Deep Learning I: from shallow to deep

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A classification task

Changing the pipeline of classification

Neural networks: from shallow to deep

Motivation and definitions Linear function, loss function, optimization Simple Neural Network

Convolutional Neural Networks Current Architectures

Guidelines for training

Learning guarantees and alternatives

A classification example

Task: learn how to distinguish two types of images:

- desert;
- ► beach.

Objective: given annotated images, develop a model able to classify unseen images into one of those classes.



- Features: set of values extracted from images that can be used to measure the (dis)similarity between images Any suggestion?
 - the two most frequent colors as a descriptor



- Classifier: a model build using labeled examples (images for which the classes are known). It must be able to predict the class of a new image. Any suggestion?
 - A linear classifier, for instance!



- Examples used to build the classifier : training set.
- Training data is seldom linearly separable
- Therefore there is a training error



► The model, or classifier, can then be used to predict/infer the class of new data.



- How good is the model? Let us test, for new data (not seen before), the classifier error rate
- Labelled examples in this stage compose the test set.



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Classic image recognition pipeline



History of methods for computer vision

- Color, shape and texture descriptors (1970-2000)
- Scale invariant features (>1999)
- Histogram of Gradients (>2005)
- Bag of Features (>2004)
- Spatial Pyramid Matching (>2006),

- 1. Descriptor grid: HoG, LBP, SIFT, SURF
- 2. Fisher Vectors projection
- 3. Spatial Pyramid Matching
- 4. Classification Algorithm

Not so versatile!

Breakthrough: annotated data available



ImageNet Challenge: \sim 1.4 million images, 1000 classes.

CNNs now dominate image classification



Previously...



New recognition pipeline: feature learning



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Guidelines for training Learning guarantees and alternative We want to find a function in the form f(x) = y — the meaning of those are dependent on the task!

Image classification

- Data available: pairs (images, labels) from desert, beach and mountain,
- ► Input: RGB image in the form x,
- Output: predicted label y (e.g. mountain) assigned to the input image.

Anomaly detection in Credit Card transactions

- > Data available: legitimate transactions from a given client,
- Input: real-valued data including transaction location, currency, value, timestamp, in form of x,
- Output: probability y of observing a fraudulent (anomalous) transaction.

Machine Learning

A more broad area that includes DL. Algorithms aims to infer f() from a space of admissible functions given training data.

- "shallow" methods often infer a single function f(.).
- e.g. a linear function $f(x) = w \cdot x + b$,
- Common algorithms: The Perceptron, Support Vector Machines, Logistic Classifier, etc.

Machine Learning (ML) vs Deep Learning (DL)

Deep Learning

Involves learning a sequence of representations via composite functions.

Given an input x_1 several intermediate representations are produced:

 $egin{aligned} {\bf x}_2 &= f_1({f x}_1) \ {f x}_3 &= f_2({f x}_2) \ {f x}_4 &= f_3({f x}_3) \end{aligned}$

The output is achieved by several L nested functions in the form:

. . .

 $f_L(\cdots f_3(f_2(f_1(\mathbf{x}_1, W_1), W_2), W_3)\cdots, W_L),$

 W_i are hyperparameters associated with each function *i*.

A shallow linear classifier



Linear classifier for image classification

- Input: image (with N × M × 3 numbers) vectorized into column x
- Classes: cat, turtle, owl
- Output: class scores

$$\begin{array}{c} \mathbf{001} \ \mathbf{073} \\ \mathbf{227} \ \mathbf{082} \end{array} = \mathbf{x} = [1, 73, 227, 82] \end{array}$$

 $f(\mathbf{x}, W) = s \quad
ightarrow$ 3 numbers with class scores

 $\begin{aligned} & \mathcal{W}\mathbf{x} + \mathbf{b} \\ \begin{bmatrix} 0.1 & -0.25 & 0.1 & 2.5 \\ 0 & 0.5 & 0.2 & -0.6 \\ 2 & 0.8 & 1.8 & -0.1 \end{bmatrix} \times \begin{bmatrix} 1 \\ 73 \\ 227 \\ 82 \end{bmatrix} + \begin{bmatrix} -2.0 \\ 1.7 \\ -0.5 \end{bmatrix} = \begin{bmatrix} -337.3 \\ -38.6 \\ 460.30 \end{bmatrix} \end{aligned}$

Linear classifier for image classification



cat	-337.3	380.3	8.0
owl	460.3	160.3	26.3
turtle	38.6	17.6	21.8

We need:

- a loss function that quantifies undesired scenarios in the training set
- ► an **optimization algorithm** to find *W* so that the loss function is minimized!

- We want to optimize some function to produce the best classifier
- This function is often called loss function,

Let (x_i, y_i) be a training example: x_i are the features, y is the label, and f(.) a classifier that maps any x_i into a class using parameters W.

A loss for a single example is some function in the form:

$$\ell(f(W, \mathbf{x}_i), y_i) \tag{1}$$

Linear classifier for image classification

In practice, we measure the loss \mathcal{L} , over a set X, Y of N examples. Common functions are:

Mean squared error (continuous values)

$$\mathcal{L}(f(W, X, Y) = \mathcal{L}(\hat{Y}, Y) = \frac{1}{N} \sum_{i=1}^{N} (\begin{array}{c} y_i \\ y_i \end{array})^2$$

Cross entropy (bits or probability vectors)

$$\mathcal{L}\left(\hat{Y},Y
ight) = rac{1}{N}\sum_{i=1}^{N}y_i\log\hat{y}_i + (1-\hat{y}_i)\log(1-\hat{y}_i)$$

A linear classifier we would like



Minimizing the loss function

Use the slope of the loss function over the space of parameters! For each dimension j:

$$\frac{df(x)}{dx} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta}$$
$$\frac{d\ell(f(w_j, \mathbf{x}_i))}{dw_j} = \lim_{\delta \to 0} \frac{f(w_j + \delta, \mathbf{x}_i) - f(w_j, \mathbf{x}_i)}{\delta}$$

We have multiple dimensions, therefore a gradient (vector of derivatives).

We may use:

- 1. Numerical gradient: approximate
- 2. Analytic gradient: exact

Gradient descent — search for the valley of the function, moving in the direction of the negative gradient.

Changes in a parameter affects the loss (ideal example)







W	$w_i + \delta$	dwi
$\left[\begin{array}{c} 0.1,\\ -0.25,\\ 0.1,\\ 2.5,\\ 0,\\ \dots,\\ -0.1 \end{array}\right]$	$\left[\begin{array}{c} 0.1, \\ -0.25 + 0.001, \\ 0.1, \\ 2.5, \\ 0, \\ \dots, \\ -0.1 \end{array}\right]$	$\left[\begin{array}{c} -0.97, \\ 0.0, \\ , \\ , \\ , \\ , \ \end{array}\right]$
$\ell(f(W)) = 2.31298$	$\ell(f(W')) = 2.31298$	$(f(w_i+\delta)-f(w_i))/\delta$

W	$w_i + \delta$	dwi
$\left[\begin{array}{c} 0.1,\\ -0.25,\\ 0.1,\\ 2.5,\\ 0,\\ \dots,\\ -0.1 \end{array}\right]$	$\left[\begin{array}{c} 0.1,\\ -0.25,\\ 0.1+0.001,\\ 2.5,\\ 0,\\\ -0.1\end{array}\right]$	$\begin{bmatrix} -0.97, \\ 0.0, \\ +1.61, \\ -, \\ -, \ \\ - \end{bmatrix}$
$\ell(f(W)) = 2.31298$	$\ell(f(W1)) = 2.31459$	$(f(w_i+\delta)-f(w_i))/\delta$

W	$w_i + \delta$	dwi
$\left[\begin{array}{c} 0.1,\\ -0.25,\\ 0.1,\\ 2.5,\\ 0,\\ \dots,\\ -0.1 \end{array}\right]$	$\left[\begin{array}{c} 0.1,\\ -0.25,\\ 0.1,\\ 2.5,\\ 0,\\\ -0.1 \end{array}\right]$	$\begin{bmatrix} -0.93, \\ 0.0, \\ -1.61, \\ +0.02, \\ +0.5, \ \\ -3.7 \end{bmatrix}$
$\ell(f(W)) = 2.31298$	$\ell(f(W')) = 2.08720$	$(f(w_i+\delta)-f(w_i))/\delta$

It is hard to compute the gradient, when N is large.

SGD:

Approximate the sum using a **minibatch** (random sample) of instances: something between 32 and 512. Because it uses only a fraction of the data:

- ► fast
- often gives bad estimates on each iteration, needing more iterations

Neuron

- ▶ input: several values (e.g. organized in a vector)
- output: a single value x.
- each input is associated with a weight w (connection strength)
- often there is a bias value b (intercept)
- ▶ to learn is to adapt the parameters: weights w and b
- ▶ function *f*(.) is called activation function (transforms output)


Some activation functions



- Algorithm that recursively apply chain rule to compute weight adaptation for all parameters.
- Forward: compute the loss function for some training input over all neurons,
- Backward: apply chain rule to compute the gradient of the loss function, propagating through all layers of the network, in a graph structure

A simple problem: digit classification

Neural Network with Single Layer



A simple problem: digit classification

$\begin{bmatrix} x_{0,0} & x_{0,1} & x_{0,2} & \dots & x_{0,783} \\ x_{1,0} & x_{0,1} & x_{1,2} & \dots & x_{0,783} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{63,0} & x_{63,1} & x_{63,2} & \dots & x_{63,783} \end{bmatrix}.$	$\begin{bmatrix} w_{0,0} \\ w_{1,0} \\ w_{2,0} \\ \vdots \\ w_{783,0} \end{bmatrix}$	W _{0,1} W _{1,1} W _{2,1} : W _{783,1}	···· ··· ··· ···	$w_{0,9}$ $w_{1,9}$ $w_{2,9}$ \vdots $w_{783,9}$	$+ [b_0 \ b_1 \ b_2 \ \ b_9$
--	--	---	---------------------------	--	------------------------------

$$\mathbf{Y} = \text{softmax}(\mathbf{X} \cdot \mathbf{W} + \mathbf{b})$$
$$\mathbf{Y} = \begin{bmatrix} y_{0,0} & y_{0,1} & y_{0,2} & \dots & y_{0,9} \\ y_{1,0} & y_{1,1} & y_{1,2} & \dots & y_{1,9} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_{63,0} & y_{63,1} & y_{63,2} & \dots & y_{63,9} \end{bmatrix}$$

"Deep" NN with two hidden layers



$^{\prime\prime}\text{Deep}^{\prime\prime}$ NN with two hidden layers : Input



"Deep" NN with two hidden layers : Hidden layer 1



"Deep" NN with two hidden layers : Hidden layer 2



$^{\prime\prime}\text{Deep}^{\prime\prime}$ NN with two hidden layers : output



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"LeNet" architecture



New terminology:

- Convolutional layer
- Pooling
- Feature (or Activation) maps
- Fully connected (or Dense) layer

Convolutional layer





e.g. $32\times32\times3$

Filter (neuron) *w* with $P \times Q \times D$, e.g. $5 \times 5 \times 3$ (keeps depth)

Each neuron/filter performs a convolution with the input image

Centred at a specific pixel, we have, mathematically

 $w^T x + b$

Convolutional layer: local receptive field



Convolutional layer: feature maps



Convolutional layer

 Feature maps after convolution with filters followed by an activation function (e.g. ReLU) are stacked, forming a tensor.



Convolutional layer: input x filter x stride

The convolutional layer must take into account

- input size
- filter size
- convolution stride

The MNIST example: now hidden layers are conv layers





The MNIST example: now hidden layers are conv layers



Convolutional layer: zero padding

In practice, zero padding is used to avoid losing borders. Example:

- input size: 10×10
- filter size: 5×5
- convolution stride: 1
- zero padding: 2
- ▶ output: 10 × 10

General rule: zero padding size to preserve image size: (P - 1)/2Example: $32 \times 32 \times 3$ input with P = 5, s = 1 and zero padding z = 2

Output size: $(N_I + (2 \cdot z) - P)/s + 1 = (32 + (2 \cdot 2) - 5)/1 + 1 = 32$

Convolutional layer: number of parameters

Parameters in a convolutional layer is $[(P \times P \times d) + 1] \times K$:

- ▶ filter weights: $P \times P \times d$, d is given by input depth
- number of filters(neurons): K (each processes input in a different way)
- ► +1 is the bias term

Example, with an image input $32 \times 32 \times 3$:

- ▶ Conv Layer 1: P = 5, K = 8
- ▶ Conv Layer 2: P = 5, K = 16
- ▶ Conv Layer 3: *P* = 1, *K* = 32
- # parameters Conv layer 1: $[(5 \times 5 \times 3) + 1] \times 8 = 608$
- ▶ # parameters Conv layer 2: $[(5 \times 5 \times 8) + 1] \times 16 = 3216$
- ▶ # parameters Conv layer 3: $[(1 \times 1 \times 16) + 1] \times 32 = 544$

Operates over each feature map, to make the data smaller Example: max pooling with downsampling factor 2 and stride 2.





Others can be used such as average pooling

Using convolutional layer with larger strides may substitute pooling

Pooling layer

Reducing the image size allows the filter to operate in larger regions, performing multirresolution processing.



Example: reducing image while fixing 5×5 filter.

Convolutional layer: convolution + activation + pooling



- ► Convolution: as seen before
- Activation: ReLU
- Pooling: maxpooling

Dense layers and output



Dense of fully connected (FC) layer:

- ► As in a regular Multilayer Perceptron
- A neuron operates over all values of previous layer

Output (also dense) layer:

each neuron represents a class of the problem

Visualization





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AlexNet (Krizhevsky, 2012)

- ▶ 60 million parameters.
- ▶ input 224 × 224
- conv1: K = 96 filters with $11 \times 11 \times 3$, stride 4,
- conv2: K = 256 filters with $5 \times 5 \times 48$,
- conv3: K = 384 filters with $3 \times 3 \times 256$,
- conv4: K = 384 filters with $3 \times 3 \times 192$,
- conv5: K = 256 filters with $3 \times 3 \times 192$,
- ▶ fc1, fc2: K = 4096.



VGG 19 (Simonyan, 2014)

- ► +layers, -filter size = less parameters
- ▶ input 224 × 224,
- ▶ filters: all 3 × 3,
- ▶ conv 1-2: K = 64 + maxpool
- ▶ conv 3-4: K = 128 + maxpool
- ▶ conv 5-6-7-8: K = 256 + maxpool
- ▶ conv 9-10-11-12: *K* = 512 + maxpool
- ▶ conv 13-14-15-16: K = 512 + maxpool
- ▶ fc1, fc2: *K* = 4096



GoogLeNet (Szegedy, 2014)

- 22 layers
- Starts with two convolutional layers
- Inception layer ("filter bank"):
 - filters 1×1 , 3×3 , $5 \times 5 + \max$ pooling 3×3 ;
 - reduce dimensionality using 1×1 filters.
 - 3 classifiers in different parts
- Blue = convolution,
- Red = pooling,
- Yellow = Softmax loss fully connected layers
- Green = normalization or concatenation



GoogLeNet: inception module



- $\blacktriangleright~1\times 1$ convolution reduces the depth of previous layers by half
- this is needed to reduce complexity (e.g. from 256 to 128 d)
- concatenates 3 filters plus an extra max pooling filter (because).

Inception modules (V2 and V3)

multiple 3×3 convs. flattened conv.

decrease size









Residual Network — ResNet (He et al, 2015)

Reduces number of filters, increases number of layers (34-1000). **Residual** architecture: add identity before activation of next layer.



Comparison



Thanks to Qingping Shan www.qingpingshan.com

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Guidelines for training Learning guarantees and alternatives
Batch Stochastic Gradient Descent

- Mini-batch size: default is around 16, but more might be used to speed-up.
- Loss, validation and training error: plot values for each epoch or for each number of iterations.
- Learning rate: adjust learning rate with *decay*, for smoother convergence.

Learning rate: fixed small step



w

Learning rate: large step



w

Learning rate: decaying step



w

Examples of Optimizers

- regular SGD: widely used, need to define proper learning rate and decaying,
- RMSProp: which employ the concept of momentum (next gradients depend on previous ones)
- Adam: that estimate the learning rate based on the current and previous gradient values

Convergence and training set

- Clean data: cleaniness of the data is very important (each class must be well defined, low rate of label errors),
- Data augmentation: generate new examples by perturbation of existing ones (e.g. noise, affine transformations),

Regularization: on loss functions

$$\ell(W) = \frac{1}{N} \sum_{i=1}^{N} \ell_i(x_i, y+i, W) + \frac{1}{\lambda R(W)}$$
$$\nabla_W \ell(W) = \frac{1}{N} \sum_{i=1}^{N} \nabla_W \ell_i(x_i, y+i, W) + \lambda \nabla_W R(W)$$

Regularization will help the model to keep it simple. Possible methods:

•
$$L2 : R(W) = \sum_i \sum_j W_{i,j}^2$$

• $L1 : R(W) = \sum_i \sum_j |W_{i,j}|$

Alternative methods that help convergence and prevent overfitting

- Dropout: randomly turn off a percentage of the neurons during *training*.
 - activation of some neurons are randomly set to zero at every iteration,
 - ► can be seen as to "bootstrap" (statistics technique) training,
 - prevents memorization.

Alternative methods that help convergence and prevent overfitting

- ▶ Batch normalization: z-score normalization over all data
 - subtract the mean, divide by the standard deviation of all batch examples,
 - performed before/after layer processing.
 - for deep nets, it is employed before every block (e.g. residual block, inception block, etc.),

Errors when defining the space of admissible functions



Errors when defining the space of admissible functions



Important stuff to look into...

- Are n training examples enough to ensure learning in a given CNN architecture?
- \blacktriangleright Minimum sample size to ensure convergence within some numerical threshold γ
- Generalisation bound given some probability error δ

Marcus (2018) in Deep Learning: a critical appraisal: "... systems that rely on deep learning frequently have to generalize beyond specific data ... the ability of formal proofs to guarantee high-quality performance is more limited." CNNs are easily fooled: adversarial examples can be created to attack or break the model



Zhang et al (2017)

"... our experiments establish that state-of-the-art convolutional networks (...) trained with stochastic gradient methods *easily fit a random labeling* of the training data."

UNDERSTANDING DEEP LEARNING REQUIRES RE-THINKING GENERALIZATION

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Abstract

Despite their massive size, successful deep artificial neural networks can exhibit a

Pre-trained Neural Networks

- Fine-tuning
- Off-the-shelf feature extraction

Finetuning

Classification (finetuning)

 Data similar to ImageNet: freeze most Conv Layers, train output (or other) top layers from scratch



 Data unsimilar to ImageNet: freeze lower Conv Layers, train output and intermediate layers from scratch



Guidelines for new data

Feature extraction for image classification and retrieval

- Input data and get activation values of higher Conv and/or dense layers
- Apply some dimensionality reduction: e.g. PCA, Product Quantization, etc. after extraction
- ► Use external classifier: e.g. SVM, Random Forest, etc.



- Deep Learning is not a panacea;
- Low interpretability;
- There are important concerns about generalization of Deep Networks;
- However those methods can be really useful for finding representations;
- Many challenges and research frontiers for more complex tasks.

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