Foundations of modern NN

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¹More content at https://erwanscornet.github.io/, Teaching section.

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 - Hyperparameters
- 2 MLP Regularization
 - Dropout
 - Batch normalization
 - Early stopping
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 - Convolution layer
 - Pooling layer
 - A variety of CNNs
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- Foundations of RNN
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 - GRU and LSTM
 - Truncated backpropagation
 - A RNN application



Supervised learning





Outline

Neural Network - MLP

- Architecture
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McCulloch and Pitts neuron - 1943

["A logical calculus of the ideas immanent in nervous activity", McCulloch and Pitts 1943]

In 1943, portrayed with a simple electrical circuit by neurophysiologist Warren McCulloch and mathematician Walter Pitts.

A McCulloch-Pitts neuron takes binary inputs, computes a weighted sum and returns 0 if the result is below threshold and 1 otherwise.



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Donald Hebb took the idea further by proposing that neural pathways strengthen over each successive use, especially between neurons that tend to fire at the same time.

[The organization of behavior: a neuropsychological theory, Hebb 1949]

Neural network with one hidden layer



Generic notations:

- $W_{i,j}^{(\ell)}$: weights between the *j* neuron in the $\ell 1$ layer and the *i* neuron of the ℓ layer.
- $b_j^{(\ell)}$: bias of the *j* neuron of the ℓ layer.
- $a_j^{(\ell)}$: output of the *j* neuron of the ℓ layer.
- $z_j^{(\ell)}$: input of the *j* neuron of the ℓ layer, such that $a_j^{(\ell)} = \sigma(z_j^{(\ell)})$.

How to find weights and bias?



Optimization

Gradient descent algorithm

The gradient of a function $f : \mathbb{R}^p \to \mathbb{R}$ in θ denoted as $\nabla f(\theta)$ is the vector of partial derivatives

$$\nabla f(\theta) = \begin{pmatrix} \frac{\partial f}{\partial \theta_1} \\ \vdots \\ \frac{\partial f}{\partial \theta_p} \end{pmatrix}$$

Gradient descent

- Initialize $\theta^{(0)}$ and t = 0.
- While not convergence do

$$\bullet \ \theta^{(t+1)} = \theta^{(t)} - \eta \nabla f(\theta^{(t)})$$

$$t = t + 1.$$

Gradient Descent Algorithm

- The prediction of the network is given by $f_{\theta}(\mathbf{x})$.
- Empirical risk minimization on a batch $B \subset \{1, ..., n\}$: Solve $\underset{\theta}{\operatorname{argmin}} R_B(\theta)$ with $R_B(\theta) = \frac{1}{|B|} \sum_{i \in B} \ell(Y_i, f_{\theta}(\mathbf{X}_i)).$
- Computationally more efficient than using the full data set.

Stochastic Gradient descent

- Divide the data set into batches B₁,..., B_{iter}
- ▶ Initialize $\theta^{(0)}$ and t = 0.
- While not convergence do
 - * $\ell = t[iter]$
 - $\star \ \theta^{(t+1)} = \theta^{(t)} \eta \nabla R_{B_{\ell}}(\theta^{(t)})$
 - * t = t + 1

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 - * t = t + 1

How to compute $\nabla_{\theta} \ell_i$ efficiently?

Backprop Algorithm

How to compute $\nabla_{\theta} \ell_i$ efficiently?

A Clever Gradient Descent Implementation

- Popularized by Rumelhart, McClelland, Hinton in 1986.
- Can be traced back to Werbos in 1974.
- Nothing but the use of chain rule derivation with a touch of dynamic programing.
- Key ingredient to make the Neural Networks work!
- Still at the core of Deep Learning algorithm.

Backpropagation idea



Backpropagation equations

Neural network with L layers, with vector output, with quadratic cost

$$C = \frac{1}{2} \|y - a^{(L)}\|^2.$$

By definition,

$$\delta_j^{(\ell)} = \frac{\partial C}{\partial z_j^{(\ell)}}.$$

The four fundamental equations of backpropagation are given by

$$\delta^{(L)} = \nabla_a C \odot \sigma'(z^{(L)}), \tag{1}$$

$$\delta^{(\ell)} = \left(\left(w^{(\ell+1)} \right)^{\mathsf{T}} \delta^{(\ell+1)} \right) \odot \sigma'(z^{(\ell)}) \tag{2}$$

$$\frac{\partial C}{\partial b_i^{(\ell)}} = \delta_j^{(\ell)} \tag{3}$$

$$\frac{\partial C}{\partial w_{j,k}^{(\ell)}} = a_k^{(\ell-1)} \delta_j^{(\ell)}.$$
(4)

Backpropagation Algorithm

Let

$$\delta_j^{(\ell)} = \frac{\partial C}{\partial z_j^{(\ell)}},$$

where $z_j^{(\ell)}$ is the entry of the neuron *j* of the layer ℓ .

Neural network training

(a) Initialize randomly the weights and biases in the network.

(b) For all training samples $(x_i)_{i \in B}$ in the batch B,

- Feedforward: Send all samples of the batch through the network and store the values of activation function and its derivative, for each neuron.
- **Output loss:** Compute the neural network loss average on all samples of the batch.
- **O** Backpropagation (BP): Compute recursively the vectors $\delta^{(\ell)}$ starting from $\ell = L$ to $\ell = 1$ with BP equations (1) and (2). Compute the gradient with BP equations (3) and (4).
- **Optimization:** Update the weights and biases using a gradient-based optimization procedure, using the gradient previously computed.

(c) Repeat step (b) until some convergence criterion is reached.

Playing with neural network: http://playground.tensorflow.org/

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What to set in a neural network?



What to set in a neural network?



Number of hidden layers/neurons

- No particular rules for choosing the number of layers or the number of neurons per layer.
- Read research papers related to the task you want to solve and test the architecture they propose.
- You may want to change the architecture a bit to see how it influences the performance.
- Beware: there exist many rules of thumbs which are not supported by evidence (either practical or theoretical).
- Use data-driven strategies:
 - Network pruning following the procedure training/pruning/training/pruning/...
 ["What is the state of neural network pruning?", Blalock et al. 2020]
 - More complex evolutionary algorithms
 ["AgEBO-Tabular: Joint Neural Architecture and Hyperparameter Search with Autotuned Data-Parallel Training for
 Tabular Data", Egele et al. 2020]

Sigmoid activation function



Figure: Sigmoid activation function $\boldsymbol{\sigma}$

$$\sigma: x \mapsto \frac{\exp(x)}{1 + \exp(x)}$$

Comments:

- Saturated function due to horizontal asymptotes:
 - Gradient is close to zero in these two areas (±∞)
 - Rescaling the inputs of each layer can help to avoid these areas.
- Sigmoid is not a zero-centered function
 - Rescaling data
- Computing exp(x) is a bit costly

Rectified Linear Unit (ReLU)



Figure: Rectified Linear Unit (ReLU)

$ReLU: x \mapsto max(0, x)$

Comments:

- $\bullet~$ Not a saturated function in $+\infty$
- But saturated (and null!) in the region $x \le 0$
- Computationally efficient
- Empirically, convergence is faster than sigmoid/tanh.
- Plus: biologically plausible

More on ReLU

The idea of ReLU in neural networks seems to appear in ["Cognitron: A self-organizing multilayered neural network"; "Neocognitron: A self-organizing neural network model for a mechanism of visual pattern recognition", Fukushima 1975; Fukushima and Miyake 1982].



Figure: Good parameter initialization - ReLU is active



Figure: Bad parameter initialization - ReLU outputs zero

ReLU output can be zero but positive initial bias can help.

Related to biology ["Deep sparse rectifier neural networks", Glorot, Bordes, et al. 2011]:

- Most of the time, neurons are inactive.
- when they activate, their activation is proportional to their input.

Output units

• Linear output unit:

$$\hat{y} = W^T h + b$$

 \rightarrow Linear regression based on the new variables *h*.

- Sigmoid output unit, used to predict $\{0, 1\}$ outputs: $\mathbb{P}(Y = 1|h) = \sigma(W^T h + b),$ where $\sigma(t) = e^t/(1 + e^t)$.
 - \rightarrow Logistic regression based on the new variables h.
- Softmax output unit, used to predict $\{1, \dots, K\}$: softmax $(z)_i = \frac{e^{z_i}}{\sum_{i=1}^{K} e^{z_k}}$

where, each z_i is the activation of one neuron of the previous layer, given by $z_i = W_i^T h + b_i$.

 \rightarrow Multinomial logistic regression based on the new variables *h*.

Cost functions

• Mean Square Error (MSE)

$$\frac{1}{n}\sum_{i=1}^{n}\ell(Y_i,f_{\theta}(\mathbf{X}_i)) = \frac{1}{n}\sum_{i=1}^{n}(Y_i-f_{\theta}(\mathbf{X}_i))^2$$

Mean Absolute Error

$$\frac{1}{n}\sum_{i=1}^{n}\ell(Y_i,f_{\theta}(\mathbf{X}_i)) = \frac{1}{n}\sum_{i=1}^{n}|Y_i - f_{\theta}(\mathbf{X}_i)|$$

• Cross entropy (or negative log-likelihood):

$$\ell(y_i, f_{\theta}(\mathbf{x}_i)) = -\log\left([f_{\theta}(\mathbf{x}_i)]_{y_i}\right)$$
(5)

Prevent saturation phenomenon:

$$-\log(\mathbb{P}(Y=y_i|\mathbf{X}=\mathbf{x}_i)) = -\log(\sigma((2y-1)(W^Th+b))), \tag{6}$$

with

$$\sigma(t) = \frac{e^t}{1+e^t}$$

Usually, saturation occurs when $(2y-1)(W^Th+b) \ll -1$. In that case, $-\log(\mathbb{P}(Y = y_i|X))$ is linear in W and b which makes the gradient easy to compute, and the gradient descent easy to implement.

Weight initialization

Idea: the variance of the input should be the same as the variance of the output.

Let w_j be any weight between layer j and layer j + 1.

He et al. initialization

["Delving deep into rectifiers: Surpassing human-level performance on imagenet classification", He et al. 2015] Initialize bias to zero and weights randomly using

$$w_j \sim \mathcal{N}\left(0, rac{\sqrt{2}}{n_j}
ight),$$

where n_j is the size of layer j.

Avier initialization

["Understanding the difficulty of training deep feedforward neural networks", Glorot and Bengio 2010] Initialize bias to zero and weights randomly using

$$w_j \sim \mathcal{U}\left[-rac{\sqrt{6}}{\sqrt{n_j+n_{j+1}}},rac{\sqrt{6}}{\sqrt{n_j+n_{j+1}}}
ight],$$

where n_j is the size of layer j \rightarrow Not theoretically valid for ReLU

Bonus: ["All you need is a good init", Mishkin and Matas 2015]

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Regularizing to avoid overfitting



Avoid overfitting by imposing some constraints over the parameter space.

Reducing variance and increasing bias.

Overfitting

Many different manners to avoid overfitting:

- Penalization (L1 or L2) Replacing the cost function \mathcal{L} by $\tilde{\mathcal{L}}(\theta, X, y) = \mathcal{L}(\theta, X, y) + \text{pen}(\theta)$.
- Soft weight sharing see CNN lecture Reduce the parameter space artificially by imposing explicit constraints.
- Dropout

Randomly kill some neurons during optimization and predict with the full network.

- Batch normalization Renormalize a layer inside a batch, so that the network does not overfit on this particular batch.
- Early stopping Stop the gradient descent procedure when the error on the validation set increases.

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Dropout



Dropout refers to dropping out units (hidden and visible) in a neural network, i.e., temporarily removing it from the network, along with all its incoming and outgoing connections.

Each unit is independently dropped with probability

- p = 0.5 for hidden units
- $p \in [0, 0.5]$ for input units, usually p = 0.2.

["Improving neural networks by preventing co-adaptation of feature detectors", Hinton, N. Srivastava, et al. 2012]

Dropout



Dropout algorithm

Training step. While not convergence

Inside one epoch, for each mini-batch of size m,

- Sample *m* different mask. A mask consists in one Bernoulli per node of the network (inner and entry nodes but not output nodes). These Bernoulli variables are *i.i.d.*. Usually
 - \star the probability of selecting an hidden node is 0.5
 - ★ the probability of selecting an input node is 0.8
- For each one of the *m* observation in the mini-batch,
 - ★ Do a forward pass on the masked network
 - ★ Compute backpropagation in the masked network
 - ★ Compute the average gradient
- O Update the parameter according to the usual formula.

Prediction step.

Use all neurons in the network with weights given by the previous optimization procedure, times the probability p of being selected (0.5 for inner nodes, 0.8 for input nodes).
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Batch normalization

The network converges faster if its input are scaled (mean, variance) and decorrelated. ["Efficient backprop", LeCun, Bottou, Orr, et al. 1998]

Hard to decorrelate variables: requiring to compute covariance matrix.

["Batch normalization: Accelerating deep network training by reducing internal covariate shift", loffe and Szegedy 2015]

Ideas:

- Improving gradient flows
- Allowing higher learning rates
- Reducing strond dependence on initialization
- Related to regularization (maybe slightly reduces the need for Dropout)

Algorithm

See ["Batch normalization: Accelerating deep network training by reducing internal covariate shift", loffe and Szegedy 2015]

• For every neuron k in the first layer, which outputs $x_i^{(k)}$ for the *i*th observation,

$$\begin{aligned}
\mathbf{\Phi} \quad \mu_{B}^{(k)} &= \frac{1}{m} \sum_{i=1}^{m} x_{i}^{(k)} \\
\mathbf{\Phi} \quad \sigma_{B,k}^{2} &= \frac{1}{m} \sum_{i=1}^{m} (x_{i}^{(k)} - \mu_{B}^{(k)})^{2} \\
\mathbf{\Phi} \quad \hat{x}_{i}^{(k)} &= \frac{x_{i}^{(k)} - \mu_{B}^{(k)}}{\sqrt{\sigma_{B,k}^{2} + \varepsilon}} \\
\mathbf{\Phi} \quad y_{i}^{(k)} &= \gamma^{(k)} \hat{x}_{i}^{(k)} + \beta^{(k)} \equiv BN_{\gamma^{(k)},\beta^{(k)}}(x_{i}^{(k)})
\end{aligned}$$

2 $y_i^{(k)}$ is fed to the next layer and the procedure iterates.

- Backpropagation is performed on the network parameters including (γ^(k), β^(k)) for all k = 1,..., H₁, where H₁ ∈ N is the number of neurons in the first layer.
- For inference, compute the average over many training batches \mathcal{B} of size m: $\mathbb{E}_{\mathcal{B}}[x^{(k)}] = \mathbb{E}_{\mathcal{B}}[\mu_{\mathcal{B}}^{(k)}] \text{ and } \mathbb{V}_{\mathcal{B}}[x^{(k)}] = \frac{m}{m-1}\mathbb{E}_{\mathcal{B}}[\sigma_{\mathcal{B},k}^2].$

③ For inference, replace every function $x^{(k)} \mapsto BN_{\gamma^{(k)},\beta^{(k)}}(x^{(k)})$ in the network by

$$\mathbf{x}^{(k)} \mapsto \gamma \left(\frac{\mathbf{x}^{(k)} - \mathbb{E}_{\mathcal{B}}[\mathbf{x}^{(k)}]}{\sqrt{\mathbb{V}_{\mathcal{B}}[\mathbf{x}^{(k)}] + \varepsilon}} \right) + \beta^{(k)}.$$

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Early stopping

Idea:

- Store the parameter values that lead to the lowest error on the validation set
- Return these values rather than the latest ones.



Early stopping algorithm

Parameters:

- patience *p* of the algorithm: number of times to observe no improvement on the validation set error before giving up;
- the number of steps *n* between evaluations.

How to implement early stopping?

- First idea: use early stopping to determine the best number of iterations *i*^{*} and train on the whole data set for *i*^{*} iterations.
- Second idea: use early stopping to determine the best parameters and the training error at the best number of iterations. Starting from θ^* , train on the whole data set until the error matches the previous early stopping error.

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Neural Network reborn

Renewed interest in 2006: ["A fast learning algorithm for deep belief nets", Hinton, Osindero, et al. 2006] Propose a way to train deep neural nets:

- Train the first layer.
- Add a layer on top of it and train only this layer.
- Repeat the process until the network is deep enough.
- Use this network as a warm start to train the whole network.

Technical reasons for this new growing interest:

- Larger datasets
- More powerful computers
- Small number of algorithmic changes
 - MSE replaced by cross-entropy
 - ReLU (Fukushima, 1975, 1980)

Using classical networks for images?

No, for two reasons:

- Do not take into account the spatial organization of pixels (if the pixels are permuted, the output of the network would be the same, whereas the image would change drastically)
- Non robust to image shifting

Idea:

- Apply local transformation to a set of nearby pixels (spatial nature of image is used)
- Repeat this transformation over the whole image (resulting in a shift-invariant output)

Not a new idea: trace back to perceptron and studies about the visual cortex of a cat. The cat is able to

- detect oriented edges, end-points, corners (low-level features)
- combine them to detect more complex geometrical forms (high-level features)

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Convolutional neural networks (CNNs)

- Neural networks that use convolution instead of matrix product in one of the layers
- A CNN layer typically includes 3 operations: convolution, activation and pooling
- Using the more general idea of **parameters sharing**, instead of **full connection** (convolution instead of matrix product)

Convolution operator in neural networks is as follows

$$O(i,j) = (I \star K)(i,j) = \sum_{k} \sum_{l} I(i+k,j+l)K(k,l)$$

- I is the input and K is called the kernels
- The kernel K will be learned (replaces the weights W in a fully connected layer)

• Size of the input image is $8 \times 8 \times 1$ (height, width, depth)



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- \bullet Size of the kernel is $3\times 3\times 1$





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- \bullet Size of the kernel is $3\times3\times1$



Convolution - RGB

- Size of the input image is $8 \times 8 \times 3$ (height, width, depth)
- \bullet Size of the kernel is $3\times 3\times 3$



Warning: every filter is small spatially (along width and height), but extends through the full depth of the input volume.

Convolution - RGB

- Size of the input image is $8 \times 8 \times 3$ (height, width, depth)
- \bullet Size of the kernel is $3\times3\times3$



Warning: every filter is small spatially (along width and height), but extends through the full depth of the input volume.

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Parameters of convolutional layer 1/4

Four hyperparameters control the size of the output volume: the kernel size, the depth of the output volume, the stride and the zero-padding.

• The size of the kernel (typically 3×3 , 5×5).



Parameters of convolutional layer 2/4

Four hyperparameters control the size of the output volume: the kernel size, the depth of the output volume, the stride and the zero-padding.

- The size of the kernel,
- The depth of the output volume, i.e., the number of filters/activation maps/feature maps.



Parameters of convolutional layer 3/4

Four hyperparameters control the size of the output volume: the kernel size, the depth of the output volume, the stride and the zero-padding.

- The size of the kernel,
- The depth of the output volume,
- The stride, i.e., of how many pixels do we move the filter horizontally and vertically. Usually, stride is equal to one (rarely to two, and even more rarely larger).



Parameters of convolutional layer 4/4

Four hyperparameters control the size of the output volume: the kernel size, the depth of the output volume, the stride and the zero-padding.

- The size of the kernel,
- The depth of the output volume,
- The stride,
- The size of the zero-padding, i.e. the number of zeros we add to the borders of the image. This can be used to obtain a constant image size between the input and the output.



How to choose zero-padding?

Let

- *I* the height/width of the input
- *O* the height/width of the output
- P the size of the zero-padding
- *K* the height/width of the filter
- S the stride

What is the relation between these quantities? How do we choose the zero-padding to obtain an output of the same size as the input?

How to choose zero-padding?

Let

- *I* the height/width of the input
- O the height/width of the output
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- *K* the height/width of the filter
- *S* the stride

What is the relation between these quantities? How do we choose the zero-padding to obtain an output of the same size as the input?

$$O = \left\lfloor \frac{2P + I - K}{S} \right\rfloor + 1$$

Why convolution?

- Same transformation applied to all parts of the image (takes into account the spatial dependence between pixels and object-shift invariance)
- Input image contains millions of pixel values, but we want to detect small meaningful features such as edges with kernels that use only few hundred of pixels
- When using a matrix product, all input and output units are connected, whereas convolution connects only output neurons with several pixels of the input image.

Convolution involves weight sharing (a form of regularization) and requires less parameters which improves memory, is more statistically efficient and computationally faster.

Sparse connections



- Left: when using matrix multiplication, all outputs are connected to all inputs. We say that **connectivity is dense**
- Right: in a convolution with a kernel of width 3, only three outputs are affected by the input x. We say that the **connectivity is sparse**

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Pooling

The Pooling Layer operates independently on every depth slice of the input and resizes it spatially, using the max function.



Parameters:

- Stride S = 2
- Spatial extend F = 2

Usually, S = F = 2 and more rarely F = 3, S = 2 (overlapping pooling).

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The Pooling Layer operates independently on every depth slice of the input and resizes it spatially, using the max function.



Parameters:

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Parameters:

- Stride S = 2
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- Pooling layers compute each pixel of the output as a summary statistic of neighboring input pixels at the corresponding location.
- The most widely used is the max aggregation, called max-pooling
- Pooling helps the representation to become approximately invariant to small translations of the input
- If a small translation is applied, output of the layer is almost unchanged
- Very useful if we care more about the presence of some feature than its position in the image: for face detection (presence of eyes is more important than where they are)
- Pooling also allows to handle inputs with different sizes: pictures can have different sizes, but the output classification layer must be of fixed size































A possible architecture of a CNN



A convolutional layer operates on the feature maps output by the pooling layer. Each kernel is a volume whose depth equals the depth of the input volume.



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At the end of the network, the feature maps are flattened in order to apply a classic neural networks.



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The full architecture is summarized below.



Outline

- Neural Network MLP
 - Architecture
 - Hyperparameters
- 2 MLP Regularization
 - Dropout
 - Batch normalization
 - Early stopping

3 Foundations of CNN

- Convolution layer
- Pooling layer
- A variety of CNNs
- Applications

4 Foundations of RNN

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- A RNN application

CNN Taxonomy



See this very detailed review paper ["A survey of the recent architectures of deep convolutional neural networks", Khan et al. 2020]

Comparison of several CNN



["An analysis of deep neural network models for practical applications", Canziani et al. 2016]

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Pose estimation - Deeppose

["Deeppose: Human pose estimation via deep neural networks", Toshev and Szegedy 2014]



Action recognition

["Actions and attributes from wholes and parts", Gkioxari et al. 2015]



Object detection - Exhaustive search vs segmentation

Bottom-up grouping generates hierarchical nested partitioning of the input image.

["Mean shift: A robust approach toward feature space analysis"; "Efficient graph-based image segmentation", Comaniciu and Meer 2002; Felzenszwalb and Huttenlocher 2004]



Object detection - R-CNN - Regions with CNN features

One of the most famous object proposal based CNN detector is Region-based CNN (R-CNN) by Girshick, Jeff Donahue, et al. 2014, aiming at

- localizing objects with a deep network
- training a high-capacity model with only a small quantity of annotated detection data



- Generating category-independent region proposals via selective search.
- Training large CNN that extracts a fixed-length feature vector from each region (Supervised pre-training on the large auxiliary dataset ILSVRC, followed by domainspecific fine-tuning on the small dataset PASCAL).
- Learning a set of class- specific linear SVMs.

Object detection - R-CNN - Regions with CNN features



YOLO

["You only look once: Unified, real-time object detection", Redmon et al. 2016]

The whole detection pipeline is a single network which predicts bounding boxes and class probabilities from the full image in one evaluation, and can be optimized end-to-end directly on detection performance.



Drawback Fails to detect small numerous objects.

Figure 2: The Model. Our system models detection as a regression problem. It divides the image into an $S \times S$ grid and for each grid cell predicts *B* bounding boxes, confidence for those boxes, and *C* class probabilities. These predictions are encoded as an $S \times S \times (B * 5 + C)$ tensor.

YOLO



Videos

Object tracking They propose a target-specific CNN for object tracking, where the CNN is trained incrementally during tracking with new examples obtained online. They employ a candidate pool of multiple CNNs as a data-driven model of different instances of the target object.

["Deeptrack: Learning discriminative feature representations online for robust visual tracking", Li et al. 2016] https://pjreddie.com/darknet/yolo/

Pose/Action recognition They use the two stream CNN (spatial /temporal) on the localized parts of the human body and show the aggregation of part-based local CNN descriptors can effectively improve the performance of action recognition.

["P-cnn: Pose-based cnn features for action recognition", Chéron et al. 2015]

["End-to-end learning of deformable mixture of parts and deep convolutional neural networks for human pose estimation",

W. Yang et al. 2016]

https://www.youtube.com/watch?v=MKVvQK8FawE

["Segnet: A deep convolutional encoder-decoder architecture for image segmentation", Badrinarayanan et al. 2015] https://www.youtube.com/watch?v=CxanE_W46ts

["Realtime multi-person 2d pose estimation using part affinity fields", Cao et al. 2016] https://www.youtube.com/watch?v=pW6nZXeWlGM

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RNNs offer a lot of variability



RNNs offer a lot of variability



- Vanilla Neural Networks
- Image Captioning: image/sequence of words
- Sentiment classification: sequence of words/sentiment
- Translation: sequence of words/sequence of words
- Video classification on frame level: sequence of images/sequence of labels

RNNs offer a lot of variability



- ANNs can't deal with sequential or "temporal" data
- ANNs lack memory
- ANNs have a fixed architecture: fixed input size and a fixed output size
- RNNs are more "biologically realistic" because of recurrent connectivities found in the visual cortex of the brain

Definition of RNN

- \bullet Input layer Data comes sequentially: $\textbf{x}_1, \textbf{x}_2, \ldots$
- Hidden Layer Hidden state of the network at time t: \mathbf{h}_t
- Output layer For the input x_t , the prediction is given by \hat{y}_t



Definition of RNN



Hidden neuron:

$$\mathbf{h}_t = \tanh(W_{HH}\mathbf{h}_{t-1} + W_{IH}\mathbf{x}_t + \mathbf{b}_h)$$

Output neuron:

$$\hat{y}_t = \operatorname{softmax}(W_{HO}\mathbf{h}_t + \mathbf{b}_{out})$$

Deep RNN



(c) Hidden to hidden and output.

y,



(d) Stack of hidden states.

Bi-directional RNN



Figure: bi-directional recurrent neural network (BRNN)

$$\mathbf{y}_t = W_{\overrightarrow{HO}} \overrightarrow{\mathbf{h}_t} + W_{\overleftarrow{HO}} \overleftarrow{\mathbf{h}_t} + \mathbf{b}_o$$

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The backpropagation equation is given by

$$\frac{\partial L_{T}}{\partial W_{HH}} = \frac{\partial L_{T}}{\partial \hat{y}_{T}} \sum_{k=1}^{T} \frac{\partial \hat{y}_{T}}{\partial \mathbf{h}_{T}} \Big(\prod_{m=k+1}^{T} \frac{\partial \mathbf{h}_{m}}{\partial \mathbf{h}_{m-1}} \Big) \frac{\partial \mathbf{h}_{k}}{\partial W_{HH}}$$

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Improving hidden units in RNN

Output gate (for reading) $\mathbf{o}_t = \sigma(W_{o,h}\mathbf{h}_{t-1} + W_{o,x}\mathbf{x}_t + \mathbf{b}_o)$

Input gate (for writing) $\mathbf{i}_t = \sigma(W_{i,h}\mathbf{h}_{t-1} + W_{i,x}\mathbf{x}_t + \mathbf{b}_i)$ Forget gate (for remembering) $\mathbf{f}_t = \sigma(W_{f,h}\mathbf{h}_{t-1} + W_{f,x}\mathbf{x}_t + \mathbf{b}_f)$

Candidate hidden state. $\tilde{\mathbf{h}}_t = \tanh(W_h(\mathbf{o}_t \odot \mathbf{h}_{t-1}) + W_x \mathbf{x}_t + \mathbf{b})$

The final state \mathbf{h}_t is given by

$$\mathbf{h}_t = \mathbf{f}_t \odot \mathbf{h}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{h}}_t.$$

Warning: the forget gate is used for forgetting, but it actually operates as a remember gate: 1 in a forget gate means remembering everything not forgetting everything.

Improving hidden units in RNN: failure

The previous hidden units described by

$$\mathbf{h}_t = \mathbf{f}_t \odot \mathbf{h}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{h}}_t$$

fail.

Two problems:

- The forget gate and the input gate are not synchronized at the beginning of the training, which can cause the hidden states to become large and unstable.
- Since the hidden state is not bounded, the gates can be saturated, which implies difficulties to train the network.

Empirical evidence:

["LSTM: A search space odyssey", Greff et al. 2017]

Gated Recurrent Unit

One way to circumvent this issue is to specify explicitly the dependence structure between the forget gate and the writing gate.

For example, we can set the forget gate to 1 minus the writing gate:

$$\mathbf{h}_t = (1 - \mathbf{i}_t) \odot \mathbf{h}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{h}}_t.$$

In that case, the new hidden state h_t is a weighted average of the previous hidden state h_{t-1} and the newly created candidate \tilde{h}_t .

Consequently, \mathbf{h}_t is bounded if \mathbf{h}_{t-1} and $\tilde{\mathbf{h}}_t$ are, which is the case using bounded activation functions.

This is exactly the Gated Recurrent Unit.

Gated Recurrent Unit





Reset gate (read gate) $\mathbf{r}_t = \sigma(W_{r,b}\mathbf{h}_{t-1} + W_{r,x}\mathbf{x}_t + \mathbf{b}_r)$

Update gate (forget gate) $\mathbf{z}_t = \sigma(W_{z,h}\mathbf{h}_{t-1} + W_{z,x}\mathbf{x}_t + \mathbf{b}_z)$ Candidate hidden state $\tilde{\mathbf{h}}_t = \tanh(W_h(\mathbf{r}_t \odot \mathbf{h}_{t-1}) + W_x \mathbf{x}_t + \mathbf{b})$

 $\begin{array}{l} \mathsf{Hidden \ state} \\ \mathbf{h}_t = \mathbf{z}_t \odot \mathbf{h}_{t-1} + (1 - \mathbf{z}_t) \odot \tilde{\mathbf{h}}_t \end{array}$

Long Short Term Memory (LSTM)

LSTM is another way to circumvent the issue of unboundedness of internal states. ["Long short-term memory", Hochreiter and Jürgen Schmidhuber 1997]



LSTM equations:

$$\begin{split} \mathbf{i}_t &= \sigma(W_{i,h}\mathbf{h}_{t-1} + W_{i,x}\mathbf{x}_t + b_i) \\ \mathbf{o}_t &= \sigma(W_{o,h}\mathbf{h}_{t-1} + W_{o,x}\mathbf{x}_t + b_o) \\ \mathbf{f}_t &= \sigma(W_{f,h}\mathbf{h}_{t-1} + W_{f,x}\mathbf{x}_t + b_f) \\ \mathbf{g}_t &= \tanh(W_{g,h}\mathbf{h}_{t-1} + W_{g,x}\mathbf{x}_t + b_g) \end{split}$$

$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \mathbf{g}_t$$

Hidden state

$$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{c}_t)$$

The prediction of the network at time t only depends on \mathbf{h}_t and not on \mathbf{c}_t .

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Backpropagation



Problem: one gradient step is too costly. It requires a pass through the entire data set.

Truncated backpropagation



Choose a small number of steps (usually 100) and back-propagate only onto these data.

Truncated backpropagation



Propagate the weights and use backpropagation on the second batch of data.

Truncated backpropagation



Pursue...

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Image Captioning: Neural Image Caption

["Show and tell: A neural image caption generator", Vinyals et al. 2015]



Image Captioning: Neural Image Caption



Aim:

$$heta^{\star} \in rgmax_{ heta} \sum_{(l,S)} \log(p(S|l))$$

where I is the input image and S the sentence describing the image. Since the sentence length can be arbitrary long, the log probability is rewritten as

$$\log(p(S|I)) = \sum_{t=0}^{N} p(S_t|I, S_0, \dots, S_{t-1}).$$

Image Captioning: Neural Image Caption

Inference time. Two approaches:

- Sampling: sample the first word using p_1 then use this word as input to sample the second word according to p_2 . Repeat the process until the network produces a stop word.
- BeamSearch: Choose the k best sentences of length t then use this set to generate the k best sentences of length t + 1.

How to compare two sentences? Example:

- Candidate: the the the the the the
- Reference 1: the cat is on the mat
- Reference 2: There is a cat on the mat

Metric:

- Precision : 7/7
- BLEU (bilingual evaluation understudy): 2/7 (maximum number of times a word is encountered in any reference sentence)

["BLEU: a method for automatic evaluation of machine translation", Papineni et al. 2002]
Image Captioning: Neural Image Caption

A person riding a motorcycle on a dirt road.



A group of young people playing a game of frisbee.



A herd of elephants walking across a dry grass field.



Two dogs play in the grass.



Two hockey players are fighting over the puck.



A close up of a cat laying on a couch.



A skateboarder does a trick on a ramp.



A little girl in a pink hat is



A red motorcycle parked on the side of the road.



A dog is jumping to catch a frisbee.



A refrigerator filled with lots of food and drinks.



A yellow school bus parked



Describes without errors

Describes with minor errors

Somewhat related to the image

Germanized to the image

Figure 5. A selection of evaluation results, grouped by human rating.

["Show, attend and tell: Neural image caption generation with visual attention", K. Xu et al. 2015]



Predicted sequence of words: $\{y_1, \ldots, y_C\}, y_i \in \mathbb{R}^K$, where K is the size of the dictionary.

Image features: $\{a_1, \ldots, a_L\}$, where $a_i \in \mathbb{R}^D$ is a feature corresponding to a small precise area in the image (extraction from a early layer of a CNN).

$$\begin{pmatrix} \mathbf{i}_t \\ \mathbf{f}_t \\ \mathbf{o}_t \\ \mathbf{g}_t \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \tau \\ \tanh \end{pmatrix} T_{D+m+n,n} \begin{pmatrix} \mathbf{E}\mathbf{y}_{t-1} \\ \mathbf{h}_{t-1} \\ \mathbf{z}_t \end{pmatrix}$$
$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \mathbf{g}_t$$
$$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{c}_t).$$

 $\hat{\mathbf{z}}_{t} = \sum_{i=1}^{L} s_{t,i} \mathbf{a}_{i},$ where $s_{t,i} = 1$ if position *i* in the image should be selected at time *t*. $\mathbb{P}[s_{t,i} = 1 | s_{j < t}, \mathbf{a}] = \alpha_{t,i},$ $e_{ti} = f_{att}(\mathbf{a}_{i}, \mathbf{h}_{t-1}),$ $\alpha_{t,i} = \frac{\exp(e_{ti})}{\sum_{i} \exp(e_{ti})}.$

Figure 2. Attention over time. As the model generates each word, its attention changes to reflect the relevant parts of the image. "soft" (top row) vs "hard" (bottom row) attention. (Note that both models generated the same captions in this example.)



Figure 3. Examples of attending to the correct object (white indicates the attended regions, underlines indicated the corresponding word)



A woman is throwing a frisbee in a park,



A dog is standing on a hardwood floor.



A stop sign is on a road with a mountain in the background.



A little girl sitting on a bed with a teddy bear.



A group of people sitting on a boat in the water.



A giraffe standing in a forest with trees in the background.

Figure 5. Examples of mistakes where we can use attention to gain intuition into what the model saw.



A large white bird standing in a forest.



A woman holding a clock in her hand.



A man wearing a hat and a hat on a skateboard.



A person is standing on a beach with a surfboard.



A woman is sitting at a table with a large pizza.



A man is talking on his cell phone while another man watches.

The End!²



²More content at https://erwanscornet.github.io/, Teaching section.

5 Famous CNN

- LeNet (1998)
- AlexNet (2012)
- ZFNet (2013)
- VGGNet (2014)
- GoogLeNet (2014)
- ResNet (2016)
- DenseNet (2017)
- Many other CNN



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LeNet

["Generalization and network design strategies", LeCun et al. 1989]

["Gradient-based learning applied to document recognition", LeCun, Bottou, Bengio, et al. 1998]





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AlexNet

["Imagenet classification with deep convolutional neural networks", Krizhevsky et al. 2012]

Ingredients:

- Activation function (ReLU)
- Local Response Normalization (LRN)
- Overlapping pooling (3 \times 3 window with a stride S = 2 which reduces overfitting)
- Dropout
- Data augmentation



Numerical results

Model	Top-1 (val)	Top-5 (val)	Top-5 (test)
SIFT + FVs[7]	_	_	26.2%
1CNN	40.7%	18.2%	_
5CNNs	38.1%	16.4%	16.4%
1CNN^*	39.0%	16.6%	_
7CNNs*	36.7%	15.4%	15.3%

- First line is the second runner-up.
- Second and third lines are results output by the averaging over 1 or 5 CNN described before.
- Last two lines correspond to networks with an extra convolutional layer after the last pooling layer which has been trained on Image Net Fall 2011 then "fine-tuned" on the ImageNet 2012 data base.

AlexNet has a very similar architecture to LeNet, but is deeper, bigger, and features Convolutional Layers stacked on top of each other: previously, pooling layers followed immediately each convolutional layer.

Results



Figure 4: (Left) Eight ILSVRC-2010 test images and the five labels considered most probable by our model. The correct label is written under each image, and the probability assigned to the correct label is also shown with a red bar (if it happens to be in the top 5). (Right) Five ILSVRC-2010 test images in the first column. The remaining columns show the six training images that produce feature vectors in the last hidden layer with the smallest Euclidean distance from the feature vector for the test image.



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ZFNet: Improve upon AlexNet

["Visualizing and understanding convolutional networks", Zeiler and Fergus 2014]



Aim at finding out what the different feature maps are searching for in order to obtain a better tuning of network architecture.

In ZFNet, feature maps are not divided across two different GPU. Thus connections between layers are less sparse than for AlexNet.

Deconvnet

Find the pixels that maximize the activation of a given feature map.

How? Invert the network.

Precisely:

- Choose a layer
- Choose a feature map
- Run the network on a validation set
- Choose the image maximizing the activation of this feature map
- "Backpropagate" this activation to obtain a stylized image in the pixel space



Results



Top 9 activations in a random subset of feature maps across the validation data, projected down to pixel space using the previous deconvolutional network approach.

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Tiny VGGnet

["Very deep convolutional networks for large-scale image recognition", Simonyan and Zisserman 2014b]



Convolutional layers:

- \bullet Small receptive field: 3 \times 3 (smallest ones capable of capturing the notion of top/down, left/right!)
- Stride of 1
- Spatial resolution is preserved after convolution

Insightful remark...

If you stack 3 convolutional layers with receptive fields 3×3 , you obtain a convolutional layer with receptive fields 7×7 . What is the interest?

- **()** Stack of 3 convolutional layers of size 3×3 : complexity of $3 \times \times 3 \times 3 = 27$.
- **②** One standard convolutional layer of size 7×7 : complexity of 49.

In the first case, we cannot obtain every possible layer: the resulting object is a decomposition of three consecutive convolutional layers. There are less possibilities hence less parameters.



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GoogLeNet

["Going deeper with convolutions", Szegedy, W. Liu, et al. 2015]

Aim.

Increasing the depth and width of state-of-the-art convolutional neural networks while keeping the number of parameters small:

- Can approximate more complex functions
- while being robust to overfitting and computationally appealing.

How.

- Specifically, use of 1×1 convolution layers to reduce the number of parameters + apply filters of different sizes 3×3 , 5×5 or 3×3 max pooling (on each feature maps).
- use auxiliary classifiers

Details.

- All convolution layers use ReLU activation functions.
- Same spatial resolution for each feature map.

GoogLeNet - Inception module

Same spatial resolution for each feature map.

Use of 1×1 convolution layers to reduce the number of parameters then apply filters of different sizes 3×3 , 5×5 or 3×3 max pooling (on each feature maps).







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ResNet (2016)

["Deep residual learning for image recognition", He et al. 2016]









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DenseNet

["Densely Connected Convolutional Networks.", G. Huang et al. 2017]



Figure: A deep DenseNet with three dense blocks. The layers between two adjacent blocks are referred to as transition layers and change feature-map sizes via convolution and pooling



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Inception V2-V3

Based on GoogLeNet Inception module

["Rethinking the inception architecture for computer vision", Szegedy, Vanhoucke, et al. 2016]



New ideas:

- Using asymmetric convolutions 1 × n and n × 1 (for n = 3, 5, 7) can be useful in the middle layers of the networks for feature maps of size m × m (for 12 ≤ m ≤ 20).
- Label smoothing using a uniform distribution over labels

Xception

["Xception: Deep learning with depthwise separable convolutions", Chollet 2017]

Stands for "Extreme Inception" and builds upon Inception module in GoogLeNet.



The main ideas:

- $\bullet~\mbox{Perform}~1\times 1$ convolutions
- Apply 3×3 (or other filter size) convolutions to each previous feature map (the one created by 1×1 convolutions) separately.

 \rightarrow Decoupled the depth (1 \times 1 convolutions) and the spatial transformations (convolutions on each feature map separately).

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