Neural Networks and Learning from Data

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Disclaimer

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Learning in Deep Architectures

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Gradient-related Issues

- The gradient with respect to the weights of the network is directly proportional to the delta terms, that are updated with the following rule (**BackProp**)

$$\delta_j^{\ell-1} = \frac{\partial o_j^{\ell-1}}{\partial a_j^{\ell-1}} \sum_i \delta_i^{\ell} w_{ij}^{\ell}$$

- Let us consider a sigmoidal activation function, for which $\frac{\partial o_j^{\ell-1}}{\partial a_j^{\ell-1}} \in (0, 0.25]$
  - Weight are generally randomly initialized, usually getting values smaller than 1 (absolute value). As a result, the value of the gradient will be progressively downscaled (**vanishing gradients**)
  - On the other hand, gradient could also **explode** when weights are very large
    - (or when using activation functions with large derivatives)

Gradient-related Issues (2)

- Some work-arounds
  - **Rectifiers** (*ReLu* activations)
    - Constant derivative in each linear region (equal to 1, or to 0)
    - It reduces the vanishing gradient effect (when we consider the linear region with derivative 1)

$$\sigma(a) = \max(0, a)$$

  - **Gradient Clipping**
    - When the norm of the gradient is too large (above a certain threshold) it is clipped to a given value
    - It helps with exploding gradients

$$\|\nabla \texttt{obj}\| \leq \tau$$

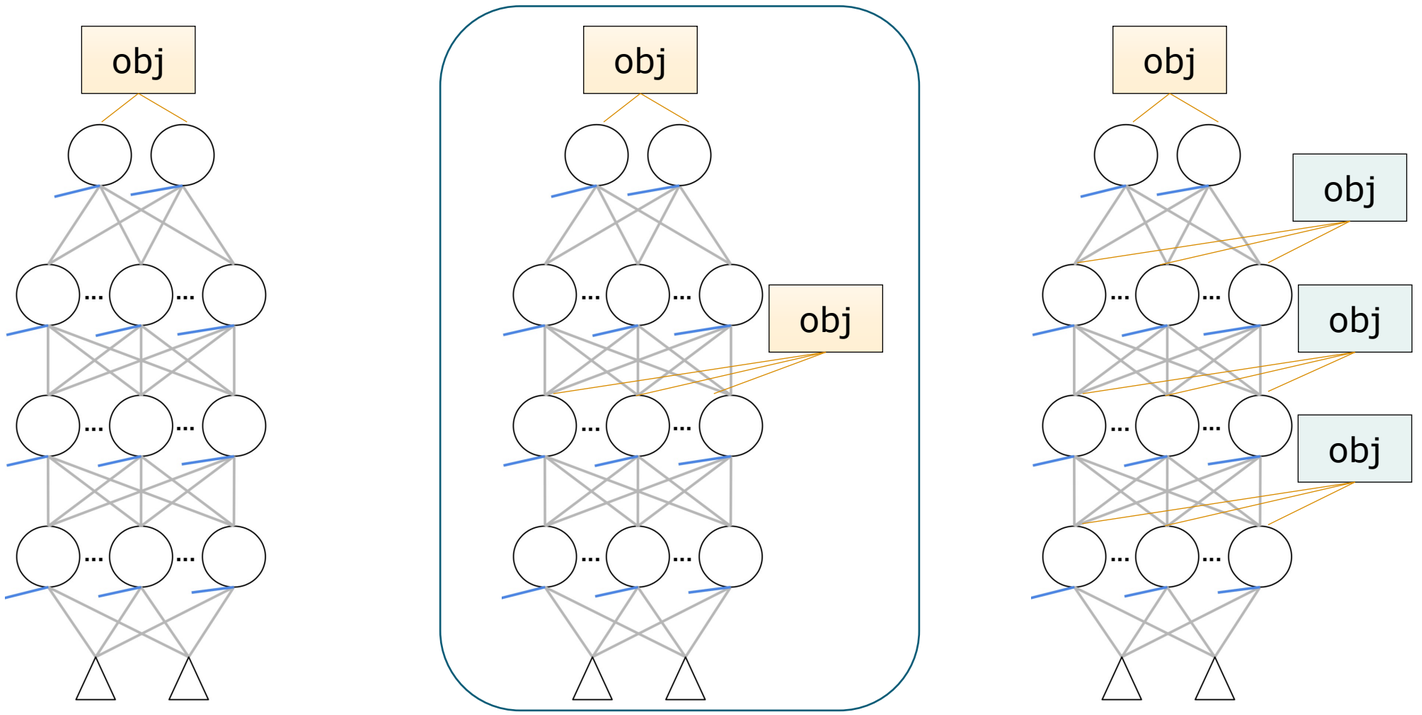
    - Simplified clipping: coordinate-wise clipping (warning, the direction of the gradient is lost!)

$$\frac{\partial \texttt{obj}}{\partial w_{ij}^{\ell}} = \max\left(\min\left(\frac{\partial \texttt{obj}}{\partial w_{ij}^{\ell}}, \tau\right), -\tau\right)$$

  - Accurate choice of the *loss function*, of the weight *initialization* routine, …

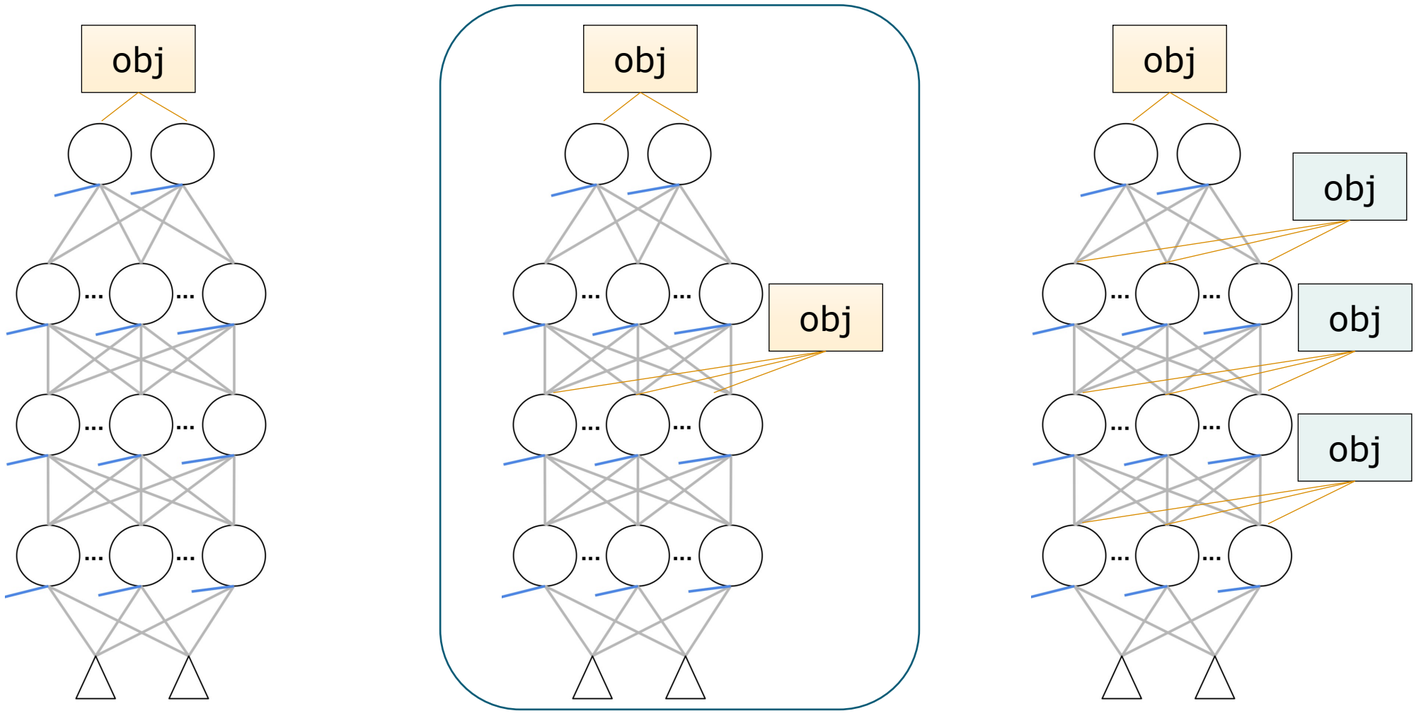
Gradient-related Issues (3)

- Some work-arounds
  - **Introduce objective functions that are closer to the lower layers**
    - It reduces the vanishing gradient effect
    - *Which objective functions?*



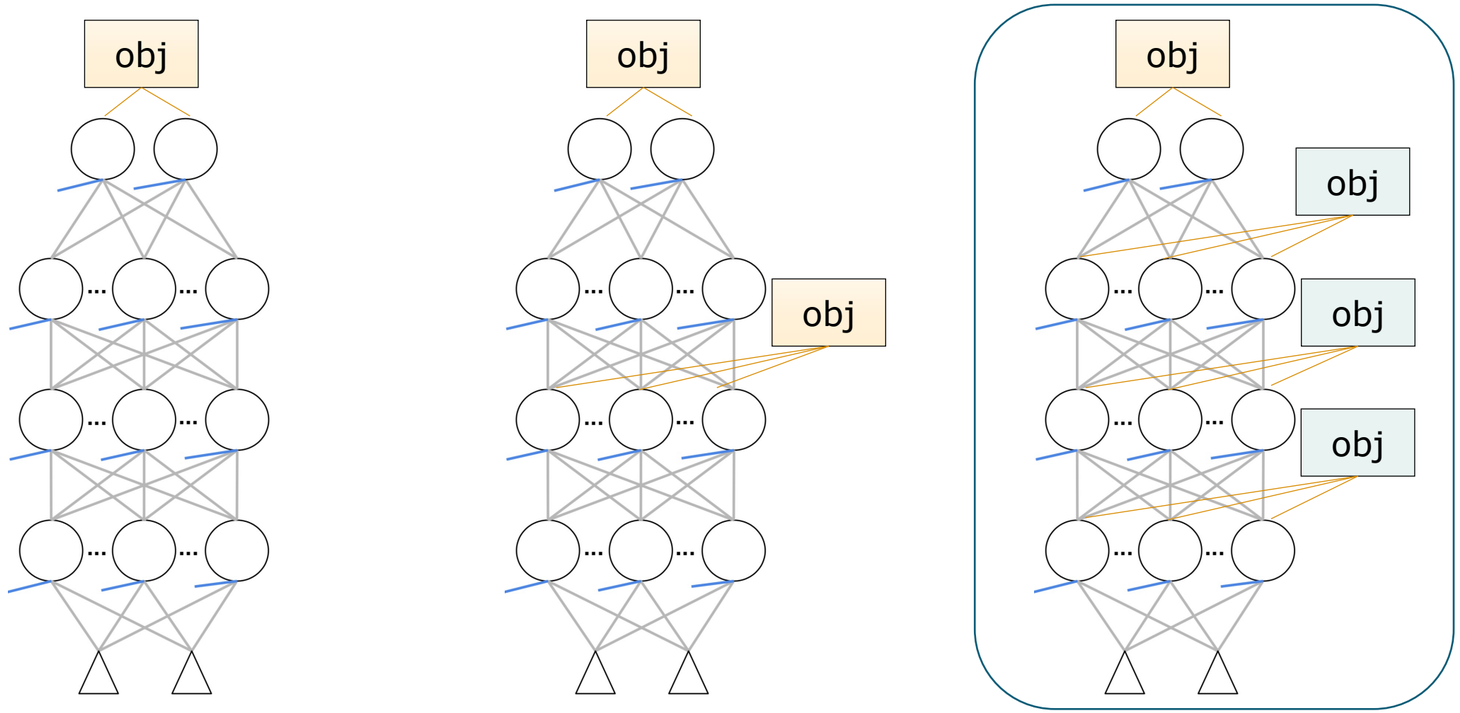
Gradient-related Issues (4)

- Some work-arounds
  - **Introduce objective functions that are closer to the lower layers**
    - Sometimes, enforcing a *downscaled* instance of the same classification loss the we use on top the network can *sometimes* help in speeding-up the development of discriminative representations



Gradient-related Issues (5)

- Some work-arounds
  - **Introduce objective functions that are closer to the lower layers**
    - Another popular solution, is to use *unsupervised learning* to train the network in a **layer-wise** fashion



Layer-wise Training

- **A more generic definition of training set**
  - We are given a training set with *n* supervised pairs, where $\boldsymbol{x}_i$ is a training example and $\boldsymbol{y}_i$ is its target (supervision)
  - The training set *might* also include *other* examples without any targets (blank)

$$T = \{(\mathbf{x}_i, \mathbf{y}_i)\,,\ i = 1, \ldots, n\} \cup \{(\mathbf{x}_j, \texttt{blank})\,,\ j = 1, \ldots, m\}$$

  - There is some precious information in the way the data is *distributed* (ignoring the targets), that can be used to pre-train the network in a layer-wise fashion
  - Some regularities in the data can be discovered in an unsupervised way

- **Layer-wise training**
  - Train the first layer using an *unsupervised* objective, then *freeze* it
  - Train the next layer using, an *unsupervised* objective, then *freeze* it, and so on…
  - Finally, **fine-tune** the whole network using the classic *supervised* loss
    - Exploiting the supervised portion of the training data

Layer-wise Training: Stacked Autoencoders

- **Autoencoder**: neural architecture that learns to reconstruct the input signal (under some conditions)
  - As a basic example, consider a neural network with
    - Single hidden layer
    - Number of output units equal to the number of dimensions of the input
    - Linear output activation

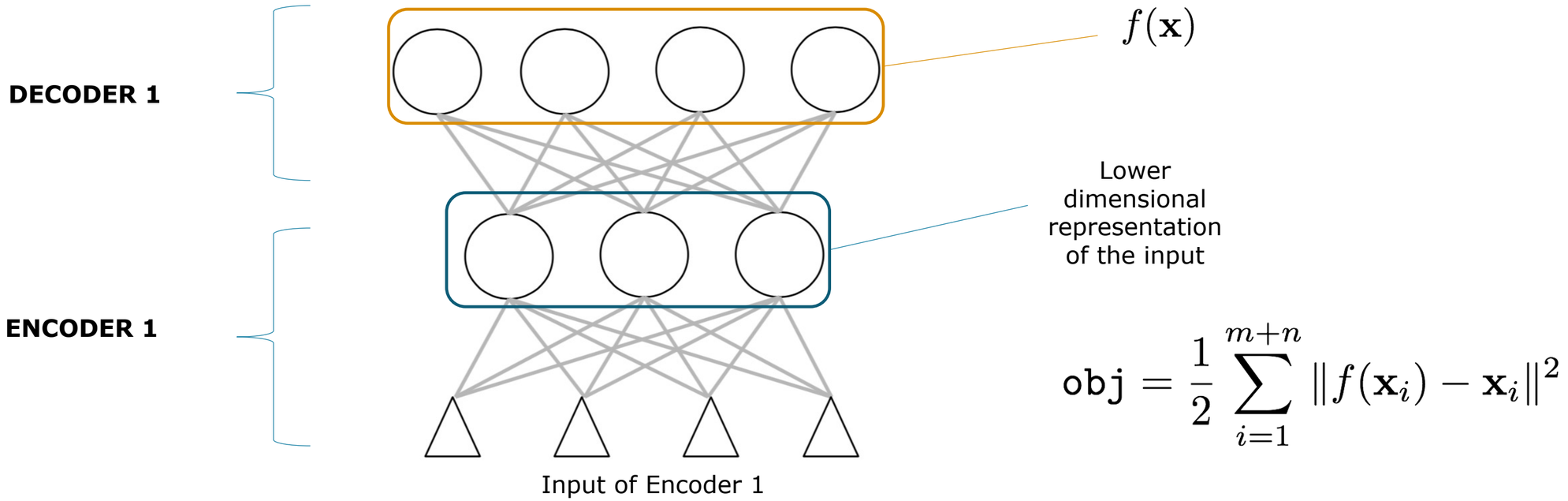
  - **Reconstruction loss**

$$\texttt{obj} = \frac{1}{2} \sum_{i=1}^{m+n} \left\| f(\mathbf{x}_i) - \mathbf{x}_i \right\|^2$$

(the sum is intended to go over all the available training points (being them supervised or not))

Layer-wise Training: Stacked Autoencoders (2)

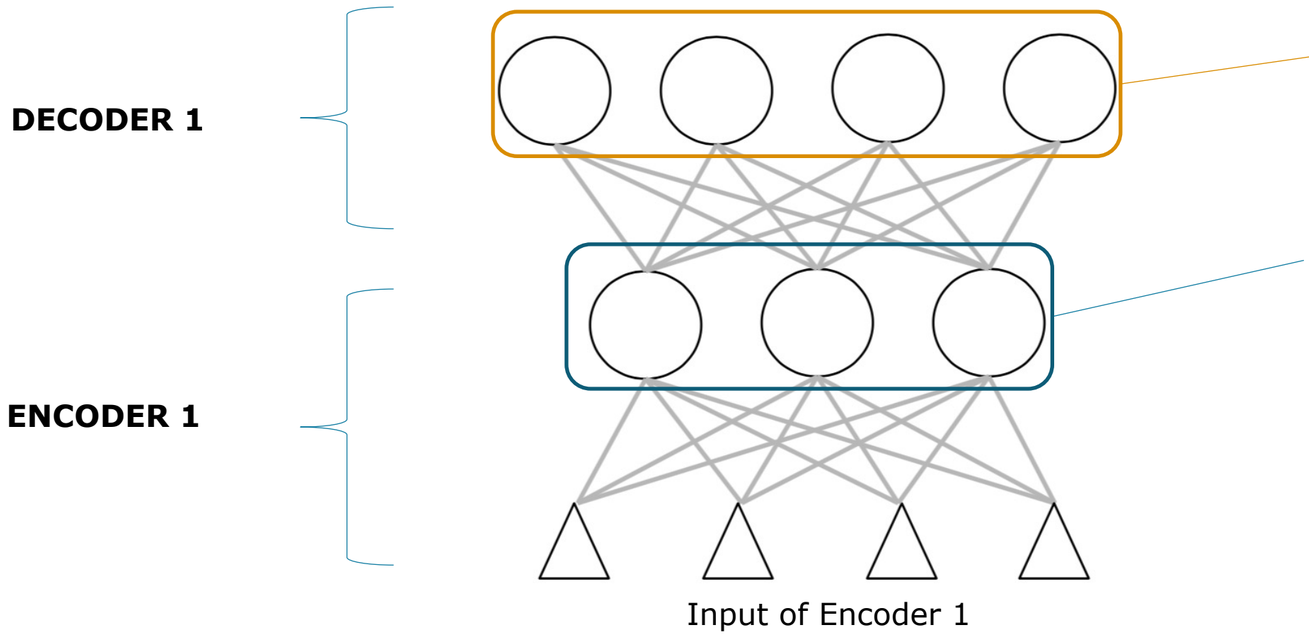
- Consider the case of autoencoders that projects the input onto a lower-dimensional space, before re-constructing it
  - There exists different types of autoencoders, with different architectural constraints



$$\texttt{obj} = \frac{1}{2}\sum_{i=1}^{m+n} \|f(\mathbf{x}_i) - \mathbf{x}_i\|^2$$

Layer-wise Training: Stacked Autoencoders (3)

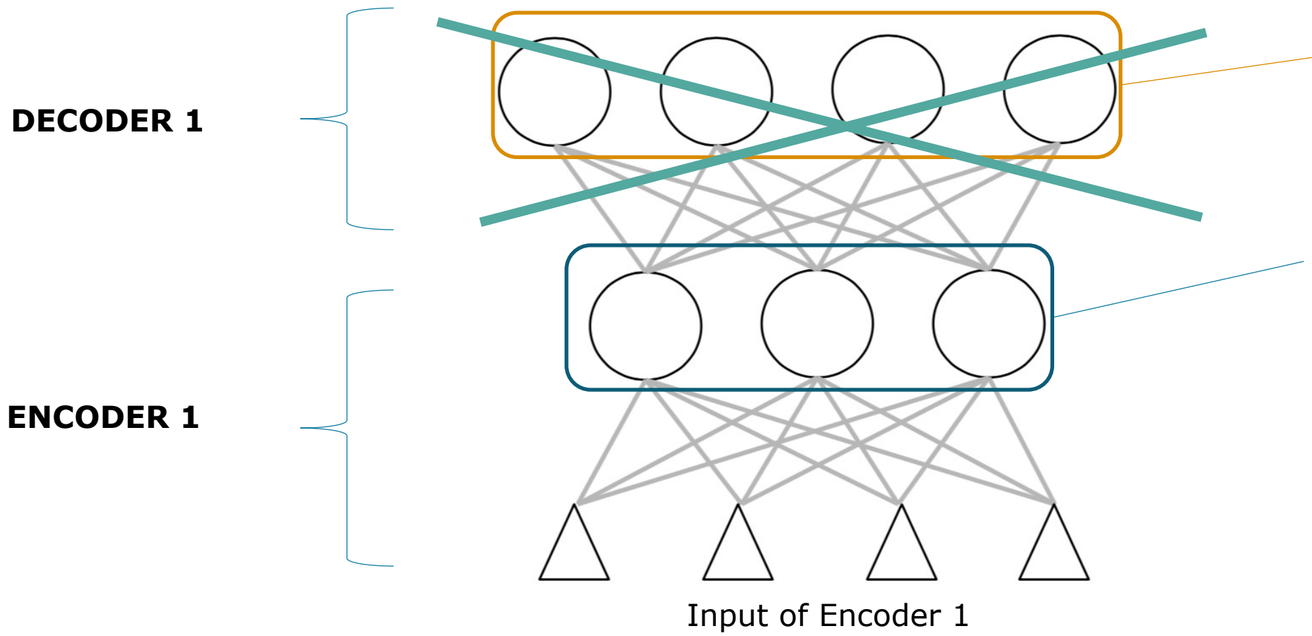
- The autoencoder is enforced to represent the data into a lower dimensional representation, thus discarding not-useful information
  - Similar examples are likely to be projected onto similar lower-dimensional representations



$$\texttt{obj} = \frac{1}{2}\sum_{i=1}^{m+n} \|f(\mathbf{x}_i) - \mathbf{x}_i\|^2$$

Layer-wise Training: Stacked Autoencoders (4)

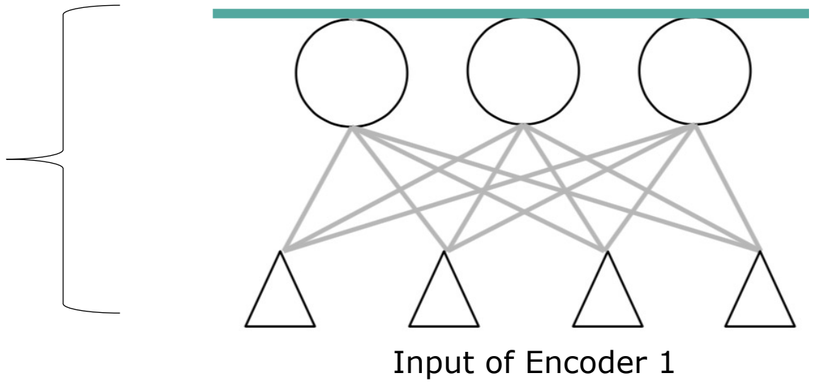
- Once the autoencoder has been trained, we can *remove the decoder*, and learn a new autoencoder, progressively building (layer-wise) a deep architecture



$$\texttt{obj} = \frac{1}{2}\sum_{i=1}^{m+n} \|f(\mathbf{x}_i) - \mathbf{x}_i\|^2$$

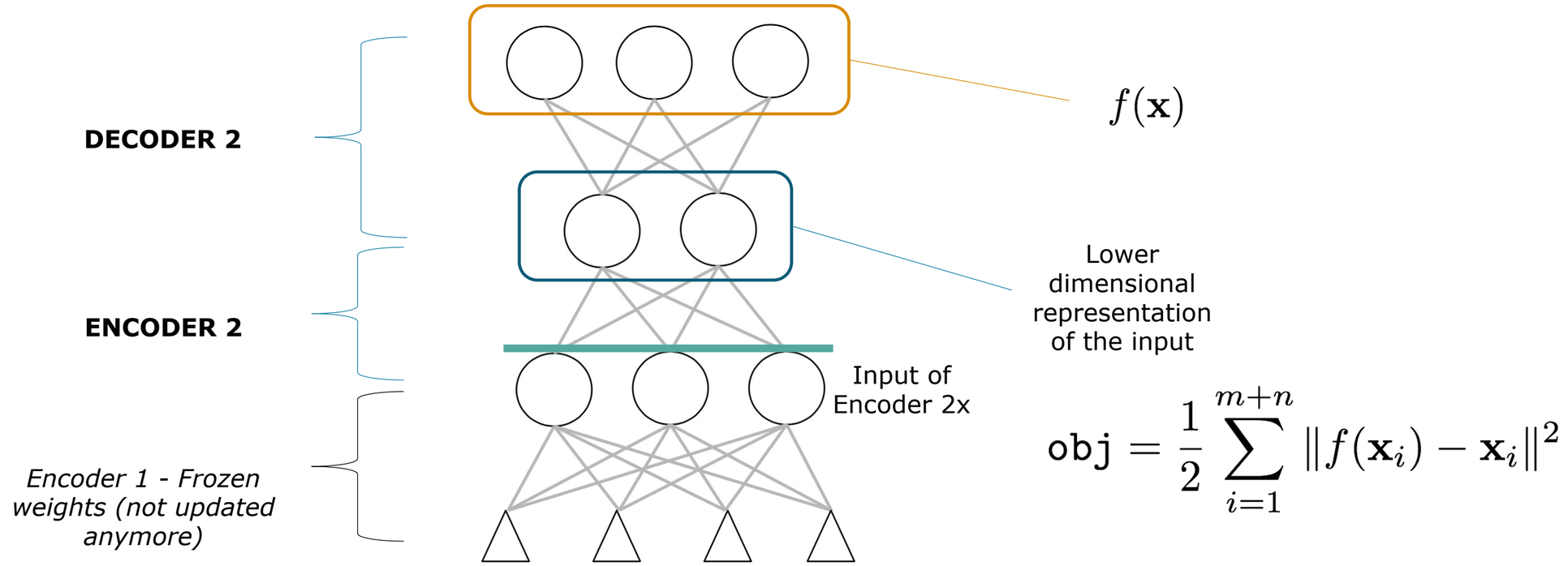
Layer-wise Training: Stacked Autoencoders (4)

- The weights of the encoder are kept **frozen** (that means the will not get updated by the following operations)



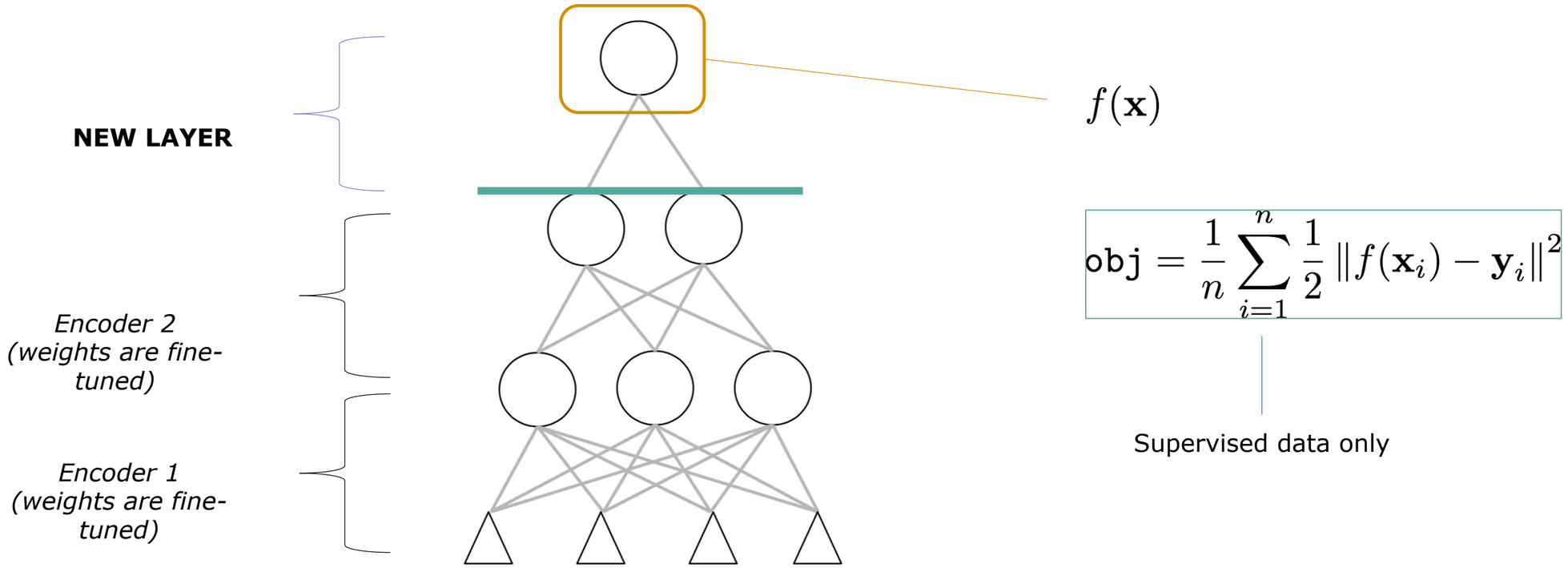
Layer-wise Training: Stacked Autoencoders (5)

- We can repeat the process and learn a new autoencoder that encodes/decodes the output of the just-learnt layer, progressively building (layer-wise) a deep architecture



Layer-wise Training: Stacked Autoencoders (6)

- Finally, the whole network can be **fine-tuned** using the available supervised data (*all the network weights are updated*)



Training Deep Networks: Weight Decay

- **Weight Decay**: a simple instance of L2-norm regularization
  - It improves the development of "regular/smoother" solutions, enhancing the generalization quality of the network and reducing overfitting

$$\texttt{obj} = \sum_j \texttt{loss}(x_i, y_i) + \sum_{h=1}^{\ell} \lambda_h \|\hat{\mathbf{w}}^h\|^2$$

This vector is flattened version of the weight matrix of layer h

  - The second element of the summation depends on a number of positive small scalar coefficients (lambdas), user-selected (it might involve only a sub-portion of the layers)
  - The norm is computed on the vector of all the weights in layer *h*
  - It favors solution with small weights

$$\frac{\partial \texttt{obj}}{\partial w_{ij}^h} = \sum_j \frac{\partial \texttt{loss}(x_i, y_i)}{\partial w_{ij}^h} + 2\lambda_h w_{ij}^h$$

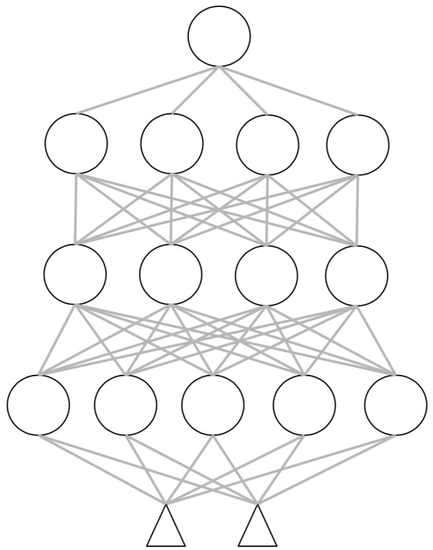
What we saw so far

New term

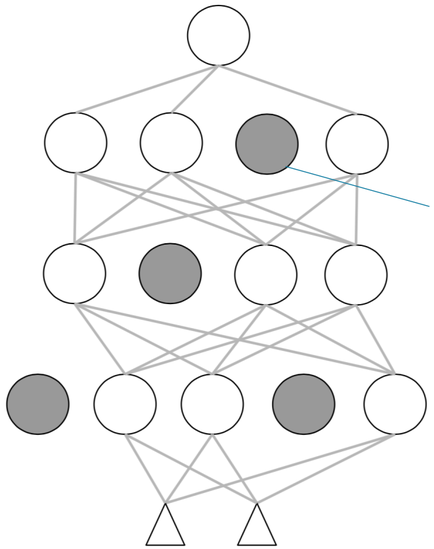
Training Deep Networks: Dropout

- **Dropout**: randomly drop units in training epochs (with a certain probability)
  - Dropped units are ignored (different units are dropped at different time instants)
  - Noisy training ➔ More robust layers
    - Layers are enforced to be robust to the dynamic dropping of the neurons that are inputs of the layer
    - It can be seen as a form of regularization
    - It reduces overfitting

Neural Net



Dropping some units



Selecting the Optimal Architecture

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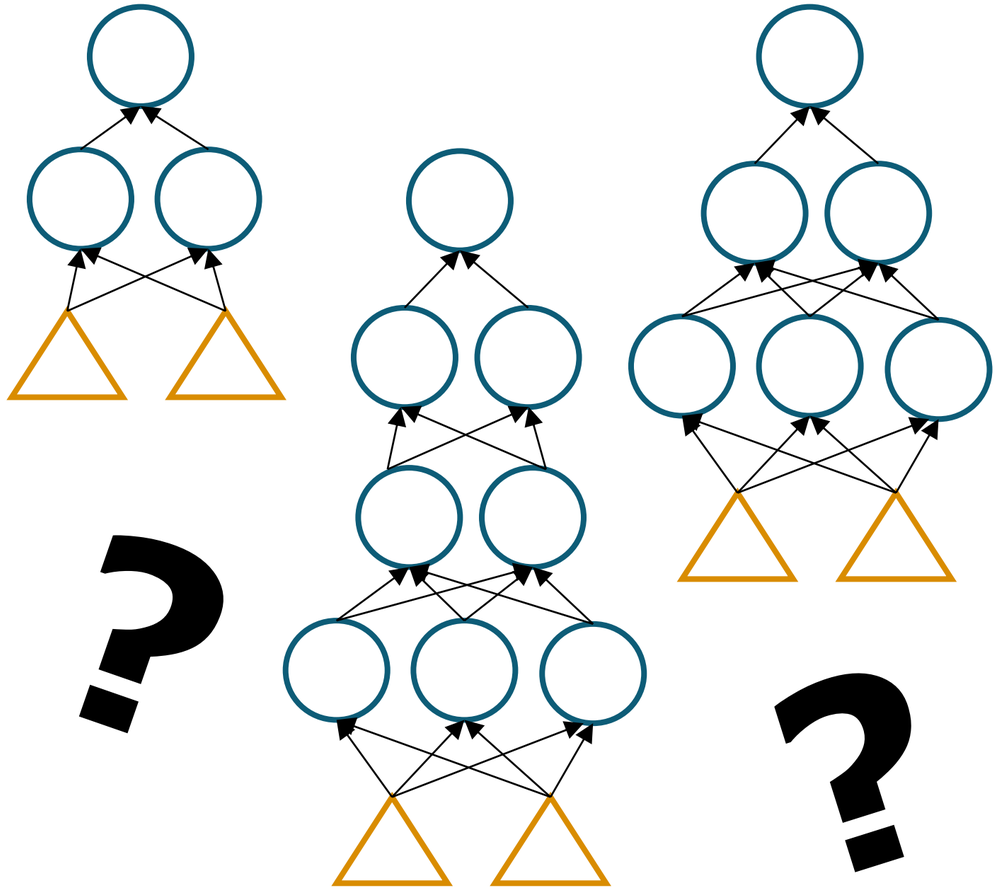
Which Architecture?

- We are given a learning problem and we want to approach it with neural networks:
  - *How many layers do we need?*
  - *How many neurons on each layer?*
  - *Which activation functions?*
  - *What about the appropriate learning rate?*
  - *How many epochs should we run the training procedure?*
  - *Which initialization of the weights?*



Which Architecture? (2)

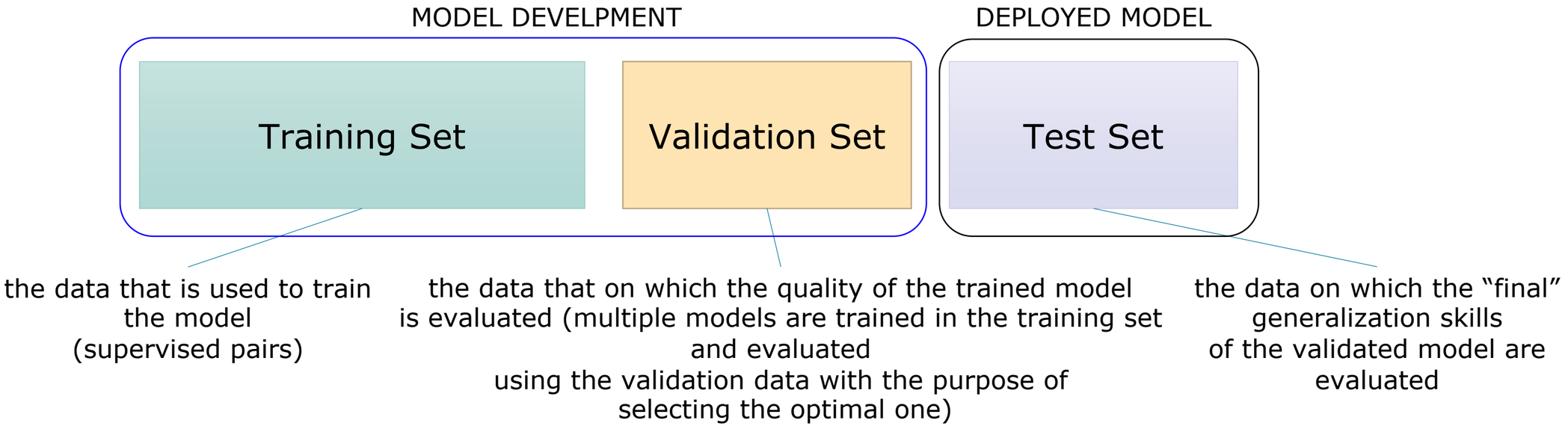
- Let us consider an award-winning network in the context of Computer Vision (object categorization)
  - The so-called ResNet model
  - **152 layers**
  - It is not a classical MLP as the ones we described in this course, but it is helpful to give an idea of how many layers researchers are experimenting in some Deep Learning problems
- Is this the best network to use?

*The the number of layers, and, more generally, the activation functions, learning rates, etc., are **task-dependent***

(we will generically talk about "network architecture", that is meant to include all these elements)

Data Splits

- The problem of determining the optimal architecture is usually solved by *training and evaluating multiple network architectures*, discovering the best one
  - Before diving into further details, it is important to remark the common data sets that are used when training and evaluating machine learning models



Data Splits (2)

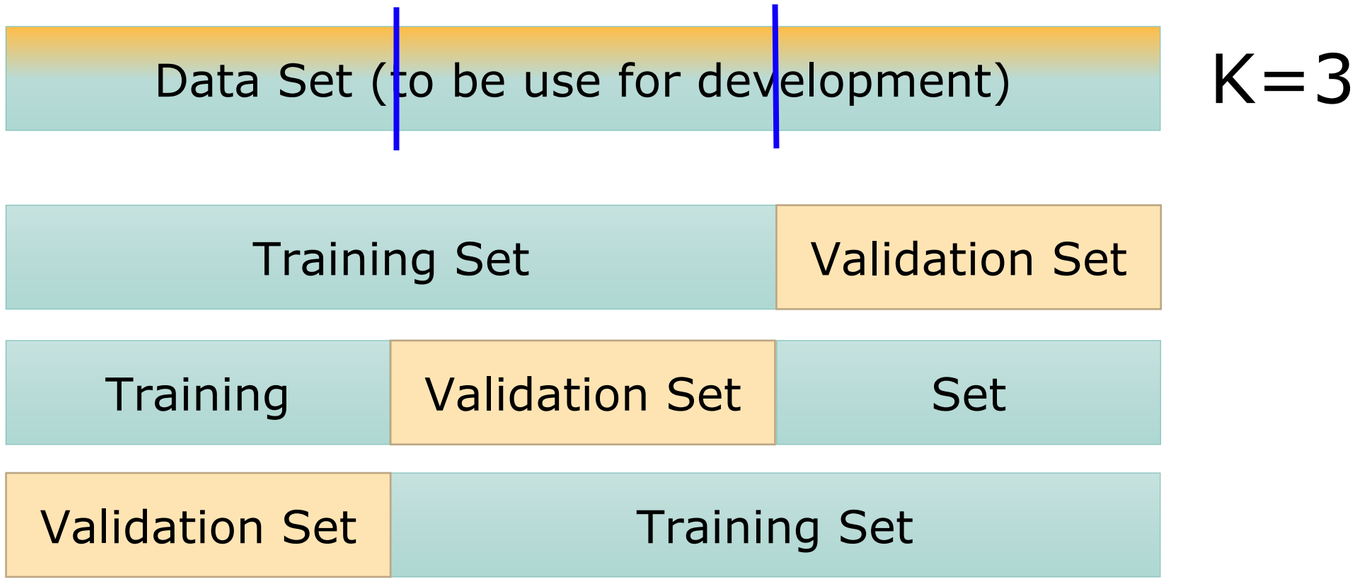
- When we are exposed to real-world problems, we do not have the use of training, validation, test set, but just a single dataset

- For example, a company might provide you a **dataset** that you are expected to use to develop you model, and they are keeping the **test data** as a private resource of the company, that the company will use to evaluate your work
  - Let's focus on such scenario…

We have to use these data to train the network(s) and find the best one

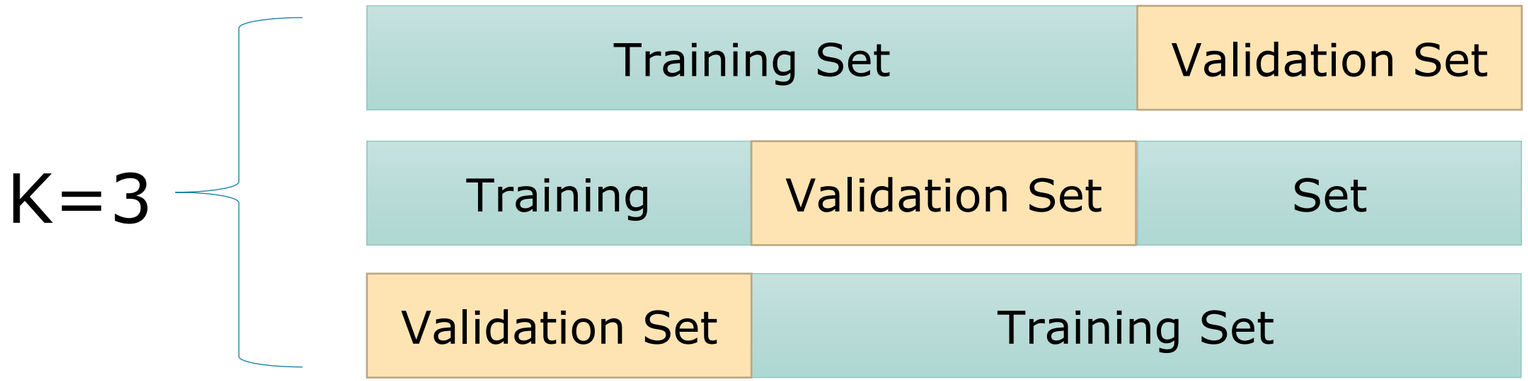
K-Fold Cross-Validation

- K-fold Cross-Validation is a very simple procedure that allows us to split the available data into multiple pairs *(training, validation set)*
  - The data is randomized and divided into *k* portions (**folds**) of equal size (balanced)
  - One fold is used as validation set, the other *k-1* are the training set



K-Fold Cross-Validation (2)

- For each neural architecture
  - We have *k* training sets and *k* validation sets
  - We train the model *k* times and we measure the performance (in the validation data) *k* times - then we can average the results to have a unique index that we can use to compare to different architectures



Measuring Performance

- We also have to define a way to measure the performance of the network
- In classification tasks, the most straightforward way is to use the **accuracy**
  - The number of right predictions divided by the total number of predictions that were computed

$$\texttt{accuracy} = \frac{\#\left[\texttt{prediction} = \texttt{class\_label}\right]}{\#\texttt{predictions}}$$

- It does not take into account the distribution of data over classes
  - For example, if your dataset has 90% of examples of class A and 10% of class B, a classifier that always outputs class A will get 0.9 of accuracy (90%)!
  - We can compute the accuracy on each class independently, and then average the results
    - Macro accuracy

Measuring Performance (2)

- Let's consider a binary classification problem (two classes, A and B)
- Let's describe the problem as the one of determining if an input example belongs to class A or not (then, of course, it will belong to class B)
  - Class A: *positive class*
  - Class B: *negative class*

- We can compute some useful measures, that are about the positive class:
  - TP: #**True Positives**
    - #Examples that were correctly classified as belonging to class A
  - FP: #**False Positives**
    - #Examples that were incorrectly classified as belonging to class A
  - TN: #**True Negatives**
    - #Examples that were correctly classified as not-belonging to class A
  - FN: #**False Negatives**
    - #Examples that were incorrectly classified as not-belonging to the class A

Measuring Performance (3)

- **Confusion Matrix**: the matrix that compares predictions and labels, counting the number of instances that falls in each of the 2x2=4 cases

Label	Prediction
A	A
A	B
A	B
B	B
B	B
B	A
B	B
B	A
B	A

PREDICTIONS

LABELS (SUPERVISIONS)

	A	B
A	1	2
B	3	3

PREDICTIONS

LABELS (SUPERVISIONS)

	A	B
A	TP	FN
B	FP	TN

Measuring Performance (4)

- We can use TP, FP, TN, FN to compute the following measures:

Already defined (right/true predictions on the total number of predictions)

$$\text{Accuracy} = \frac{TP+TN}{TP+FP+TN+FN}$$

$$\text{Precision} = \frac{TP}{TP+FP}$$

It measures "how good is the system when generating a positive decision" (if the system predicts the positive class for all the examples of that class, precision is 1)

$$\text{Recall} = \frac{TP}{TP+FN}$$

It is related to the tendency of the system of predicting the positive class (if the system ALWAYS predict such class, recall is 1)

$$\text{F-Measure (F1 Score)} = \frac{2 \cdot \text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$$

It mixes precision and recall (it is in [0,1])

Measuring Performance (5)

- In the multi-class case it is straightforward to compute the **confusion matrix**, that will a *c-by-c* matrix, where *c* is the number of classes

PREDICTIONS

LABELS (SUPERVISIONS)	A	B	C
A	…	…	…
B	…	…	…
C	…	…	…

PREDICTIONS

LABELS (SUPERVISIONS)	A	B	C
A	TP_A	FN_A	
B	FP_A	TN_A	
C			

PREDICTIONS

LABELS (SUPERVISIONS)	A	B	C
A	TN_C		FP_C
B			
C	FN_C		TP_C

Measuring Performance (5)

- Precision, Recall, F1 can be computed *for the predictor of each class*
  - **Precision of class *i***: divide the element in position *(i,i)* by the sum of the *i-th* row
  - **Recall of class *i***: divide the element in position *(i,i)* by the sum of the *i-th* column

- It is pretty common to average the **F1**'s of the *c* classes in order to have a single, multi-class index, if needed
  - Macro averaging

PREDICTIONS

LABELS (SUPERVISIONS)	A	B	C
A	TP_A	FN_A	
B	FP_A	TN_A	
C			

Selecting the Best Architecture

- Finding the optimal neural architecture for the considered task requires several trainings
  - It is a **costly** procedure, frequently underestimated by people that approach Machine Learning for the first time

- We have to try a **large number** of configurations with significantly different properties

- Several possible strategies
  - "Random" search (evaluate a batch of different configurations)
  - **Grid search** (next slide)
  - A mixture of both of random and grid search (next slide)

Selecting the Best Architecture (2)

- Grid search
  - Define the parameters that will be involved in the search procedure
    - Examples: Learning rate, number of layers, activation functions, …
  - For each of them, define a list of different values to evaluate
    - Example: Learning rate = [0.01, 0.001, 0.000001]
  - Test all the possible combinations of grid values

- Grid search is time consuming and it quickly becomes unfeasible
  - Coarse-to-fine search: define coarse grids and find the best configuration, then define new grids composed of values that are close to the ones of such configuration (**fine tune**)

- Another possible strategy consists in trying randomly selected configurations
  - And then **fine tune** the best one

Selecting the Best Architecture (3)

- Multiple trainings must be executed on the same architecture, given **different initializations of the weights**
  - The network accuracy can be averaged over the multiple training instances
  - In some tasks, especially in the ones that exploit large-scale fully supervised data, the quality of the solution is pretty stable with respect to different initialization

Selecting the Best Architecture (4)

- Frequently underestimated constraints in the selection of the optimal architecture are
  - The hardware-spec of the target machine in which the model will be deployed
  - The hardware-spec of the machine that will be used to train the network
- It is useless to train a large model if we are going to deploy it in a machine were each prediction would take a long time or where the available memory is not enough to store the trained model
- It is also useless to select large/deep models that would make the training times prohibitive
  - Evaluate smaller models or on subsets of the training data
  - Then make a last, long-term, training attempt using the whole training data or increasing the number of units in the selected model