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- Introduction to Neural Networks
  - Feed-Forward Neural Networks
  - Hyper-parameters
- Optimization
- Regularization

Machine learning, big data and artificial intelligence – Block 4

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Evaluation assignment 2

- Took too much time (roughly 26h) - how to solve this? Hints? remove subtasks?
- More teaching on code
- The bugs...
- Minor comments:
  - xgboost video
  - bigger diff between RF and bagging
  - more focus on the assignment on the lecture

Grading of assignment 1

- Why is SGD important?
- Differece between unsupervised and supervised learning. Task or experience?

Masters thesis proposals

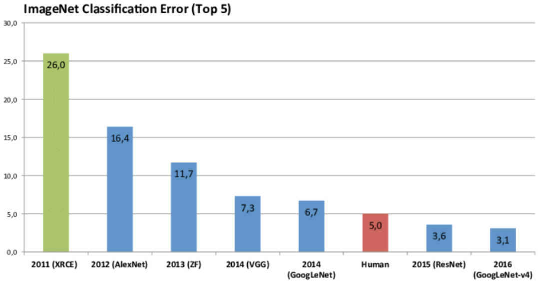
1. Evaluation of probabilistic programming frameworks
2. Predicting introductions in Swedish parliamentary protocols using BERT
3. Topic model inference: (Stochastic) variational inference and Gibbs sampling
4. Will Svenska akademins ordlista (SAOL) improve Swedish word embeddings?
5. Fine-tune a language model (BERT) on EDGAR-CORPUS
6. OCR-error detection using image and text classification

This week's lecture

- Feed-Forward Neural Networks

The Hype: Computer Vision

Figure: ImageNet performance (Roessler, 2019)



The Hype: Speech Recognition

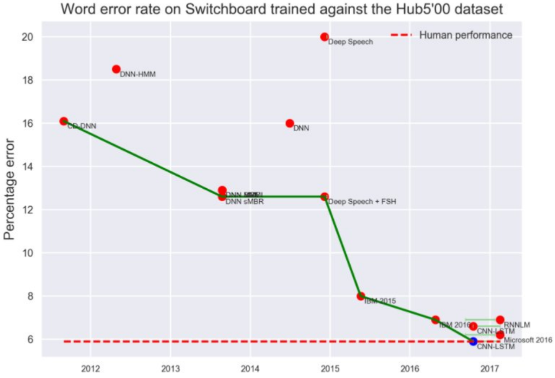


Figure: Speech recognition performance (source: `https://eff.org/ai/metrics`)

The Hype: Natural Language Processing

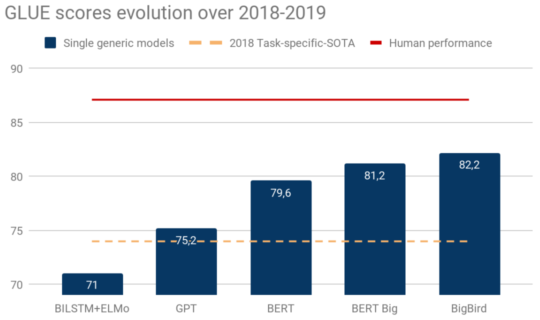


Figure: General Language Understanding (source: `https://www.programmersought.com/article/4251948498/`)

Work is very much ongoing:

`https://gluebenchmark.com/leaderboard`

The Hype

- Although - Neural Networks is not a silver bullet

The Hype

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- Remember the Bayes error

The Hype

- Although - Neural Networks is not a silver bullet
- Remember the Bayes error
- Some times a linear regression (or Random Forest) is enough

The Feed-Forward Network

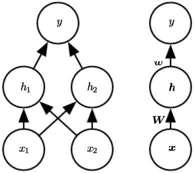

Figure 6.2: An example of a feedforward network, drawn in two different styles. Specifically, this is the feedforward network we use to solve the XOR example. It has a single hidden layer containing two units. *(Left)*In this style, we draw every unit as a node in the graph. This style is very explicit and unambiguous but for networks larger than this example it can consume too much space. *(Right)*In this style, we draw a node in the graph for each entire vector representing a layer's activations. This style is much more compact.

Figure: A simple feed-forward network (Goodfellow et al, 2017)

Important concepts:

Layers, neurons, input, output, weights, bias, architecture

Different Architectures for Different Purposes

- Different networks for different purposes
  - Convolutional Neural Networks: Computer Vision

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Different Architectures for Different Purposes

- Different networks for different purposes
  - Convolutional Neural Networks: Computer Vision
  - Recurrent Neural Networks: Speech Audio (?)
  - Transformers/Attention: Textual data
- The Neural Network Zoo: `https://www.asimovinstitute.org/neural-network-zoo/`

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Areas of Use: All fields

- Supervised learning
- Unsupervised learning
- Reinforcement learning

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Why and when neural nets?

- Learning feature representations
- Needs a lot of data to learn complex representations
- Good for sensor data (high-dimensional)

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Why and when neural nets?

- Learning feature representations
- Needs a lot of data to learn complex representations
- Good for sensor data (high-dimensional)
- When should we not use neural networks?

Learning Representations

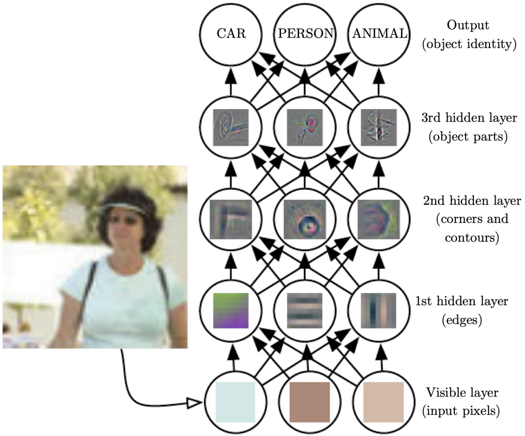

Figure: Learning representations can be crucial (Goodfellow et al, 2017, Fig. 1.2)

The Feed-Forward Network

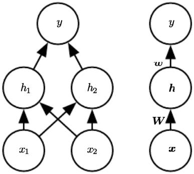

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Figure: A simple feed-forward network (Goodfellow et al, 2017, Fig. 6.2)

In mathematical notation:

$$\mathbf{w}^T g(\mathbf{W}^T \mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2$$

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The Feed-Forward Network

A feed-forward network for one observation (x_i).

$$\underbrace{\mathbf{h}_1}_{1\times k_1} = g_1(\underbrace{\mathbf{x}^T}_{1\times p}\underbrace{\mathbf{W}_1}_{p\times k_1} + \underbrace{\mathbf{b}_1}_{1\times k_1})$$

$$\vdots$$

$$\underbrace{\mathbf{h}_l}_{1\times k_l} = g_l(\underbrace{\mathbf{h}_{l-1}^T}_{1\times k_{l-1}}\underbrace{\mathbf{W}_l}_{k_{l-1}\times k_l} + \underbrace{\mathbf{b}_l}_{1\times k_l})$$

$$\vdots$$

$$\underbrace{\hat{\mathbf{y}}}_{1\times m} = g_L(\underbrace{\mathbf{h}_{L-1}^T}_{1\times k_{l-1}}\underbrace{\mathbf{W}_L}_{k_{l-1}\times m} + \underbrace{\mathbf{b}_L}_{1\times m})$$

$$\hat{y} = f_L(f_{L-1}(\ldots f_1(x)\ldots))$$

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Activation functions (g_l)

- Sometimes use notation σ as in $\sigma(Wh + b)$

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- Historically $g(z)$ has been the sigmoid or or hyperbolic tangent (tanh)
- Now, usually variants of Rectified linear unit (ReLU)
  - $g(z) = \max 0, z$
  - Easier to estimate with SGD
  - Easier for deep models
- Last activation is the output function g_L, usually a softmax (if classification)

$$f(z_i) = \frac{e^{z_i}}{\sum_{j=1}^{J} e^{z_j}}$$

Activation functions (g_l)

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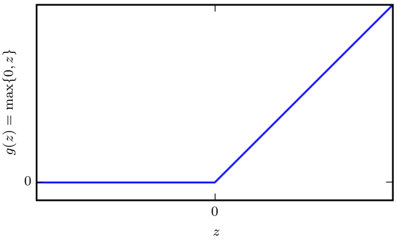

Figure: Rectified Linear Unit (Goodfellow et al, 2017, Fig. 6.3)

Universal Approximation Theorem

"A feed-forward neural network with a linear output layer and at least one hidden layer with any 'squashing' activation function can approximate any Borel measurable function from one finite-dimensional space to another with any desired non-zero amount of error, provided that the network is given enough hidden units." (Goodfellow et al. 2017, p. 198)

- Also holds for ReLU
- No garantuee we can learn the network
- No garantuee that it will generalize
- No indication of how large the network need to be

Hyper-parameters in feed-forward networks

- The number of layers
- The number of neurons
- Activation functions
- The type of layers (CNN, MaxPooling, Multi-head attention)

How to choose parameters

- Trial and error on validation sets
- Art rather than science
- Specialized approaches (Bayesian Optimization)

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- Trial and error on validation sets
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- Grid search (combinatorical explosion)
  - Really bad with many parameters with less effects
  - If we have 5 irrelevant parameters we try 3 values for: 125 training per relevant run
  - Instead use...

How to choose parameters

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  - Instead use...
- Random search

Grid search vs. Random Search

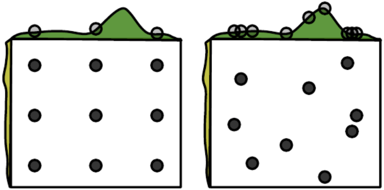

Figure: Grid search and random search (Goodfellow et al, 2017, Fig. 11.2)

Optimization of Neural Networks

- Difficult problem
- Many local minima (weight space symmetry)
- Platueas and sadel points
  - Gradient is small - but not a minimum or maximum
  - Sadel points increases with the number of dimensions (?)
  - Large areas with small change in cost function

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Optimization of Neural Networks II

- A lot of parameters (W and b)
- Usually a lot of data

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- A lot of parameters (W and b)
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- Stochastic Gradient Descent, commonly
  - Adam

Optimization of Neural Networks II

- A lot of parameters (W and b)
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- Stochastic Gradient Descent, commonly
  - Adam
- To compute gradients: backpropagation
  - Chain-rule for derivatives

Initial values

- We need to have starting values for SGD - non-trivial
- Bad initial values might
  - Bad convergence (local optimum)
  - Numerical problems
- We want to break symmetry between layers
- Initialization can be seen as a hyperparameter
- Good practice
  - Initialize values randomly close to zero (uniform or normal)

Neural Networks in Practice: TensorFlow and Keras

- Tensorflow
  - Framework for large-scale machine learning and Neural Networks
  - Developed by Google
  - Computational graphs
  - Handles:
    - Computing gradients for Neural Networks
    - Enable simple use of graphical processing units (GPU) and Tensor processing Units (TPU)
    - Used in both research and production
- Keras
  - Syntax for 'building' Neural Networks
  - Platform independent (ish)

Regularization of Neural Networks

- Reduce traing error but improve test/validation error

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Weight decay / Norm penalty

- Let
$$\tilde{J}(W, b) = J(W, b) + \alpha\Omega(W)\,,$$
where $J(W, b)$ is the cost function and $\alpha\Omega(W)$ is the penalty for the weight matrices.
- α is the strength of the penalty.

Weight decay / Norm penalty

- Let

$$\Omega_1(W) = \sum_i \sum_j |w|_{i,j} ,$$

and

$$\Omega_2(W) = \sum_i \sum_j w_{i,j}^2 ,$$

be the L_1 and L_2 regularization respectively.

- We can then get the cost function

$$\tilde{J}(W, b) = J(W, b) + \sum_l \alpha_l \Omega_2(W_l) ,$$

Weight decay / Norm penalty

- Lets define the cost function as

$$\begin{aligned}\tilde{J}(w) &= J(w) + \alpha\Omega_2(w) \\ &= J(w) + \alpha w^T w\end{aligned}$$

- Then the gradient update becomes

$$\nabla_w \tilde{J}(w) = \nabla_w J(w) + 2\alpha w$$

- To update our weights with gradient descent

$$\begin{aligned}w &\leftarrow w - \epsilon(\nabla_w J(w) + 2\alpha w) \\ w &\leftarrow (1 - 2\alpha\epsilon)w - \epsilon\nabla_w J(w)\end{aligned}$$

Weight decay / Norm penalty

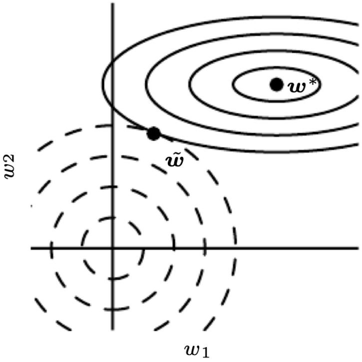

Figure: L_2 regularization (Goodfellow et al, 2017, Fig. 7.1)

Early Stopping

- Stop optimization early based on validation error
- Rerun to that number of epochs (hyperparameter)
- Can be shown to be quivalent (under strict assumptions) to L_2 regularization

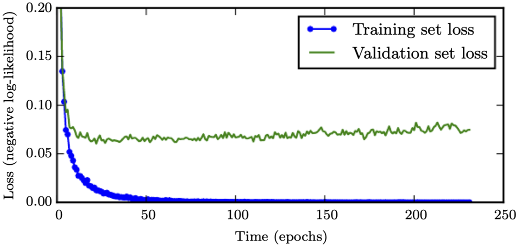

Figure: Early Stopping (Goodfellow et al, 2017, Fig. 7.3)

Early Stopping

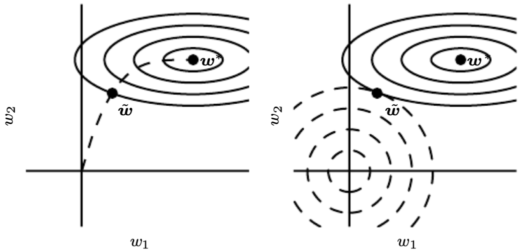

Figure: Early Stopping (Goodfellow et al, 2017, Fig. 7.4)

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Dropout

- In each iteration:
  - Sample an indicator I_i for each node i
  - Set the value h_i to 0 with probability p
- The dropout probability is typically 0.8 for input nodes and 0.5 for hidden nodes
- Forces the network to
  - not rely on individual nodes
  - spread out the weights over more nodes
- Can be seen as an ensamble method

Dropout

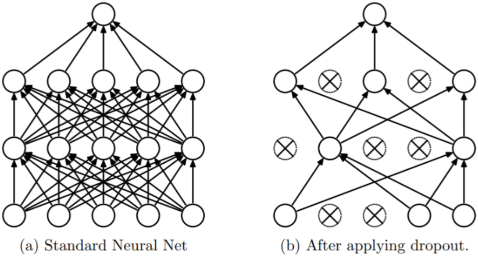

Figure 1: Dropout Neural Net Model. **Left**: A standard neural net with 2 hidden layers. **Right**: An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

Figure: Dropout (Srivastava et al, 2014)

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Other regularization techniques

- In CNN: Dataset augmentation
- Get more data...