MO434 - Deep Learning
Art of Training Deep Neural Networks

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Agenda

- Preparing data for training, validation, and test.
- Selecting a DNN architecture and its hyperparameters.
- Dealing with loss gradient instabilities.
- Further speeding up convergence.
- Scheduling the learning rate and avoiding under/overfitting
- Training and evaluating NNs in practice.

Data preparation

- A dataset $\mathcal{Z} = (X, Y)$ must be randomly divided into training (X_{tr}, Y_{tr}), validation (X_{vl}, Y_{vl}), and test (X_{ts}, Y_{ts}) sets by simulating the real distribution of samples.

- While (X_{tr}, Y_{tr}) is used to train the DNN, its validation on (X_{vl}, Y_{vl}) provides insights about training that guide the choice of the DNN's hyperparameters.

- $(X_{ts}, Y_{ts}$ is reserved to evaluate how well the DNN performs on unseen data.

- One may use a k-fold cross validation by dividing $(X_{tr}, Y_{tr}) \cup (X_{vl}, Y_{vl})$ into k parts, holding each part per time for (X_{vl}, Y_{vl}) and using the remaining samples for (X_{tr}, Y_{tr}). However, multiple splits of $\mathcal{Z}$ should be used to measure mean and standard deviation on the test sets.

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Let's see a simple example of data preparation ▸ DATA PREPARATION

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- However, more complex problems require too many neurons per hidden layer to be solved by shallow networks.
- Deep neural networks can be created with three or more hidden layers, but those dense layers with too many weights are difficult to be optimized.
- Convolutional layers have considerably reduced that number of weights, making viable and successful the use of DNNs.

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Ironically, except for NAS, architecture learning is still a feature engineering task.

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- We need methods to build effective DNNs with minimum human effort in data annotation [6, 7, 8, 9] and, ideally,
- from scratch guided by data visualization, optimization criteria, and user intervention [10, 11, 12].

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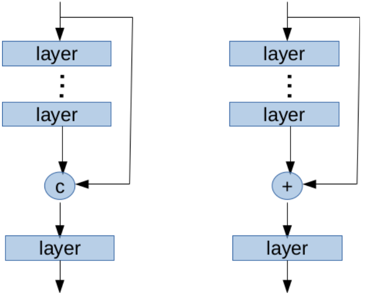
- Concatenation or addition of a previous layer input to the output of a subsequent layer is a way to avoid the vanishing gradient problem.



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- The weights of each layer may be randomly generated by a normal distribution with mean 0 and variance σ^2 or by a uniform distribution from $-r$ to $+r$, with $r = \sqrt{3\sigma^2}$.

Initialization	activation function	σ^2
Xavier/Glorot	None, tanh, logistic, softmax	$1/fan_{avg}$
He	ReLU and variants	$2/fan_{in}$
LeCun	SELU	$1/fan_{in}$

where fan_{in} and fan_{out} are the numbers of input and output channels, $fan_{avg} = \frac{fan_{in}+fan_{out}}{2}$.

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- Let $\boldsymbol{x}^{(i)}$ be the i-th feature vector of a batch $\mathcal{B} \subset X_{tr}$.

- Batch normalization creates a new feature vector $\boldsymbol{z}^{(i)}$ as follows.

$$
\begin{aligned}
\boldsymbol{\mu}_{\mathcal{B}} &\leftarrow \frac{1}{|\mathcal{B}|}\sum_{i=1}^{|\mathcal{B}|}\boldsymbol{x}^{(i)} \\
\boldsymbol{\sigma}^2_{\mathcal{B}} &\leftarrow \frac{1}{|\mathcal{B}|}\sum_{i=1}^{|\mathcal{B}|}\left(\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_{\mathcal{B}}\right)^2
\end{aligned}
$$

Dealing with loss gradient instabilities

$$\boldsymbol{z}^{(i)} \quad \leftarrow \quad \boldsymbol{\gamma} \otimes \frac{\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_{\mathcal{B}}}{\sqrt{\boldsymbol{\sigma}^2_{\mathcal{B}} + \epsilon}} + \boldsymbol{\beta}$$

where

- $\boldsymbol{\gamma}$ is a scale parameter vector for the layer, with one scale value per input.
- $\otimes$ is element-wise multiplication.
- $\boldsymbol{\beta}$ is a shift parameter vector for the layer, with one shift value per input.
- ϵ is typically 10^{-5} to avoid division by zero.

obs: all operations are element-wise from now on.

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- Using pretrained layers (backbone) from another network to generate an input to the current network with the remaining layers for training is another way to treat gradient instabilities and speed up convergence (transfer learning).

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- Finally, momentum and faster optimizers than SGD can be used to speed up convergence.

Further speeding up convergence

A momentum α (e.g., 0.9) can reduce oscillation in the loss values as follows.

$$\begin{aligned}\Delta \boldsymbol{w}_j^r(i) &\leftarrow \alpha \Delta \boldsymbol{w}_j^r(i-1) - \mu \sum_{s \in \mathcal{B} \subset \mathcal{Z}_{tr}} \delta_j^r(s) \boldsymbol{y}^{r-1}(s), \\ \boldsymbol{w}_j^r(i+1) &\leftarrow \boldsymbol{w}_j^r(i) + \Delta \boldsymbol{w}_j^r(i).\end{aligned}$$

For the sake of simplicity, these equations may be rewritten as

$$\begin{aligned}\boldsymbol{m} &\leftarrow \alpha \boldsymbol{m} - \mu \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}), \\ \boldsymbol{\theta} &\leftarrow \boldsymbol{\theta} + \boldsymbol{m}.\end{aligned}$$

where μ is the learning rate, $\boldsymbol{m}$, $\boldsymbol{\theta}$ and $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$ represent updates, weights and the gradient of the loss function during training.

Further speeding up convergence

Faster optimizers essentially estimate and correct the gradient vector towards a local minimum of the loss function.

- Nesterov Accelerated Gradient (NAG).

$$
\begin{aligned}
\boldsymbol{m} &\leftarrow \alpha\boldsymbol{m} - \mu\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta} + \alpha\boldsymbol{m}), \\
\boldsymbol{\theta} &\leftarrow \boldsymbol{\theta} + \boldsymbol{m}.
\end{aligned}
$$

- RMSProp.

$$
\begin{aligned}
\boldsymbol{s} &\leftarrow \rho\boldsymbol{s} + (1-\rho)\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \otimes \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}), \\
\boldsymbol{\theta} &\leftarrow \boldsymbol{\theta} - \mu\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \oslash \sqrt{\boldsymbol{s} + \epsilon}.
\end{aligned}
$$

where $\otimes$ and $\oslash$ are element-wise multiplication and division, respectively, $\rho = 0.9$, $\epsilon = 10^{-10}$, $\boldsymbol{m}$ and $\boldsymbol{s}$ initialized with zeros.

Further speeding up convergence

- Adam, Nadam, and AdaMax.

$$
\begin{aligned}
\boldsymbol{m} &\leftarrow \beta_1\boldsymbol{m} - (1-\beta_1)\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}),\\
\boldsymbol{s} &\leftarrow \beta_2\boldsymbol{s} + (1-\beta_2)\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \otimes \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}),\\
\hat{\boldsymbol{m}} &\leftarrow \frac{\boldsymbol{m}}{1-\beta_1^t},\\
\hat{\boldsymbol{s}} &\leftarrow \frac{\boldsymbol{s}}{1-\beta_2^t},\\
\boldsymbol{\theta} &\leftarrow \boldsymbol{\theta} + \mu\hat{\boldsymbol{m}} \oslash \sqrt{\hat{\boldsymbol{s}} + \epsilon}.
\end{aligned}
$$

where $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-7}$, $t \geq 1$ is the iteration, first $\boldsymbol{m}$ and second $\boldsymbol{s}$ momenta are initialized with zeros. Nadam is Adam with the Nesterov trick $\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta} + \beta_1\boldsymbol{m})$ and AdaMax replaces the second equation by $\boldsymbol{s} \leftarrow \max\{\beta_2\boldsymbol{s}, \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})\}$.

Scheduling the learning rate and avoiding under/overfitting

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- Strategies to change the learning rate during training are called learning schedules – e.g., $\mu^{(t)} = \mu^{(0)}0.1^{t//s}$ drops it by a factor of 10 at every s iterations.

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- Strategies to change the learning rate during training are called learning schedules – e.g., $\mu^{(t)} = \mu^{(0)}0.1^{t//s}$ drops it by a factor of 10 at every s iterations.

- By starting from a very low learning rate $\mu^{(0)}$ (e.g., low accuracy on $\mathcal{Z}_{tr}$ - underfitting) and increasing it at every s iterations until $\mu^{(t)}$, when we observe high accuracy on $\mathcal{Z}_{tr}$ and low accuracy on $\mathcal{Z}_{vl}$ (overfitting), we may estimate the best learning rate as $\mu^{(t-\delta)}$ (e.g., $\delta = 1$).

Scheduling the learning rate and avoiding under/overfitting

Recall our loss $J = \sum_{s \in \mathcal{B} \subset \mathcal{Z}_{tr}} \mathcal{E}(s)$ per batch. Overfitting can be avoided by regularization techniques.

- L1 and L2.

$$\begin{aligned}
\mathcal{E}(s) &= -\sum_{j=1}^{N_L} y_j(s) \log(y_j^L(s)) + 0.01 \sum_{r=1}^{L} \sum_{j=1}^{N_r} \|\mathbf{w}_j^r\|, \\
\mathcal{E}(s) &= -\sum_{j=1}^{N_L} y_j(s) \log(y_j^L(s)) + 0.0001 \sum_{r=1}^{L} \sum_{j=1}^{N_r} \|\mathbf{w}_j^r\|^2.
\end{aligned}$$

- Max-Norm, which rescales by $s \in (0, 1]$ (lower s, more regularization) the weights after each update – i.e., $\mathbf{w}_j^r \leftarrow s \frac{\mathbf{w}_j^r}{\|\mathbf{w}_j^r\|}$.
- Dropout, which before any layer $r \in [1, L]$ sets its weights $\mathbf{w}_j^r \leftarrow 0$ with probability $p \in [0.1, 0.5]$ at every training step.

Training and evaluating NNs in practice

To fix all we have learned, let's project and evaluate our first neural network with images. ▸ FirstDeepNeuralNetwork.

- We will understand the role of the validation set – it allows you to avoid underfitting and overfitting.
- The next step is an introduction to image analysis, so we can understand the success of DNNs in this field.
- We will then see that convolutional layers play a crucial role to make feasible the training of DNN models for image analysis.

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