabla f_{\ell}\left[A_{i}(\ell)\right] W_{\ell+1}^{T} z_{i}(\ell+1) \quad \ell=0, \ldots, L-1
\end{aligned}
$$

$$
\text { - } W \leftarrow W+\lambda \frac{\partial \mathcal{L}}{\partial W}
$$

## Weight update

$$
W_{\ell} \leftarrow W_{\ell}+\lambda \sum_{i=1}^{n} z_{i}(\ell) x_{i}^{T}(\ell-1)
$$

## Support Vector Machine (Max-Margin Classifier) <br> $\operatorname{minimize}_{\beta_{0}, \beta_{1}, \ldots, \beta_{p}}\|\beta\|^{2}:=\sum_{j} \beta_{j}^{2}$

subject to $y_{i}\left(\beta_{0}+\beta_{1} x_{i 1}+\ldots+\beta_{p} x_{i p}\right) \geq 1$ for all $i$



Vladmir Vapnik, 1994

Convex optimization + Reproducing Kernel Hilbert Spaces (Grace Wahba etc.)

## MNIST Challenge Test Error: SVM vs. CNN LeCun et al. 1998



Simple SVM performs
as well as Multilayer
Convolutional Neural
Networks which need careful tuning (LeNets)

Second dark era for NN: 2000s


## LeNe†



Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

- Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. Proceedings of the IEEE, november 1998.


## Fully Connected Layer

## $32 \times 32 \times 3$ image -> stretch to $3072 \times 1$



## Convolution



## Convolution Layer: a first (blue) filter



activation map



## Convolution Layer: a second (green) filter



## Convolution Layer

For example, if we had $65 \times 5$ filters, we'll get 6 separate activation maps:
activation maps


We stack these up to get a "new image" of size $28 \times 28 \times 6$ !

## Stride

## $7 \times 7$ Input Volume



7×7 Input Volume

$5 \times 5$ Output Volume

$3 \times 3$ Output Volume


## A Closer Look at Convolution: stride=1


$7 x 7$ input (spatially) assume $3 \times 3$ filter
$7 \times 7$ input (spatially) assume $3 \times 3$ filter


7

$7 x 7$ input (spatially) assume $3 \times 3$ filter
$7 \times 7$ input (spatially) assume $3 \times 3$ filter
$=>5 \times 5$ output

## A Closer Look at Convolution: stride=2



7


7x7 input (spatially)
assume $3 \times 3$ filter
applied with stride 2


Output size:
( N - F ) / stride + 1
e.g. $N=7, F=3$ :
stride $1=>(7-3) / 1+1=5$
stride $2=>(7-3) / 2+1=3$
stride $3=>(7-3) / 3+1=2.33: \$
$7 x 7$ input (spatially) assume $3 \times 3$ filter applied with stride 2 => $3 \times 3$ output!

## A Closer Look at Convolution: Padding


e.g. input $7 \times 7$
$3 \times 3$ filter, applied with stride 1 pad with 1 pixel border => what is the output?

## 7x7 output!

in general, common to see CONV layers with stride 1, filters of size FxF, and zero-padding with (F-1)/2. (will preserve size spatially)
e.g. $F=3$ => zero pad with 1

F = 5 => zero pad with 2
F = 7 => zero pad with 3

## ConvNet:



Stride $=1$
Padding $=0$

## Formula: NewlmageSize = <br> floor((lmageSize - Filter + 2*Padding)/Stride + 1)

Summary To summarize, the Conv Layer:

- Accepts a volume of size $W_{1} \times H_{1} \times D_{1}$
- Requires four hyperparameters:
- Number of filters $K$,
- their spatial extent $F$,
- the stride $S$,
- the amount of zero padding $P$.
- Produces a volume of size $W_{2} \times H_{2} \times D_{2}$ where:
- $W_{2}=\left(W_{1}-F+2 P\right) / S+1$
- $H_{2}=\left(H_{1}-F+2 P\right) / S+1$ (i.e. width and height are computed equally by symmetry)
- $D_{2}=K$
- With parameter sharing, it introduces $F \cdot F \cdot D_{1}$ weights per filter, for a total of $\left(F \cdot F \cdot D_{1}\right) \cdot K$ weights and $K$ biases.
- In the output volume, the $\boldsymbol{d}$-th depth slice (of size $W_{2} \times H_{2}$ ) is the result of performing a valid convolution of the $d$-th filter over the input volume with a stride of $S$, and then offset by $d$-th bias.


## ReLU

- Non-saturating function and therefore faster convergence when compared to other nonlinearities
- Problem of dying neurons



## Max Pooling

Single depth slice

$x \nmid$| 1 | 1 | 2 | 4 |
| :---: | :---: | :---: | :---: |
| 5 | 6 | 7 | 8 |
| 3 | 2 | 1 | 0 |
| 1 | 2 | 3 | 4 |

max pool with $2 \times 2$ filters and stride 2

| 6 | 8 |
| :--- | :--- |
| 3 | 4 |

## 2000-2010: The Era of SVM, Boosting, ...

 as nights of Neural Networks

## Decision Trees and Boosting


－Breiman，Friedman，Olshen，Stone，（1983）：CART
－＂‘The Boosting problem＂（M．Kearns \＆L．Valiant）： Can a set of weak learners create a single strong learner？（三个臭皮匠顶个诸葛亮？）
－Breiman（1996）：Bagging
－Freund，Schapire（1997）：AdaBoos $\dagger$
－Breiman（2001）：Random Forests


## Around the year of 2012...

Speech Recognition: TIMIT
TIMIT Speech Recognition Dataset


## Computer Vision: ImageNe†

- ImageNet (subset):
- 1.2 million training images
- 100,000 test images
- 1000 classes
- ImageNet large-scale visual recognition Challenge



## Depth as function of year



## AlexNet (2012): Architecture

- 8 layers: first 5 convolutional, rest fully connected
- ReLU nonlinearity
- Local response normalization
- Max-pooling
- Dropout



## AlexNet (2012): Dropout


(a) Standard Neural Net

(b) After applying dropout.

Source: [Srivastava et al., 2014]

- Zero every neuron with probability $1-p$
- At test time, multiply every neuron by $p$


## VGG (2014) [Simonyan-Zisserman'14]

- Deeper than AlexNet: 11-19 layers versus 8
- No local response normalization
- Number of filters multiplied by two every few layers
- Spatial extent of filters $3 \times 3$ in all layers
- Instead of $7 \times 7$ filters, use three layers of $3 \times 3$ filters
- Gain intermediate nonlinearity
- Impose a regularization on the $7 \times 7$ filters


[^0]
## ResNet (2015) [HGRS-15]

- Solves problem by adding skip connections
- Very deep: 152 layers
- No dropout
- Stride
- Batch normalization


Source: Deep Residual Learning for Image Recognition


## Batch Normalization


(Assume $\mathrm{X}[\mathrm{NxD}]$ is data matrix, each example in a row)

## Batch Normalization

Algorithm 2 Batch normalization [loffe and Szegedy, 2015] Input: Values of $x$ over minibatch $x_{1} \ldots x_{B}$, where $x$ is a certain channel in a certain feature vector
Output: Normalized, scaled and shifted values $y_{1} \ldots y_{B}$

$$
\begin{aligned}
& \text { 1: } \mu=\frac{1}{B} \sum_{b=1}^{B} x_{b} \\
& \text { 2: } \sigma^{2}=\frac{1}{B} \sum_{b=1}^{B}\left(x_{b}-\mu\right)^{2} \\
& \text { 3: } \hat{x}_{b}=\frac{x_{b}-\mu}{\sqrt{\sigma^{2}+\epsilon}} \\
& \text { 4: } y_{b}=\gamma \hat{x}_{b}+\beta
\end{aligned}
$$

- Accelerates training and makes initialization less sensitive
- Zero mean and unit variance feature vectors


## BatchNorm at Test

Input: Values of $x$ over a mini-batch: $\mathcal{B}=\left\{x_{1 \ldots m}\right\}$; Parameters to be learned: $\gamma, \beta$
Output: $\left\{y_{i}=\mathrm{BN}_{\gamma, \beta}\left(x_{i}\right)\right\}$

$$
\begin{array}{rlr}
\mu_{\mathcal{B}} & \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_{i} & \text { // mini-batch mean } \\
\sigma_{\mathcal{B}}^{2} & \leftarrow \frac{1}{m} \sum_{i=1}^{m}\left(x_{i}-\mu_{\mathcal{B}}\right)^{2} & \text { // mini-batch variance } \\
\widehat{x}_{i} & \leftarrow \frac{x_{i}-\mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^{2}+\epsilon}} & \text { // normalize } \\
y_{i} & \leftarrow \gamma \widehat{x}_{i}+\beta \equiv \mathrm{BN}_{\gamma, \beta}\left(x_{i}\right) & \text { // scale and shift }
\end{array}
$$

## Note: at test time BatchNorm layer functions differently:

The mean/std are not computed based on the batch. Instead, a single fixed empirical mean of activations during training is used.
(e.g. can be estimated during training with running averages)

## Complexity vs. Accuracy of Different Networks



## Deep Learning Softwares

- Pyłorch (developed by Yann LeCun and Facebook):
- http://pytorch.org/tutorials/
- Tensorflow (developed by Google based on Caffe)
- https://www.tensorflow.org/tutorials/
- Theano (developed by Yoshua Bengio)
- http://deeplearning.net/software/theano/tutorial/
- Keras (based on Tensorflow or Pytorch)
- https://www.manning.com/books/deep-learning-withpython?a aid=keras\&a bid=76564dff


## Show some examples by jupyter notebooks

Thank you!



[^0]:    Source: https://blog.heuritech.com/2016/02/29/

