



Machine learning – Block 3

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Department of Statistics, Uppsala University

Autumn 2024

- 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



Evaluation assignment 2

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- **Neural Networks in Practice**

- Challenging - hard to find the right level of hints



This week's lecture

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



On this weeks assignment

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



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Section 2

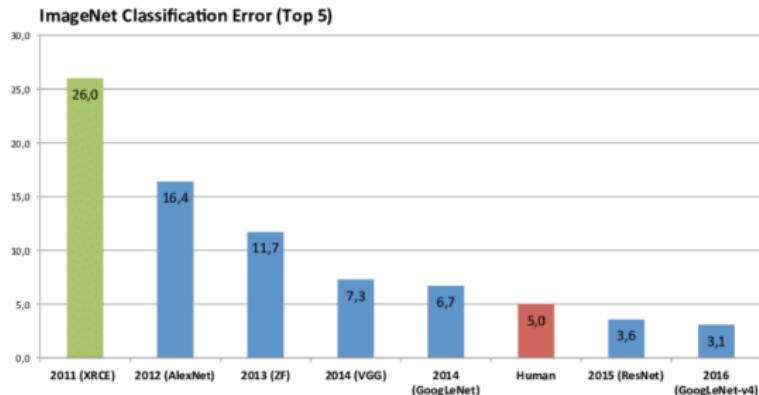
Introduction



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The Hype: Computer Vision

Figure: ImageNet performance (Roessler, 2019)





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The Hype: Speech Recognition

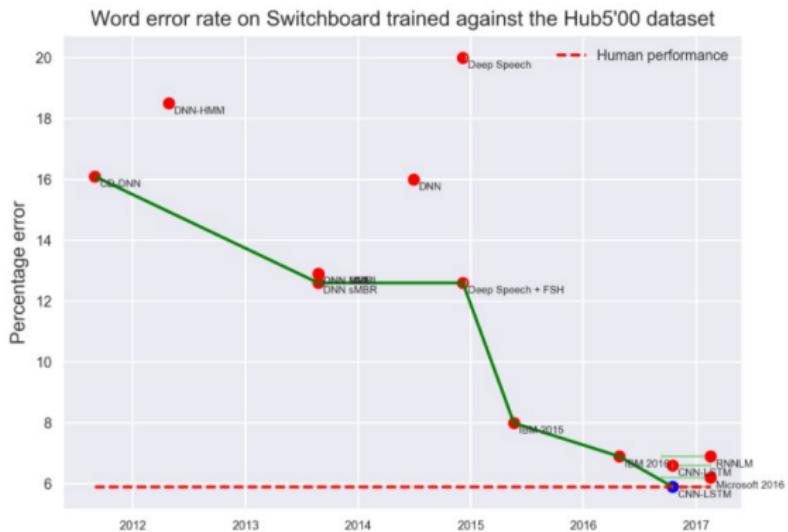


Figure: Speech recognition performance (source:
<https://eff.org/ai/metrics>)



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The Hype: Natural Language Processing

GLUE scores evolution over 2018-2019

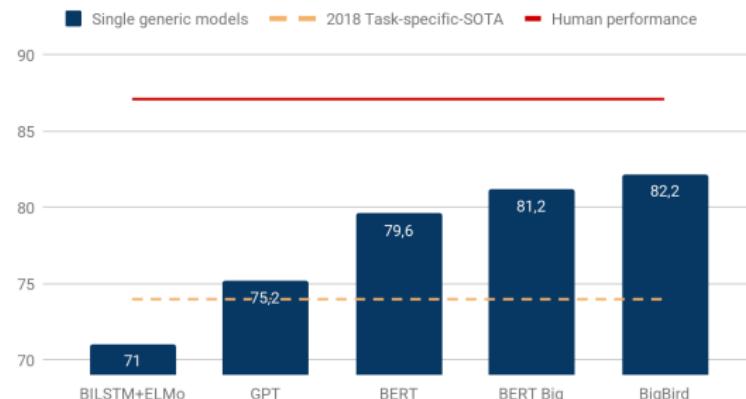


Figure: General Language Understanding (source:
<https://www.programmersought.com/article/4251948498/>)

Work is very much ongoing:

<https://gluebenchmark.com/leaderboard>



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The Hype: Large Language Models

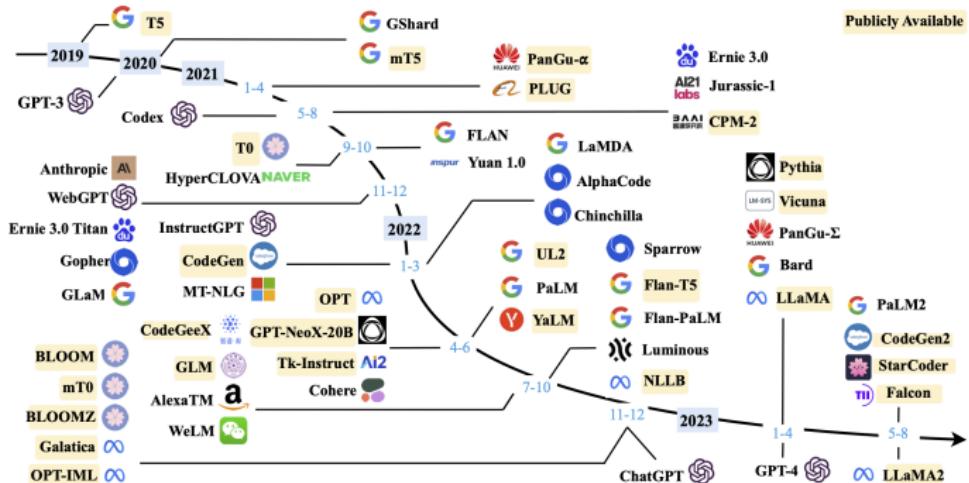


Figure: Large Language Models timeline (Zhao et al (2023))



The Hype

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



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- 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

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- Supervised learning
- Self-Supervised learning
- Unsupervised learning
- Reinforcement learning



Why and when neural nets?

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- 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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- 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

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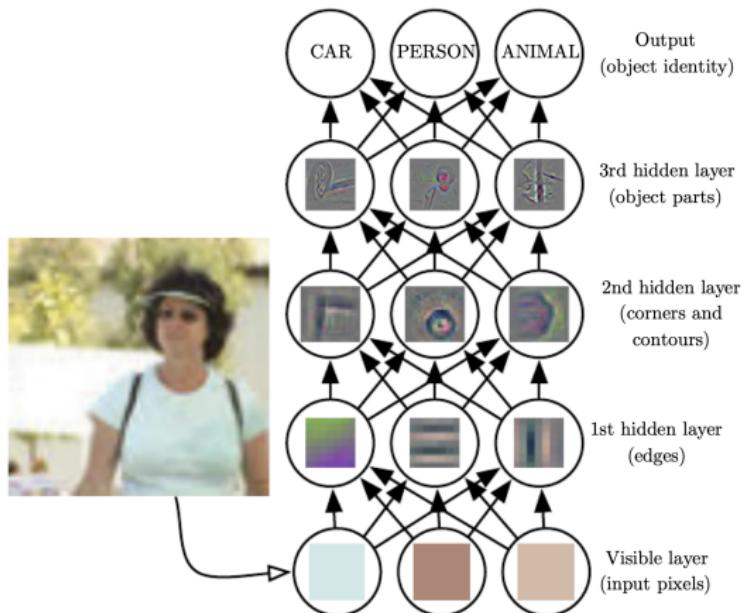


Figure: Learning representations can be crucial (Goodfellow et al, 2017, Fig. 1.2)



Different Network Architectures for Different Purposes

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



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- Different networks for different purposes
 - **Feed-Forward Neural Network:** Basic building block
 - **Convolutional Neural Networks:** Computer Vision



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- 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



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The Feed-Forward Network

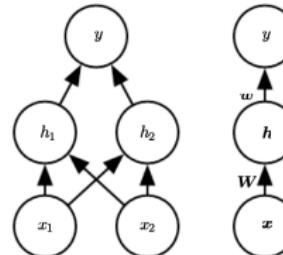


Figure 6.2: An example of a feedforward network, drawn in two different styles. Specifically, this is the feedforward network we use to solve the XOR example. It has a single hidden layer containing two units. (*Left*) In this style, we draw every unit as a node in the graph. This style is very explicit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



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The Feed-Forward Network

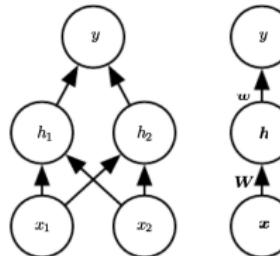


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Figure: A simple feed-forward network (Goodfellow et al, 2017, Fig. 6.2)

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

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

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

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

$$\mathbf{x}_i = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

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

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

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The Feed-Forward Network

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

$$\begin{aligned}\underbrace{\mathbf{h}_1}_{1 \times k_1} &= g_1(\underbrace{\mathbf{x}^T}_{1 \times p} \underbrace{\mathbf{W}_1}_{p \times k_1} + \underbrace{\mathbf{b}_1}_{1 \times k_1}) \\ &\vdots \\ \underbrace{\mathbf{h}_I}_{1 \times k_I} &= g_I(\underbrace{\mathbf{h}_{I-1}^T}_{1 \times k_{I-1}} \underbrace{\mathbf{W}_I}_{k_{I-1} \times k_I} + \underbrace{\mathbf{b}_I}_{1 \times k_I}) \\ &\vdots \\ \underbrace{\hat{\mathbf{y}}}_{1 \times m} &= g_L(\underbrace{\mathbf{h}_{L-1}^T}_{1 \times k_{L-1}} \underbrace{\mathbf{W}_L}_{k_{L-1} \times m} + \underbrace{\mathbf{b}_L}_{1 \times m})\end{aligned}$$
$$\hat{y} = f_L(f_{L-1}(\dots f_1(x)\dots))$$



Output units (g_L)

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- Depend on the data y



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Output units (g_L)

- Depend on the data y
- Linear units for regression

$$\hat{y} = \mathbf{w}\mathbf{h} + \mathbf{b}$$



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Output units (g_L)

- Depend on the data y
- Linear units for regression

$$\hat{y} = \mathbf{w}\mathbf{h} + \mathbf{b}$$

- Bernoulli units for binary classification

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

where

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

i.e. the logistic or sigmoid function.



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Output units (g_L)

- Multinoulli units for multi-class classification

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

where

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



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where

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

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



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



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Activation functions (g_I)

- Sometimes use notation σ as in $\sigma(Wh + b)$
- Historically $g(z)$ has been the **sigmoid** or or hyperbolic tangent (\tanh)

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

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



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

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



Activation functions (g_I): ReLU

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

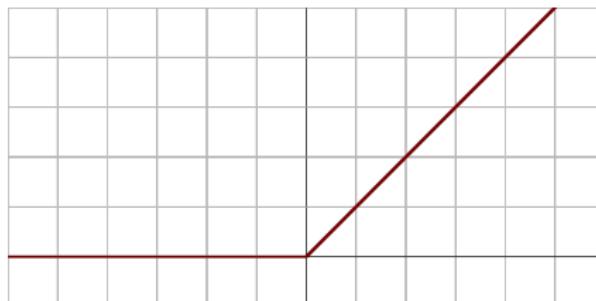


Figure: Rectified Linear Unit (Wikipedia)



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Activation functions (g_I): GeLU

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

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

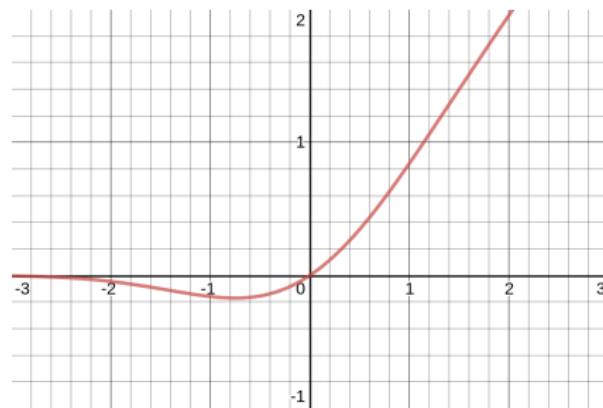


Figure: Gaussian Error Linear Unit (Wikipedia)



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Activation functions (g_I): ELU

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

where α is commonly 1.

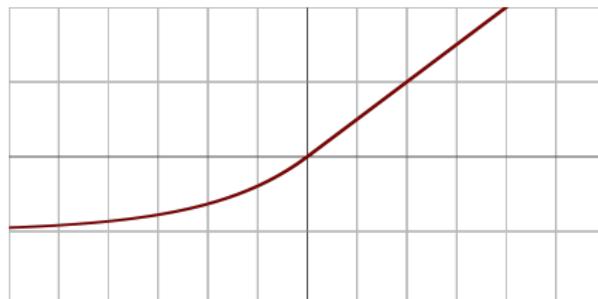


Figure: Exponential Linear Unit (Wikipedia)



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



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- **Architecture:** the overall structure of the network
 - **Choices:**
 - How many layers?
 - How many hidden units in each layer?
 - Activation functions?
 - **Note!** Output units is defined by both the **data** and by design



Universal Approximation Theorem

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



Universal Approximation Theorem

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 - But...
 - No guarantee we can **learn** the network



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- A feedforward network with a **single layer** of sufficient size is can to represent any function.
 - Also holds for ReLU (under some assumptions)
 - But...
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 - No garantuee that it will **generalize**



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Depth matters

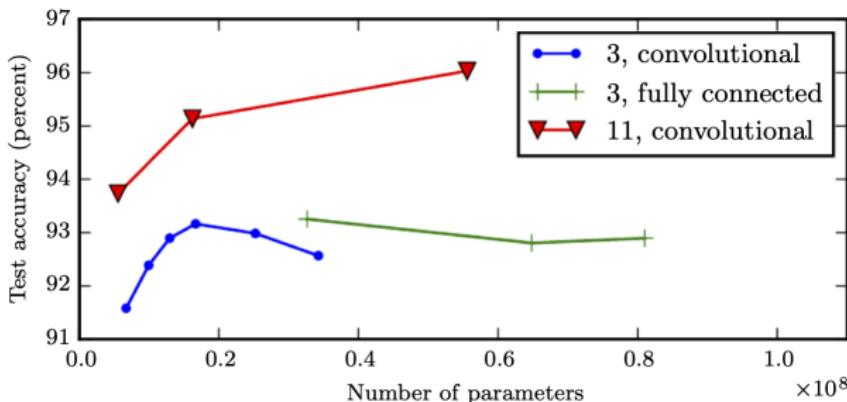


Figure: Effect of depth on accuracy (Goodfellow et al, 2017, Fig. 6.3)



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Depth matters II

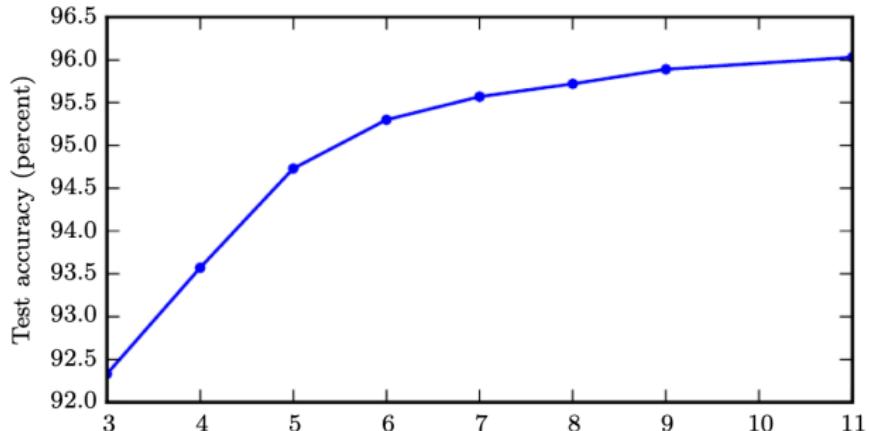


Figure: Depth vs. no of parameters (Goodfellow et al, 2017, Fig. 6.6)



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



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



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



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 - Really bad with many parameters with less effects
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 - Instead use...
 - Random search



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Grid search vs. Random Search

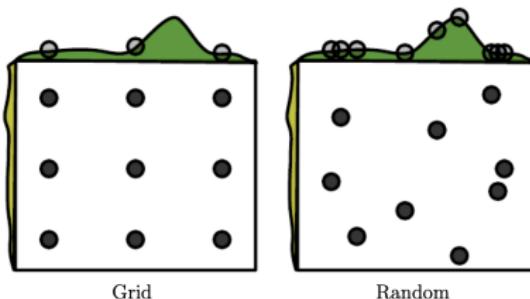


Figure: Grid search and random search (Goodfellow et al, 2017, Fig. 11.2)



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Section 4

Regularization



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- Reduce training error but **improve generalization error**



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- Reduce training error but **improve generalization error**
- Neural Networks are extremely flexible / high model capacity



Regularization of Neural Networks

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



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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.



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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

$$\tilde{J}(W, b) = J(W, b) + \sum_I \alpha_I \Omega_2(W_I),$$



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

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



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Weight decay / Norm penalty

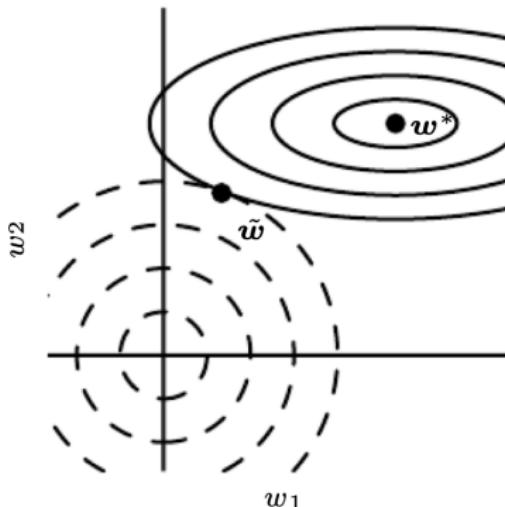


Figure: L_2 regularization (Goodfellow et al, 2017, Fig. 7.1)



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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



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Multi-Task Learning

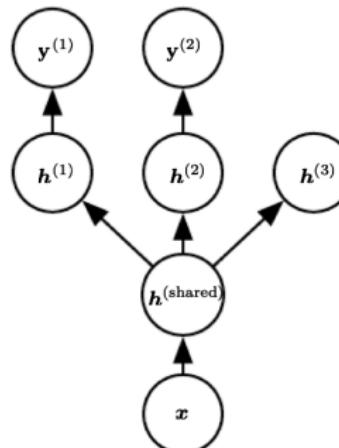


Figure: Multi-task learning (Goodfellow et al., 2017, Fig 7.2)

- Common in Pre-Trained Language Models (Transformers)



Early Stopping

- Stop optimization early based on validation error

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Early Stopping

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

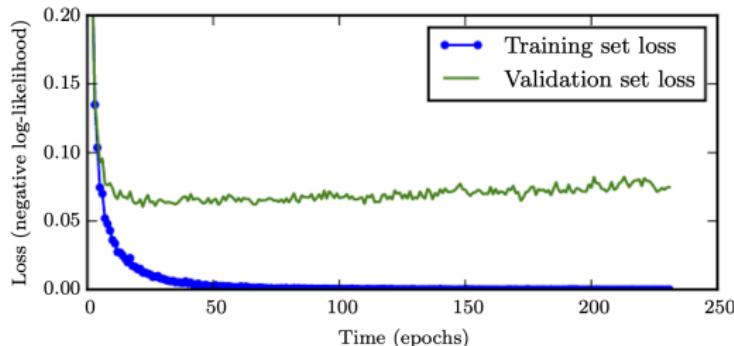


Figure: Early Stopping (Goodfellow et al, 2017, Fig. 7.3)

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



Early Stopping

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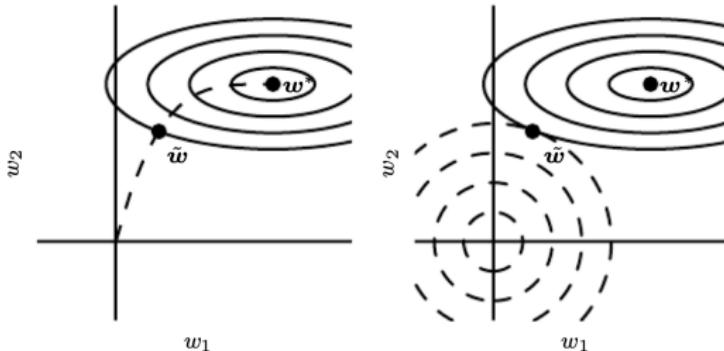


Figure: Early Stopping (Goodfellow et al, 2017, Fig. 7.4)



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- 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 ensemble method



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Dropout

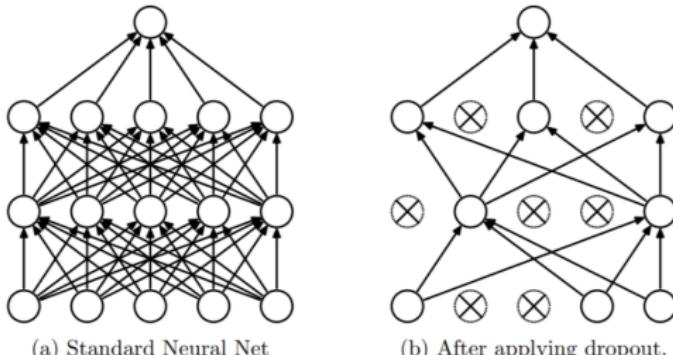


Figure 1: Dropout Neural Net Model. **Left:** A standard neural net with 2 hidden layers. **Right:** An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

Figure: Dropout (Srivastava et al, 2014)



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But...

The best regularizer is...



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



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Section 5

Optimization of Neural Networks



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

$$J(\theta) = \sum_i^N L(\text{NN}(x_i|\theta), y_i) + \Omega(\theta),$$

where L is the observation level loss, $\text{NN}()$ is our neural network and Ω is the regularization term.



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Neural Network Learning

- Usually, a lot of data and many parameters ($\theta = (W, b)$)
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$$J(\theta) = \sum_i^N L(\text{NN}(x_i|\theta), y_i) + \Omega(\theta),$$

where L is the observation level loss, $\text{NN}()$ is our neural network and Ω is the regularization term.

- **Learning Target:** Find $\hat{\theta}$ that minimize the **generalization error**



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- 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



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- Stochastic Gradient Descent methods

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

- In practice, better optimizers are used:

- Adam
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- To compute gradients ($\hat{\nabla} J(\theta_{t-1})$):

- **Backpropagation** algorithm (chain-rule for derivatives)



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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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- Neural Networks cost function $J(\theta)$ are (usually) **not a convex** function
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- **When will this be a problem?**
- A problem if local optima has a **high cost/bad performance**



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- We can have local minima
- **When will this be a problem?**
- A problem if local optima has a **high cost/bad performance**
- **Good thing:** This is probably not the situation!
- Many practitioners believe this is a problem
- **Diagnosis:** Plot the gradient norm, $\mathbf{g}^T \mathbf{g}$, where $\mathbf{g} = \hat{\nabla} J(\theta)$



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- Neural Networks cost function $J(\theta)$ are (usually) **not a convex** function
 - We can have local minima
 - **When will this be a problem?**
 - A problem if local optima has a **high cost/bad performance**
 - **Good thing:** This is probably not the situation!
 - Many practitioners believe this is a problem
 - **Diagnosis:** Plot the gradient norm, $\mathbf{g}^T \mathbf{g}$, where $\mathbf{g} = \hat{\nabla} J(\theta)$



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Problems: Plateaus and Saddle Points

- Another problem is **saddle points**

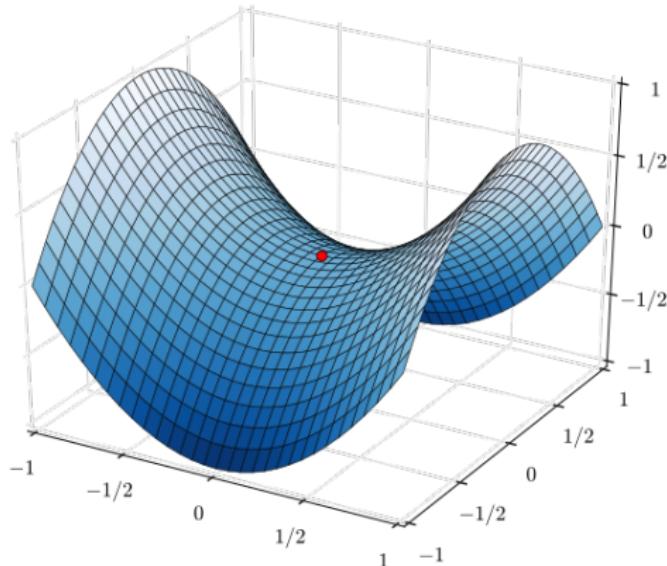


Figure: Saddle point for $z = x^2 - y^2$ (Wikipedia)

- What is the gradient in a saddle point?



Problems: Plateaus and Saddle Points

- In a saddle point the Hessian is **indefinite**, both positive and negative eigenvalues

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Problems: Plateaus and Saddle Points

- In a saddle point the Hessian is **indefinite**, both positive and negative eigenvalues
- A local minimum: Hessian is **positive definite**, only positive eigen values



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Problems: Plateaus and Saddle Points



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Problems: Plateaus and Saddle Points

- In a saddle point the Hessian is **indefinite**, both positive and negative eigenvalues
- A local minimum: Hessian is **positive definite**, only positive eigen values
- In random functions of **high dimension**: **most points are saddle points**
- **Intuition:** In random functions the sign of the eigen values of the Hessian is **random**
- 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



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- **Intuition:** In random functions the sign of the eigen values of the Hessian is random
- 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



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Problems: Cliffs

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

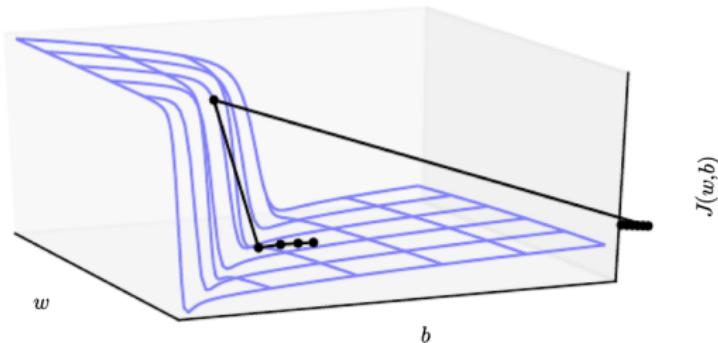


Figure: Cliff (Goodfellow et al., 2017, Fig. 8.3)

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



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Problems: Exploding 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

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

- The gradient is scaled wrt $\text{diag}(\lambda)^t$



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- Cliffs is an example of gradient explosion
- **Mitigation for gradient explosion:** Gradient clipping



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- The gradient is scaled wrt $\text{diag}(\lambda)^t$
- Cliffs is an example of gradient explosion
- **Mitigation for gradient explosion:** Gradient clipping
- Common problem in **Recurrent neural networks**



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- We need to have **starting values** for gradient descent



Initial values

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- We need to have **starting values** for gradient descent
- Initialization can be seen as a hyperparameter



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Initial values

- We need to have **starting values** for gradient descent
- Initialization can be seen as a hyperparameter
- Bad initial values might
 - Bad convergence (local optimum)
 - Numerical problems



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- We need to have **starting values** for gradient descent
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 - We want to **break symmetry** between layers
 - Otherwise the same units will be updated in the same way (deterministically)



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 - We want to **break symmetry** between layers
 - Otherwise the same units will be updated in the same way (deterministically)
 - Good practice
 - Initialize values randomly close to zero (uniform or normal)



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Section 6

Neural Networks in Practice



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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 TensorFlow 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)
- TensorFlow Probability is a probabilistic programming framework using TF





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(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





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Keras

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

