Deep Learning (BEV033DLE) Lecture 6 Weight initialisation, batch normalisation, data augmentation

Czech Technical University in Prague

- Weight initialisation
- Batch normalisation
- Data augmentation
- Transfer learning

(1) Initialising all weights and biases with zero is not a good idea. Why?

Side step: symmetries and gradients:

Consider a scalar function f(w) that is invariant to the linear mapping $B \colon \mathbb{R}^n \to \mathbb{R}^n$, i.e. f(Bw) = f(w). Its gradient ∇f has the property

$$\nabla f(Bw) = B^{-T} \nabla f(w),$$

which follows from

$$\left\langle \nabla f(Bw), u \right\rangle \coloneqq \lim_{t \downarrow 0} \frac{f(Bw + tu) - f(Bw)}{t} \stackrel{!}{=} \left\langle \nabla f(w), B^{-1}u \right\rangle$$

What happens if SGD is started from an invariant point $w_0 = Bw_0$ and $B^{-T} = B$ holds?

$$B[w_0 - \alpha \nabla f(w_0)] = w_0 - \alpha \nabla f(Bw_0) = w_0 - \alpha \nabla f(w_0)$$

The new point w_1 will be again invariant, i.e. $Bw_1 = w_1$. We need to break the symmetry!

Invariance w.r.t. permutations



Gradient of a mirror symmetric function





(2) Initialise all weights and biases randomly from a uniform (or normal) distribution.

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- o.k. for shallow networks,
- not o.k. for deep networks!



Left: node statistics for layers of a deep FFN with ReLU units, all weights initialised from a normal distribution.

Middle and right: this can lead to vanishing/exploding gradients and "dead units" during learning

(3) **Proper initialisation:** Initialise weights/biases so that each neuron has activation statistic (over the dataset) with certain mean and variance.

Example 1 (Glorot & Bengio, 2010). Analyse variance of neuron outputs and backprop gradients under the following simplifying assumptions

• Tanh activation function f(x) in linear regime, i.e., $f(x) \approx x$

Neuron outputs as well as gradient components are i.i.d.

Start from a single neuron $y = w^T x$, $x \in \mathbb{R}^n$. Assume

$$lacksymbol{\circ}$$
 x_i are i.i.d. with $\mathbb{E}[x_i]=0$ and $\mathbb{V}[x_i]=\chi$

$$lacksymbol{\circ}~w_i$$
 are i.i.d. with $\mathbb{E}[w_i]=0$ and $\mathbb{V}[w_i]=\omega$

It follows that $\mathbb{E}[y] = 0$ and $\mathbb{V}[y] = n\omega\chi$.



Example 1 (cont.). Consider now a feedforward network with Tanh activation and assumptions as above. For layer k with n_k nodes, denote neuron outputs by x^k and gradients by ∇^k . Denote the variance of weights in layer k by ω_k .

- forward: $\mathbb{V}[x_i^k] = n_{k-1}\omega_k \mathbb{V}[x_j^{k-1}]$ We want $\mathbb{V}[x_i^k] \approx \mathbb{V}[x_j^{k-1}]$, i.e. $n_{k-1}\omega_k = 1$.
- $\label{eq:started} \bullet \ \text{backward:} \ \mathbb{V}[\nabla_i^k] = n_{k+1} \omega_{k+1} \mathbb{V}[\nabla_j^{k+1}] \\ \text{We want} \ \mathbb{V}[\nabla_i^k] \approx \mathbb{V}[\nabla_j^{k+1}] \text{, i.e.} \ n_k \omega_k = 1$
- Compromise: Set $\omega_k = \frac{2}{n_{k-1}+n_k}$. Assuming that the inputs x^0 have zero mean and unit variance, initialise the weights randomly by $w_{ij}^k \sim \mathcal{N}(0, \sqrt{\omega_k})$.

Similar considerations for ReLU activation lead to a different scheme (He et al., 2015)





Batch normalisation

(Joffe & Szegedy, 2015) Motivation:

- Keep control over neuron activation statistics during training
- Alleviate the need of specialised initialisation variants
- Regularise learning & pre-condition gradients

Batch normalisation: Denote by $\mathcal{B} \subset \mathcal{T}^m$ a mini-batch of training examples and by a_i the activation of a network unit $a_i = \sum_j w_{ij} x_j$. Re-parametrise it (stochastically) by using its statistic over mini-batches

$$\mu_{\mathcal{B}} = \mathbb{E}_{\mathcal{B}}[a_i] \quad \sigma_{\mathcal{B}}^2 = \mathbb{V}_{\mathcal{B}}[a_i]$$
$$\hat{a}_i = \frac{a_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \varepsilon}}$$
$$a_i \leftarrow \gamma \hat{a}_i + \beta \equiv BN_{\gamma,\beta}(a_i)$$

 $igstarrow \gamma_i$, eta_i are learnable parameters

- $\mu_{\mathcal{B}}$ and $\sigma_{\mathcal{B}}$ have to be differentiated w.r.t. network parameters
- exponentially weighted averages of $\mu_{\mathcal{B}}$ and $\sigma_{\mathcal{B}}$ are kept during training and used for inference.



Batch normalisation

Technical implementation of batch normalisation in PyTorch: A layer BatchNorm1d that

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- takes a tensor x with dimension [batchsize, channels] on input and returns a tensor y with same dimension on output,
- has learnable parameters γ and β for each channel (init: $\gamma = 1$, $\beta = 0$)
- keeps running averages of the batch statistic $\mu_{\mathcal{B}}$ and $\sigma_{\mathcal{B}}$ for each channel,
- depending on its state (train, eval) uses either the batch statistics or the saved running averages to compute its outputs.

For convolutional networks: use the layer BatchNorm2d, which computes statistics over batchsize and spatial dimensions.

Batch normalisation:

- alleviates the need of special weight initialisation since it implements the scheme (3) discussed above for the first mini batch,
- the neuron outputs for a particular training example depend on the outputs of the other examples in the mini-batch, which in turn is stochastic.
- can be seen as stochastic re-parametrisation of weights and gradient preconditioning

$$w \to \gamma \frac{w}{\sigma_{\mathcal{B}}} \qquad b \to \gamma \frac{(b - \mu_{\mathcal{B}})}{\sigma_{\mathcal{B}}} + \beta$$

Data augmentation

Goals of data augmentation:

 Artificially enlarge the training set – an attempt to bound the generalisation error (i.e. prevent overfitting). 8/11

• Enforce invariance of the predictor w.r.t. certain transformations of the input space.

Technically: online augmentation generates new data on the fly, whereas offline augmentation stores augmented datasets.

We discuss it here in context of image processing (classification, segmentation . . .)

(Image) data augmentation: Create new images from a single training image

- geometric transformations: flip, crop, rotate, non-linear transformations, . .
- photometric transformations: color space transformations, histogram changes, . . .
- kernel transforms: sharpening, blurring, . . .
- noise: pixel-wise independent noise, jitter, random erasing, . . .

Data augmentation





Available libraries & methods: Augmentor, Albumentations, DeepAugment, GAN based style transfer, ...

Transfer Learning: pre-training & fine-tuning

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Transfer learning: pre-training + fine-tuning

- You want to train a predictor for a complex recognition task, but suffer from lack of training data.
- A predictor for a different task has been successfully trained on a large dataset.
- The domains of the two tasks are similar.

We can use the following approach

- Use the first layers of the network that implements the predictor for the other task.
- Add your layers on top
- Learn the network on your data, if necessary apply early stopping to prevent overfitting. This can be done in two ways
 - (1) freeze the parameters of the transferred layers
 - (2) fine-tuning: learn parameters of all layers

Transfer Learning: pre-training & fine-tuning

Example 2 (Yosinski et al., NIPS 2014). Randomly split the 1000 Image-Net classes intervector two groups with 500 classes: datasets A and B. Learn BnB, BnB^+ , AnB and AnB^+ networks. Here: letters indicate the task of the pre-trained/transfer network, n is the layer number and + indicate the fine-tuning variant.



blue: BnB, BnB^+ red: AnB, AnB^+