Notes on INFO8010 - Deep Learning

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This document contains notes and additional readings for self-study.

Lecture 4: Computer Vision

- Misc.
 - On cross-entropy
 - * (Wiki page) Cross Entropy
 - * A Gentle Introduction to Cross-Entropy for Machine Learning
 - * Liangjie Hong: Notes on Logistic Loss Function
- Classification
 - Image augmentation
 - Use pre-trained models for fine tuning and transfer learning
 - Large networks trained for classification are heavily re-used for object detection and semantic segmentation tasks.
- Object Detection
 - YOLO for object detection
 - * EPFL EE-559, 8-3: Object Detection
 - R-CNN
 - * Dive into Deep Learning 13.8. Region-based CNNs (R-CNNs)
 - Takeaways
 - * One-stage detectors (YOLO, SSD, RetinaNet, etc) are fast for inference not as accurate.
 - * Two-stage detectors (Fast R-CNN, Faster R-CNN, R-FCN, Light head R-CNN, etc) are usually slower but are more accurate.
 - * Both depend on engineering decisions.
- Segmentation
 - Task: partitioning an image into regions of different semantic categories at pixel level.
 - Fully convolutional network(FCN) and transposed convolution
 - * CS231n, Lecture 11, 2018.
 - Mask R-CNN
 - * Object detection combined with mask prediction enables instance segmentation.
 - * Dive into Deep Learning 13.8.4 Mask R-CNN

Lecture 5: Training Neural Networks

- Gradient descent
 - GD, SGD, mini-batch SGD
 - Rely on assumptions on 1) the magnitude of the local curvature to set the step size, and 2) *isotropy* in gradient so the step size makes sense in all directions
- Wolfe conditions ensures that both the loss function decreases sufficiently and the slope reduces sufficiently. However, line search will be too expensive for DL, and might lead to local minimum / overfitted solution.
- Momentem
 - Use momentum to add inertia in the choice of the step direction
 - Nesterov momentem
- Adaptive learning rate: without the assumption of istropic gradient
 - Per-parameter methods: AdaGrad, RMSProp, Adam
 - Scheduling
- Some additional reading on optimization: (Sebastian Ruder) An overview of gradient descent optimization algorithms
- Initialization
 - Principles
 - * Break symmetry
 - * Control variance of activation across layers during forward and backward pass
 - Xavier initialization
- Normalization
 - Batch normalization
 - Layer normalization

Lecture 6: Recurrent Neural Networks

- Some of the notes were added by reviewing EPFL EE-559, 12.1 Recurrent Neural Networks, 12.2 LSTM and GRU
- Types of tasks
 - Classification: sequence to classes
 - Synthesis: real values to sequence
 - Translation: sequence to sequence
- Temporal convolutions
- Recurent neural networks
 - Structure
 - * maintain a recurrent state updated at each time step (a function of state the previous step, input of the current step, and weights), $\mathbf{h}_t = \phi(\mathbf{x}_t, \mathbf{h}_{t-1}; \theta)$. So if $\mathbf{x} \in \mathbb{R}^D$ and $\mathbf{h} \in \mathbb{R}^Q$, then $\phi : \mathbb{R}^D \times \mathbb{R}^Q \to \mathbb{R}^Q$
 - * Predictions can be computed at any step from the recurrent state $y_t = \psi(\mathbf{h}_t; \theta)$.

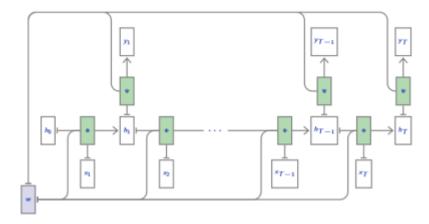


Figure 1: RNN

* Elman netoworks apply non-linear activation functions as ϕ and ψ

$$h_t = \text{ReLU}(W_{x(\times h)}\mathbf{X}_t + W_{(h \times h)}h_{t-1} + b_{(h)}), \quad y_T = W_{(h \times y)}h_T + b_{(y)}$$

- Stacked RNN
 - * Since RNNs can be viewed as layers producing sequences of activations, and can be stacked
- Bidirectional RNNs. RNNs can be made bidirectional. run the same single direction RNN twice from both end and concatenate the states.
- Gating
 - * Similar to the skip connections in ResNet, RNN cells can include pass-throughs so recurrent state does not go repeatedly through a squashing non-linearity.
 - * *forget gate*: current state update be a per-component weighted average of its previous value and a full update, with the weighting depending on input and the previous state.

We can improve our minimal example with such a mechanism, from our simple

$$h_t = \mathsf{ReLU}\left(W_{(x\ h)} \times_t + W_{(h\ h)} h_{t-1} + b_{(h)}\right) \qquad \text{(recurrent state)}$$
o
$$\bar{h}_t = \mathsf{ReLU}\left(W_{(x\ h)} \times_t + W_{(h\ h)} h_{t-1} + b_{(h)}\right) \qquad \text{(full update)}$$

$$z_t = \mathsf{sigm}\left(W_{(x\ z)} \times_t + W_{(h\ z)} h_{t-1} + b_{(z)}\right) \qquad \text{(forget gate)}$$

$$h_t = z_t \odot h_{t-1} + (1 - z_t) \odot \bar{h}_t \qquad \text{(recurrent state)}$$

Figure 2: rnn: forget gate

- LSTM is able to learn long-term dependencies, and the core idea is to use cell state and erase/update/output
 gates for cell state information.
 - * See Understanding LSTM Networks by Colah
 - * Mathematical formulation of a LSTM cell

The recurrent state is composed of a "cell state" c_t and an "output state" h_t . Gate f_t modulates if the cell state should be forgotten, i_t if the new update should be taken into account, and o_t if the output state should be reset.

$$\begin{split} f_t &= \operatorname{sigm} \left(W_{(x-f)} x_t + W_{(h-f)} h_{t-1} + b_{(f)} \right) & \text{(forget gate)} \\ i_t &= \operatorname{sigm} \left(W_{(x-f)} x_t + W_{(h-f)} h_{t-1} + b_{(f)} \right) & \text{(input gate)} \\ g_t &= \tanh \left(W_{(x-c)} x_t + W_{(h-c)} h_{t-1} + b_{(c)} \right) & \text{(full cell state update)} \\ c_t &= f_t \odot c_{t-1} + i_t \odot g_t & \text{(cell state)} \\ o_t &= \operatorname{sigm} \left(W_{(x-o)} x_t + W_{(h-o)} h_{t-1} + b_{(o)} \right) & \text{(output gate)} \\ h_t &= o_t \odot \tanh(c_t) & \text{(output state)} \end{split}$$

As pointed out by Gers et al. (2000), the forget bias $b_{(f)}$ should be initialized with large values so that initially $f_t \simeq 1$ and the gating has no effect.

This model was extended by Gers et al. (2003) with "peephole connections" that allow gates to depend on $c_{\varepsilon-1}$.

Figure 3: lstm: math

- * A visualization of a (two-layer) LSTM
- GRU (gated recurren unit) uses two (instead of three as in LSTM) gates (update/reset), and it performs similarly to LSTM but with fewer parameters (although LSTM is strictly stronger).
 - * Mathematical formulation of a GRU cell
- Graident

Several such "cells" can be combined to create a multi-layer LSTM.

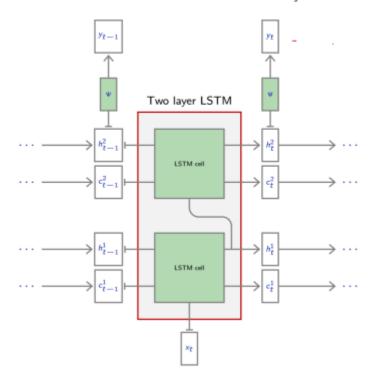


Figure 4: lstm: diagram

The LSTM were simplified into the Gated Recurrent Unit (GRU) by Cho et al. (2014), with a gating for the recurrent state, and a reset gate.

$$\begin{split} r_t &= \operatorname{sigm} \left(W_{(x-r)} x_t + W_{(h-r)} h_{t-1} + b_{(r)} \right) & \text{(reset gate)} \\ z_t &= \operatorname{sigm} \left(W_{(x-z)} x_t + W_{(h-z)} h_{t-1} + b_{(z)} \right) & \text{(forget gate)} \\ \bar{h}_t &= \tanh \left(W_{(x-h)} x_t + W_{(h-h)} (r_t \odot h_{t-1}) + b_{(h)} \right) & \text{(full update)} \\ h_t &= z_t \odot h_{t-1} + (1-z_t) \odot \bar{h}_t & \text{(hidden update)} \end{split}$$

Figure 5: GRU: math

* Note that gated units prevent gradients from vanishing, but not from exploding, which can be solved using **gradient norm clipping** (scaling of the norm).

$$\tilde{\triangledown f} = \frac{\triangledown f}{||\triangledown f||}\min(||\triangledown f||,\delta)$$

- * Orthogonal initialization (of the weight matrix) will guarantee that activations will neigher vanish nore explode.
- Applications
 - Sentiment analysis
 - * Document-level modeling for sentiment analysis (= text classification), with stacked, bidirectional and gated recurrent networks. (Duyu Tang et al, 2015)
 - Language models
 - * Language as Markov Chain $p(\mathbf{w}_t|\mathbf{w}_{1:t-1})$
 - * An instance of sequence synthesis where predictions are computed at all time steps
 - * Text generation (Max Woolf 2018)
 - Sequence synthesis
 - Neural machine translation (Google's Neural Machine Translation System: Bridging the Gap between Human and Machine Translation)
 - Text-to-speech synthesis
- Beyond sequences
 - Neural computers
 - Programs as neural nets
 - Graph neural network
- Reference
 - Kyunghyun Cho, "Natural Language Understanding with Distributed Representation", 2015

Lecture 7: Auto-encoders and generative models

- An auto-encoder is a composite function made of
 - encoder f from the original space \mathcal{X} to a latent space \mathcal{Z}
 - decoder g to map back to \mathcal{X}
 - such that $g \circ f$ is close to the identity on the data, i.e. $\mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})}[||\mathbf{x} g \circ f(\mathbf{x})||^2] \approx 0$
 - Training an auto-encoder consists of minimizing this loss function to find the best parameterization of f and g.
- Interpolation on latent space can be made to get an intuition of the learned latent representation.
- Denoising auto-encoders
 - The goal is to optimize $h = g \circ f : \mathcal{X} \to \mathcal{X}$ such that a perturbation $\tilde{\mathbf{x}}$ is restored to \mathbf{x} .
 - A weakness of denoising auto-encoder is that the posterior $p(\mathbf{x}|\tilde{\mathbf{x}})$ may be multi-modal.
- Generative models
 - a probabilistic model that can be used to simulate the data, $\mathbf{x} \sim p(\mathbf{x}; \theta)$.
 - Applications
 - * Supper-resolution, Compression, text-to-speech
 - * Proteomics, drug discovery, astronomy
 - * Planning, exploration, model-based RL
 - The decoder g can be assessed by introducing a density model q over the latent space \mathcal{Z} for sampling and mapping back into the data space \mathcal{X} . (e.g., Gaussian $q(\mathbf{z}) = \mathcal{N}(\hat{\mu}, \hat{\Sigma})$)
 - Sampled and generated results are not satisfactory because the density model p on the latent space is too simple and inadequate.
- Variational inference (VI)
 - A prescribed latent variable model that defines a joint probability $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z})$
 - Bayes rule gives $p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{p(\mathbf{x})}$, which is intractable for integrating over \mathbf{x} .
 - VI turns the posterior inference into an optimization problem that minimize the KL divergence between $p(\mathbf{z}|\mathbf{x})$ and the approximation $q(\mathbf{z}|\mathbf{x};\nu)$
 - * See slides pp. 44 pp.47 for details of the KL divergence, evidence lower bound objective (ELBO), and the optimization setups.

- * ELBO encourages distributions to place their mass on configurations of latent variables that explain the oberved data, and close to the prior.
- Variational auto-encoders
 - Variational auto-encoder is a deep latent model where
 - * $p(\mathbf{x}|\mathbf{z};\theta)$ is parameterized with a **generative network** NN_{θ} (decoder) that takes input $\mathbf{z} \in \mathcal{Z}$ and outputs parameters $\phi = NN_{\theta}(\mathbf{z})$ to the data distribution, i.e.

$$\mu, \sigma = \text{NN}_{\theta}(\mathbf{z}), \quad p(\mathbf{x}|\mathbf{z}; \theta) = \mathcal{N}(\mathbf{x}; \mu, \sigma^2 \mathbf{I})$$

* The approximate posterior $q(\mathbf{z}|\mathbf{x};\varphi)$ is parameterized with an **inference network** NN_{φ} (encoder) that takes as input \mathbf{x} and outputs parameters $\nu = \mathrm{NN}_{\varphi}(x)$ to the approximate posterior. E.g.

$$\mu, \sigma = NN_{\varphi}(\mathbf{x}), \quad q(\mathbf{z}|\mathbf{x}; \varphi) = \mathcal{N}(\mathbf{z}; \mu, \sigma^2 \mathbf{I})$$

- We use variational inference to jointly optimize the generative and inference networks.
 - * Doing so involves Monte Carlo integration (for computing gradients of the ELBO w.r.t. θ) and reparameterization trick + Monte Carlo (for computing gradients of ELBO w.r.t. φ)

Lecture 8: Generative Adversarial Networks

- Generative adversarial networks (GANs)
 - Two-player game
 - * Generator network $g(\cdot; \theta) : \mathcal{Z} \to \mathcal{X}$ with prior $p(\mathbf{z})$ on latent space, thereby inducing a generative distribution

$$\mathbf{x} \sim q(\mathbf{x}; \theta) \iff \mathbf{z} \sim p(\mathbf{z}), \mathbf{x} = g(\mathbf{z}; \theta)$$

- * Discriminative network $d(\cdot; \phi) : \mathcal{X} \to [0, 1]$ as a classifier to distinguish between true samples $\mathbf{x} \sim p(\mathbf{x})$ and generated samples $\mathbf{x} \sim q(\mathbf{x}; \theta)$
- Objective of GANs
 - * Use cross-entropy loss for d and we have the value function (log-likelihood)

$$V(\phi, \theta) = \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})}[\log d(\mathbf{x}; \theta)] + \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})}[1 - d(q(\mathbf{z}; \theta); \phi))]$$

- * The ultimate goal is $\theta^* = \arg\min_{\theta} \max_{\phi} V(\phi, \theta)$
- * Mathematically θ^* is minimum $\iff p(\mathbf{x}) = q(\mathbf{x}; \theta)$, that is, the corresponding generative model can perfectly reproduce the true data distribution.
- Learning process
 - * Alternating SGD

$$\theta \leftarrow \theta - \gamma \nabla_{\theta} V(\phi, \theta); \quad \phi \leftarrow \phi - \gamma \nabla_{\phi} V(\theta, \phi)$$

- * For each step of θ we can take k steps on ϕ to make the classifier near optimal
- * Computing ∇_{θ} requires backprop through d before computing the partial derivatives w.r.t. g's internals.
- Open problems
 - * Training standard GAN often results in pathological behaviors due to
 - · Oscillations without convergence
 - · Vanishing gradients
 - · Mode collapse: g models well on a small sub-population concentrating on a few modes of the data distribution.
 - · Performance diffucult to assess in practice.
- Wasserstein GANs
 - Original GAN as defined above suffers from vanishing gradients, especially when initialy $\mathbf{x} \sim q(\mathbf{x}; \theta)$ can be so bad that the response of d saturates, meaning d is nearly perfect there fore $V(\phi, \theta) = ...(definedabove)$ has near-zero gradients which halts the optimization.
 - * One of the reason for the setback is that Jensen-SHannon divergence poorly accounts for the metric structure of the space.
 - Wasserstein GAN uses Wasserstein-1 distance

$$\theta^* = \arg\min_{\theta} W_1(p(\mathbf{x}||q(\mathbf{x};\theta))) = \arg\min_{\theta} \max_{\phi: ||d(\cdot;\phi)||_L \le 1} \mathbb{E}_{\mathbf{x} \sim p(\mathbf{x})}[d(\cdot;\phi)] - \mathbb{E}_{\mathbf{x} \sim q(\mathbf{x};\theta)[d(\mathbf{x};\theta)]}$$

- * In this case, $d: \mathcal{X} \to \mathbb{R}$ is a critic function that satisfies 1-Lipschitzness.
- * See Arjovsky et al (2017) and Gulrajani et al (2017) for details.
- As a result, Wasserstein GANS benefit from
 - * A meaningful loss metric
 - * Improved stability (no mode collapse is observed)
- Convergence of GANs
 - TODO: this section (from pp. 39 54) is skipped for now, with some brief notes as follows:
 - * GANs suffer from saddle point, see Ferenc Huszár, GANs are Broken in More than One Way, 2017 for details
 - * The loss function of Vanilla GANs and Wisserstein GANs can be unified to analyse the convergence.
 - * Reference: Mescheder et al, 2018. Which Training Methods for GANs do actually Converge?
- State of the art
 - Progress: Wasserstein GANs as baseline + Gradient Penalty (Gulrajani 2017) + quite a few other tricks
 - BigGANs
 - * Brock et al, 2018: Large Scale GAN Training For High Fidelit Natural Image Synthes
 - StyleGAN
 - * V1: Karras et al, 2018
 - * V2: Karras et al, 2019
- Applications
 - The prior $p(\mathbf{z})$ of the latent space need not be a random noise distribution
 - Image-to-image translation: CycleGANs (Zhu et al, 2017)
 - Nvidia: Stroke of Genius: GauGAN Turns Doodles into Stunning, Photorealistic Landscapes
 - Captioning
 - Text-to-image synthesis
 - * Zhang et al, 2017: StackGAN: Text to Photo-realistic Image Synthesis with Stacked Generative Adversarial Networks
 - Music generation
 - * MuseGAN (Dong et al, 2018)
 - Accelerating scientific simulators
 - * Learning particle physics (Paganini et al, 2017)
 - * Learning cosmological models (Rodriguez et al, 2018)
 - * Brain reading (Shen et al, 2018)

Supplementary Notes

This section contains reading notes for lecture 12 - 13 of the EPFL EE-559 – Deep Learning course as supplementary materials to the INFO8010 course.

Recurrent models and NLP

- 12.3. Word embeddings and translation
 - Motivation: To devise a proper density model for sequence of words when vocabularies are usually of the order of $10^4 10^6$ words, a standard strategy is to embed words into a geometrical space and exploit regularities for further statistical modeling.
 - Continuous Bag of Words (CBOW, Mikolov et al., 2013a)
 - * In this model, the embedding vectors are chosen so that a word can be [linearly] predicted from the sum of the embeddings of words around it.
 - * Negative sampling on the correct class and randomly sample the incorrect classes.
 - * Uses (variant of) logistic loss
 - Skip-gram
 - * Optimizes the embedding so that a word can be predicted by any individual word in its context.
 - Sequence-to-sequence translation
 - * Diagram

If the corpus is "The black cat plays with the black ball.", we will get the following word IDs:

The corpus will be encoded as

the black cat plays with the black ball
$$0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 0 \quad 1 \quad 5$$

and the data and label tensors will be

		Words					IDs			c	W
the	black	cat	plays	with	0	1	2	3	4	0, 1, 3, 4	2
black	cat	plays	with	the	1	2	3	4	0	1, 2, 4, 0	3
cat	plays	with	the	black	2	3	4	0	1	2, 3, 0, 1	4
plays	with	the	black	ball	3	4	0	1	5	3, 4, 1, 5	0

Figure 6: CWOB example

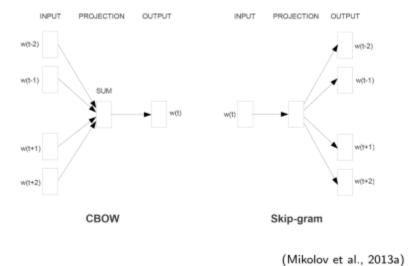


Figure 7: Skip gram diagram

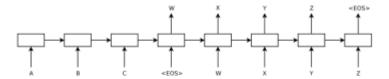


Figure 1: Our model reads an input sentence "ABC" and produces "WXYZ" as the output sentence. The model stops making predictions after outputting the end-of-sentence token. Note that the LSTM reads the input sentence in reverse, because doing so introduces many short term dependencies in the data that make the optimization problem much easier.

* Evaluation standard: **BLEU** (bilingual evaluation understudy) score that counts the fraction of groups of one, two, three and four words (aka "n-grams") from the generated sentence that appear in the reference translations.

Attention models

Resrouces

- EPFL EE-559 Deep Learning EE-559 "Deep Learning", taught by François Fleuret in the School of Engineering of the École Polytechnique Fédérale de Lausanne, Switzerland.
- Dive into Deep Learning: An interactive deep learning book with code, math, and discussions, based on the NumPy interface.
- Notes of deep learning specialization, good for reviewing the fundamentals of DL.