QML-Mod2-Classical Machine Learning

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Indice

1 Introduction to classical machine learning -22/03/2025

Despite maybe we were not aware but we've already trained models, in our life, with machine learning algorithms: an example is given by the tools asking the users to spot cars, traffic signals, etc. in some website before entering them. An other example is given by all the filters that one can apply before taking a picture while using social media.

Artificial Intelligence vs Machine Learning vs Deep Learning

- artificial intelligence: any technique that enables computers to mimic human intelligence. It includes machine learning
- machine learning: a subset of AI that includes techniques that enable machines to improve at tasks with experience. It includes deep learning
- deep learning: a subset of machine learning based on neural networks that permit a machine to train itself to perform tasks

Machine learning includes two kinds of modalities to train the algorithm: supervised and unsupervised learning. In the latter we don't give any label to the algorithm and we let it to find itself the correct answer to the given problem.
An example of machine learning algorithm is to be found in surgical data science, where AI is at service of surgeons.
The choice of the best algorithm to apply has to be done considering the dimension and the type of data one has to manage.

$$\text{machine learnign}\begin{cases}\text{Unsupervised learning}\begin{cases}\text{Clustering}\end{cases}\\ \text{Supervised learning}\begin{cases}\text{Classification}\\ \text{Regression}\end{cases}\end{cases}$$

The goal of supervised training is mapping inputs in outputs. The difference between classification and regression is that the first one does a prediction of discrete outputs while the second one does a prediction of continuous outputs.
The main problem with unsupervised learning is that evaluating its performance is not always immediate.
Note that one can combine supervised and unsupervised learning.

1.1 Input data

Standard algorithms of ML usually take as inputs features and characteristics extracted from the data set. Those features are handcrafted or manually extracted.

The data is divided in a training set and a validation set. An algorithm is subject to underfitting of the data set if it has a poor performance on the training set. Otherwise it is said being subject to overfitting is it works well with the data training but has poor results with data of the validation set.
After having tested the algorithm with data from training and validation sets, we go to another phase of the analysis which implies the use of a third data set called test set.

Cross validation strategy : one can repeat the whole training of the model swapping every time the data from one set to another (what was first, for example, in the training set now will go in the validation set).

Generalization In Machine Learning, generalization refers to a model's ability to perform well on unseen data, meaning data that was not used during training. A well-generalized model captures the underlying patterns in the data rather than memorizing specific examples, allowing it to make accurate predictions on new inputs. Poor generalization can lead to overfitting (where the model performs well on training data but poorly on new data) or underfitting (where the model fails to learn meaningful patterns from the training data).
A **bias** is a distortion of the training data which is propagated in the algorithm. The goals related to the supervised training are a low error during training, validation and testing phases. The selection of the algorithm is based on:

- velocity of the training
- storage capacity
- accuracy on new data prediction
- transparency and interpretability

1.2 Practical examples of ML

- **Logistic regression**: the model is trained to predict the probability of a binary choice.
- **k nearest neighbor (kNN)**: is a pattern recognition algorithm based on distance of the data. If a subject A has, for example, characteristic close to the one of a subject B, then probably they are associated to the same category.

The ML learning model, in the training phase, learns a set of rules which depends both on the data set and a fixed combination of hyperparameters. The automatic learning of a model is not a single process, in necessary to experiment different models fixing different values of the hyperparameters.

```python
from sklearn.ensemble import RandomForestClassifier

rf_clf = RandomForestClassifier(n_estimators=?, max_depth=?)
```

Imports the RandomForestClassifier model from the scikit-learn library. This model is a supervised learning algorithm based on decision trees. Creates an instance of the Random Forest classifier with two key parameters:

- `n_estimators=?`: defines the number of trees in the forest (typically between 10 and 1000).
- `max_depth=?`: sets the maximum depth of the trees (can be `None` to allow them to grow until all leaves are pure).

1.3 Cross validation and hyperparameter tuning

We divide the training and the validation set in multiple sets so that the model can be trained with all the available data. **Cross validation** is statistical method used to estimate the ability of different models of performing automatic learning. This procedure is done by defining a parameter k which represents the number of sets in which every set is subdivided. We can perform cross validation for hyperparameter tuning in either inner loops or outer loops.

Accuracy: $\frac{TP+TN}{TP+FP+FN+TN}$

Recall (Sensitivity/True positive rate): $\frac{TP}{TP+FN}$

Precision: $\frac{TP}{TP+FP}$

Specificity: $\frac{TN}{TN+FP}$

F1 score: $2 \times \frac{Precision \times Recall}{Precision + Recall}$

ROC Curve & AUC (Area under the curve)

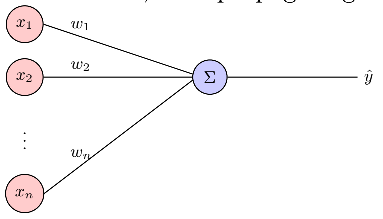
- **ROC curve:** Plot true positive rate (recall) vs. False Positive rate [...]
- **AUC** Probability [...]

2 Introduction to deep learning -28/03/2025

2.1 Training an artificial neural network

Modeling problems the first example is defining the position of a car whose positions is given exactly by $d(t) = d_0 + vt$. This problem is fully solvable. That is not always the case; indeed, a problem could be characterized by a large number of variables. The problem with working with large number of variables is that not always every variable has the same importance as the other. The problem, can be reduced to: $y = \alpha x_1 + \beta x_2 + \gamma x_3$.
Machine learning allow to solve complex problems in which we can easily tell what variables are involved in it.
Another problem that could be modeled is image recognition.
In ML we have a phase that does not appear in deep learning which is feature education: in traditional ML, model require pre-computed features that are manually designed based on domain knowledge. This feature engineering requires human expertise to identify the most relevant attributes for a given task.
Deep learning eliminates the need for manual feature extraction by learning hierarchical representations directly from raw data. Using AI networks, DL can automatically detect patterns at multiple levels of abstraction.

Artificial Neural Networks Biologically, neurons are unique cells that can communicate with one another, thus propagating information.



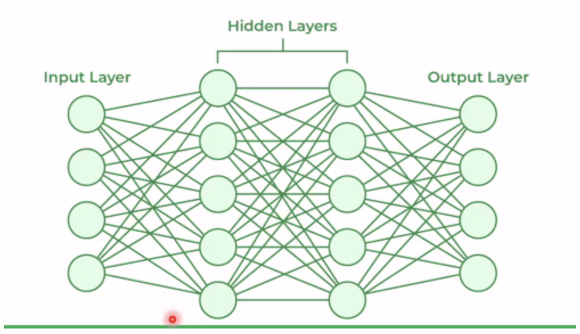
It receives n inputs, each scaled by a factor (weights), ad it sums them all scaled by a bias factor:

$$y = \sum_{i=1}^{n} w_i \times x_i + b.$$

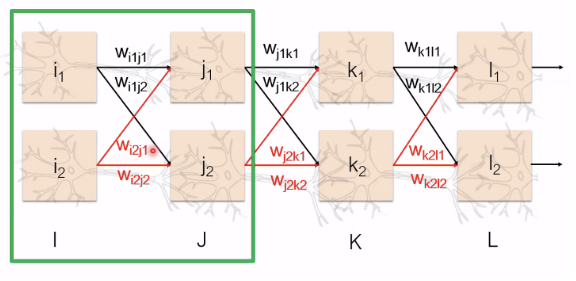
Weights and bias are the parameters of the neural network. Note that very few models are correctly modeled using linear combinations of the variables; indeed, we introduce an activate factor such that:

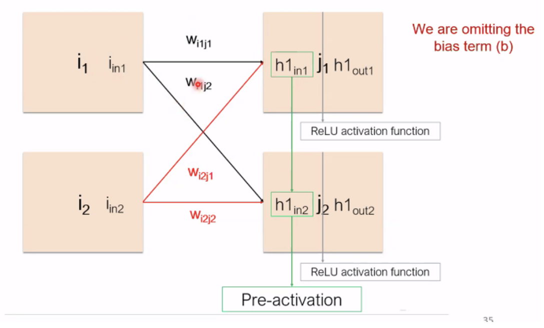
$$y = \sum_{i=1}^{n} g(w_i \times x_i + b).$$

Typical activation functions are: sigmoid, tanh, ReLU ($\max(0, x)$), Leaky ReLU ($\max(0.1x, x)$). The sigmoid and tanh functions limit the output, indeed, the output is always confined between 0 and 1.



This is what a simple neural network looks like: an input layer, a bunch of hidden layers, and an output layer. Each layer extracts information from the input and transmits it to the next one for further data processing.





$$[i_{in1} i_{in2}] \times \begin{bmatrix} w_{i1j1} w_{i1j2} \\ w_{i2j1} w_{i2j2} \end{bmatrix} = [h1_{out1} h2_{out2}]$$

What we are building is a neural architecture. All these parameters will have to be adjusted. This process is exactly what is called train of the neural network. The training process continues with making mistakes.
Let's consider the problem of predicting the cost of house: y is the real cost and $\hat{y}$ is the predicted one. y is also called ground-truth value and is used to supervise the training. The idea under the training process lays in computing the error, and what we want is indeed try to minimize this error. Error minimization is an optimization problem: I need a parameter configuration that explains the problem in the best possible way (i.e. i get as close as possible to the ground-truth value)

$$error = |y - \hat{y}|.$$

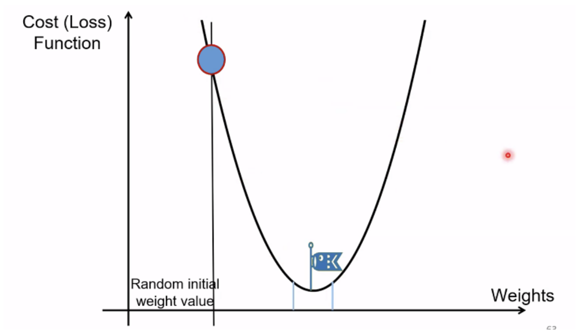
To optimize the parameters of a neural network we use the gradient method. What we always know when computing an algorithm is whether the error is increasing or decreasing.

- step 0: the error is very big
- step 1: i change the parametes
- step 2: ...

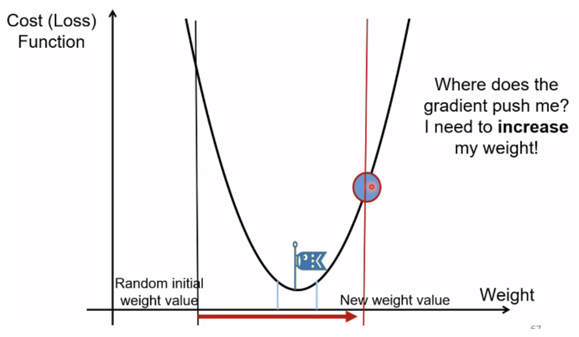
Gradient descent is the most used optimization technique to minimize the error. It means that, for each step, I compute the error and change the parameters in order to minimize the function.

$$error = f(w, b)$$

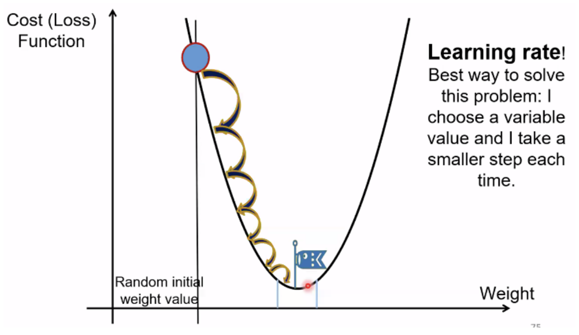
this function is called **cost function**. First order derivative (gradient) ...



Initializing the parameters randomly gives better results.


Cost (Loss) Function
Where does the gradient push me? I need to **increase** my weight!
Random initial weight value
New weight value
Weight

and so on till we reach the minimum.
In general the first step to reach the minimum is the bigger among all the steps that will be done. In this case we talk about learning rate. While "learning" we have to decrease the learning rate (i should take smaller steps) in order to reach the target.


Cost (Loss) Function
Learning rate!
Best way to solve this problem: I choose a variable value and I take a smaller step each time.
Random initial weight value
Weight

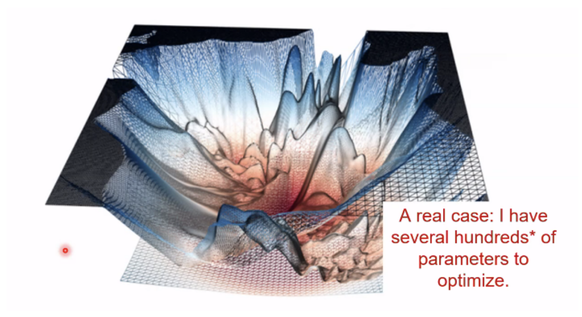
Mathematically, training a neural network means to change its parameters N times in order to minimize the cost function (error). Each update can be expressed as

$$w_{t+1} = w_t - \eta \times \nabla error$$

where η is the learning rate and $\nabla error$ is the gradient of the cost function with respect to w. A typical loss function is the MSE. The only constraint that we impose to the loss functions is to be differentiable everywhere. The error can be computed only from the output of the layers.

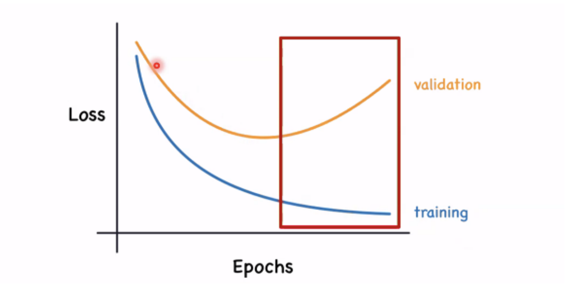
$$\frac{dE_1}{dw_{k1l1}} = \frac{dE_1}{dO_{out1}} \times \frac{dO_{out1}}{dO_{in1}} \times \frac{dO_{in1}}{dw_{ikl1}}$$

For a forward pass of information we have an error back-propagation. This kind of neural network is called fully connected.


A real case: I have several hundreds* of parameters to optimize.

Usually, what we need is a dataset, i.e. a set of (x,y) samples where x is the input and y is the output. The dataset is divided in three sub-sets: a training set, a validation set and a test set. The training process involves parameters optimization on the same training samples several times, or epochs.
AI does not really "learns": it just finds patterns. It's like a student who only studies math by doing every exercise on the book but never reads a page of theory. How can we make sure that the student is learning and not just memorizing? During the test, the student has no way to learn new knowledge because it has no supervision. [...]. Therefore, our neural network needs to perform well both on the training set and on the two test sets. What happens if it doesn't? The loss function on the training set has a very nice trend: as the network is iteratively optimized on the training sample, its error on these samples decreases. However, the loss function on the validation test doesn't seem as good: while the student improves with those "training" exercises, they make a lots of mistakes during the exam.
Two things are never to be expected:

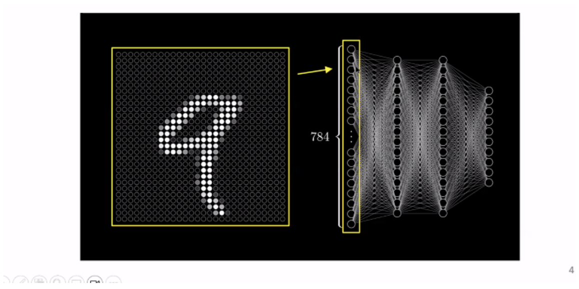
- no error or 100% accuracy
- better results in validation



However, we should minimize the distance between training and validation performance: **overfitting**.

2.2 Artificial neural networks: tasks

Regression: predict a number from a continuous set of numbers. An example is given by the prediction of the cost of a house.
Classification: predict a number from a discrete set of numbers.
The number of neurons in the input and output layers will depend on the task. In regression, we need to predict one number: one neuron is needed. The optimal number of neurons in the hidden layer (as well as the number of hidden layers) cannot be assessed a priori. The more the neurons and the layers, the more abstract information we can extract from the input data.
Check out the following site: playground tensorflow
Binary classification Classification is the most studied problem in DL. The MNIST dataset is on of the most famous one: our network needs to classify the input image as one of the 10 possible labels (the digits 0-9).



Check out: The stilwell brain
...
For classification, a perfect loss function is (binary) cross-entropy.

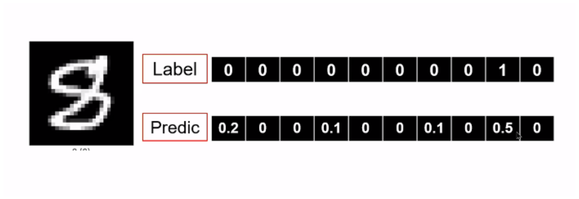


Figura 1: Note: 0.6 instead of 0.5

I want my prediction to be a probability distribution. The sum of all my elements needs to be 1. In the case of a odd vs even prediction the binary classification will give more precise results.

Loss function: Binary cross enrtopy

$$-\sum_{j=1}^{M} y_j \log(p(y_j))$$

$$-\sum_{i=1}^{N} y_i \log(p(y_i)) + (1 - y_i) \log(1 - p(y_i))$$

Final activation: softmax

In order to obtain a probability distribution, I need to use the softmax activation function in the outer layer.

$$\begin{bmatrix} 1.3 \\ 5.1 \\ 2.2 \\ 0.7 \\ 1.1 \end{bmatrix} = \left[\frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}} \right] = \begin{bmatrix} 0.02 \\ 0.9 \\ 0.05 \\ 0.01 \\ 0.02 \end{bmatrix}$$

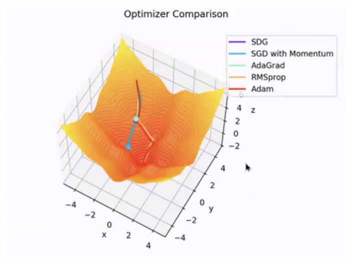
Metric: accuracy

$$\begin{bmatrix} \text{True positive (TP)} & \text{False Positive (FP)} \\ \text{False Negative (FN)} & \text{True Negative (TN)} \end{bmatrix}$$

where

- Recall $= \frac{\sum TP}{\sum TP+FN}$
- Precision $= \frac{\sum TP}{\sum TP+FP}$
- Accuracy $= \frac{\sum TP+TN}{\sum TP+FP+FN+TN}$

Optimizer: Adam (Adaptive moment estimator)



3 Advanced topics -29/03/2025

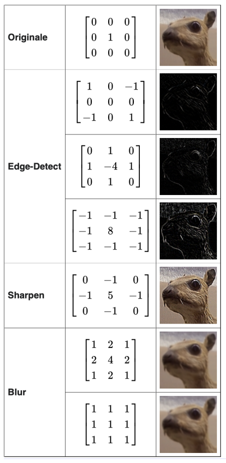
3.1 Convolutions from scratch

Edge detection is an old but gold problem in computer vision that involves detecting edges in an image to determinate object boundaries and thus separate the object of interest.
An edge is a point of rapid change of intensity of the image function. The gradient points in the direction of the most rapid increase.
Using filters (aka matrices) is possible defining the edges in an image. An example is given by:

$$\begin{bmatrix} 1 & 0 & -1 \\ 1 & 0 & -1 \\ 1 & 0 & -1 \end{bmatrix}$$

A **convolution** (of images) is simply an elementary multiplication of two matrices followed by a sum:

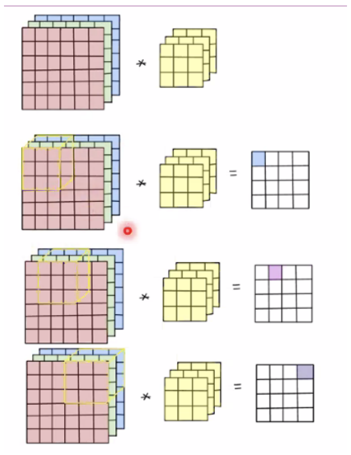
- take two matrices (which both have the same dimension)
- multiply them, element by element
- add up the elements



Originale	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	
Edge-Detect	$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	
	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	
	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$	
Sharpen	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
Blur	$\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	
	$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	

An image is just a multidimensional matrix, but unlike traditional matrices, images (RGB) can also have a depth. The kernel should be thought as a small matrix. It is common to define the kernel by hand to achieve various image processing functions, edge detection, etc. The question the arises: is there a way to automatically learn these type of filters? Of course there is: **CNN**.

Kernel Most of the kernels we usually see are $N \times N$ square matrices. We use an odd kernel dimension to ensure that there is a valid integer coordinate in the center of the image.
The process of "sliding" a convolutional kernel over an image and storing the output decreases the spatial dimensions of the output data. This decrease in spatial dimension is simply a side effect of applying convolutions to images. However, in most cases, we want the output image to be the same size as the input image. To ensure this, we apply padding.
The fact that the output is smaller than the input does not seem to be a big problem: we did not lose much data because most of the important features are located in the central area of the input. The only case when losing this information is a real problem is when much information in concentrated on border of the image. Padding could be done using zero elements or just copies of the border.
For an image we have:



The number of channels in the image must match the number of channels in the filter.
In convolutional neural networks, convolutional layers are not only applied to input data, such as pixel values, but can also be applied to the output layers. The sequence of convolutional layers allows a hierarchical breakdown of the input. Consider that filters operating directly on the raw pixel values will learn to extract low level features from the starting image, such as lines. The abstraction of characteristics to ever higher orders increases with network depth.
Kernel size The kernel size defines the convolution field of view.
Padding The padding defines how the edge of a sample is handled.
Stride The stride defines the size of the kernel step when passing through the image. Although the default setting is usually 1, you can use a stride of 2 to downsample an image (this is used to improve the features of the network).

3.1.1 Types of convolutions

Dilated/Atrous convolution The atrous convolutions introduce another parameter called the rate of expansion. This parameter defines the distance between values of a kernel. This way you get a wider field of view at the same computational cost. That type of convolution is use to understand large partial context.

Spatial separable convolutions A separable spatial convolution simply splits one kernel into smaller kernels. With fewer multiplications, the computational complexity decreases.

Depth-wise separable convolutions We have an RGB input image (with 3 channels). After convolutions, a feature map can have more channels (as usually happens). Each channel can be as a particular interpretation of the image. Similarly to spatial separable convolution, a deep separable convolution divides a kernel into two separate kernels that perform two convolutions: the **deep convolution** and the **point convolution**.
Width multiplier allows scaling the network's width to control the number of parameters and computation.
Resolution multiplier enables adjusting the input image resolution to further reduce computational requirements.

3.2 Convolutional neural networks

The visual cortex has hierarchical structure: LGB -> simple cells -> complex cells -> ...
We can think that these complex cells are performing an aggregation of activations.
Deep neural networks are normally organized in alternate repetitions of linear and non-linear operators. The reason for having multiple layers of this type is to build a hierarchical representation of the data.
The local pixels assemble to perform simple patterns like oriented edges.
Deep neural networks are normally organized in alternate representations of linear and non-linear operators.

3.2.1 Image classification

is the task of assigning to an input image a label belonging to pre-set set of categories.

Pro convolutional neural networks The 3D element that flows along the 3 image ...
The pixels of the feature map with the same color are from the same kernel. Both types of networks

learn by updating the weights which, in the case of fully connected networks, are the values of the connections whereas, in the case of convolutional neural networks, they are the values of the kernels.

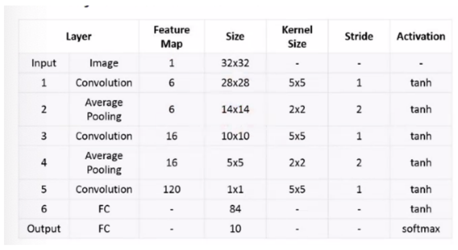
Other layers in CNNs: Pooling Pooling provides a form of translation invariance: small shift in the input can lead to the same output. Statistics over neighboring features to reduce the size of the feature maps:

- separate the image into non-overlapping subimages

- select the maximum/average/... in each layer

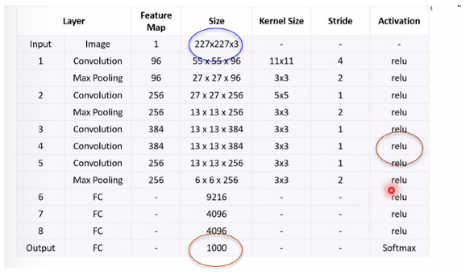
3.2.2 Architectures

- **LeNet-5** 1998



Layer		Feature Map	Size	Kernel Size	Stride	Activation
Input	Image	1	32x32	-	-	-
1	Convolution	6	28x28	5x5	1	tanh
2	Average Pooling	6	14x14	2x2	2	tanh
3	Convolution	16	10x10	5x5	1	tanh
4	Average Pooling	16	5x5	2x2	2	tanh
5	Convolution	120	1x1	5x5	1	tanh
6	FC	-	84	-	-	tanh
Output	FC	-	10	-	-	softmax

- **Alexnet** 2012



Layer		Feature Map	Size	Kernel Size	Stride	Activation
Input	Image	1	227x227x3	-	-	-
1	Convolution	96	55 x 55 x 96	11x11	4	relu
	Max Pooling	96	27 x 27 x 96	3x3	2	relu
2	Convolution	256	27 x 27 x 256	5x5	1	relu
	Max Pooling	256	13 x 13 x 256	3x3	2	relu
3	Convolution	384	13 x 13 x 384	3x3	1	relu
4	Convolution	384	13 x 13 x 384	3x3	1	relu
5	Convolution	256	13 x 13 x 256	3x3	1	relu
	Max Pooling	256	6 x 6 x 256	3x3	2	relu
6	FC	-	9216	-	-	relu
7	FC	-	4096	-	-	relu
8	FC	-	4096	-	-	relu
Output	FC	-	1000	-	-	Softmax

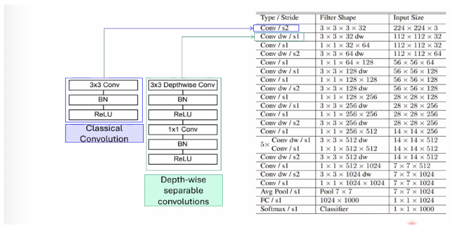
  In deep learning application, the ReLU activation feature is among the most popular. ImageNet is a large dataset of multimedia data annotated manually and divided into 1000 categories.

- **Googlenet inception** 2014
  The inception module relies on several convolutions with reduced kernel size to drastically lower the number of parameters.

- **VGG16** 2014
  Characterized by a total of 16 layers with weights, that is, of parameters which are implemented.

- **ResNet50** 2014
  Particularity: skip connections.

- **MobileNet V1**
  MobileNet is designed to be a lightweight architecture optimized for mobile and embedded devices. It uses a new type of convolutional layer, known as Depthwise Separate convolution which comprises a depthwise convolution and a pointwise convolution.

Type / Stride	Filter Shape	Input Size
Conv / s2	$3 \times 3 \times 3 \times 32$	$224 \times 224 \times 3$
Conv dw / s1	$3 \times 3 \times 32$ dw	$112 \times 112 \times 32$
Conv / s1	$1 \times 1 \times 32 \times 64$	$112 \times 112 \times 32$
Conv dw / s2	$3 \times 3 \times 64$ dw	$112 \times 112 \times 64$
Conv / s1	$1 \times 1 \times 64 \times 128$	$56 \times 56 \times 64$
Conv dw / s1	$3 \times 3 \times 128$ dw	$56 \times 56 \times 128$
Conv / s1	$1 \times 1 \times 128 \times 128$	$56 \times 56 \times 128$
Conv dw / s2	$3 \times 3 \times 128$ dw	$56 \times 56 \times 128$
Conv / s1	$1 \times 1 \times 128 \times 256$	$28 \times 28 \times 128$
Conv dw / s1	$3 \times 3 \times 256$ dw	$28 \times 28 \times 256$
Conv / s1	$1 \times 1 \times 256 \times 256$	$28 \times 28 \times 256$
Conv dw / s2	$3 \times 3 \times 256$ dw	$28 \times 28 \times 256$
Conv / s1	$1 \times 1 \times 256 \times 512$	$14 \times 14 \times 256$
5× Conv dw / s1	$3 \times 3 \times 512$ dw	$14 \times 14 \times 512$
5× Conv / s1	$1 \times 1 \times 512 \times 512$	$14 \times 14 \times 512$
Conv dw / s2	$3 \times 3 \times 512$ dw	$14 \times 14 \times 512$
Conv / s1	$1 \times 1 \times 512 \times 1024$	$7 \times 7 \times 512$
Conv dw / s2	$3 \times 3 \times 1024$ dw	$7 \times 7 \times 1024$
Conv / s1	$1 \times 1 \times 1024 \times 1024$	$7 \times 7 \times 1024$
Avg Pool / s1	Pool 7×7	$7 \times 7 \times 1024$
FC / s1	1024×1000	$1 \times 1 \times 1024$
Softmax / s1	Classifier	$1 \times 1 \times 1000$

  Batch normalization:
  $$\hat{x} = \frac{x - \mu}{\sigma},$$
  where μ is the mean of x in mini-batch and σ is the std of x in mini-batch.

- **DensNet**
  Densnet emphasizes strong feature reuse within the network through dense connections. Each layer receives inputs from all preceding layers in a dense block. Dense connections include direct connections between layers within dense blocks, reducing the number of parameters and enabling better gradient flow. Growth rate controls the number of output feature maps produced by each layer within a dense block. Compound scaling: scaled the network's depth, width and resolution uniformly to find an optimal balance model size and accuracy.

All previous CNNs have been trained on ImageNet to classify 1000 classes. This means that all CNN weights are available online. It's possible to use the pre-trained CNNs.