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- 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
  - Difficulties in Neural Network Optimization
  - Local minima
  - Plateaus and Saddle Points
  - Cliffs, exploding and vanishing gradients
  - Parameter initialization
- Neural Networks in Practice

# Machine learning – Block 3

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# This week's lecture

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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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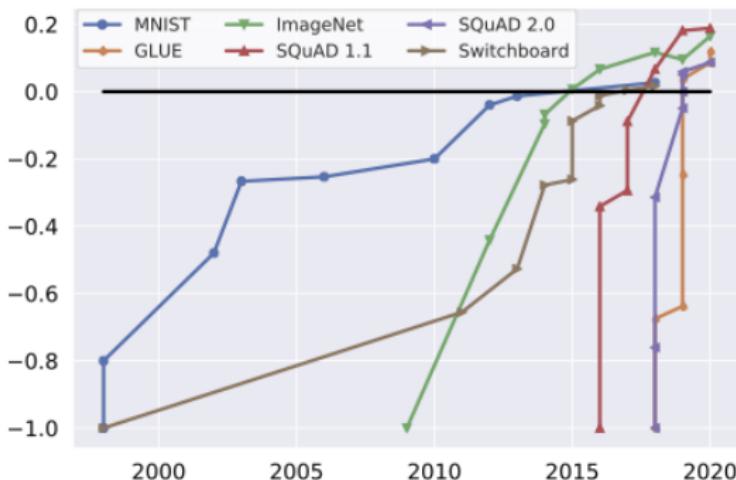
## Section 1

### Introduction



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# The Hype: Deep Learning



**Figure:** Benchmark saturation over time for popular benchmarks, normalized with initial performance at mid- minus one and human performance at zero. (Kiela et al., 2021)



# The Hype: Large Language Models

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- **GPT-3 (2020)** 175B parameters; breakthrough in general language capabilities.

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- **2021–2022: Scaling + Instruction Tuning : ChatGPT**
  - Models such as GPT-3.5, Gopher, Chinchilla, PaLM.
  - Emergence of instruction-following (ChatGPT)



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- 2023: GPT-4 Era
  - Multimodal models (image+text)
  - Open models: LLaMA, Falcon
  - Focus on safety and alignment



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- **2024: Open-Weights Explosion**
  - LLaMA-2/3, Mistral, Mixtral (MoE)
  - Efficient inference and training.
  - Training data reached internet-size.



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  - Efficient inference and training.
  - Training data reached internet-size.
- **2025: Multimodal Models**
  - Native multimodal architectures (audio–vision–text).
  - Agents: reasoning + planning + tool execution.
  - GPT-5 released



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- **Neural Networks in Practice**
  - Although - (Deep) Neural Networks are not a silver bullet



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



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  - **Neural Networks in Practice**
- Although - (Deep) Neural Networks are not a silver bullet
  - Remember the **Bayes error**
  - Sometimes a linear regression (or Random Forest) is enough



# Areas of Use

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- **Feed-Forward Neural Networks**

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- **Neural Networks in Practice**

- **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)



# Why and when neural nets?

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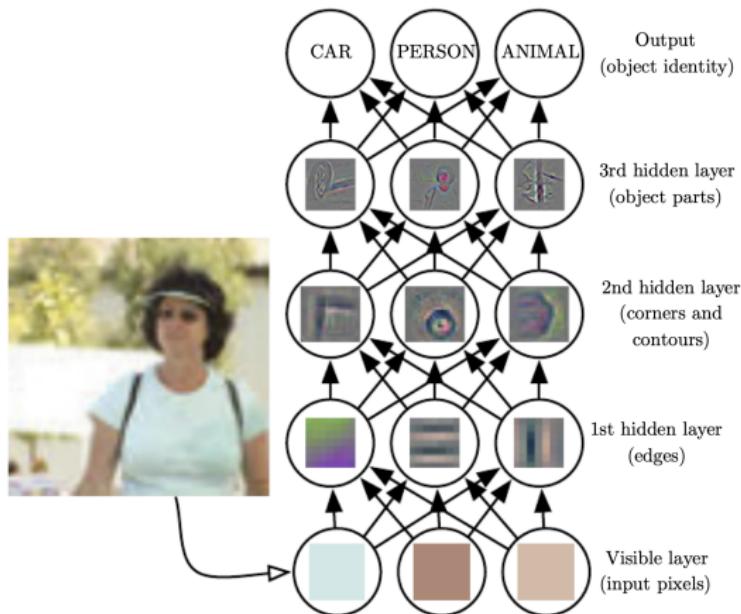
- Learning **feature representations**
- Needs a lot of data to learn **complex representations** (image, text, audio)
- Good for sensor data (high-dimensional)
- When should we **not** use neural networks?



# 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 2

### Feed-Forward Neural Networks



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# The Feed-Forward Network

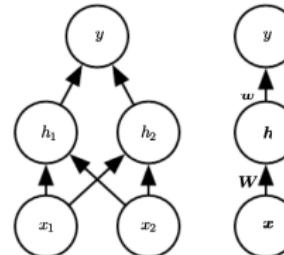


Figure 6.2: An example of a feedforward network, drawn in two different styles. Specifically, this is the feedforward network we use to solve the XOR example. It has a single hidden layer containing two units. (*Left*) In this style, we draw every unit as a node in the graph. This style is very explicit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

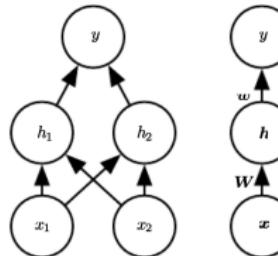


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**Figure:** A simple feed-forward network (Goodfellow et al, 2017, Fig. 6.2)

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 ( $x_i$ ).

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

⋮

$$\underbrace{\mathbf{h}_I}_{1 \times k_I} = g_I(\underbrace{\mathbf{h}_{I-1}^T}_{1 \times k_{I-1}} \underbrace{\mathbf{W}_I}_{k_{I-1} \times k_I} + \underbrace{\mathbf{b}_I}_{1 \times k_I})$$

⋮

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

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



# 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

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



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where

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



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



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# Activation functions ( $g_I$ )

---

- Sometimes use notation  $\sigma$  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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- 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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$$g_{\text{ReLU}}(z) = \max(0, z)$$

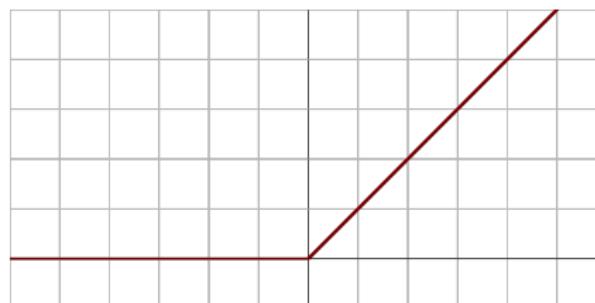


Figure: Rectified Linear Unit (Wikipedia)



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# Activation functions ( $g_I$ ): GeLU

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

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

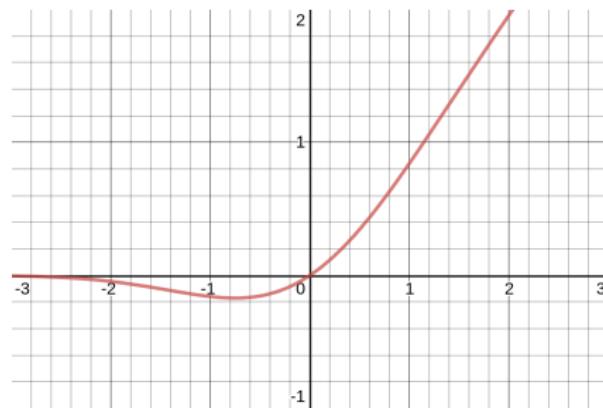


Figure: Gaussian Error Linear Unit (Wikipedia)



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## Activation functions ( $g_I$ ): ELU

$$g_{\text{ELU}}(z) = \begin{cases} \alpha(e^z - 1), & \text{if } z < 0, \\ z, & \text{if } z \geq 0. \end{cases}$$

where  $\alpha$  is commonly set to 1.

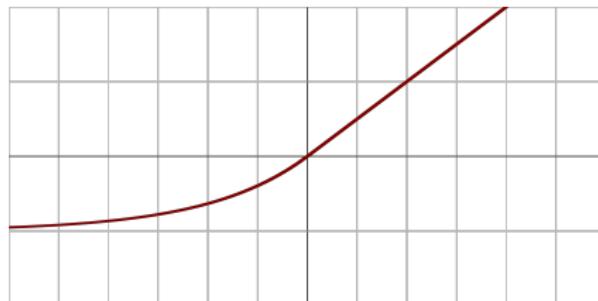


Figure: Exponential Linear Unit (Wikipedia)



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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
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    - How many layers?
    - How many hidden units in each layer?
    - Activation functions?
  - *Note!* Output units is defined by both the **data** and by design



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# Universal Approximation Theorem

---

- A feed-forward neural network with **one hidden layer** and a **non-polynomial activation** (e.g., sigmoid, tanh, ReLU) can approximate **any continuous function** on a compact set  $K \subset \mathbb{R}^n$ .



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# Universal Approximation Theorem

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- Formally, for any continuous function  $f : K \rightarrow \mathbb{R}^m$  and any  $\varepsilon > 0$ , there exists a one-hidden-layer network

$$g(x) = C \sigma(Ax + b)$$

such that

$$\sup_{x \in K} \|f(x) - g(x)\| < \varepsilon.$$



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such that

$$\sup_{x \in K} \|f(x) - g(x)\| < \varepsilon.$$

- Interpretation: The **worst-case error** between the network  $g$  and the target function  $f$  on the entire set  $K$  can be made **arbitrarily small** by using enough hidden units.



# Universal Approximation Theorem, but...

---

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- Neural networks are **universal function approximators**, but...



# Universal Approximation Theorem, but...

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- Neural networks are **universal function approximators**, but...
  - No guarantee we can **learn** the network



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- Neural networks are **universal function approximators**, but...
    - No guarantee we can **learn** the network
    - No guarantee that it will **generalize**



# Universal Approximation Theorem, but...

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- Neural networks are **universal function approximators**, but...
  - No guarantee we can **learn** the network
  - No guarantee that it will **generalize**
  - No indication of how large the network needs to be



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# Depth matters

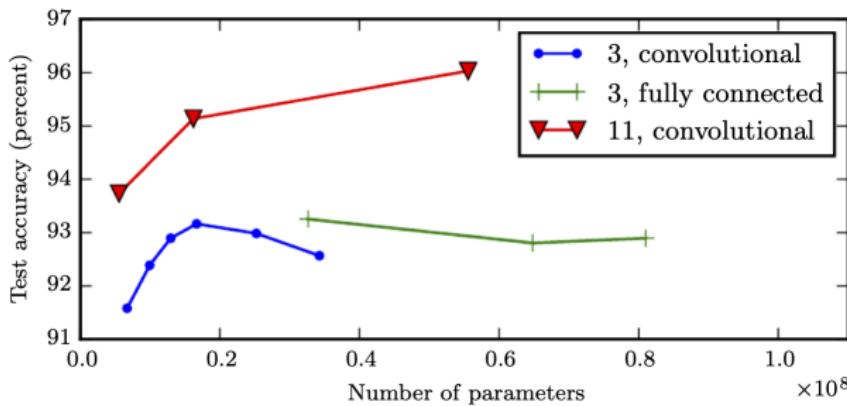


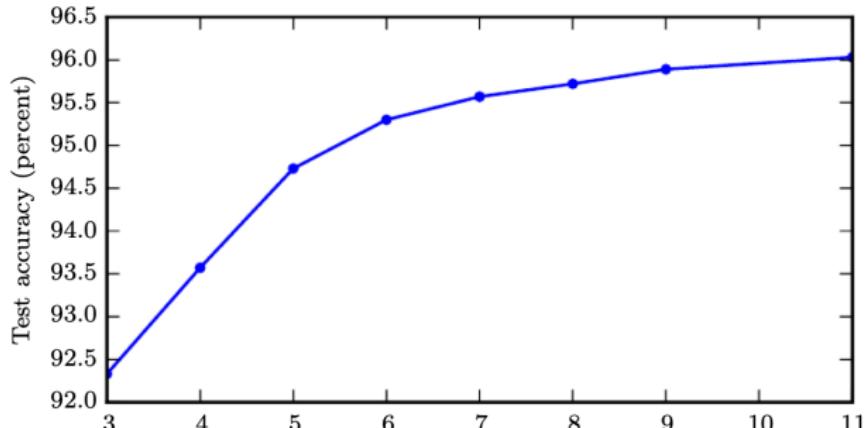
Figure: Effect of depth on accuracy (Goodfellow et al, 2017, Fig. 6.3)



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## Depth matters II



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



# How to choose architecture

---

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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)



# How to choose architecture

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- Trial and error on validation sets
  - Art rather than science
  - Specialized approaches (Bayesian optimization)
  - Grid search (combinatorial explosion)
    - Really bad if many hyperparameters has a little effect
    - If we have 5 irrelevant parameters we try 3 values for:  $125$  training per relevant run
    - Instead use...



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



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# Grid search vs. Random Search

---

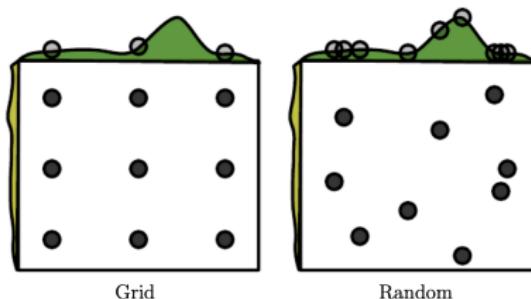


Figure: Grid search and random search (Goodfellow et al, 2017, Fig. 11.2)



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## Section 3

### Regularization



# Regularization of Neural Networks

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



# Regularization of Neural Networks

---

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- 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.

- $\alpha$  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

---

- Let's 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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- Then the gradient update becomes

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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

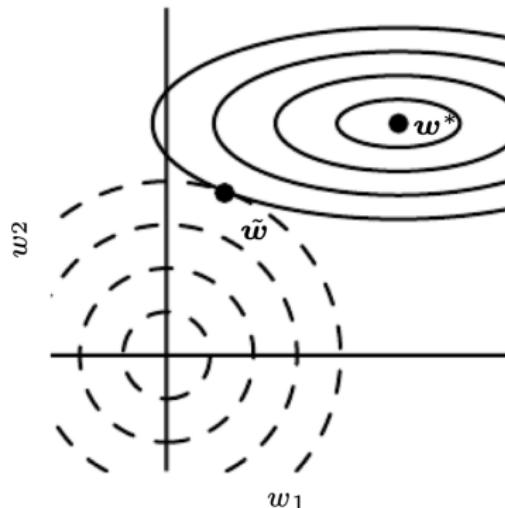


Figure:  $L_2$  regularization (Goodfellow et al, 2017, Fig. 7.1)



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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

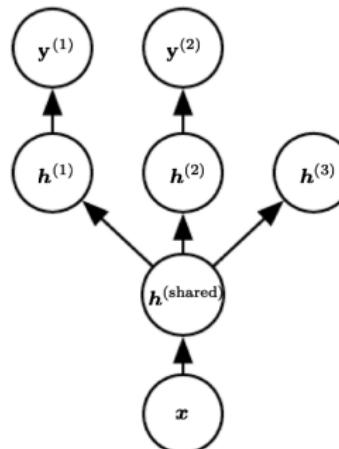


Figure: Multi-task learning (Goodfellow et al., 2017, Fig 7.2)

- 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)

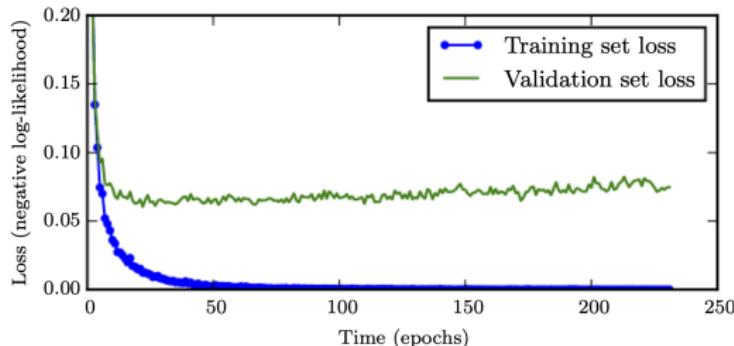


Figure: Early Stopping (Goodfellow et al, 2017, Fig. 7.3)

- 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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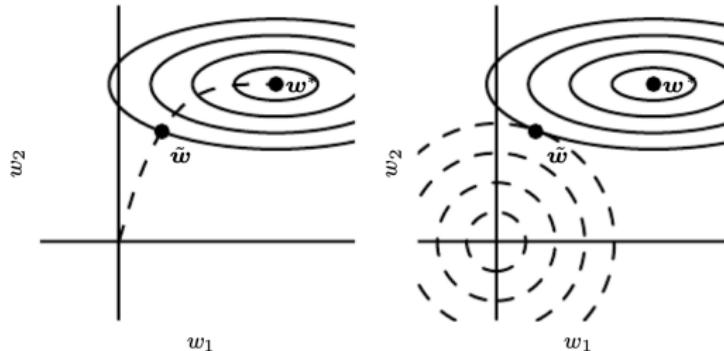


Figure: Early Stopping (Goodfellow et al, 2017, Fig. 7.4)



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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 (dropout rate) is typically 0.2 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



# Dropout

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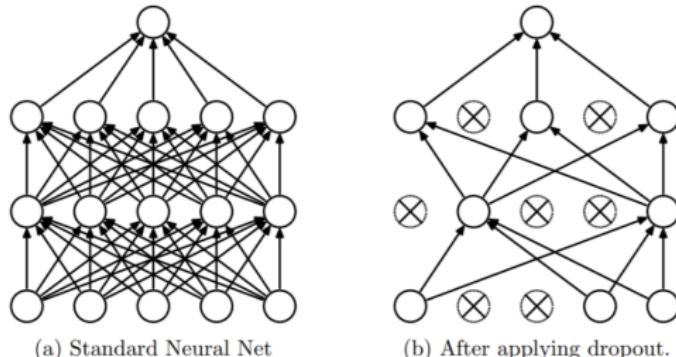


Figure 1: Dropout Neural Net Model. **Left:** A standard neural net with 2 hidden layers. **Right:** An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

**Figure: Dropout (Srivastava et al, 2014)**



# But...

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The best regularizer is...



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



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# Optimization of Neural Networks



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



# Neural Network Learning

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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  $\Omega$  is the regularization term.



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

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



# Optimization of Neural Networks

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- Stochastic Gradient Descent methods

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

where  $\eta_t$  denotes the learning rate at iteration  $t$  and  $\hat{\nabla} J(\theta_{t-1})$  is an estimate of the gradient of the objective function.



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  - Adam (the main optimizer today)
  - RMSprop



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



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# Backpropagation

---

- Backpropagation provides an efficient procedure for computing all parameter gradients  $\nabla J(\theta)$  in a feed-forward neural network.
- Uses the chain rule to propagate the error backward through layers:

$$\frac{\partial J}{\partial W_l} = h_{l-1}^\top \delta_l, \quad \frac{\partial J}{\partial b_l} = \delta_l,$$

where  $\delta_l$  is the error signal at layer  $l$ .

- The algorithm consists of two passes:
  - **Forward pass:** compute

$$h_l = g_l(h_{l-1}^\top W_l + b_l)$$

for each layer  $l$ .

- **Backward pass:** compute error signals

$$\delta_l = (\delta_{l+1} W_{l+1}^\top) \odot g'_l(z_l), \quad z_l = h_{l-1}^\top W_l + b_l,$$

starting from the output layer.



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starting from the output layer.

- Enables efficient gradient-based optimization even for networks with many layers and millions of parameters.



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## Forward Pass: Simple Example

- Consider a network with one hidden layer (2 units, we skip biases for simplicity) and ReLU activation:

$$h_1 = g_1(x^\top W_1), \quad \hat{y} = w^\top h_1.$$

- Let

$$x = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \quad W_1 = \begin{bmatrix} 1 & 2 \\ -1 & 1 \end{bmatrix}, \quad w = \begin{bmatrix} 1 \\ -2 \end{bmatrix}.$$

- Compute hidden pre-activation:

$$z_1 = x^\top W_1 = \begin{bmatrix} -1 \\ 4 \end{bmatrix}.$$

- Apply ReLU:

$$h_1 = g_{\text{ReLU}}(z_1) = \max(0, z_1) = \begin{bmatrix} 0 \\ 4 \end{bmatrix}.$$

- Output:

$$\hat{y} = w^\top h_1 = -8.$$



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## Backward Pass: Simple Example

- Loss (squared error):

$$J = \frac{1}{2}(\hat{y} - y)^2, \quad y = 0, \quad \frac{\partial J}{\partial \hat{y}} = \hat{y} - y = -8.$$

- Output layer gradients:

$$\frac{\partial J}{\partial w} = \frac{\partial J}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial w} = h_1(\hat{y} - y) = \begin{bmatrix} 0 \\ -40 \end{bmatrix}.$$

- Backpropagated error signal:

$$\delta_1 := \frac{\partial J}{\partial z_1} = \frac{\partial J}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial h_1} \cdot \frac{\partial h_1}{\partial z_1} = (\hat{y} - y) w \odot g'_{\text{ReLU}}(z_1).$$

$$(\hat{y} - y) w = \begin{bmatrix} -8 \\ 16 \end{bmatrix}, \quad g'_{\text{ReLU}}(z_1) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \delta_1 = \begin{bmatrix} 0 \\ 16 \end{bmatrix}.$$

- Gradients for first layer:

$$\frac{\partial J}{\partial W_1} = \frac{\partial J}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial h_1} \cdot \frac{\partial h_1}{\partial z_1} \cdot \frac{\partial z_1}{\partial W_1} = x \delta_1^\top = \begin{bmatrix} 0 & 16 \\ 0 & 32 \end{bmatrix}.$$



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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?



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# Problems: Local Minima

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- Neural Networks cost function  $J(\theta)$  are (usually) **not a convex** function
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- **Good thing:** This is probably not the situation!



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# Problems: Plateaus and Saddle Points

- Another problem is **saddle points**

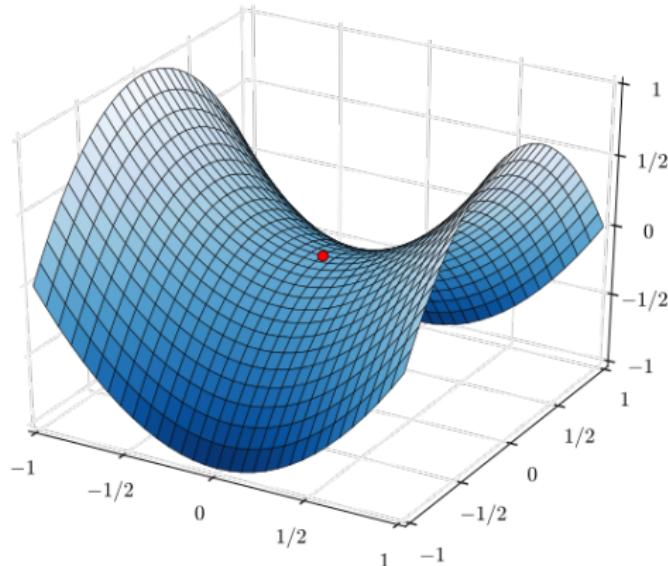


Figure: Saddle point for  $z = x^2 - y^2$  (Wikipedia)

- What is the gradient in a saddle point?



# Problems: Plateaus and Saddle Points

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

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## Problems: Plateaus and Saddle Points

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



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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

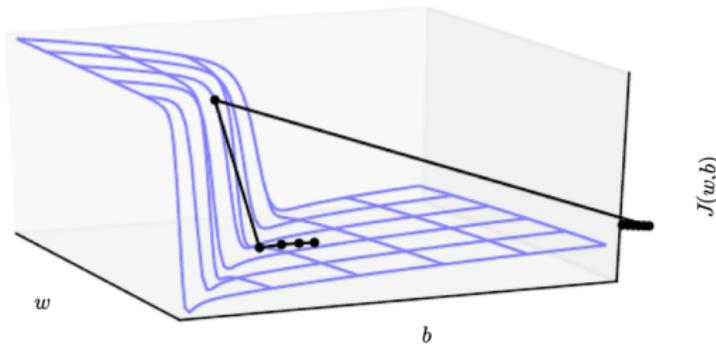


Figure: Cliff (Goodfellow et al., 2017, Fig. 8.3)

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



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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

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



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## Section 5

### Neural Networks in Practice



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# TensorFlow

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- 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

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

