Predictive Modelling - VII

Artificial Neural Networks

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Summary

- Artificial Neural Networks
- (Very Short) Introduction to Deep Learning

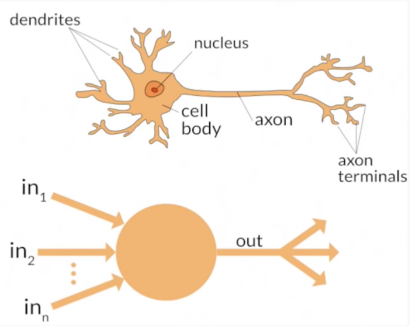
Predictive Modelling: Where we at?

- Distance-based Approaches
  - e.g. kNN
- Probabilistic Approaches
  - e.g. Naive Bayes, Bayesian Networks
- Mathematical Formulae
  - e.g. multiple linear regression
- Logical Approaches
  - e.g. CART
- Optimization Approaches
  - e.g. SVM, ANN
- Ensemble Approaches

Artificial Neural Networks

Artificial Neural Networks (ANN)

- Models with a strong biological inspiration. The brain is a highly complex structure, non linear and highly parallel.
- McCulloch e Pitts (1943) proposed the first artificial model of a neuron.
- Neuron: many-inputs / one-output unit
- Synapses: electrochemical contact between neurons

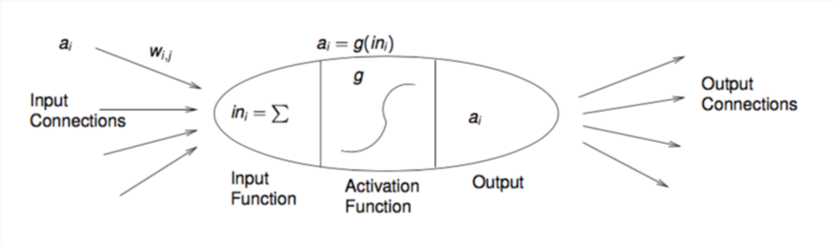


- Output of a neuron: excited or not excited
- Incoming signals from other neurons determine if the neuron shall excite ("fire")
- Output subject to attenuation in the synapses

Artificial Neural Networks (ANN)

- An artificial neural network is composed by a set of units (neurons) that are connected.
- These connections have an associated weight.
- Each unit has an activation level as well as means to update this level.
- Some units are connected to the outside world. We have input and output neurons.
- Learning within ANNs consists of updating the weights of the network connections.

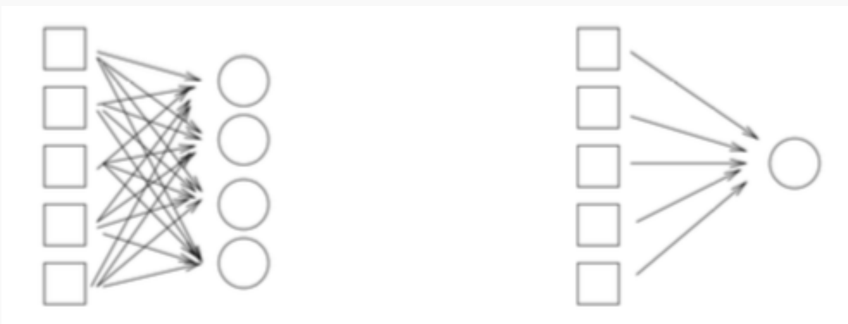
Artificial Neural Networks: Artificial Neuron



- Each unit has a very simple function:
  - receive the input impulses and calculate its ouput as a function of these impulses.
- This calculation is divided in two parts:
  - a linear combination of the inputs: $\in_i = \sum_j w_{ji} a_j + b$
  - a (typically) non-linear activation function: $a_i = g(in_i)$

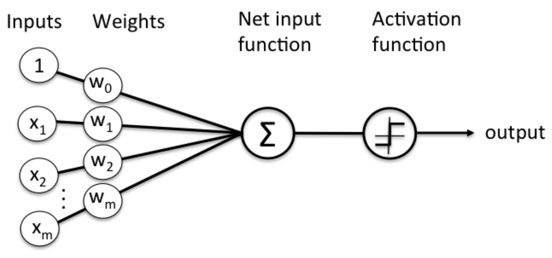
Artificial Neural Networks: Perceptron

- Rosenblatt (1958) introduced the notion of perceptron networks. This work was then further extended by Minsky and Papert (1969).
- Perceptrons are networks with an input layer and an output layer.



Artificial Neural Networks: Perceptron

Simplest Perceptron



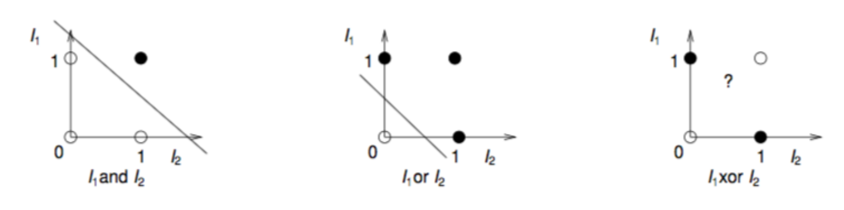
Schematic of Rosenblatt's perceptron.

- A linear classifier for binary classification problems

$$f(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w} \cdot \mathbf{x} + w_0 > 0 \\ 0 & \text{otherwise} \end{cases}$$

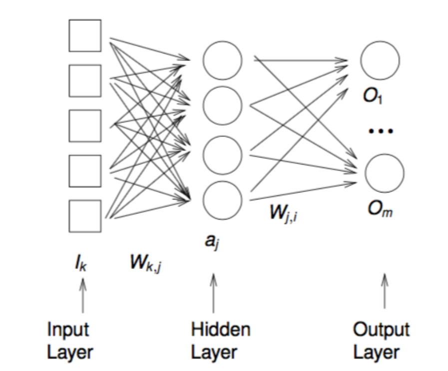
- It learns by updating the weights through delta rule with learning rate η
- $w_i(t+1) = w_i(t) + \eta(true - predicted)x_i$

Perceptrons are limited to linearly separable functions.



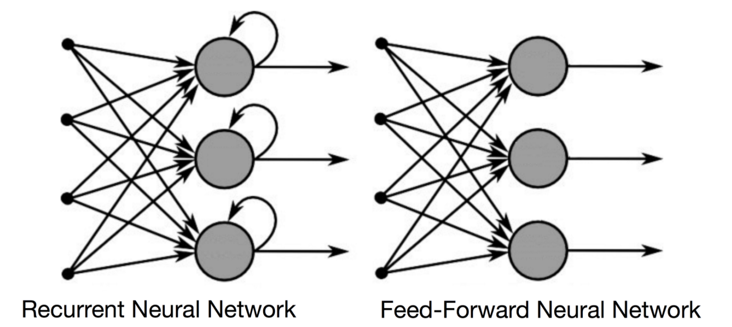
Artificial Neural Networks: Types of ANNs

- Feed-forward networks (Multilayer perceptrons)
  - networks with uni-directional connections (from input to output), and without cycles
  - each unit is connected only to units in the following layer
  - there are no connections from units on a certain layer and units on previous layers



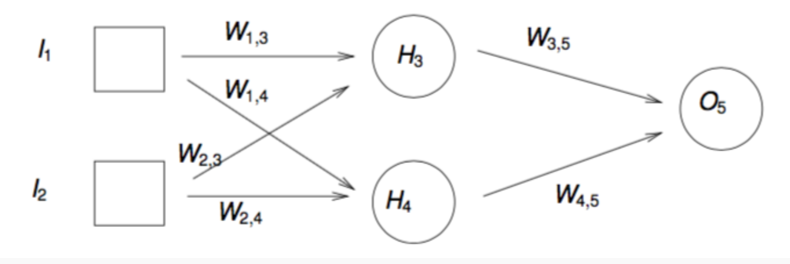
Artificial Neural Networks: Types of ANNs

- Recurrent networks
  - networks with arbitrary connections
  - due to the possible feedback effects, recurrent networks are potentially more instable, possibly exhibiting caotic behaviors
  - usually they take longer to converge



Artificial Neural Networks: Types of ANNs

- Example of a feed-forward network with one input layer (I), one hidden layer (H) and one output layer (O) with one output variable.



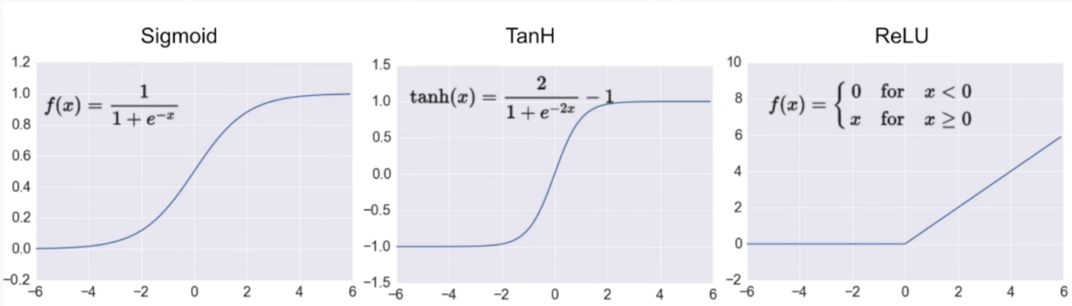
- The output can be represented as follows:

$$a_5 = g(W_{3,5}a_3 + W_{4,5}a_4) =$$
$$= g(W_{3,5}g(W_{1,3}a_1 + W_{2,3}a_2) + W_{4,5}g(W_{1,4}a_1 + W_{2,4}a_2))$$

- where $g()$ is the activation function

Artificial Neural Networks: Activation Functions

- Activation functions are used to determine the output of each node of the neural network
  - linear
  - non-linear: most commonly used as it allows the model to generalize or adapt with variety of data
- Examples



Artificial Neural Networks: Backpropagation Algorithm

- This is the most popular algorithm for learning ANNs.
- It has similarities with the learning algorithm used in perceptron networks
- Intuition:
  - each unit is responsible for a certain fraction of the error in the output nodes to which it is connected
  - thus, the error is divided according to the weight of the connection between the respective hidden and output units, thus propagating the errors backwards
- Backpropagation computes the gradient in weight space of a feedforward neural network, with respect to a loss function.

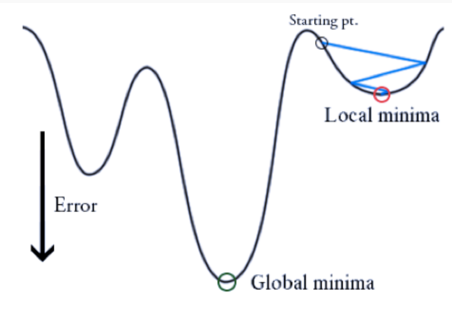
Artificial Neural Networks: Backpropagation Algorithm

The Algorithm (for one hidden layer)

- Initialize network weights (often small random values)
- Do
  - For each example in training set
    - predict the output
    - calculate the prediction error by a loss function
    - compute δ_h for all the weights from hidden layer to output layer
    - compute δ_i for all the weights from input layer to hidden layer
    - update network weights
- Until it converges
  - all examples are classified correctly or stopping criterion is satistified
- Return the network

Artificial Neural Networks: Backpropagation Algorithm

Gradient Descendent



- Stochastic Gradient Descent: instead of calculating the gradient of the full error function (which involves using the full training set), we update the weights one example at a time.
- Batch Gradient Descent: the batch size is the number of sub samples given to the network after which weights update happens.
- Both are more effective to escape from local minima.

Artificial Neural Networks: Backpropagation Algorithm

When to stop training?

- If stopping too early: risk of getting a network not yet trained.
- If stopping too late: danger of overfitting (fit noise in the data)
- Stopping criteria:
  - maximum number of iterations
  - error based on the training set
    - when the error in the training set is below a certain limit.
  - error based on a validation set (independent from the training set)
    - when the error on the validation set has reached a minimum.

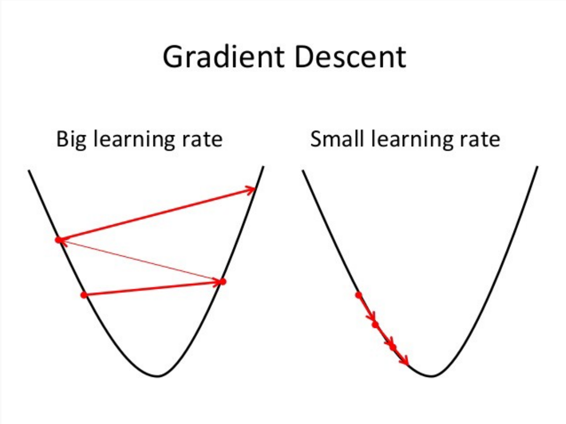
Artificial Neural Networks: Issues

Network topology

- The number of nodes in the hidden layer
  - few nodes: underfitting
  - many nodes: overfitting
  - no specific criterion exists
- Effect of learning rate
  - a small learning rate has the effect of learning times higher
  - a high learning rate may lead to non-convergence

Artificial Neural Networks: Issues

- The learning rate sets the size of the steps to obtain the direction of maximum descendent.



Artificial Neural Networks: Issues

Generalization vs Specialization trade-off

- Optimal number of hidden neurons
  - too many hidden neurons: training set is memorized, thus making the network useless on new data sets
  - not enough hidden neurons: network is unable to learn problem concept
- Overtraining
  - too much examples, the ANN memorizes the examples instead of the general idea

Artificial Neural Networks: Issues

Some relevant hyperparameters

- Network Structure
  - number of layers
  - number of neurons in each layer
  - weights initialization
  - activation function
- Training Algorithm
  - learning rate
  - number of epochs
  - early stopping criterion
  - weight decay (a regularization on the network weights)

Artificial Neural Networks: Issues

Some Tips

- Features with very different distributions of values are not convenient, given the typical activation functions.
  - Data should be standarized.
- Missing values in input features may be represented as zeros, which do not influence the neural net training process.
- Output in Multiclass Setting
  - Use one-hot encoding, there are M output neurons (1 per class),
  - For each case, the class with the highest probability value.

Artificial Neural Networks: Issues

Some Tips (cont.)

- Initialize the weights with small random values $[-0.05, 0.05]$
- Shuffle the training set between epochs, i.e. change the sequence of the examples
- The learning rate must start with a high value that decreases progressively
- Train the network several times using different initialization of the weights

Artificial Neural Networks: Wrap-Up

Use ANNs when

- Input is high-dimensional discrete or real-valued (e.g. raw sensor input)
- Output is discrete or real valued
  - Classification: use Softmax function as activation function in output layer to compute the probabilites for the classes
  - Regression: use a linear function as activation function in output layer
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant

Artificial Neural Networks: Wrap-Up

Pros

- Tolerance of noisy data
- Ability to classify patterns on which they have not been trained
- Successful on a wide range of real-world problems
- Algorithms are inherently parallel

Cons

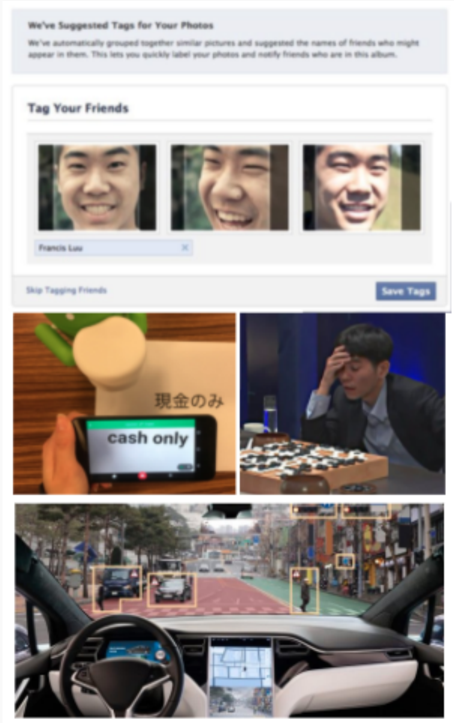
- Long training times
- Resulting models are essentially black boxes

(Very Short) Introduction to Deep Learning

A (Very Short) Introduction to Deep Learning

Deep Learning: where?

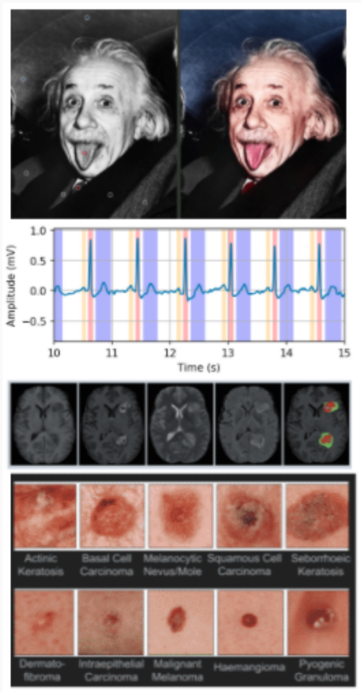
- Image recognition
  (e.g. Google, Facebook)
- Automatic text translation
  (e.g. Google Translator)
- Answers in natural language
  (e.g. ChatGPT)
- Games
  (e.g. DeepMind, AlphaGo)
- Transcript of handwritten text
- Self-driving cars



A (Very Short) Introduction to Deep Learning

Deep Learning: where?

- Image colorization, caption generation
- Classification of protein and DNA sequences
- Heart sound: classification and segmentation
- Tumor images detection from MRI, CT, X-rays
- Skin lesion classification from clinical and dermoscopic images
- Parkinson’s disease detection from voice recording



A (Very Short) Introduction to Deep Learning

- Deep learning = Deep neural networks
  - Deep = high number of hidden layers
  - Learn a larger number of parameters!
- It was made possible recently since we have:
  - Access to big amounts of (training) data
  - Increased computational capabilities (e.g., GPUs)
- Some algorithms:
  - Convolution Neural Networks (CNN)
  - Long-Short Term Memory Networks (LSTM)
  - Gated Recurrent Unit (GRU)
  - Autoencoders (AE)

Convolutional neural networks (CNNs)

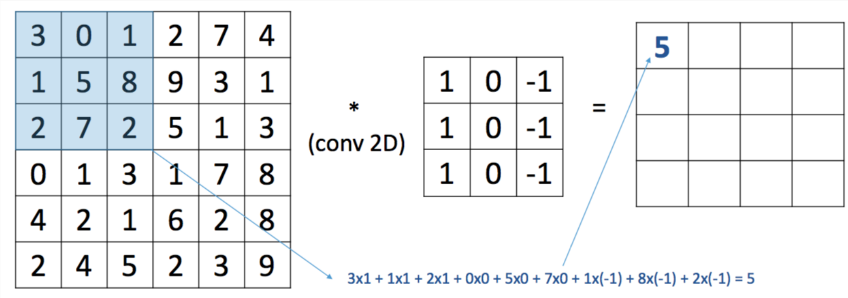
Convolution Neural Networks (CNN)

- Feedforward neural networks
- Neurons typically use the ReLU or sigmoid activation functions
- Weight multiplications are replaced by convolutions (filters)
- Change of paradigm: can be directly applied to the raw signal, without computing first ad hoc features
- Features are learnt automatically!!

Convolutional neural networks (CNNs)

Convolution

- mathematical operation between two matrices;
- the 2nd matrix is a filter that is overlapped to each position of the 1st matrix.



Convolutional neural networks (CNNs)

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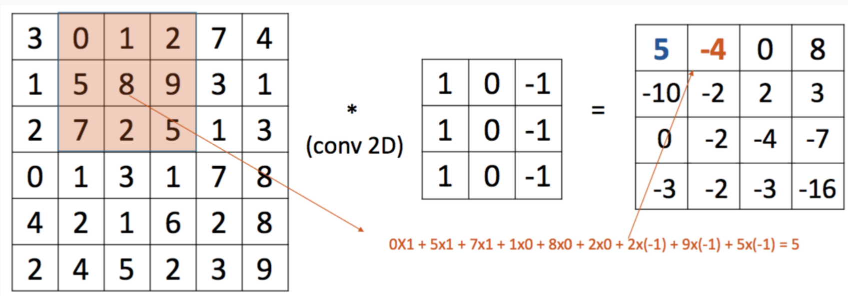
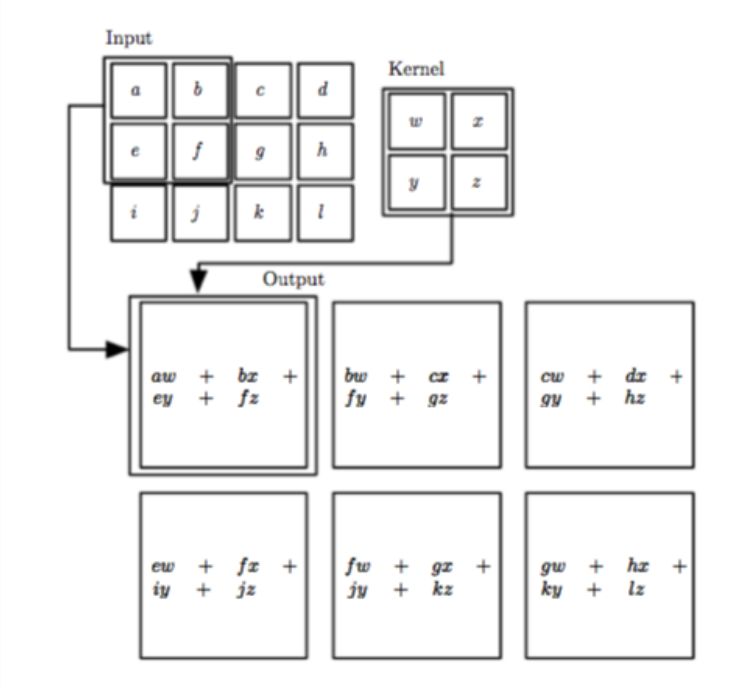


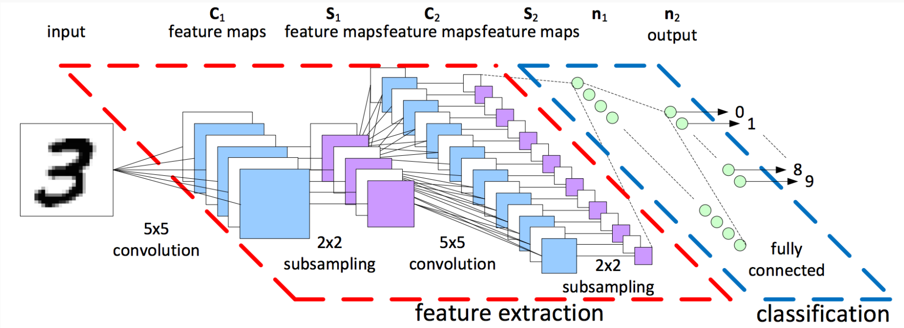
Convolutional neural networks (CNNs)

Convolution



Convolutional neural networks (CNNs)

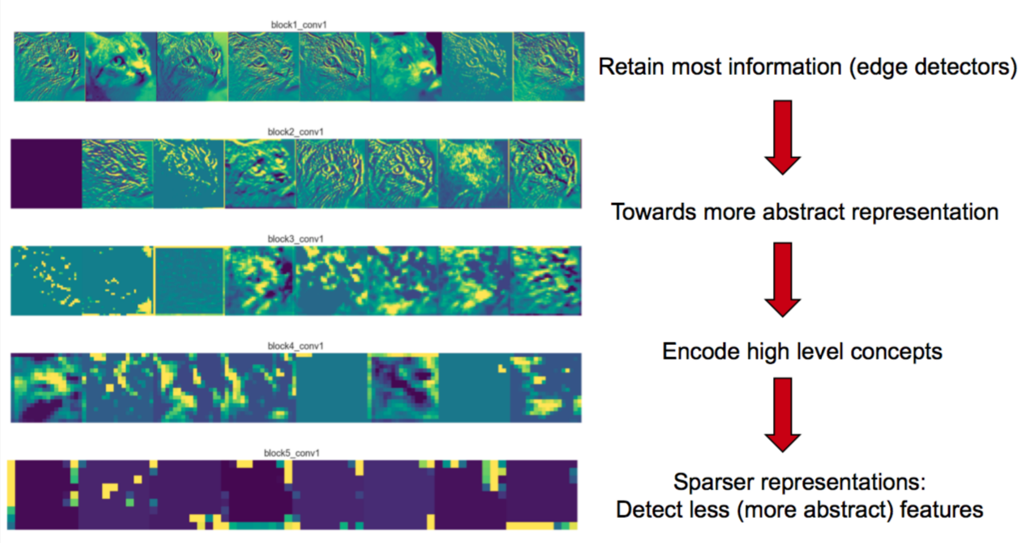
Example for Image Processing



- convolutional layers, followed by nonlinear activation and subsampling (pooling)
- output of hidden layers (feature maps) are features learnt by the CNN
- flatten fully connected layers for classification (as in “standard” NN)

Convolutional neural networks (CNNs)

Example for Image Processing: feature extraction

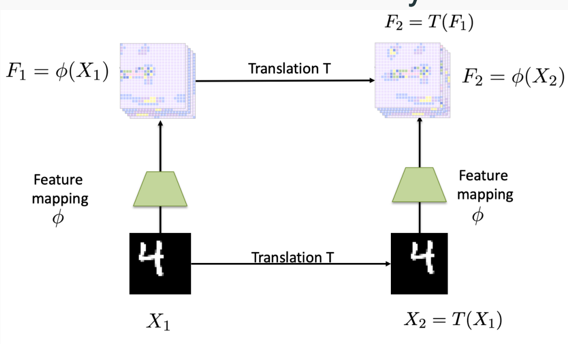


- the convolutions, applied to various zones of the image, act as filters that can detect certain patterns

Convolutional neural networks (CNNs)

Properties

- Reduced amount of parameters to learn (local features)
- More efficient than dense multiplication
- Specifically thought for images or data with grid-like topology
- Convolutional layers are equivariant to translation



- if image input is translated by a certain amount,
- the feature map is also translated
- useful for classification

- Currently state-of-the-art in several tasks

(Very Short) Introduction to Deep Learning: Wrap-Up

Great results! But...

- Like any other technique, DL does not solve all problems and will not always be the best option for any learning task.
- Difficult to select best architecture for a problem
- Require new training for each task/configuration
- (Most commonly) require a large training dataset to generalize well
  - Data augmentation, weight regularization, dropout, transfer learning, etc.
- Still not fully understood why it works so well
  - Unstable against adversarial examples

(Very Short) Introduction to Deep Learning: Wrap-Up

To know more

- Book – I.Goodfellow,Y.Bengio,and A.Courville. Deep learning. Vol.1. Cambridge: MIT press, 2016.
- Tutorial – Oxford Visual Geometry Group: VGG Convolutional Neural Networks Practical

References

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