Lecture 3: Deep Neural Networks

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Advanced Machine Learning 2022

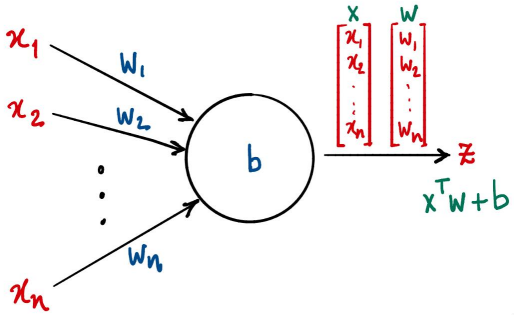
(based on slides by Madhavan Mukund)

Linear separators and perceptrons

- Perceptrons define linear separators $x^T w + b$
  - $x^T w + b > 0$, classify Yes $(+1)$
  - $x^T w + b < 0$, classify No (-1)

$x \in \mathbb{R}^n$

$n = h \times w \times 3$



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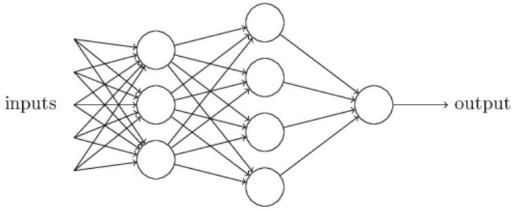

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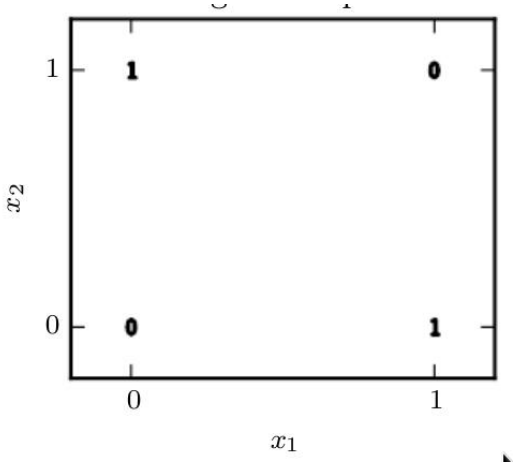

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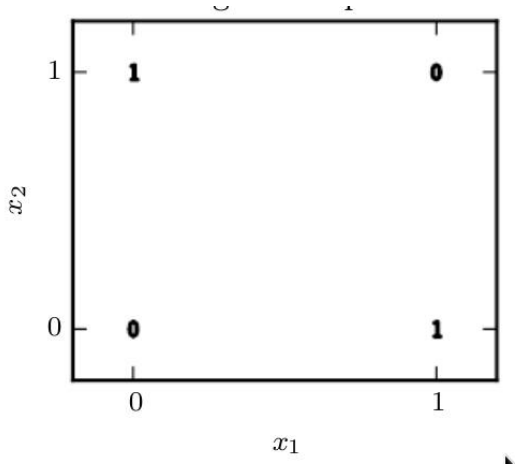

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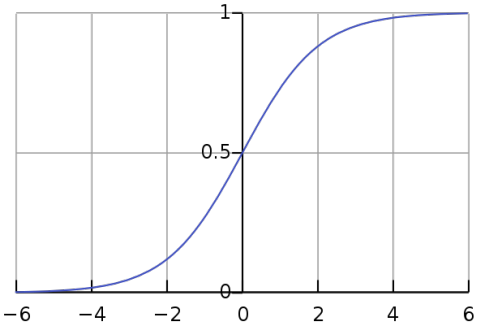
We need non-linearity!

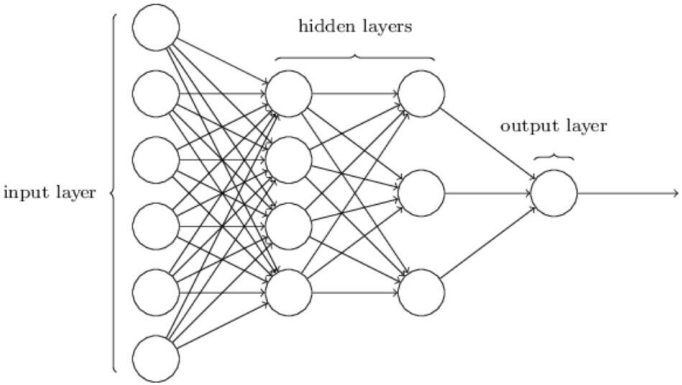
- Introduce a non-linear activation function
  - Traditionally sigmoid, $\sigma(z) = 1/(1 + e^{-z})$

This is a neuron!



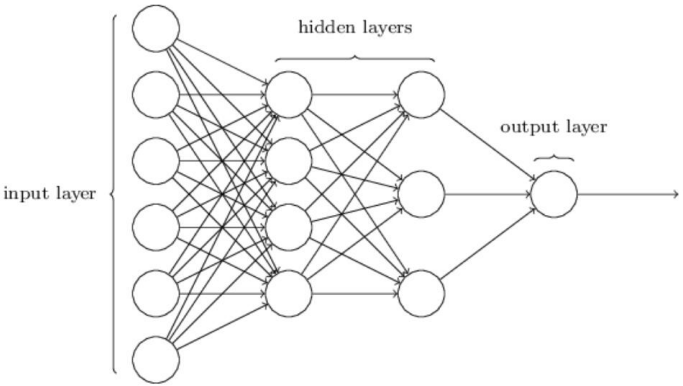
(Feed forward) Neural networks

- Acyclic network of perceptrons with non-linear activation functions
  - Universal Approximation Theorem: With just 1 hidden layer, a neural network can approximate any function for any degree of precision.
  - For a function f, it is possible to construct such a neural network.
    For example the XOR function.



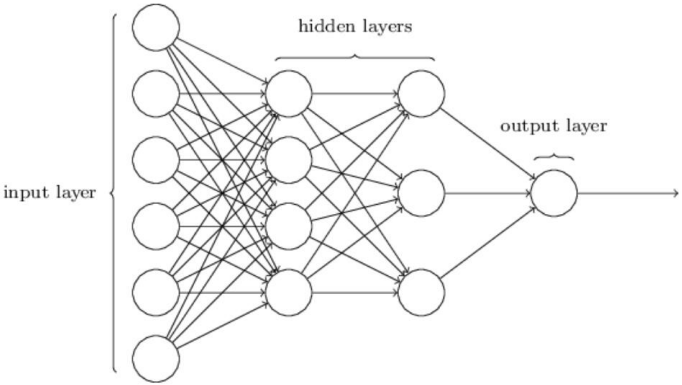
(Feed forward) Neural networks

- Acyclic network of perceptrons with non-linear activation functions
  - The Structure of the network and the value of it's Parameters θ (weights and biases of each neuron).
  - **Objective:** Given a training set S, compute a neural network with *low generalization loss.*
  - We can estimate the generalization loss using a test set T.



(Feed forward) Neural networks

- How do we compute a neural network?
  - Choose the structure of the neural network, based on the ML task at hand.
  - Initially set the weights and biases of neurons to random numbers.
  - Choose a loss-function $\ell(\theta, S)$ on the output of the neural network, e.g. Cross-Entropy Loss
  - Optimization problem: Given S find the values for θ with least $\ell(\theta, S)$.



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Highly Non-Trivial Problem!

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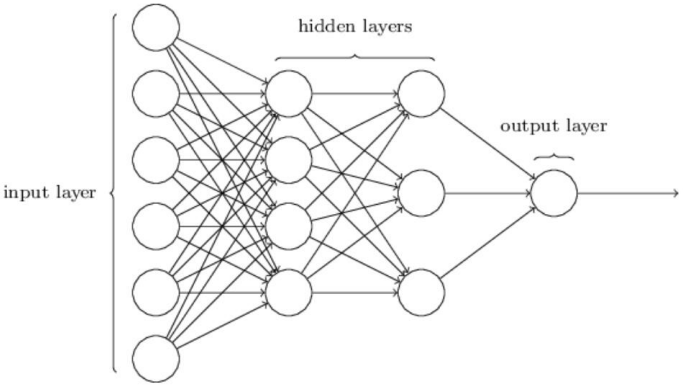
  - Optimization problem: Given S find the values for θ with least $\ell(\theta, S)$.

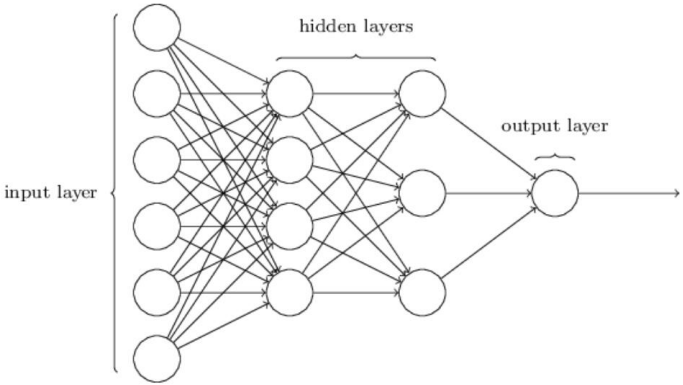
Highly Non-Trivial Problem!

  - We use the most basic optimization method: **Gradient Descent**
  - Update θ so that $\ell(\theta, S)$ decreases $\implies$ $\theta \leftarrow \theta - \alpha \cdot \frac{d\ell(\theta,S)}{d\theta}$
  - α is the learning rate



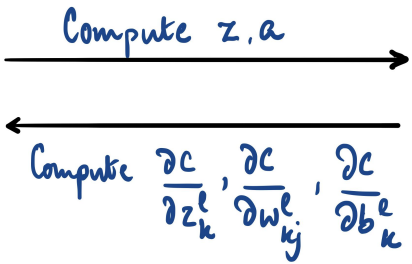
(Feed forward) Neural networks

- Acyclic network of perceptrons with non-linear activation functions
- Ingredients
  - Output layer activation function
  - Loss function for gradient descent
  - Hidden layer activation functions
  - Network architecture: Interconnection of layers
  - Initial values of weights and biases



Training a neural network

- Backpropagation — efficient implementation of gradient descent for neural networks



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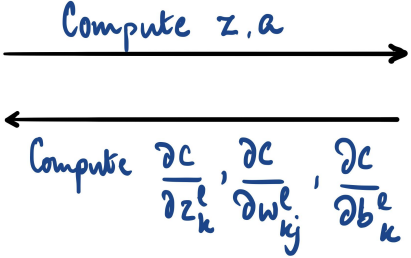
- Forward pass, compute outputs, activation values
- Backward pass, use chain rule to compute all gradients in one scan



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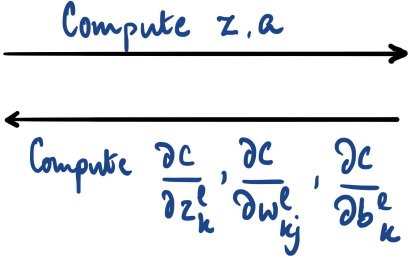
- Stochastic gradient descent (SGD)
  - Update parameters in minibatches
  - Epoch: set of minibatches that covers entire training data



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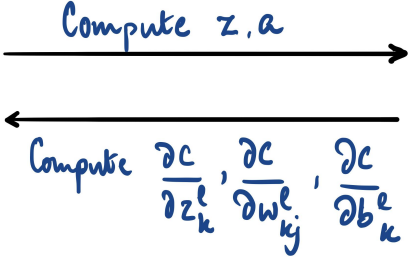
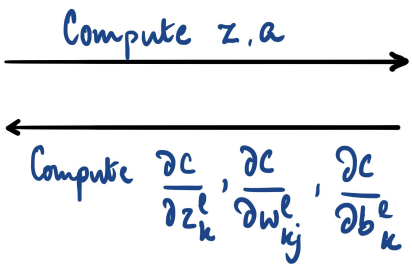
  - Epoch: set of minibatches that covers entire training data
- Difficulties: slow convergence, vanishing and exploding gradients



Unstable gradients

- Vanishing gradients — gradients become smaller towards lower layers (closer to input)
  - Gradient descent updates leave these layers' parameters virtually unchanged



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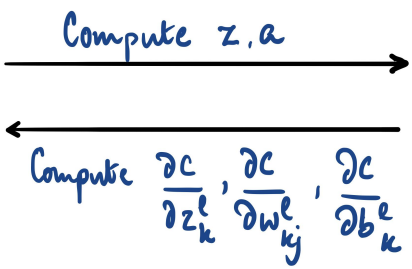

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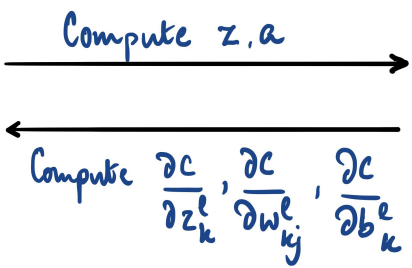

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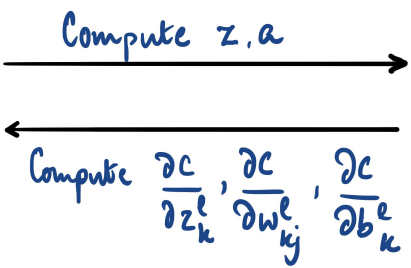
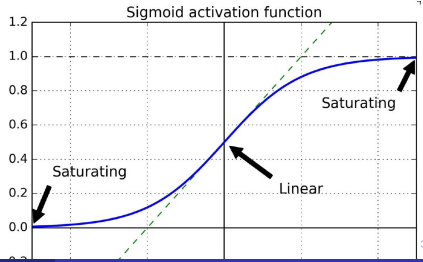
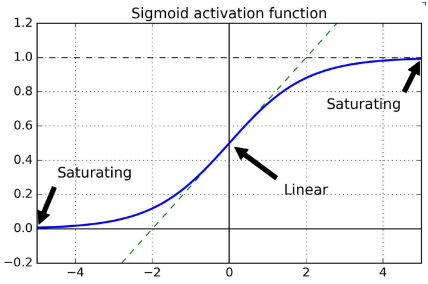
- [Xavier Glorot and Joshua Bengio, 2010]
  - Random initialization, traditionally Gaussian distribution $\mathcal{N}(0, 1)$
  - Variance keeps increasing going forward
  - Saturating sigmoid function





Initializing neural networks

- Want "signal" to flow well in both directions during backpropagation
  - Signal should not die out, explode, saturate



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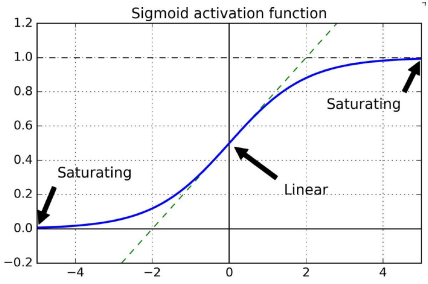

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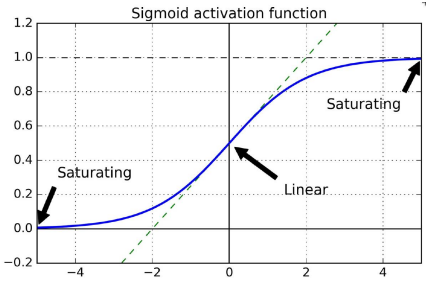
- Let $fan_{avg} = (fan_{in} + fan_{out})/2$



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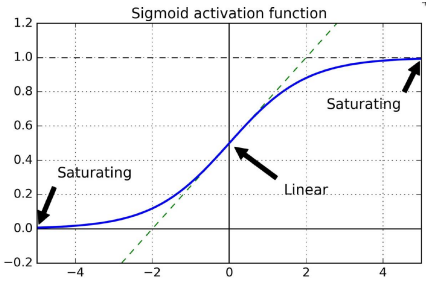
- Initialize with
  - Gaussian, $\mathcal{N}(0, 1/fan_{avg})$
  - Uniform, $\mathcal{U}(-r, r)$, $r = \sqrt{\frac{3}{fan_{avg}}}$



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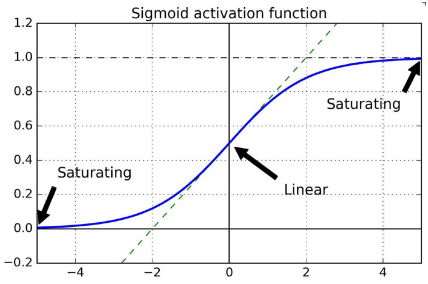

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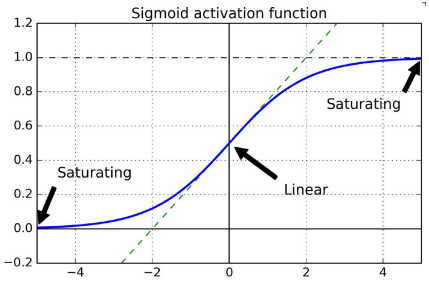
  - Equivalent if $fan_{in} = fan_{out}$



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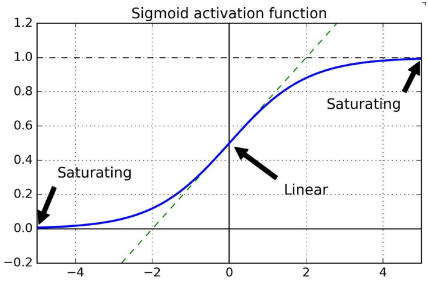
  - Equivalent if $fan_{in} = fan_{out}$
- Other choices for specific activation function
  - ReLU, [He et al, 2015], $\mathcal{N}(0, 2/fan_{in})$



Non-saturating activation functions

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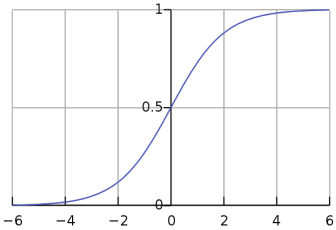

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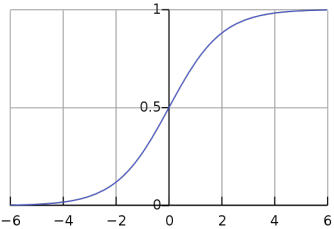
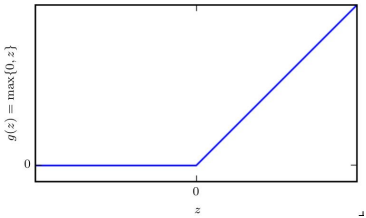
  - Fast to compute
  - Non-differentiable point not a bottleneck





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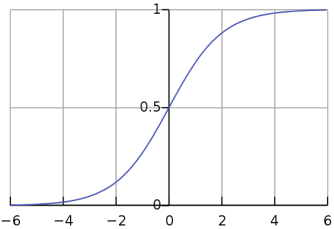
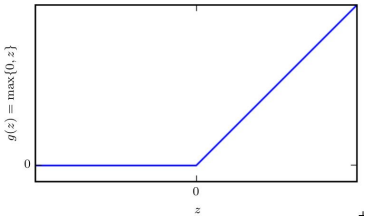
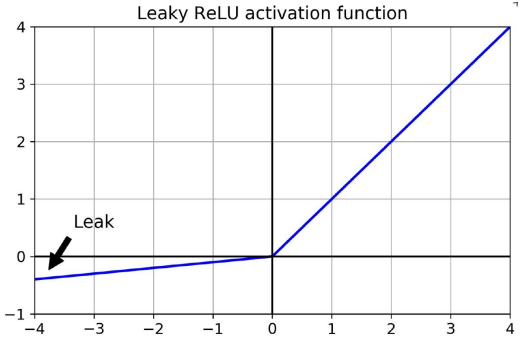
  - Fast to compute
  - Non-differentiable point not a bottleneck
- "Dying ReLU"
  - Neuron dies — weighted sum of outputs is negative for all training samples
  - With a large learning rate, half the network may die!





Non-saturating activation functions

- Leaky ReLU, $\max(\alpha z, z)$
  - "Leak" α is a hyperparameter



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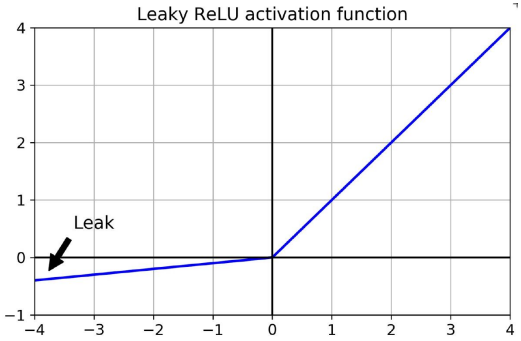
  - Fix to an average value when testing
  - Seems to work well, act as a regularizer



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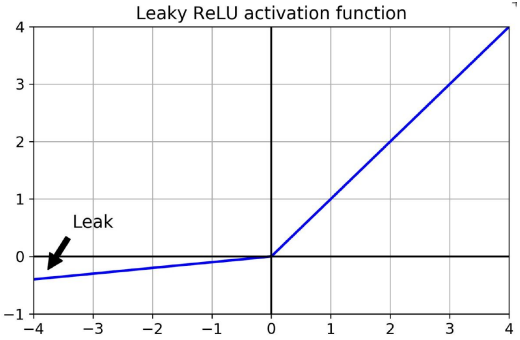
- PReLU — parametric ReLU [He et al, 2015]
  - α is learned during training
  - Often outperforms ReLU, but could lead to overfitting

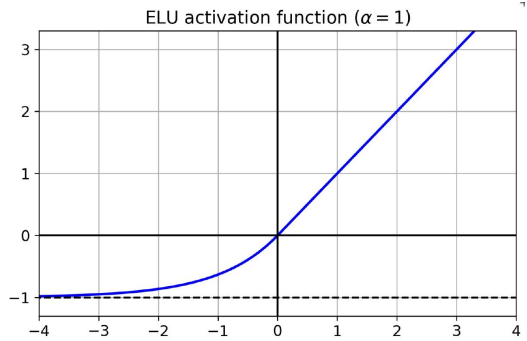


Non-saturating activation functions

- ELU — Exponential Linear Unit [Clevert et al, 2015]

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

  - Training converges faster
  - Computing exponential is slower
  - In practice, slower than ReLU

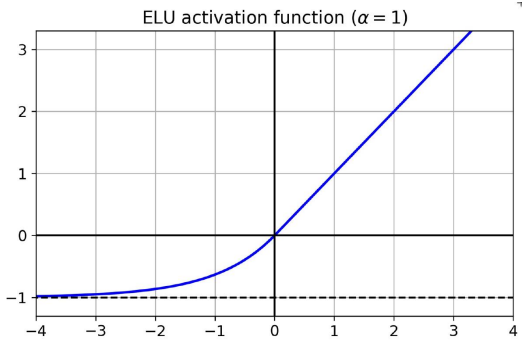


Non-saturating activation functions

- SELU — Scaled ELU
  [Klambauer et al, 2017]

$$SELU_\alpha(z) = \lambda \begin{cases} \alpha(e^z - 1) & \text{if } z < 0 \\ z & \text{if } z \geq 0 \end{cases}$$

  - Self-normalizing — output of each layer preserves mean 0 and standard deviation 1 during training
  - Use LeCun initialization, $\mathcal{N}(0, 1/fan_{in})$



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  - Zero-centre and normalize each input

$$\hat{x}_i = \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

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- Even works as a regularizer!

Transfer learning

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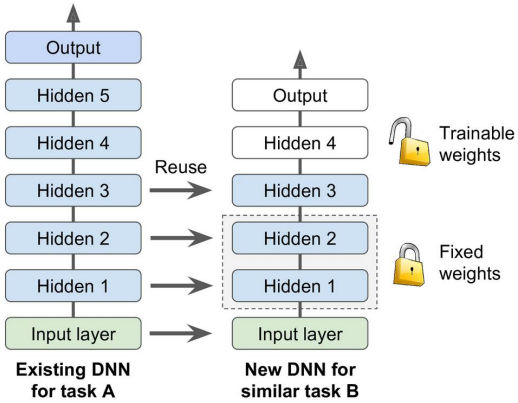

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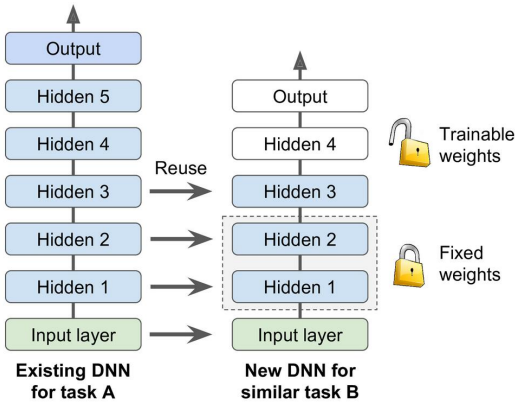

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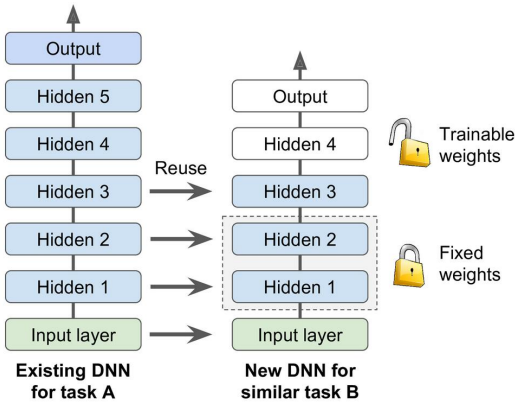

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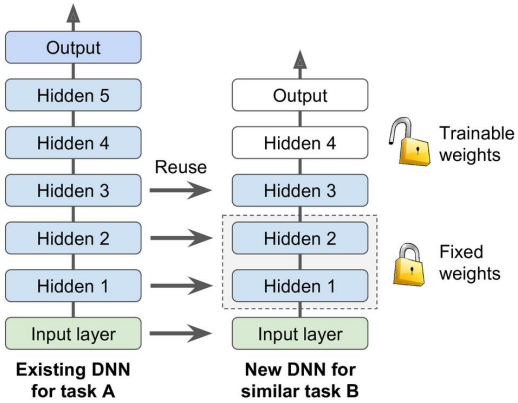

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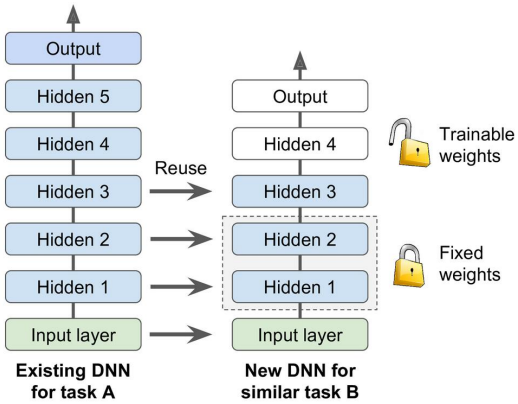

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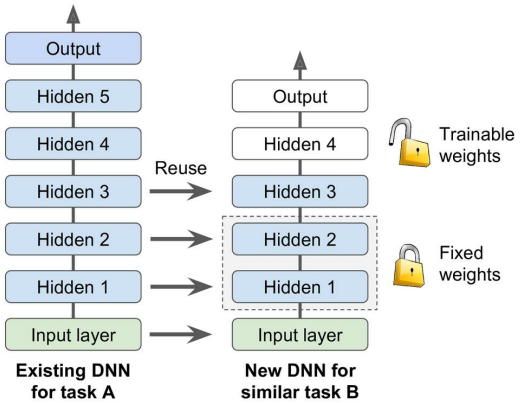

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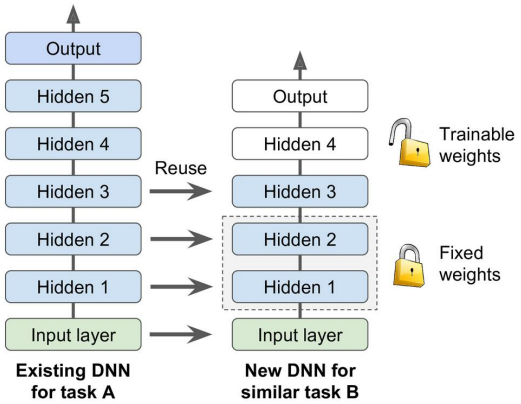

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