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Machine learning – Block 3

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Evaluation assignment 2

- Challenging - hard to find the right level of hints

This week's lecture

- Feed-Forward Neural Networks
- Regularization of Neural Networks
- Neural Network Optimization

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On this weeks assignment

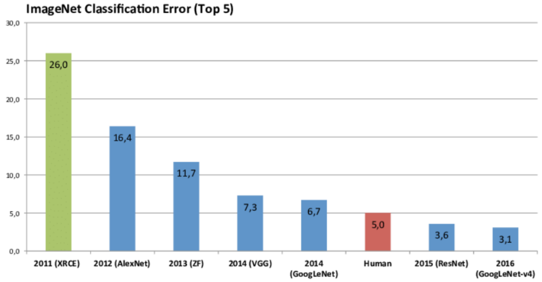
- It can be tricky to get Tensorflow and R to work. Start early and use the zoom sessions.
- Don't run Tensorflow in markdown.

Section 2

Introduction

The Hype: Computer Vision

Figure: ImageNet performance (Roessler, 2019)



The Hype: Speech Recognition

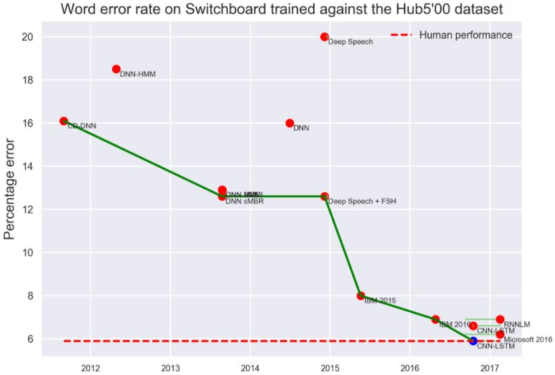


Figure: Speech recognition performance (source: `https://eff.org/ai/metrics`)

- Practicalities
- Introduction
- Feed-Forward Neural Networks
  - Feed-Forward Neural Networks
  - Output Units
  - Hidden Units
  - Architecture design
- Regularization
  - Norm penalty
  - Data augmentation
  - Multi-Task Learning
  - Early Stopping
  - Drop-out
- Optimization of Neural Networks
  - Local minima
  - Plateaus and Saddle Points
  - Cliffs, exploding and vanishing gradients
  - Parameter initialization
- Neural Networks in Practice

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The Hype: Natural Language Processing

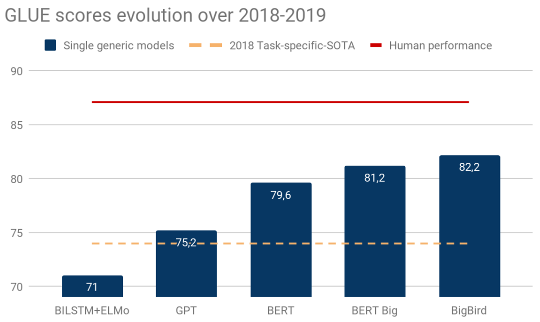

Figure: General Language Understanding (source: `https://www.programmersought.com/article/4251948498/`)

Work is very much ongoing:

`https://gluebenchmark.com/leaderboard`

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The Hype: Large Language Models

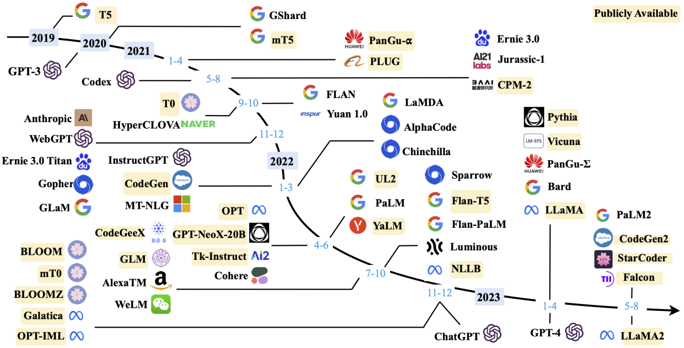

Figure: Large Language Models timeline (Zhao et al (2023)

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The Hype

- Although - Neural Networks are not a silver bullet

The Hype

- Although - Neural Networks are not a silver bullet
- Remember the Bayes error

The Hype

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

Areas of Use

- Supervised learning
- Self-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 (image, text, audio)
- 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 (image, text, audio)
- Good for sensor data (high-dimensional)
- When should we not use neural networks?

Learning Representations

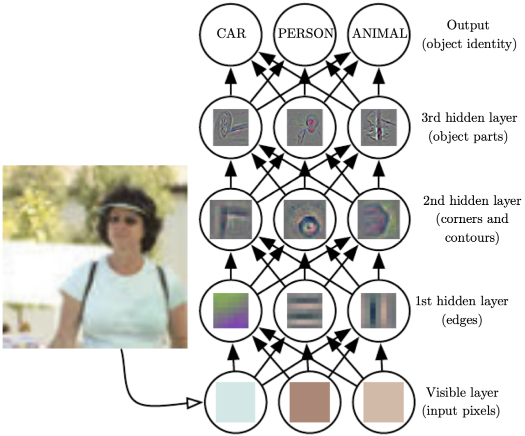

Figure: Learning representations can be crucial (Goodfellow et al, 2017, Fig. 1.2)

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Different Network Architectures for Different Purposes

- Different networks for different purposes
  - Feed-Forward Neural Network: Basic building block

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  - Convolutional Neural Networks: Computer Vision

Different Network Architectures for Different Purposes

- Different networks for different purposes
  - Feed-Forward Neural Network: Basic building block
  - Convolutional Neural Networks: Computer Vision
  - Transformer Neural Networks: Textual data/Audio/Vision (generation)
  - Diffusion Neural Networks: Image generation

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Section 3

Feed-Forward Neural Networks

The Feed-Forward Network

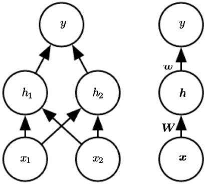

Figure 6.2: An example of a feedforward network, drawn in two different styles. Specifically, this is the feedforward network we use to solve the XOR example. It has a single hidden layer containing two units. *(Left)*In this style, we draw every unit as a node in the graph. This style is very explicit 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, Fig. 6.2)

Important concepts:

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

The Feed-Forward Network

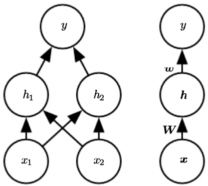

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Figure: A simple feed-forward network (Goodfellow et al, 2017, Fig. 6.2)

In mathematical notation:

$$y_i = \mathbf{w}^T \underbrace{g(\mathbf{W}^T \mathbf{x}_i + \mathbf{b}_1)}_{\mathbf{h}} + \mathbf{b}_2$$

The Feed-Forward Network

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

$$W = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, w = \begin{pmatrix} 1 \\ -2 \end{pmatrix}, b_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, b_2 = (0)$$

$$g(z) = \text{ReLU}(z) = \max(0, z)$$

$$x_i = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

$$y_i = \begin{pmatrix} 1 \\ -2 \end{pmatrix}^T \text{ReLU}\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 1 \\ -1 \end{pmatrix}\right] + (0)$$

$$y_i = \begin{pmatrix} 1 \\ -2 \end{pmatrix}^T \begin{pmatrix} 1 \\ 0 \end{pmatrix} + (0) = 1$$

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The Feed-Forward Network

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

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

$$\vdots$$

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

$$\vdots$$

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

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

Output units (g_L)

- Depend on the data y

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- Linear units for regression

$$\hat{y} = \mathbf{wh} + \mathbf{b}$$

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$$\hat{y} = \mathbf{wh} + \mathbf{b}$$

- Bernoulli units for binary classification

$$\hat{y} = \sigma(\mathbf{wh} + \mathbf{b}),$$

where

$$\sigma(z) = \frac{1}{1 + \exp(-z)},$$

i.e. the logistic or sigmoid function.

Output units (g_L)

- Multinoulli units for multi-class classification

$$\hat{\mathbf{y}} = \text{softmax}(\mathbf{wh} + \mathbf{b}),$$

where

$$\text{softmax}(\mathbf{z}) = \frac{\exp(z_j)}{\sum_j \exp(z_j)}.$$

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- Other situations: Use the negative log-likelihood, e.g. Poisson, ordinal logit, survival models

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)

$$g_{\text{sigmoid}}(z) = \frac{e^z}{e^z + 1} = \frac{1}{1 + e^{-z}}$$

$$g_{\text{tanh}}(z) = \frac{\sinh z}{\cosh z} = \frac{e^{2z} - 1}{e^{2z} + 1}$$

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- Today, variants of Rectified linear unit (ReLU) is common
  - Easier to estimate with SGD
  - Easier for deep models

Activation functions (g_l): ReLU

$$g_{\text{ReLU}}(z) = \max(0, z)$$

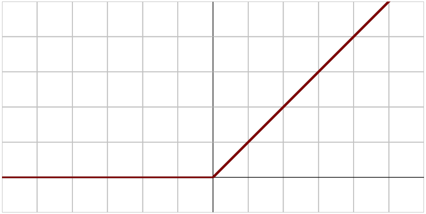

Figure: Rectified Linear Unit (Wikipedia)

Activation functions (g_l): GeLU

$$g_{\text{GeLU}}(z) = z\Phi(z)$$

where $\Phi(z)$ is a standard Gaussian.

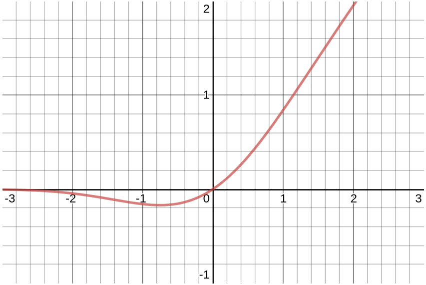

Figure: Gaussian Error Linear Unit (Wikipedia)

Activation functions (g_l): ELU

$$g_{\mathrm{ELU}}(z) = \begin{cases} \alpha\left(e^z - 1\right) & \text{if } z \leq 0 \\ z & \text{if } z > 0 \end{cases}$$

where α is commonly 1.

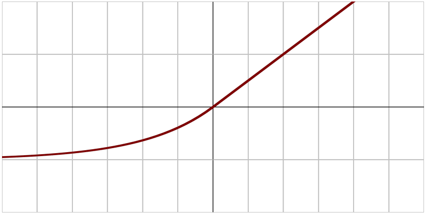

Figure: Exponential Linear Unit (Wikipedia)

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Architecture design

- Architecture: the overall structure of the network
- Choices:
  - How many layers?
  - How many hidden units in each layer?
  - Activation functions?

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- Choices:
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  - Activation functions?
- *Note!* Output units is defined by both the data and by design

Universal Approximation Theorem

- A feedforward network with a single layer of sufficient size is can to represent any function.
- Also holds for ReLU (under some assumptions)

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Depth matters

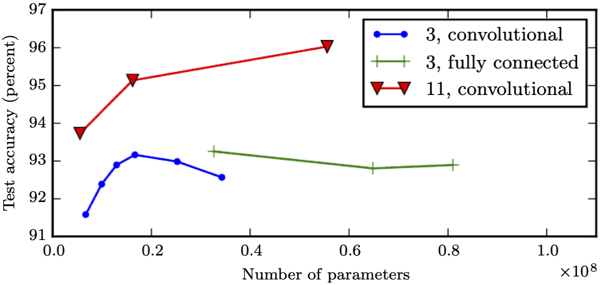

Figure: Effect of depth on accuracy (Goodfellow et al, 2017, Fig. 6.3)

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Depth matters II

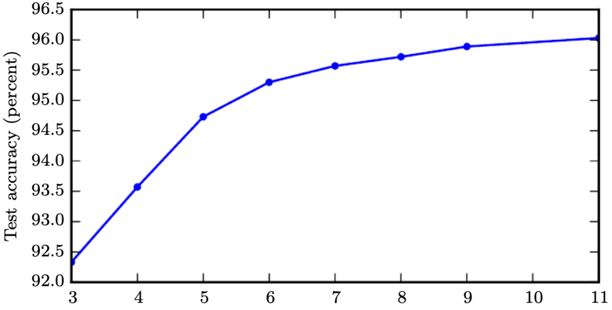

Figure: Depth vs. no of parameters (Goodfellow et al, 2017, Fig. 6.6)

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How to choose architecture

- Trial and error on validation sets
- Art rather than science

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- Trial and error on validation sets
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- Specialized approaches (Bayesian Optimization)
- 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 architecture

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  - If we have 5 irrelevant parameters we try 3 values for: 125 training per relevant run
  - Instead use...
- Random search

Grid search vs. Random Search

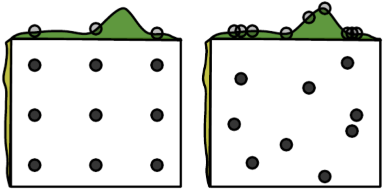

Figure: Grid search and random search (Goodfellow et al, 2017, Fig. 11.2)

Section 4

Regularization

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Regularization of Neural Networks

- Reduce traing error but improve generalization error

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- Neural Networks are extremely flexible / high model capacity

Regularization of Neural Networks

- Reduce traing error but improve generalization error
- Neural Networks are extremely flexible / high model capacity
- Regularization is important for good generalizability

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.

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

- 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

$$w \leftarrow w - \epsilon(\nabla_w J(w) + 2\alpha w)$$

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$$w \leftarrow (1 - 2\alpha\epsilon)w - \epsilon\nabla_w J(w)$$

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Weight decay / Norm penalty

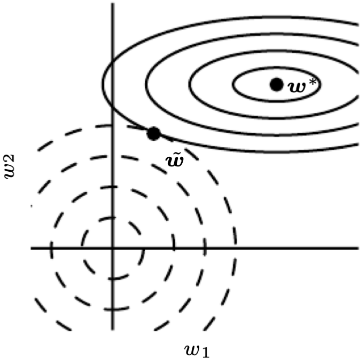

Figure: L_2 regularization (Goodfellow et al, 2017, Fig. 7.1)

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Dataset augmentation

Figure: Data Augmentation (Chollet and Allair, 2018, Fig 5.10)

- "Modify" data or inject noise
- Common in Convolutional neural networks

Multi-Task Learning

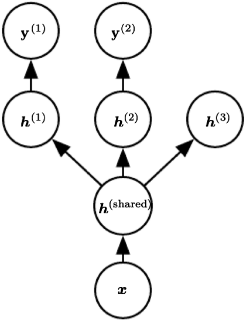

Figure: Multi-task learning (Goodfellow et al., 2017, Fig 7.2)

- Common in Large Language Models (Transformers)

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Early Stopping

- Stop optimization early based on validation error

Early Stopping

- Stop optimization early based on validation error
- Use the best iteration (hyperparameter)

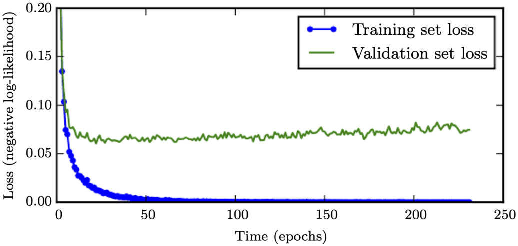


Figure: Early Stopping (Goodfellow et al, 2017, Fig. 7.3)

- Can be shown to be equivalent (under strict assumptions) to L_2 regularization (see Goodfellow et al, 2017)
- Efficient regularization

Early Stopping

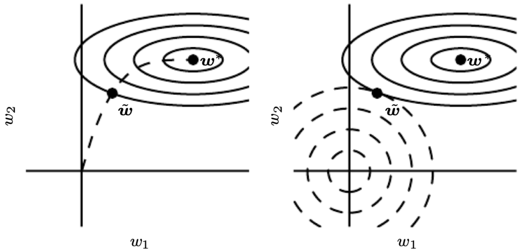
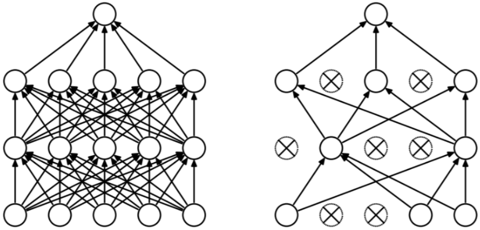


Figure: Early Stopping (Goodfellow et al, 2017, Fig. 7.4)

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



(a) Standard Neural Net (b) After applying 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)

But...

The best regularizer is...

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But...

The best regularizer is... to get more data.

Section 5

Optimization of Neural Networks

Neural Network Learning

- Usually, a lot of data and many parameters ($\theta = (W, b)$)

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Neural Network Learning

- Usually, a lot of data and many parameters ($\theta = (W, b)$)
- We usually minimize our training cost function

$$J(\theta) = \sum_{i}^{N} L(\mathrm{NN}(x_i|\theta), y_i) + \Omega(\theta)\,,$$

where L is the observation level loss, NN() is our neural network and Ω is the regularization term.

Neural Network Learning

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  where L is the observation level loss, NN() is our neural network and Ω is the regularization term.
- Learning Target: Find $\hat{\theta}$ that minimize the generalization error

Optimization of Neural Networks

- Stochastic Gradient Descent methods

$$\theta_t = \theta_{t-1} - \eta_t \hat{\nabla} J(\theta_{t-1})$$

- In practice, better optimizers are used:
  - Adam
  - RMSprop

Optimization of Neural Networks

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- In practice, better optimizers are used:
  - Adam
  - RMSprop
- To compute gradients ($\hat{\nabla} J(\theta_{t-1})$):
  - Backpropagation algorithm (chain-rule for derivatives)

Problems: Local Minima

- Neural Networks cost function $J(\theta)$ are (usually) not a convex function
- We can have local minima
- When will this be a problem?

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Problems: Plateaus and Saddle Points

- Another problem is saddle points

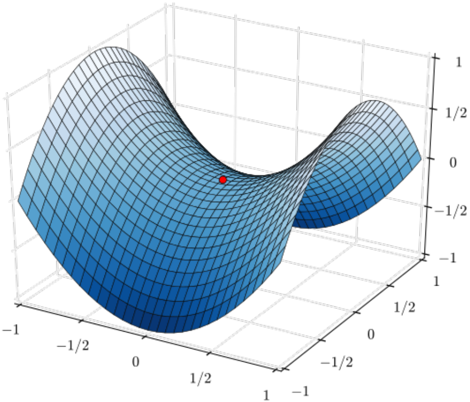

Figure: Saddle point for $z = x^2 - y^2$ (Wikipedia)

- What is the gradient in a saddle point?

Problems: Plateaus and Saddle Points

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- In random functions: eigen values become more positive in regions of lower cost. I.e. local minima more probable in low cost regions. Saddle points more common in high-cost regions
- The problem of saddle points:
  - Probably a reason why second order methods (using the Hessian) has not succeed
  - Empirically, (stochastic) gradient descent seem to escape saddle points

Problems: Cliffs

- Another problem is "cliffs" or large changes in gradients

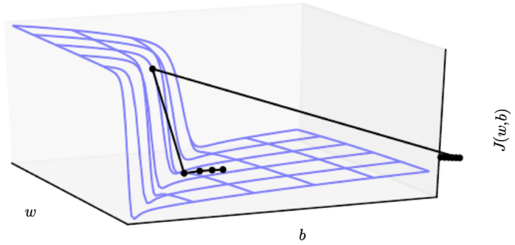

Figure: Cliff (Goodfellow et al., 2017, Fig. 8.3)

- Can undo many iterative steps
- Common in Recurrent neural networks
- Mitigation: Gradient clipping

Problems: Explodig and vanishing gradients

- In deep neural networks, gradients can vanish or explode
- As an example: We want to compute the gradient for a situation where the weights are multiplied t times. Then using eigendecomposition

$$W^t = V \mathrm{diag}(\lambda)^t V^T$$

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- Good practice
  - Initialize values randomly close to zero (uniform or normal)

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Section 6

Neural Networks in Practice

TensorFlow

- Framework for large-scale machine learning and Neural Networks
- Developed by Google
- Can be used both from R and Python
- Used in both research and production
- What Tesorflow does:
  - Computing gradients (autodiff) for Neural Networks
  - Enable use of graphical processing units (GPU) and Tensor processing Units (TPU)
  - Enable training using common optimizers (such as Adam, RMSprop)
- Tesorflow Probability is a probabilistic programming framework using TF

TensorFlow

(Py)Torch

- Similar to TensorFlow
- Developed by Meta AI
- Can be used both from R and Python
- Used in both research and production
- pyro is a probabilistic programming framework using torch

PyTorch

Keras

- Syntax for 'building' Neural Networks
- Available both in R and Python
- TensorFlow or Torch as backend