Artificial Neural Network

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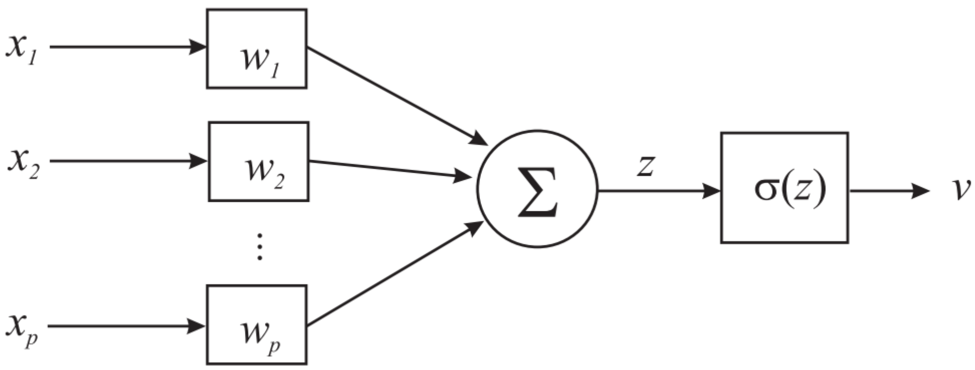
1. Introduction

1.1. Artificial Neuron



x_i: ith **input** of the neuron

w_i: adaptive **weight** (synaptic strength) for x_i

z: weighted sum of inputs:

$$z = \sum_{i=1}^{p} w_i x_i = \mathbf{w}^T \mathbf{x} + b \tag{1}$$

$\sigma(z)$: **activation function**

v: output of the neuron

1.2. Activation functions

Transformation of the input space (squeezing).

1.2.1. Projection Functions

threshold function, piece-wise linear function, tangent hyperbolic, sigmoidal, rectified linear, … function:

$$\sigma(z) = 1/(1 + \exp(-2z)) \tag{2}$$

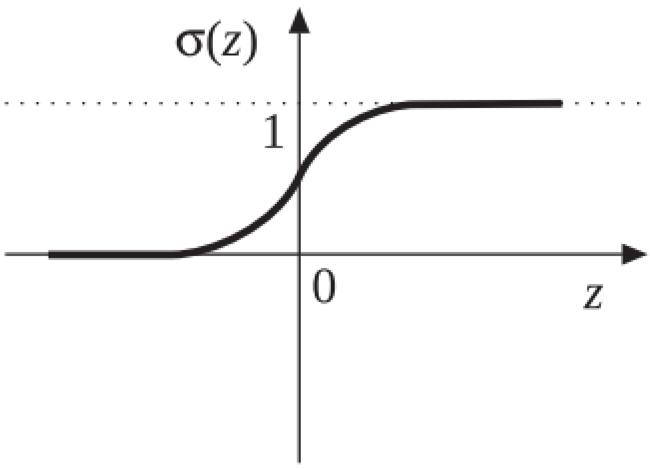
1.2.2. Kernal Functions

$$\sigma(\mathbf{x}) = \exp\left(-(\mathbf{x} - \mathbf{c})^2/s^2\right) \tag{3}$$

1.3.3. Common Choices

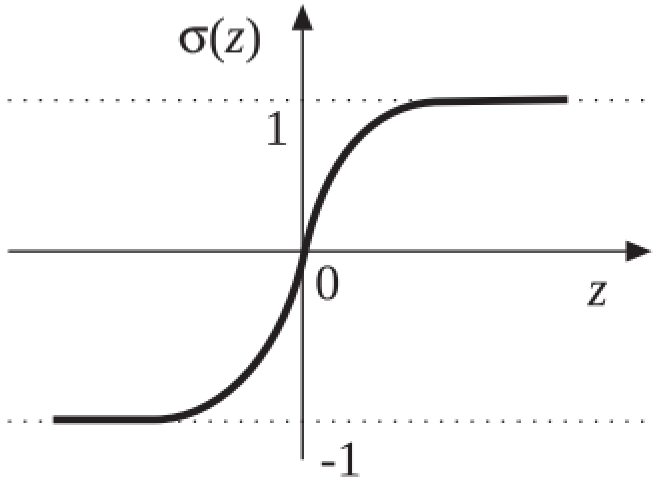
Sigmoid:

$$\sigma(z) = 1/(1 + \exp(-z)) \tag{4}$$



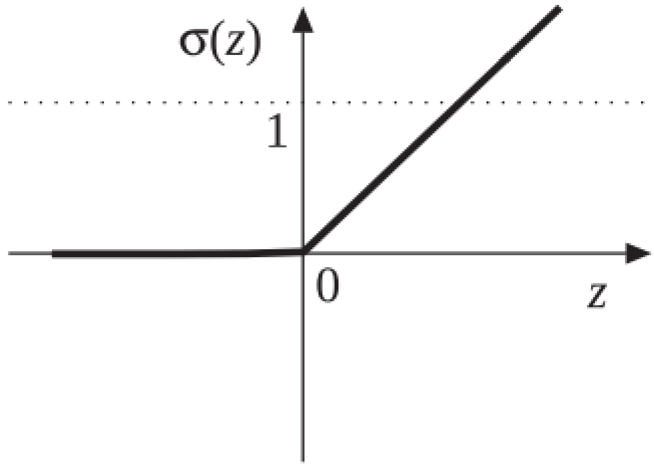
Tangent Hyperbolic:

$$\sigma(z) = \frac{2}{1 + e^{-2z}} - 1 \tag{5}$$



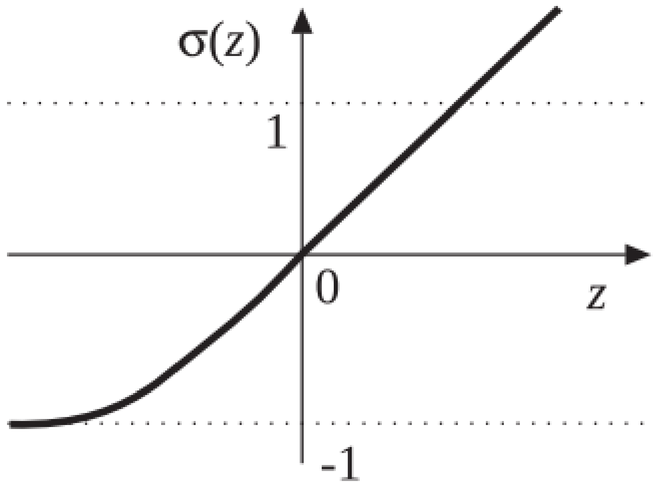
Rectified Linear Unit (ReLU):

$$\sigma(z) = \begin{cases} 0 & \text{if } z < 0 \\ z & \text{if } z \geq 0 \end{cases} \tag{6}$$



Exponential Linear Unit (ELU):

$$\sigma(z) = \begin{cases} z & \text{if } z > 0 \\ \alpha\left(e^z - 1\right) & \text{if } z \leq 0 \end{cases} \tag{7}$$



2. Simple Networks

2.1. Feedforward neural network example

- Activation of hidden-layer neuron j:

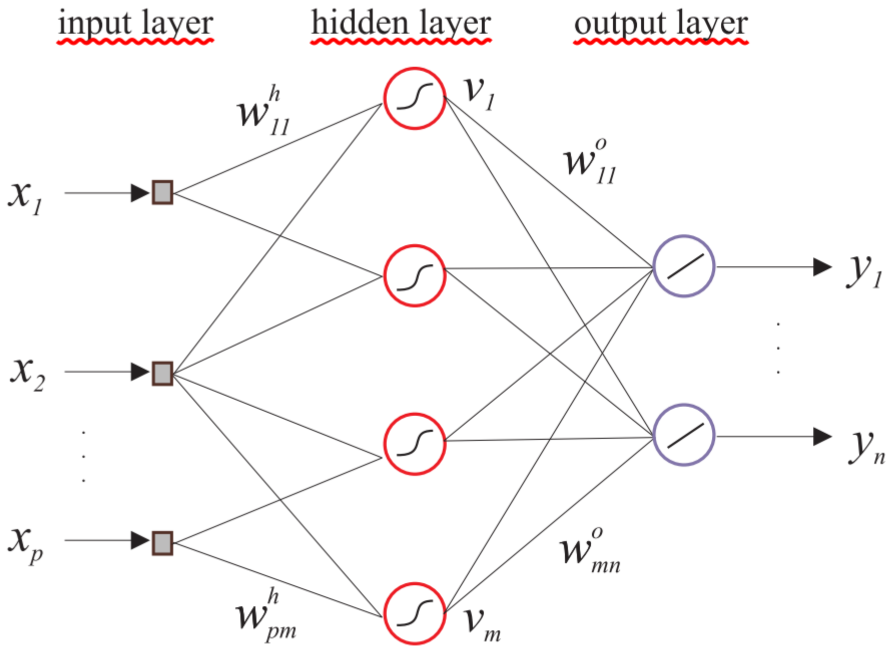
$$z_j = \sum_{i=1}^{p} w_{ij}^h x_i + b_j^h \tag{8}$$

- Output of hidden-layer neuron j

$$v_j = \sigma(z_j) \tag{9}$$

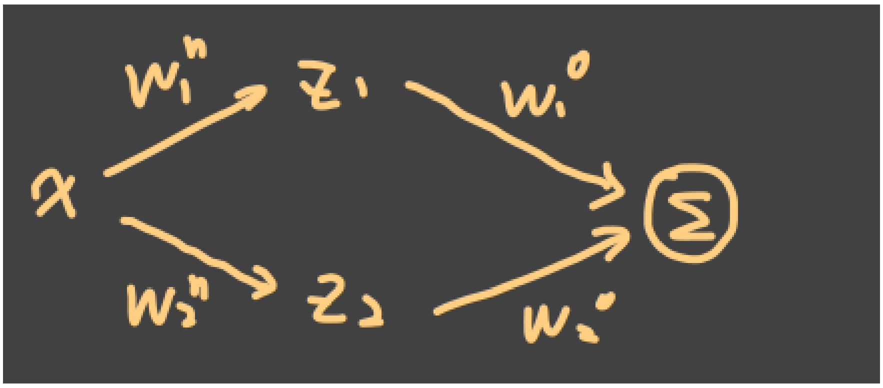
- Output of output-layer neuron l:

$$y_l = \sum_{j=1}^{m} w_{jl}^o v_j + b_l^o \tag{10}$$

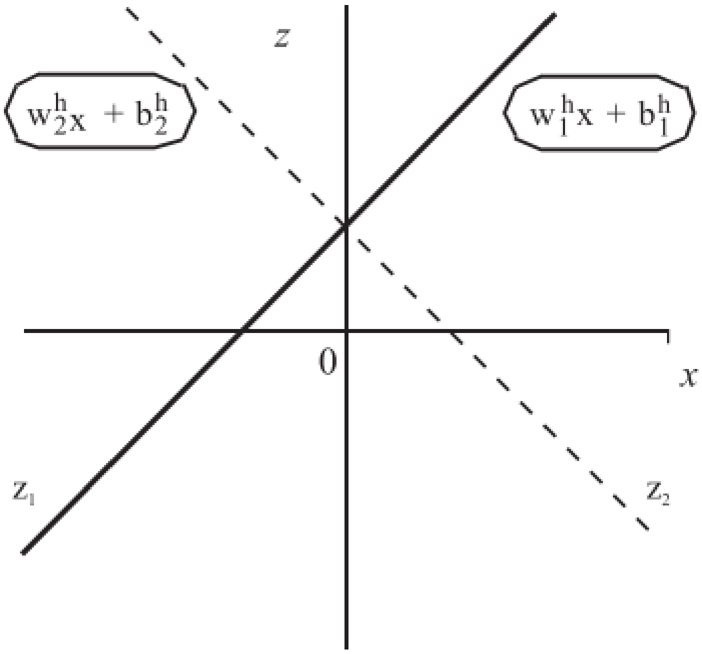


2.2. Function approximation with neural nets: examples

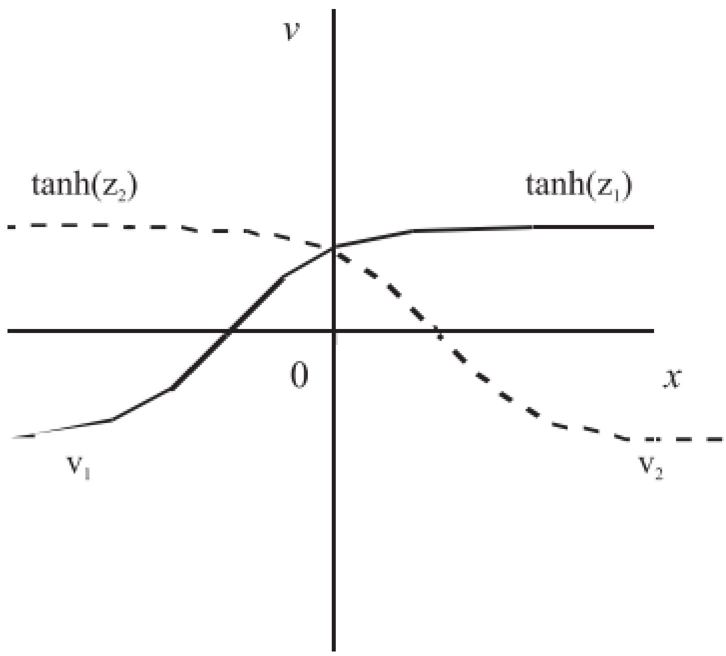
$$y = w^o_1 \tanh\left(w^h_1 x + b^h_1\right) + w^o_2 \tanh\left(w^h_2 x + b^h_2\right) \tag{11}$$

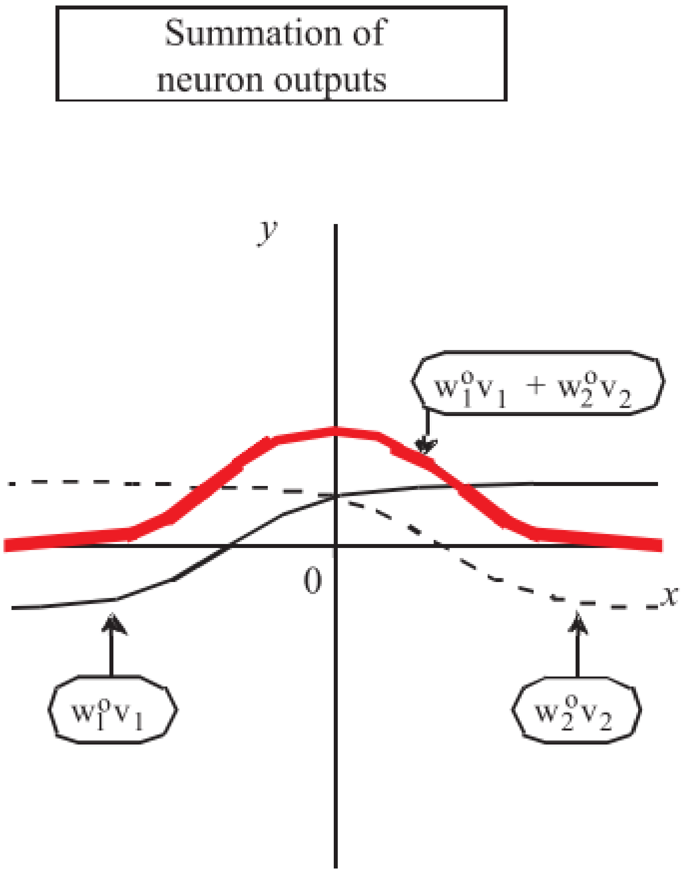


Activation (weighted summation)



Transformation through tanh





2.3. Input–Output Mapping

$$
\begin{aligned}
\mathbf{Z} &= \mathbf{X}_b \mathbf{W}^h \\
\mathbf{V} &= \sigma(\mathbf{Z}) \\
\mathbf{Y} &= \mathbf{V}_b \mathbf{W}^\circ
\end{aligned}
$$

$$
\text{with } \mathbf{X}_b = [\mathbf{X}, \mathbf{1}] \text{ and } \mathbf{V}_b = [\mathbf{V}, 1] \tag{12}
$$

Compact formula:

$$
\mathbf{Y} = \left[\sigma\left([\mathbf{X}\mathbf{1}]\mathbf{W}^h\right) \mathbf{1}\right] \mathbf{W}^\circ \tag{13}
$$

2.4. Approximation capability of neural nets

Cybenko Theorem

A feedforward neural net with **at least one hidden layer** can **approximate any** continuous nonlinear function $\mathbb{R}^p \to \mathbb{R}^n$ **arbitrarily well**, provided that **sufficient number of hidden neurons are available (not constructive**).

Barron Theorem

- A feedforward neural net **with one hidden layer** with **sigmoidal activation functions** can achieve an integrated squared error of the order

$$J = \mathcal{O}\left(\frac{1}{h}\right) \tag{14}$$

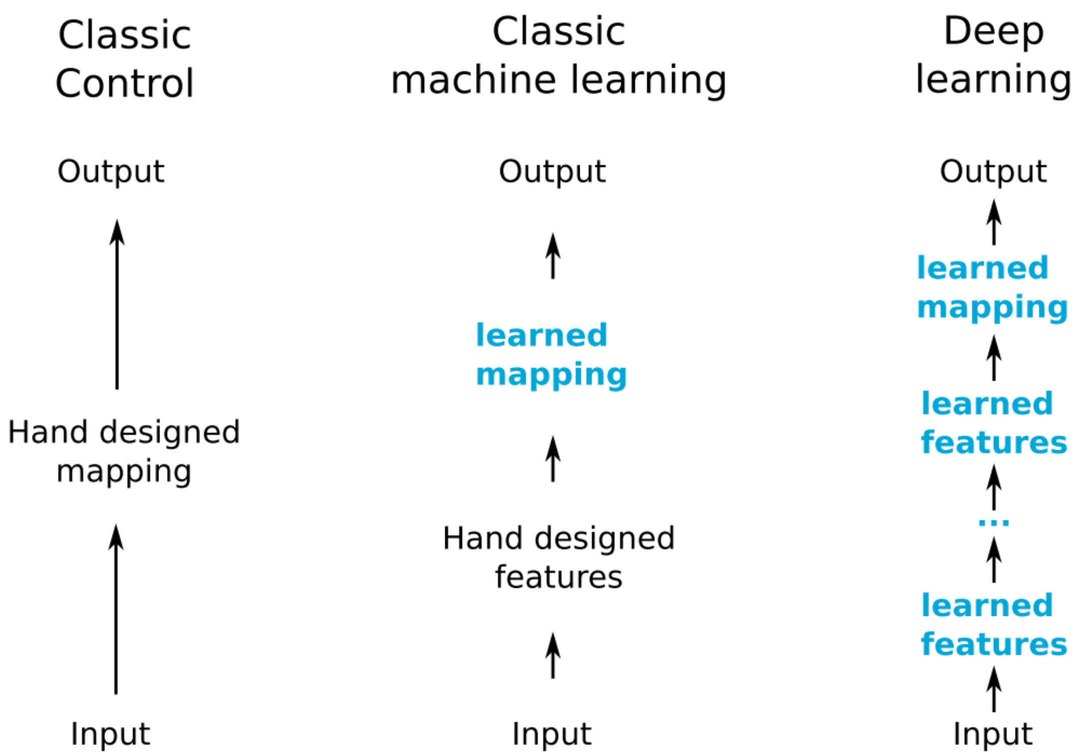
- **independently** of the dimension of the **input space p**, where **h denotes the number** of hidden neurons
- For a **basis function expansion** (polynomial, trigonometric expansion, singleton fuzzy model, etc.) with **h terms**, in which only the parameters of the linear combination are adjusted

$$J = \mathcal{O}\left(\frac{1}{h^{2/p}}\right) \tag{15}$$

Understanding

- Does mean neural networks are suitable for a range of problems with high dimensional inputs.
- Does not mean it is always possible to get near the theoretical limit.
- Does not mean adding more neurons per layer always results in a lower approximation error.
- Does not mean one layer is optimal

3. Deep Learning



4. Training

4.1. Goal

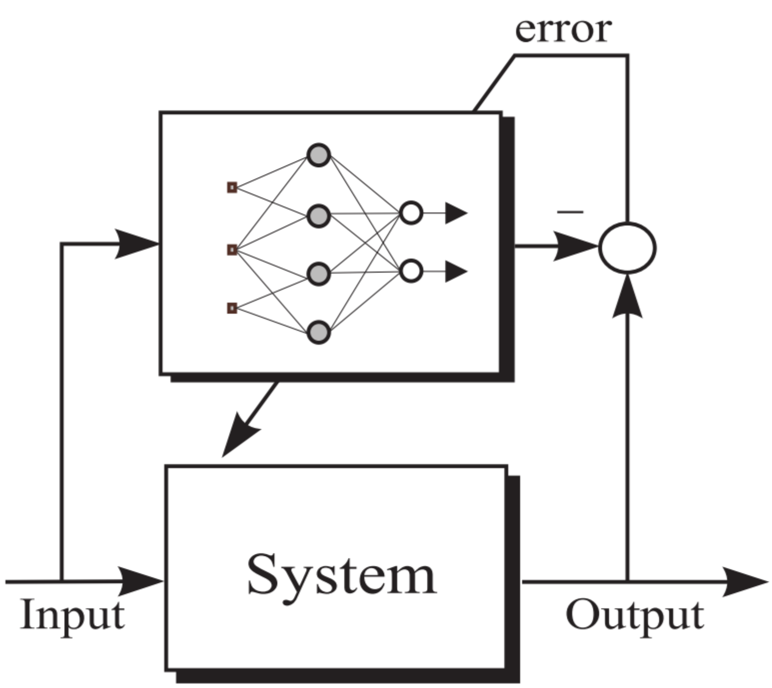
Find the **weight vector W** that minimizes some **cost function** $J(f(x;W))$ for **all (especially unseen) inputs x**.

Important Notes

When training, we always calculate th**e loss over the examples** in the dataset. We **actually want to minimize the loss over the true underlying distribution of examples (Regularization)**

Supervised Learning Example

Make a neural network approximate a known function $x \rightarrow t$ by minimizing:
$J(W) = \frac{1}{2}(f(x;W) - t)^2$



4.2. General Process

1. **Initialize** W to small random values
2. Repeat until the performance (on a separate test-set) stops improving
   a. **Forward pass**: Given an input x, calculate the neural network output $y = f(x; W)$. Then calculate the cost $J(y; t)$ of predicting y instead of the target output t.
   b. **Backward pass**: Calculate the **gradient** of the cost with respect to the weights
   $\nabla J(y(x;W), t) = \left[\frac{\partial J}{\partial w_1}, \quad \ldots, \quad \frac{\partial J}{\partial w_n} \right]^T$
   c. **Optimization step**: **Change the weights** based on the gradient to reduce the cost.

4.3. Back-Propagation

Calculate the **gradient** of the cost with respect to the weights

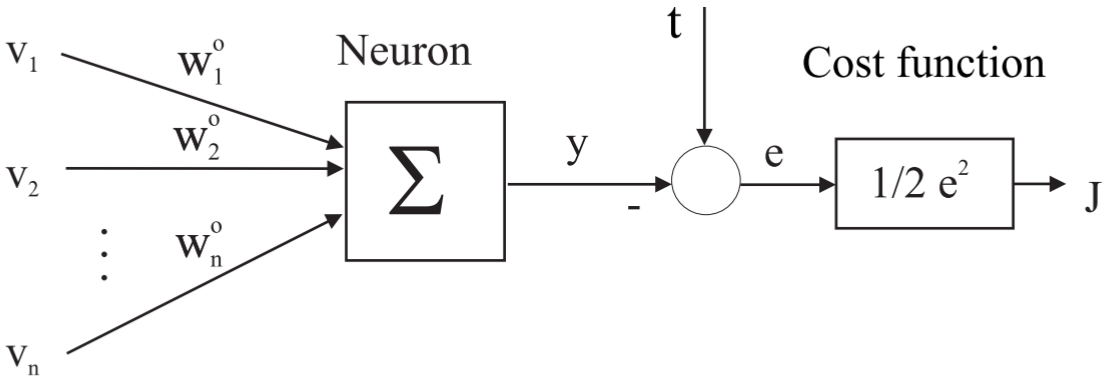
$$\nabla J(y(x;W), t) = \left[\frac{\partial J}{\partial w_1}, \quad \ldots, \quad \frac{\partial J}{\partial w_n} \right]^T \tag{16}$$

Recall Chain Rules

$$\frac{d}{dx} f\left(g_1(x), \ldots, g_k(x)\right) = \sum_{i=1}^{k} \left(\frac{d}{dx} g_i(x)\right) D_i f\left(g_1(x), \ldots, g_k(x)\right) \tag{17}$$

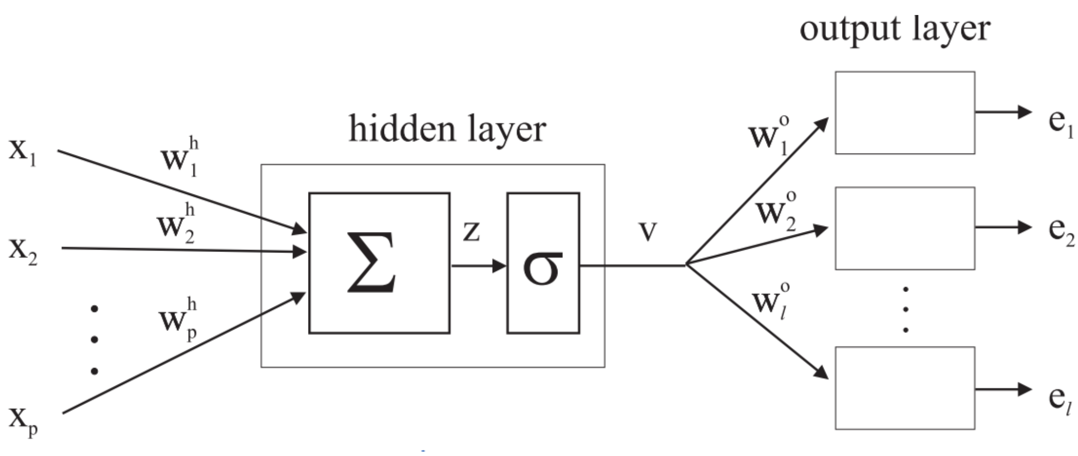
Examples

Output-layer weights example



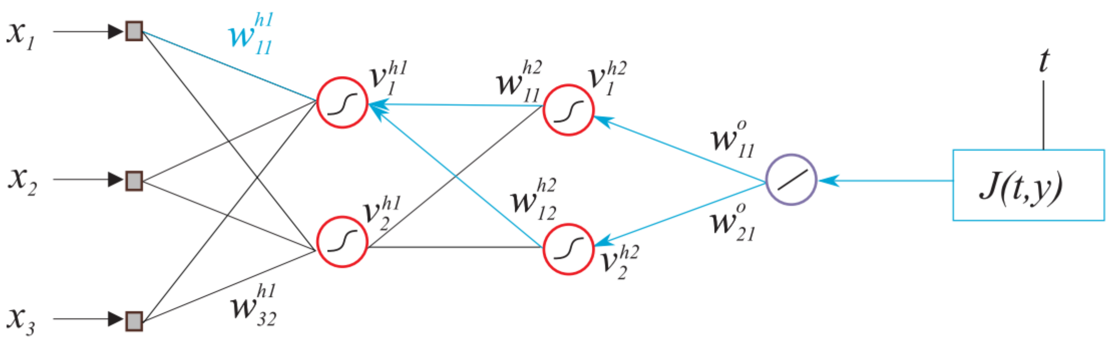
$$\begin{gathered} J = \frac{1}{2} \sum_l e_l^2, \quad e_l = t_l - y_l, \quad y_l = \sum_j w_j^o v_j \\ \frac{\partial J}{\partial w_{jl}^o} = \frac{\partial J}{\partial e_l} \cdot \frac{\partial e_l}{\partial y_l} \cdot \frac{\partial y_l}{\partial w_{jl}^o} = -v_j e_l \end{gathered} \tag{18}$$

Hidden-layer weights example



$$\begin{gathered} \frac{\partial J}{\partial w_{ij}^h} = \frac{\partial J}{\partial v_j} \cdot \frac{\partial v_j}{\partial z_j} \cdot \frac{\partial z_j}{\partial w_{ij}^h} = -x_i \cdot \sigma_j'\left(z_j\right) \cdot \sum_l e_i w_j^o \\ \frac{\partial J}{\partial v_j} = \sum_l -e_i w_{jl}^o, \quad \frac{\partial v_j}{\partial z_j} = \sigma_j'\left(z_j\right), \quad \frac{\partial z_j}{\partial w_{ij}^h} = x_i \end{gathered} \tag{19}$$

More General Example



$$\frac{\partial J}{\partial w_{11}^{h1}} = \left(\frac{\partial J}{\partial v_1^{h2}} \frac{\partial v_1^{h2}}{\partial v_1^{h1}} + \frac{\partial J}{\partial v_2^{h2}} \frac{\partial v_2^{h2}}{\partial v_1^{h1}} \right) \frac{\partial v_1^{h1}}{\partial w_{11}^{h1}} \tag{20}$$

4.4 Cost Function

Two main **criteria**:

- The minimum of the cost function $w^* = \arg\min_w J(f(w))$ should correspond to desirable behavior.

  e.g.

  $$\begin{aligned} J(y,t) &= \|y-t\|^2 \quad &: y = f(x; w^*) \rightarrow \text{ mean } t \text{ for each } x \\ J(y,t) &= \|y-t\|_1 \quad &: y = f(x; w^*) \rightarrow \text{ median of } t \text{ for each } x \end{aligned}$$

Illustration:

- the first one like minimize $(x-a)^2 + (y-a)^2$, when a is mean, the least
- the second one like "absolute distance", the median is the smallest
- The error gradient should be informative (**below are some classical examples**)
  - linear output, Minimum Square Error (MSE):

    $$y = z, \quad J = \frac{1}{2}(y-t)^2 \quad \rightarrow \frac{\partial J}{\partial z} = \frac{\partial J}{\partial y}\frac{\partial y}{\partial z} = (y-t)\cdot 1$$

  - Sigmoidal output, MSE

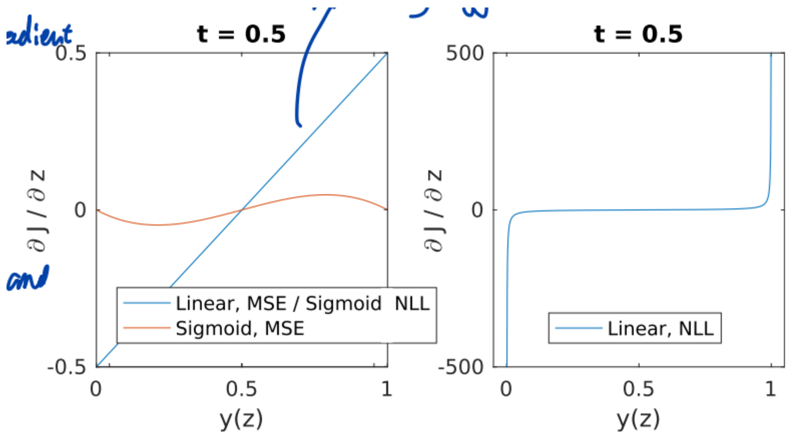
    $$y = \frac{1}{1+e^{-z}}, \quad J = \frac{1}{2}(y-t)^2,$$
    $$\rightarrow \frac{\partial J}{\partial z} = \frac{\partial J}{\partial y}\frac{\partial y}{\partial z} = (y-t)\cdot y(1-y) = \left(y^2 - ty\right)(1-y)$$

    Note: may have a problem when y=0 or y=1

  - sigmoidal output, negative log likelihood

    $$y = \frac{1}{1+e^{-z}}, \quad J = -t\ln(y) - (1-t)\ln(1-y)$$
    $$\rightarrow \frac{\partial J}{\partial z} = \frac{\partial J}{\partial y}\frac{\partial y}{\partial z} = \left(\frac{-t}{y} + \frac{1-t}{1-y}\right) y(1-y) = y - t$$

Different gradient features: $\rightarrow$ different "**aggressive**" extent to modify error and weight



4.5. (Stochastic) Gradient Descent

Basic Way to Update Weights

$$\mathbf{w}_{n+1} = \mathbf{w}_n - \alpha_n \nabla J(\mathbf{w_n}) \tag{21}$$

$$\text{where} \nabla J(\mathbf{w}) = \left(\frac{\partial J}{\partial w_1}, \frac{\partial J}{\partial w_2}, \ldots, \frac{\partial J}{\partial w_M} \right)^T$$

- **Gradient Discent:**

  use $\nabla J(\mathbf{w}) = \frac{1}{K} \sum_{i=1}^{K} \left(\frac{\partial J(t_i, f(x_i; W))}{\partial W} \right)$ with **K equal to the size of the database**

- **Stochastic Gradient Descent:**

  use $\hat{\nabla} J(\mathbf{w}) = \frac{1}{k} \sum_{i=1}^{k} \left(\frac{\partial J(t_i, f(x_i; W))}{\partial W} \right)$ with **k << K the batch size**

  - The $x_i ; t_i$ data points in the batches should be independent and identically distributed (i.i.d)
  - In practice: $k \approx 10^0 - 10^2$, $K \approx 10^4 - 10^9$

Improvement 1: Second-order gradient methods

$$J(\mathbf{w}) \approx J(\mathbf{w}_0) + \nabla J(\mathbf{w}_0)^T (\mathbf{w} - \mathbf{w}_0) + \frac{1}{2} (\mathbf{w} - \mathbf{w}_0)^T \mathbf{H}(\mathbf{w}_0)(\mathbf{w} - \mathbf{w}_0) \tag{22}$$

Update rule for the weights:

$$\mathbf{w}_{n+1} = \mathbf{w}_n - \mathbf{H}^{-1}(\mathbf{w}_n) \nabla J(\mathbf{w_n}) \tag{23}$$

- $H^{-1}\nabla J$ computes a good step for each weight, **only feasible for (very) small networks.**

Improvement 2: Momentum

increase step-size if we keep going in the same direction

$$\begin{gathered}\mathbf{v} \leftarrow \beta\mathbf{v} - \alpha\nabla J \\ \mathbf{w} \leftarrow \mathbf{w} + \mathbf{v}\end{gathered} \tag{24}$$

- the v is initialized 0, $\beta \in [0, 1)$
- if keep going in the same ∇J, then the speed will be faster
- if there once be ∇J, the later movement always keep the trend
- if one dimension (component) always positive in ∇J, then the effect on this dimension will be accumulated

Improvement 3: RMSProp

decrease step-size over time, especially if gradients are large

$$\begin{aligned}\mathbf{r} &\leftarrow \gamma\mathbf{r} + (1-\gamma)\nabla J \odot \nabla J \\ \mathbf{w} \leftarrow &\mathbf{w} - \frac{\alpha}{\sqrt{10^{-6} + \sqrt{\mathbf{r}}}} \odot \nabla J\end{aligned}$$

> $\odot$ *menas **Hadamard Product,** "element-wise product"*

- the r is initialized 0, $\gamma \in [0, 1)$

Improvement 4: ADAM

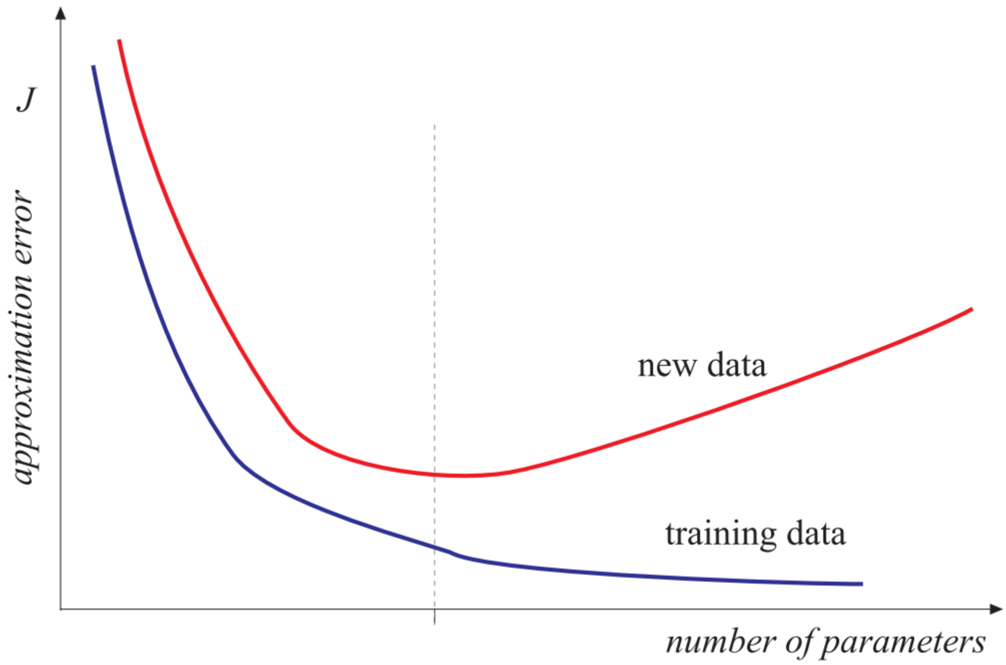
combine both previous ideas and correct for their initial bias

$$\begin{aligned}\mathbf{s} &\leftarrow \beta\mathbf{s} + (1-\beta)\nabla J \\ \mathbf{r} &\leftarrow \gamma\mathbf{r} + (1-\gamma)\nabla J \odot \nabla J \\ \hat{\mathbf{s}} &\leftarrow \tfrac{\mathbf{s}}{1-\beta^t} \\ \hat{\mathbf{r}} &\leftarrow \tfrac{\mathbf{r}}{1-\gamma^t} \\ \mathbf{w} &\leftarrow \mathbf{w} - \alpha\tfrac{\hat{\mathbf{s}}}{\sqrt{10^{-6}+\hat{\mathbf{r}}}}\end{aligned} \tag{25}$$

- Initialize s; r to 0. Choose $\beta, \gamma \in [0; 1)$: Common values: $\beta = 0.9; \gamma = 0.999$
- when time growing, the denominator of third and forth equation is larger, means, smaller change between $\hat{x}$ and x

5. Regularization & Validation

5.1. Overfitting



5.2. Validation & Cross-Validation

True Criterion

$$I = \int_X \|f(\mathbf{x}) - F(\mathbf{x})\| \mathbf{dx} \tag{26}$$

But, Usually cannot be computed as $f(x)$ **is not available**, use available data to **numerically approximate**

Cross-Validation Ways

- Regular Criterion (for two data sets)

$$\mathrm{RC}=\frac{1}{2}\left[\frac{1}{N_A}\sum_{i=1}^{N_A}\left(y^A(i)-\hat{y}_B^A(i)\right)^2+\frac{1}{N_B}\sum_{i=1}^{N_B}\left(y^B(i)-\hat{y}_A^B(i)\right)^2\right] \tag{27}$$

- Means Squared Error

$$\mathrm{MSE}=\frac{1}{N}\sum_{i=1}^{N}(y(i)-\hat{y}(i))^2 \tag{28}$$

- Variance accounted for (VAF)

Is a summary of how much of the variability of the data can be explained by a fitted regression model

$$\mathrm{VAF}=100\%\cdot\left[1-\frac{\mathrm{var}(y-\hat{y})}{\mathrm{var}(y)}\right] \tag{29}$$

> *From: https://blog.csdn.net/qq_36330643/article/details/77452951*
>
> *From: https://baike.baidu.com/item/交叉验证/8543100?fromtitle=Cross validation&fromid=18081946&fr=aladdin*

- 简单交叉验证（simple cross validation）

常识来说，Holdout 验证并非一种交叉验证，因为数据并没有交叉使用。 随机从最初的样本中选出部分，形成交叉验证数据，而剩余的就当做训练数据。 一般来说，少于原本样本三分之一的数据被选做验证数据。

- k-fold cross validation

K折交叉验证，初始采样分割成K个子样本，一个单独的子样本被保留作为验证模型的数据，其他K-1个样本用来训练。**交叉验证重复K次**，每个子样本验证一次，平均K次的结果或者使用其它结合方式，最终得到一个单一估测。这个方法的优势在于，同时重复运用随机产生的子样本进行训练和验证，每次的结果验证一次，10折交叉验证是最常用的

5.3. Test Set

The **validation set** is used to **select the right hyper-parameters,** Use a **separate test set** to verify the hyper-parameters have not been over-fitted to the validation set.

- Structure of the network
- Cost function
- Optimization parameters

5.4. Regularization

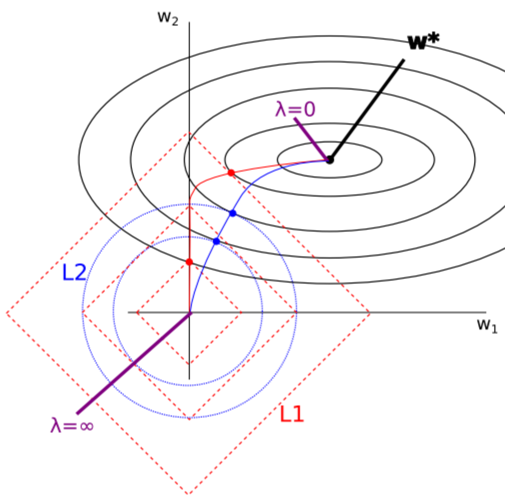
Any strategy that attempts to **improve the test performance**, but not the training performance

Weight Penalty

- Large weights in a neural network are a sign of overfitting.
- A network with large weights has very likely **learned the statistical noise** in the training data. This results in a model that is unstable, and **very sensitive** to changes to the input variables. In turn, the overfit network has **poor performance** when making predictions on new unseen data.

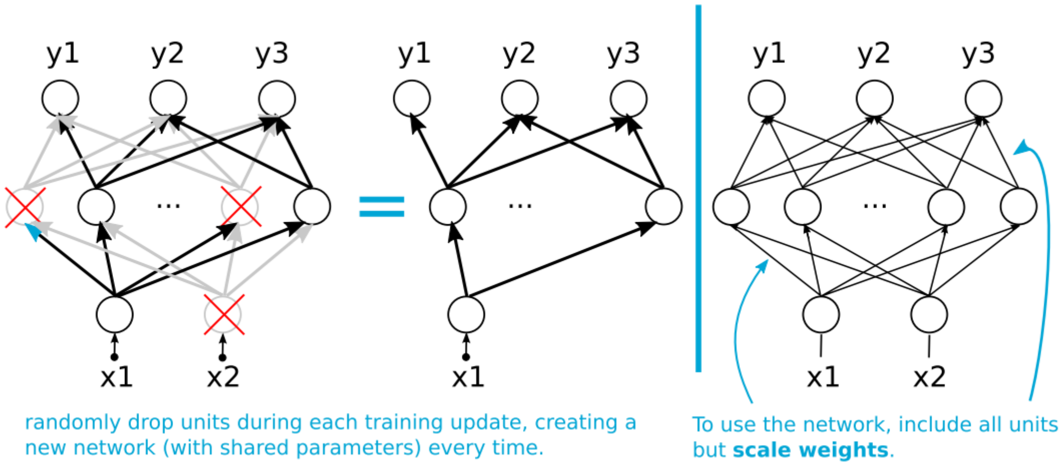
$$J_r(y, t, \mathbf{w}) = J^*(y, t) + \lambda \|\mathbf{w}\|_p^p \tag{30}$$

- p = 1: L^1 : Leads to 0-weights (sparsity, feature selection)
- p = 2: L^2 : Leads to small weights



Dropout

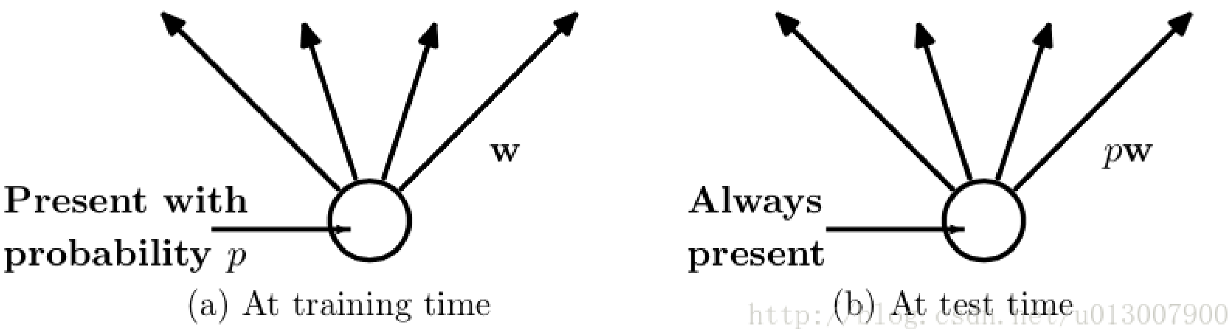
Practical approximation of an automatic ensemble method. During training, **drop out units (neurons) with probability p. During testing use all units, multiply weights by (1 – p).**



> *From: https://blog.csdn.net/u013007900/article/details/78120669/*

第一种理解方式是，在每次训练的时候使用dropout，每个神经元有百分之50的概率被移除，这样可以使得一个神经元的训练不依赖于另外一个神经元，同样也使得特征之间的协同作用被减弱。Hinton认为，过拟合可以通过**阻止某些特征的协同作用来缓解**。

第二种理解方式是，我们可以把dropout当做一种多模型效果平均的方式。对于减少测试集中的错误，我们可以将多个不同神经网络的预测结果取平均，而因为dropout的随机性，我们每次dropout后，网络模型都可以看成是一个不同结构的神经网络，而此时要训练的参数数目却是不变的，这就解脱了训练多个独立的不同神经网络的时耗问题。在测试输出的时候，将输出权重除以二，从而达到类似平均的效果。



Model ensembles

- For k models, where the errors made are zero mean, normally distributed, with variance $v = E[\epsilon_i^2]$, covariance $c = E[\epsilon_i \epsilon_j]$
- The variance of the ensemble is: $\mathbb{E}\left[\left(\frac{1}{k}\sum_i \epsilon_i\right)^2\right] = \frac{1}{k^2}\mathbb{E}\left[\sum_i \left[\epsilon_i^2 + \sum_{j\neq i}\epsilon_i\epsilon_j\right)\right] = \frac{1}{k}v + \frac{k-1}{k}c$
- When the errors are not fully correlated (c < v), the variance will reduce.

Data augmentation

Sometimes existing data **can be transformed to get more data**. Noise can be added to inputs, weights, outputs, Make noise realistic.

- e.g. rotate, noise

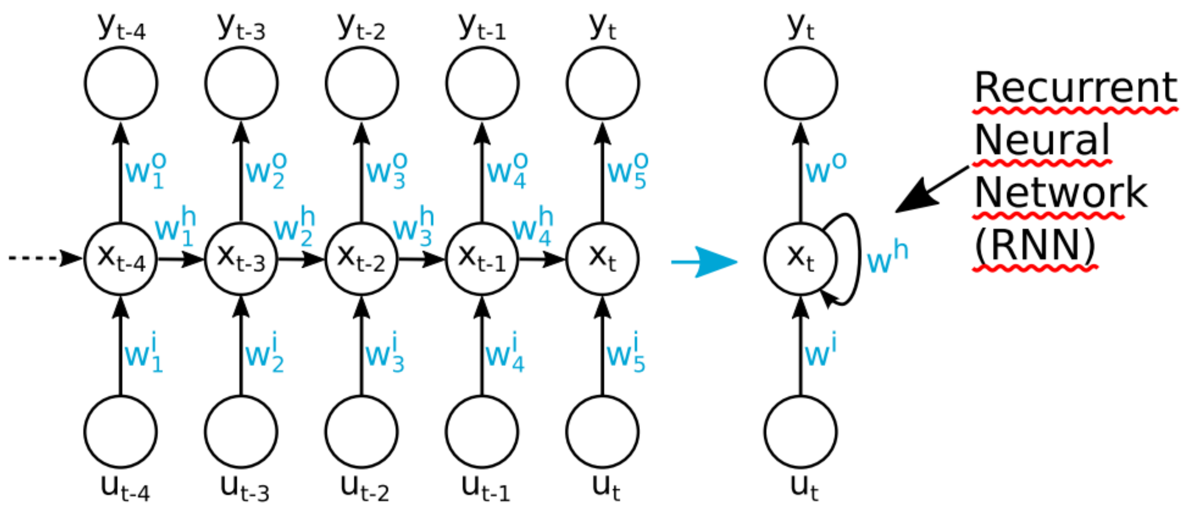
6. Specialized Network Architetures

6.1. Recurrent Neural Networks (RNN)

> *Also Refer to: https://zhuanlan.zhihu.com/p/123211148*

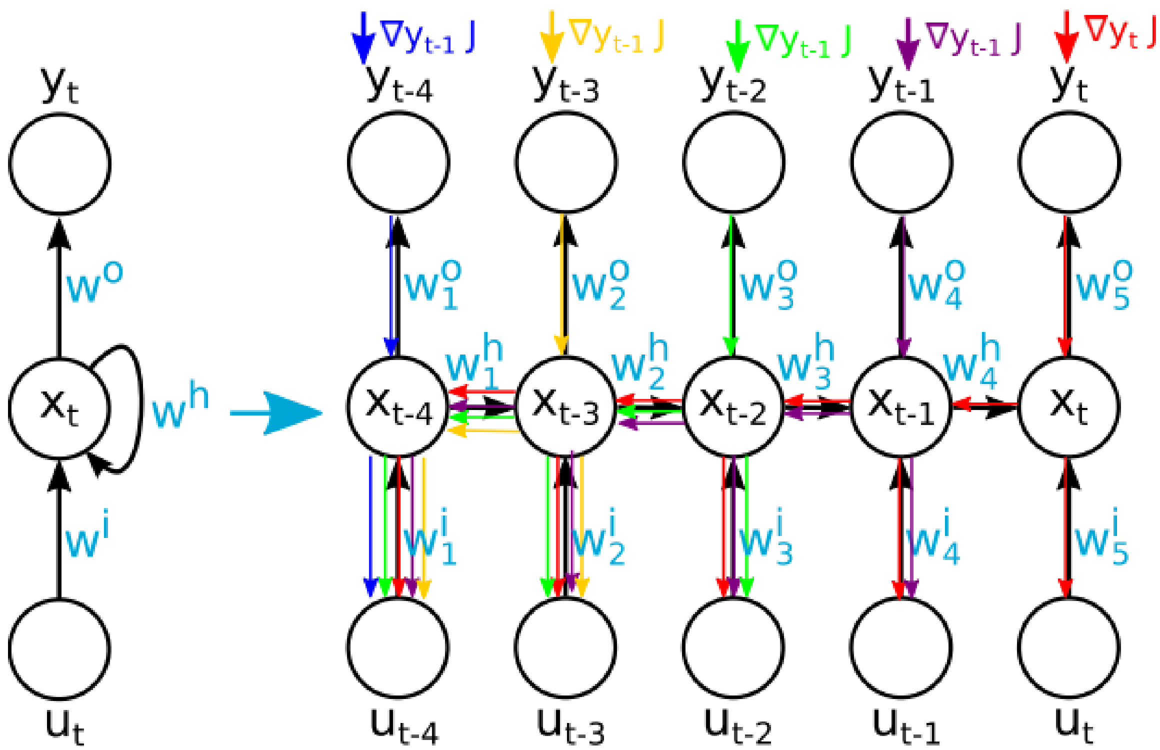
RNN对具有序列特性的数据非常有效，它能挖掘数据中的时序信息以及语义信息，利用了RNN的这种能力，使深度学习模型在解决语音识别、语言模型、机器翻译以及时序分析等NLP领域的问题时有所突破。

> *Example: sequence with time characteristic 举个例子，现在有两句话： 第一句话：I like eating apple！（我喜欢吃苹果！） 第二句话：The Apple is a great company！（苹果真是一家很棒的公司！）*



RNN training: Back Propagation Through Time (BPTT)

1. Make n copies of the network, calculate $y_1, \cdots, y_n$
2. Start at time step n and propagate the loss backwards through the unrolled networks
3. Update the weights based on the average gradient of the network copies $\nabla_w J = \frac{1}{n}\sum_{i=1}^{n} \nabla_{w_i} J$



Exploding/vanishing gradients problem

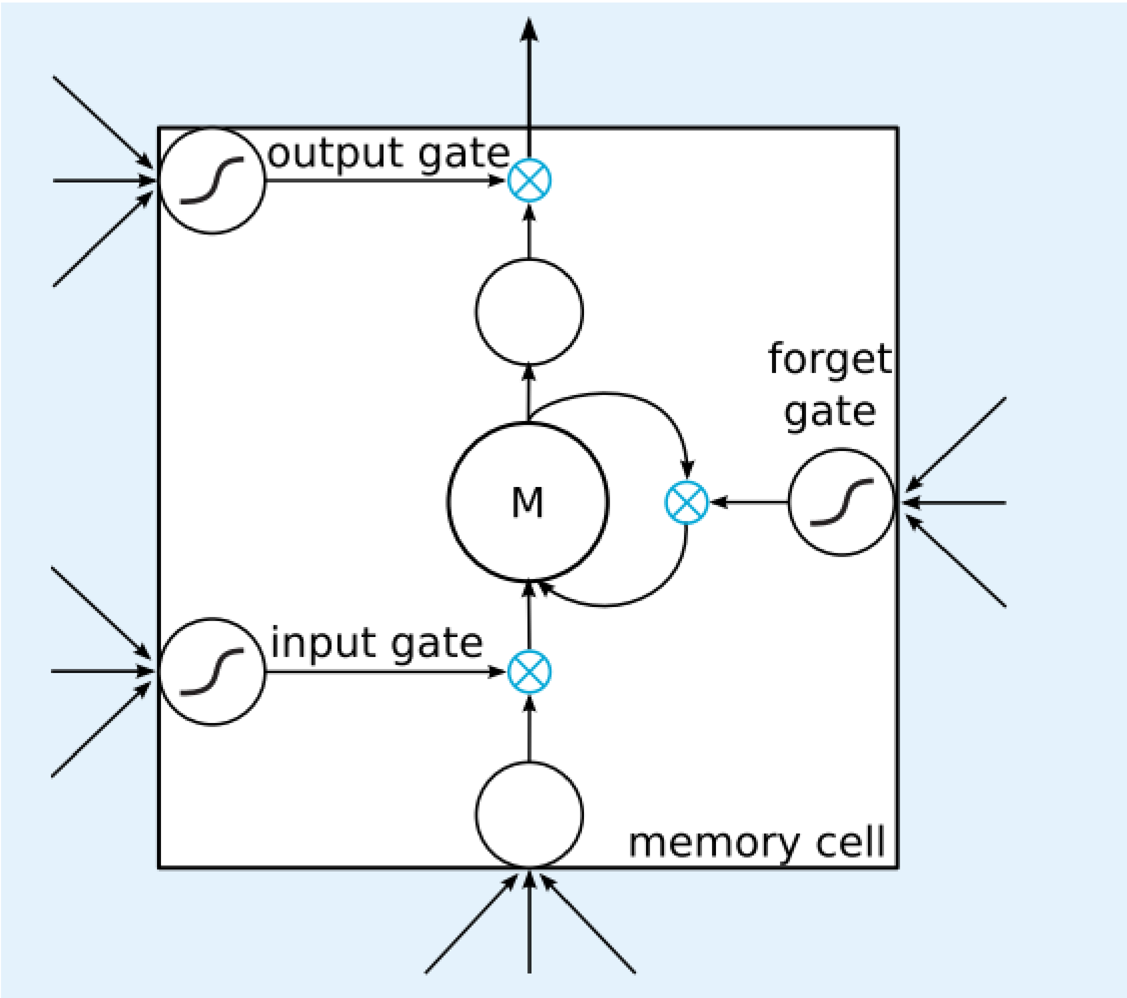
Scalar case with no input: $x_n = w^n \cdot x_0$, For $w < 1; x_n \to 0$, for $w > 1; x_n \to \infty$.

This makes it hard to learn long term dependencies

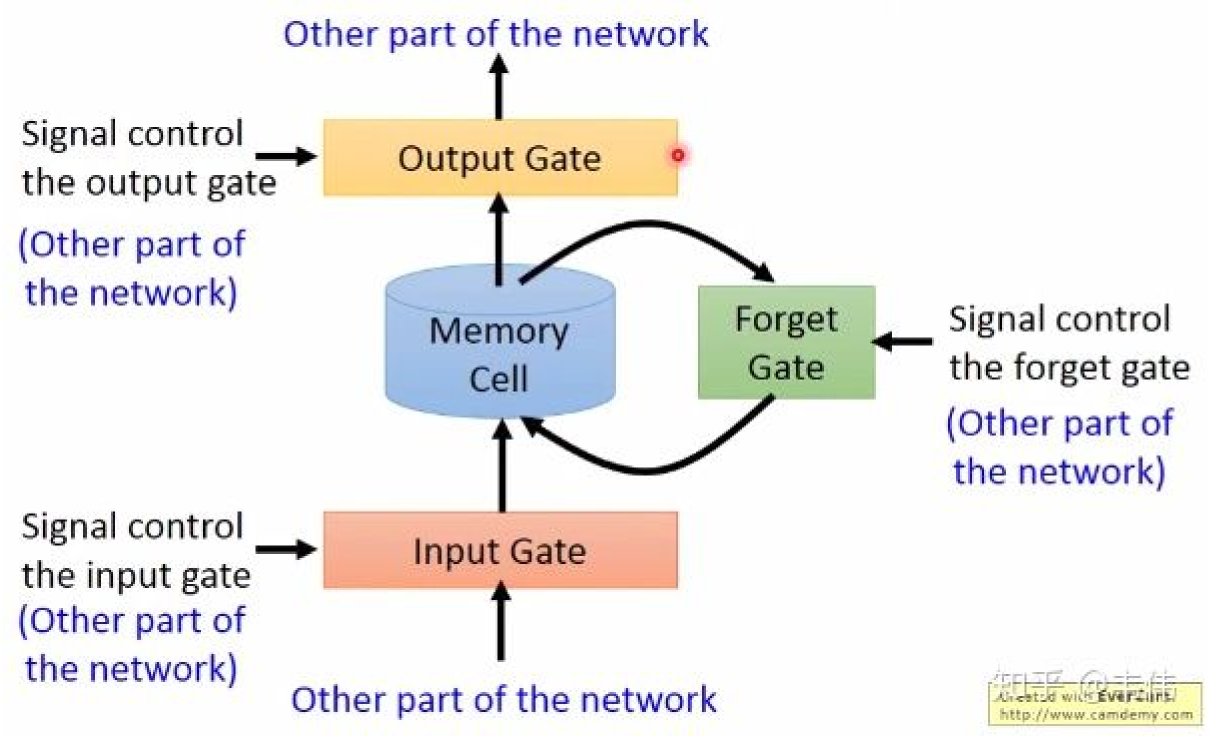
6.2. LSTM

> *Also Refer to: https://zhuanlan.zhihu.com/p/123211148*

LSTM不一样，它会**选择性的存储信息**，它有**门控装置**，它可以尽情的选择



this is a structure grarph of a **single memory cell**



- Input Gate：中文是输入门，在每一时刻从输入层输入的信息会首先经过输入门，输入门的开关会决定这一时刻是否会有信息输入到Memory Cell。
- Output Gate：中文是输出门，每一时刻是否有信息从Memory Cell输出取决于这一道门。
- Forget Gate：中文是遗忘门，每一时刻Memory Cell里的值都会经历一个是否被遗忘的过程，就是由该门控制的，如果打卡，那么将会把Memory Cell里的值清除，也就是遗忘掉。

按照上图的顺序，信息在传递的顺序，是这样的：

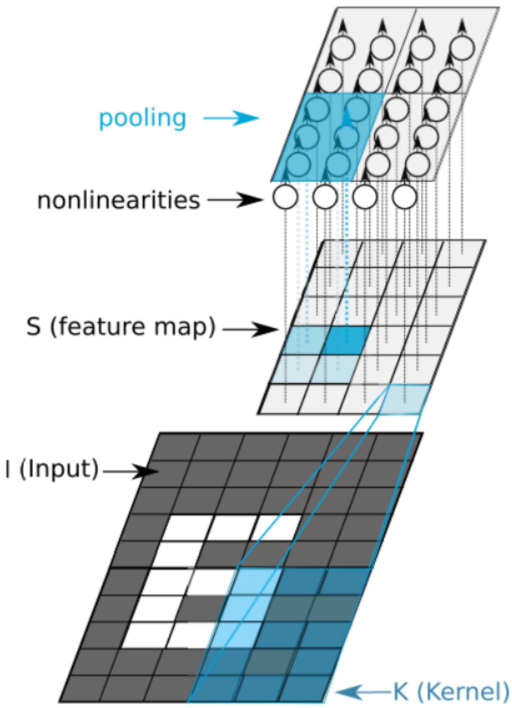
先经过输入门，看是否有信息输入，再判断遗忘门是否选择遗忘Memory Cell里的信息，最后再经过输出门，判断是否将这一时刻的信息进行输出。

6.3. Convolutional Neural Networks (CNN)

> *Also refer to: https://zhuanlan.zhihu.com/p/27908027*

Convolution & Nonlinear Detector

- Step 1: **Convolution**:
  $S(i,j) = (I * K)(i,j) = \sum_m \sum_n I(m,n)K(i-m, j-n)$
- Step 2: **Detector stage:** nonlinearities on top of the feature map
- Step 3 (*optional*) **Pooling:** Take some function (e.g. max) of an area

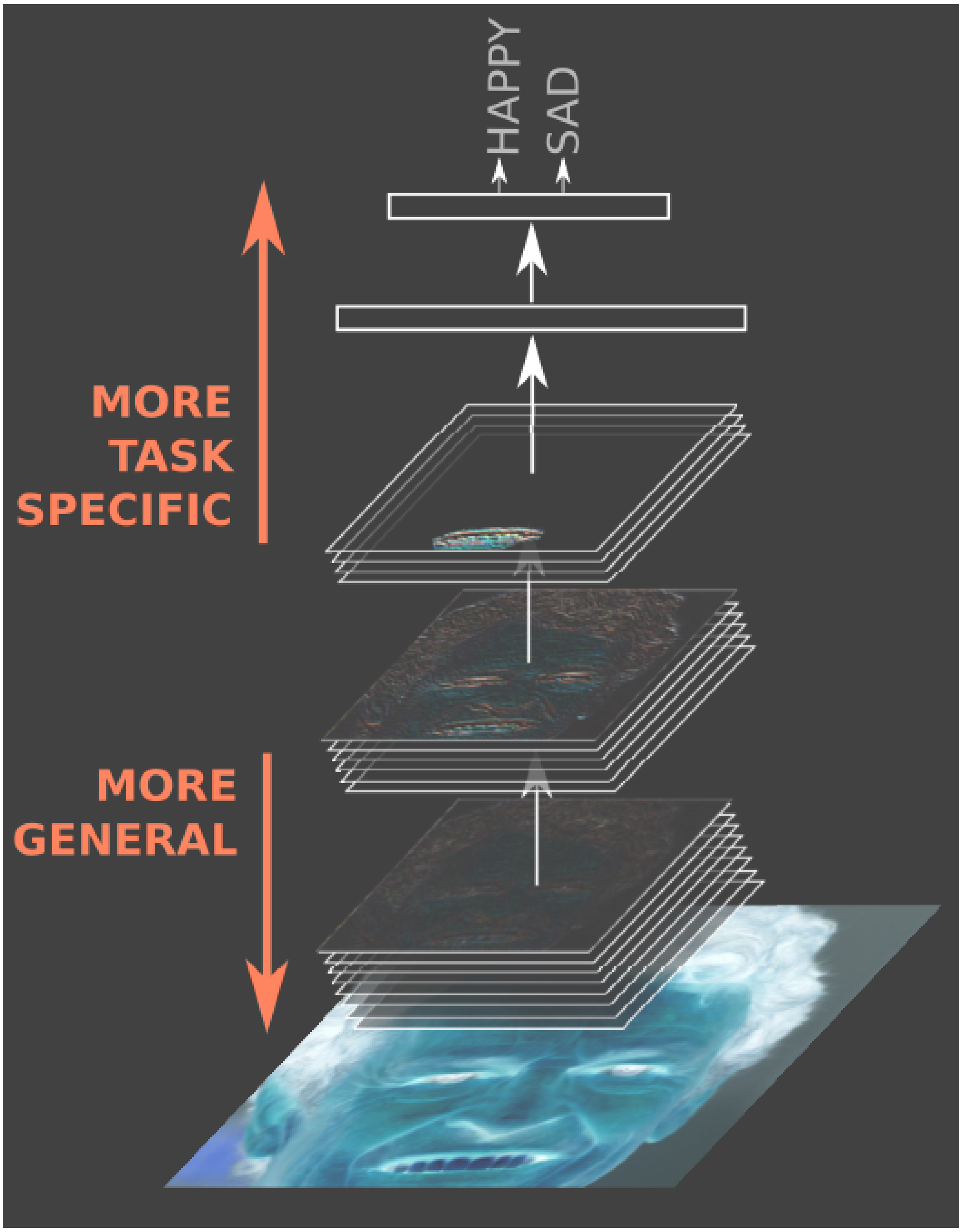


7. Unsupervised Learning

7.1. Additional Training Criteria

Inputs x are often much easier to obtain than targets t.

- For deep networks, many of the earlier layers perform very **general functions** (e.g. edge detection).
- These layers can be **trained on different tasks for which there is data.**

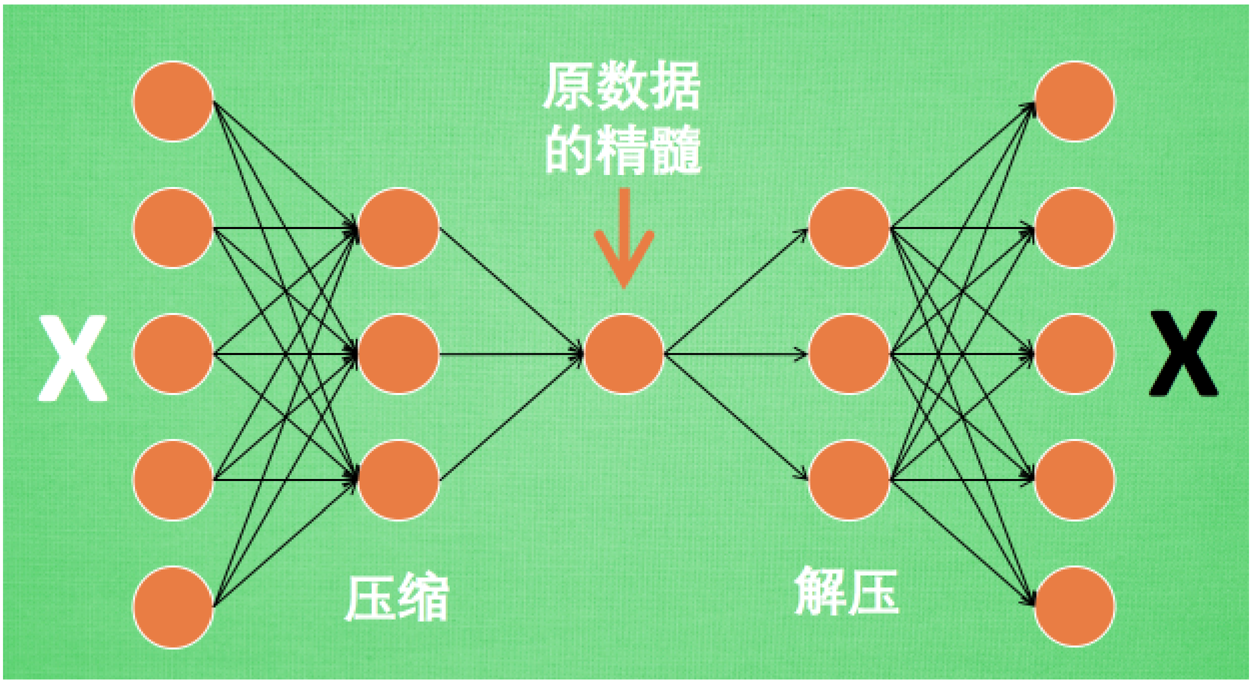


7.2. Auto Encoders

> *Also From: https://zhuanlan.zhihu.com/p/24813602*

Unsupervised Learning (UL): find some structure in input data without extra information

Auto Encoders (AE) do this by reconstructing their input



- 有时神经网络要接受大量的输入信息, 比如输入信息是高清图片时, 输入信息量可能达到上千万, 让**神经网络直接从上千万个信息源中学习是一件很吃力的工作.**
- 通过**压缩**, 提取出原图片中的**最具代表性的信息**, 缩减输入信息量, 再把缩减过后的信息放进神经网络学习. 这样学习起来就简单轻松了.
- **自编码**就能在这时发挥作用. 通过将原数据白色的X 压缩, 解压 成黑色的X, 然后通过**对比黑白 X ,求出预测误差, 进行反向传递, 逐步提升自编码的准确性.** 训练好的自编码中间这一部分就是能总结原数据的精髓.
- 从头到尾, 我们**只用到了输入数据 X, 并没有用到 X 对应的数据标签**, 所以也可以说自编码是一种非监督学习. 到了真正使用自编码的时候. 通常只会用到自编码前半部分.
- 换句话说, 自编码 可以像 主成分分析(PCA) 一样 给特征属性降维.

ENCODER

compresses the input, useful feature hierarchy for later supervised tasks.

Decoder

decompresses the input, can be used as a generative model.

7.3. Auxiliary training objectives

Auxiliary training objectives can be added

- Because they are easier and allow the optimization to make faster initial progress.

- To force the network to keep more generic features, as a regularization technique.