

Neural Networks

Tobias Scheffer

Overview

- Neural information processing.
- Deep learning.
- Feed-forward networks.
- Training feed-forward networks: back propagation.
- Parallel inference on GPUs.
- Convolutional neural networks,
- Recurrent neural networks.

Learning Problems can be Impossible without the Right Features



→ motorcycle

88	82	84	88	85	83	80	93	102	88	82	84	88	85	83	80	93	102
88	80	78	80	80	78	73	94	100	88	80	78	80	80	78	73	94	100
85	79	80	78	77	74	65	91	99	85	79	80	78	77	74	65	91	99
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22	26	22	28	40	65	64	59	34	22	26	22	28	40	65	64	59	34
24	28	24	30	37	60	58	56	66	24	28	24	30	37	60	58	56	66
21	22	23	27	38	60	67	65	67	21	22	23	27	38	60	67	65	67
23	22	22	25	38	59	64	67	66	23	22	22	25	38	59	64	67	66

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→ motorcycle

Learning Problems can be Impossible without the Right Features

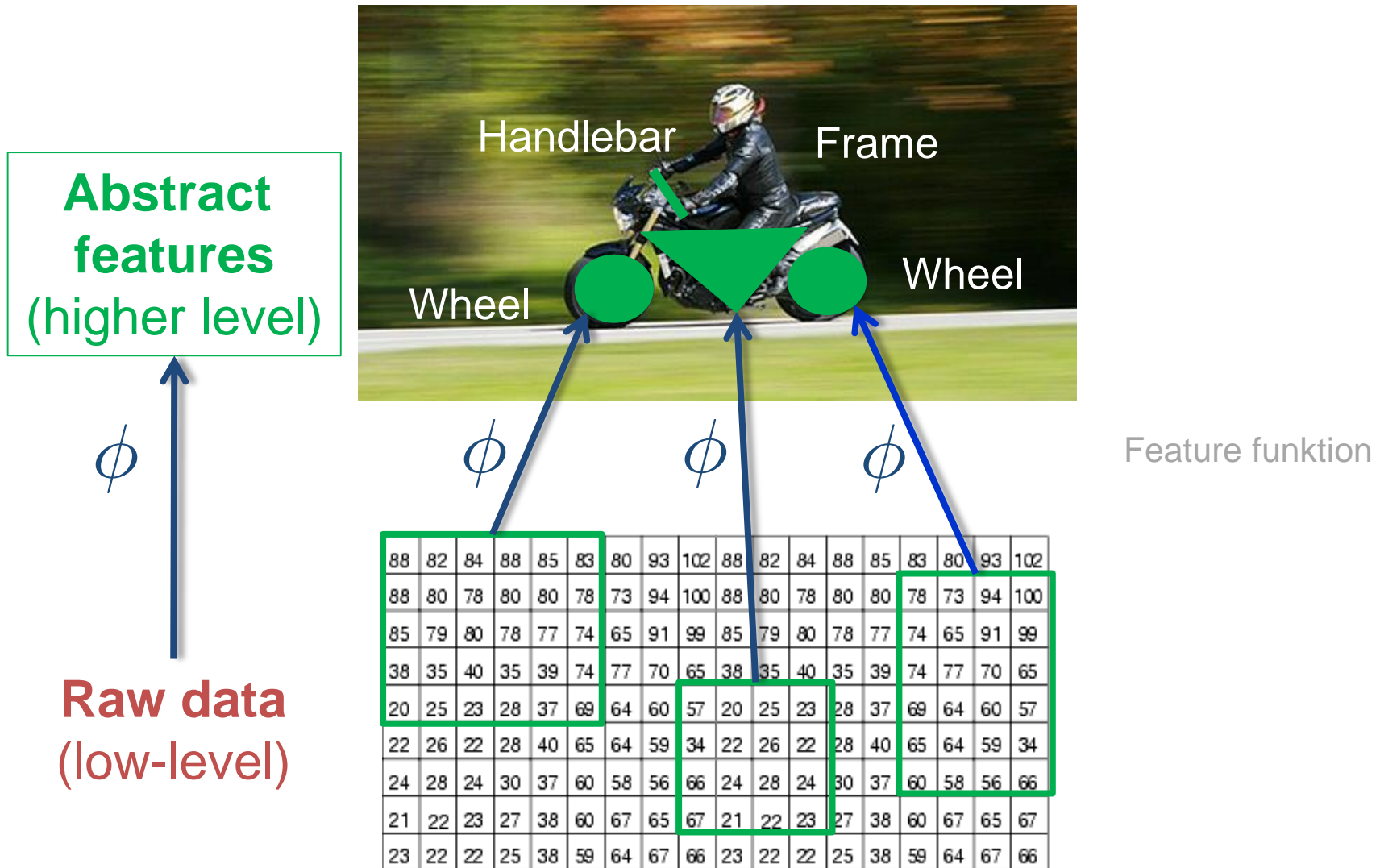


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Learning Problems can be Impossible without the Right Features



Learning Problems can be Impossible without the Right Features

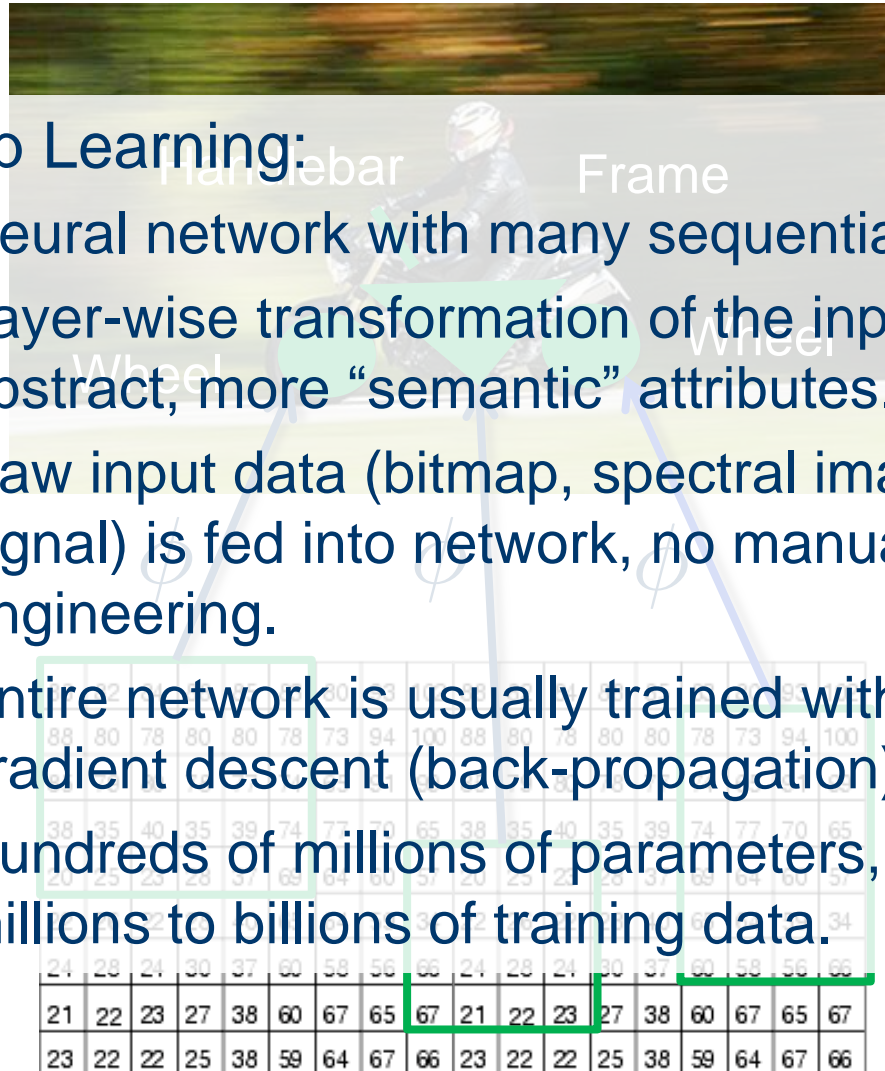
■ Deep Learning:

Abstract features
(higher level)

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Raw data
(low-level)

- ◆ Neural network with many sequential layers.
- ◆ Layer-wise transformation of the input into more abstract, more “semantic” attributes.
- ◆ Raw input data (bitmap, spectral image of audio signal) is fed into network, no manual feature engineering.
- ◆ Entire network is usually trained with stochastic gradient descent (back-propagation).
- ◆ Hundreds of millions of parameters, hundreds of millions to billions of training data.

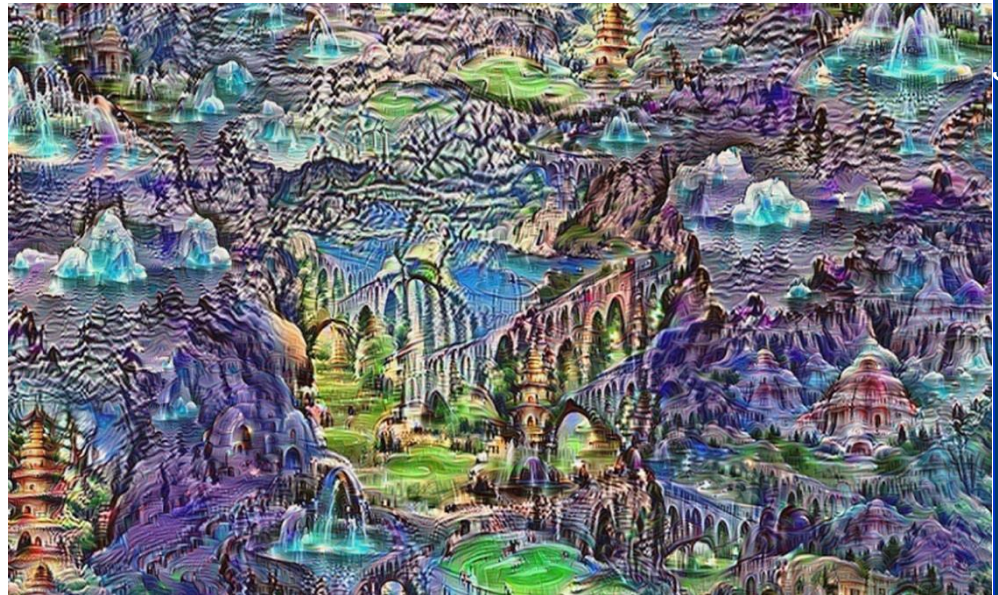


Neural Networks

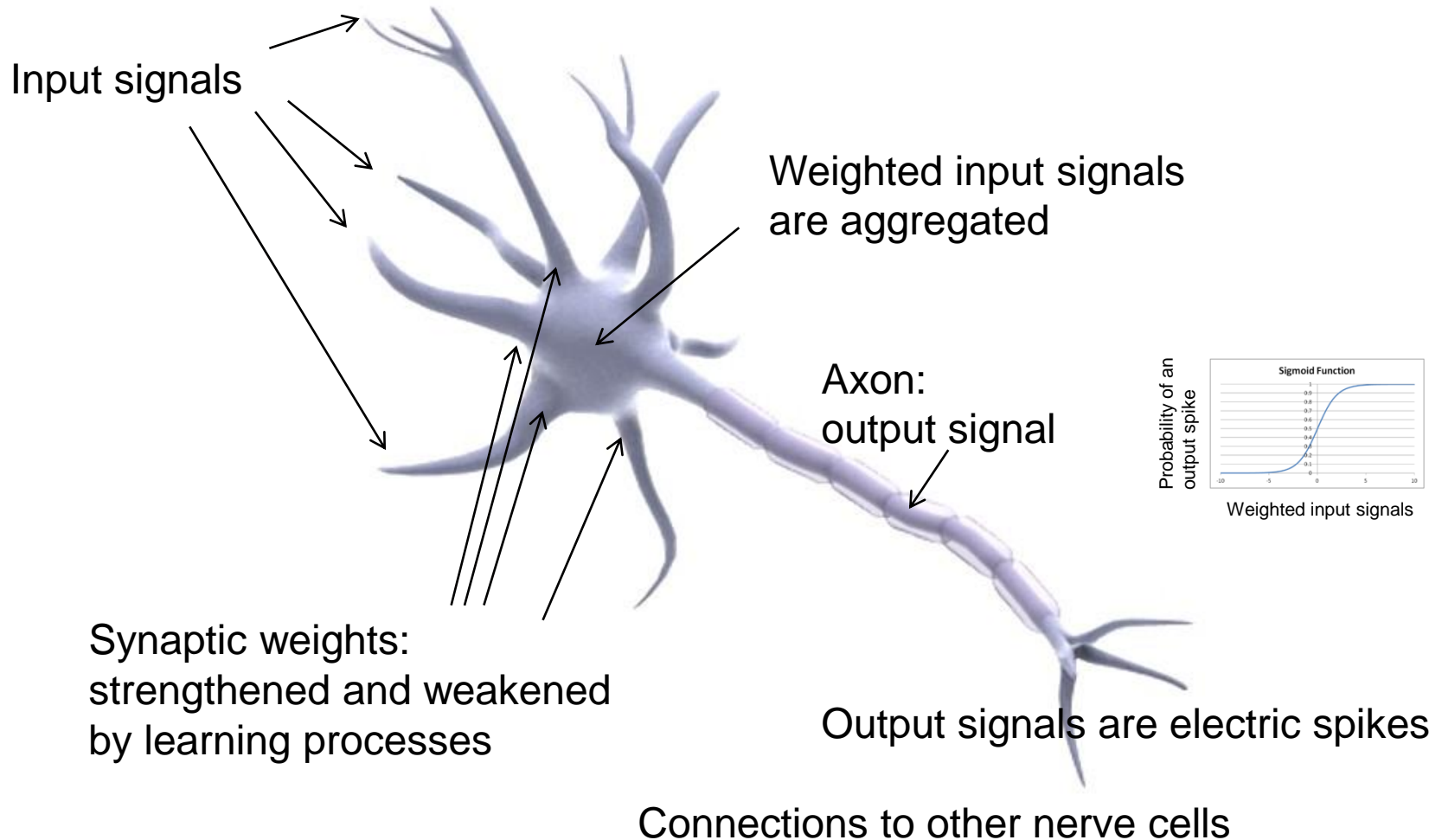
- Model of neural information processing
- Waves of popularity
 - ◆ ↑ Perceptron: Rosenblatt, 1960.
 - ◆ ↓ Perceptron only linear classifier (Minsky, Papert, 69).
 - ◆ ↑ Multilayer perceptrons (90s).
 - ◆ ↓ Popularity of SVMs (late 90s).
 - ◆ ↑ Deep learning (late 2000s).
 - ◆ Now state of the art for Speech Recognition image classification, face recognition and other problems.

Deep Learning Records

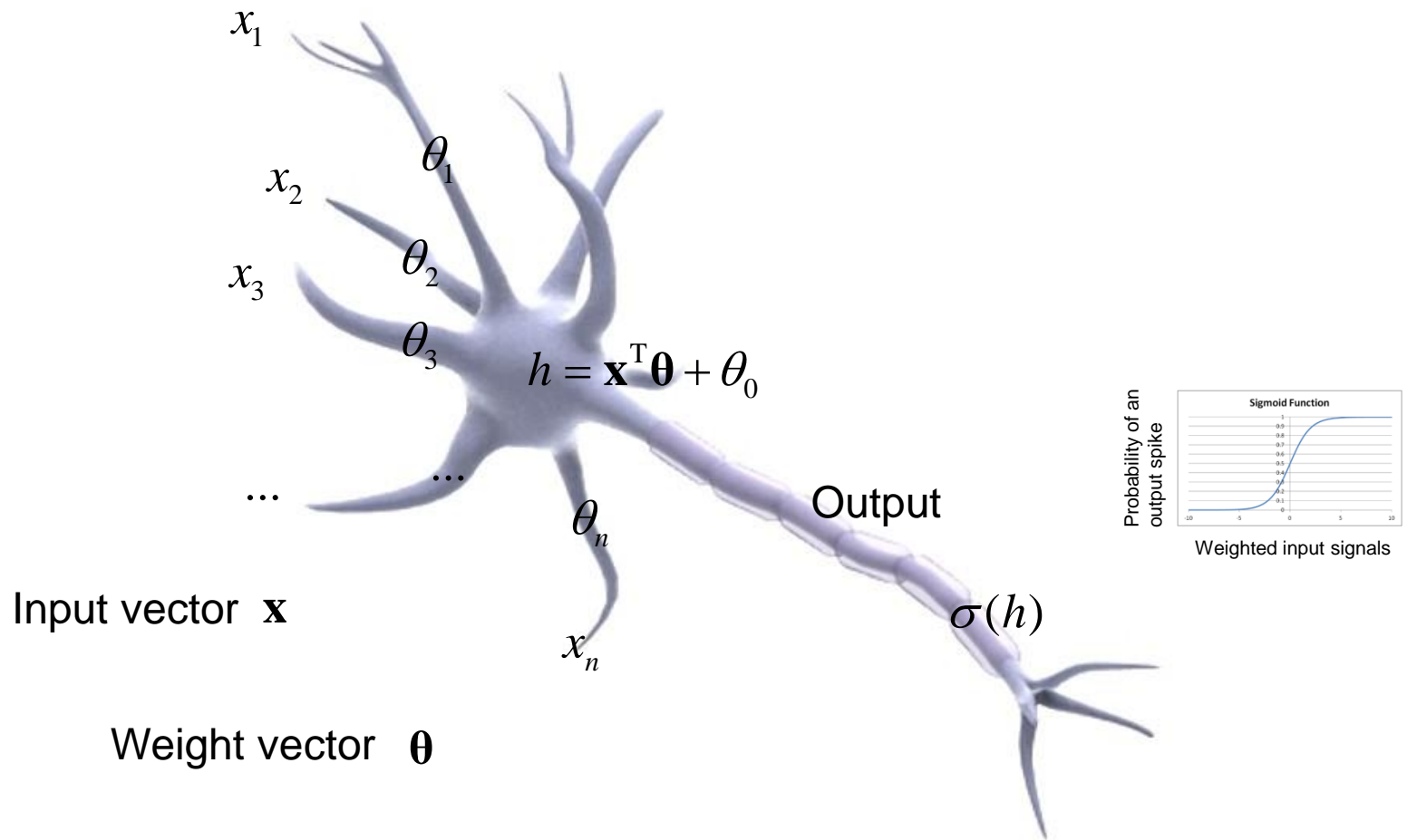
- Neural networks tend to be best-performing models whenever enough training data are available.
 - ◆ Object classification (CIFAR/NORB/PASCAL VOC-Benchmarks)
 - ◆ Video classification (various benchmarks)
 - ◆ Sentiment analysis (MR Benchmark)
 - ◆ Pedestrian detection
 - ◆ Face recognition
 - ◆ Speech recognition
 - ◆ Go (AlphaGo)



Neural Information Processing



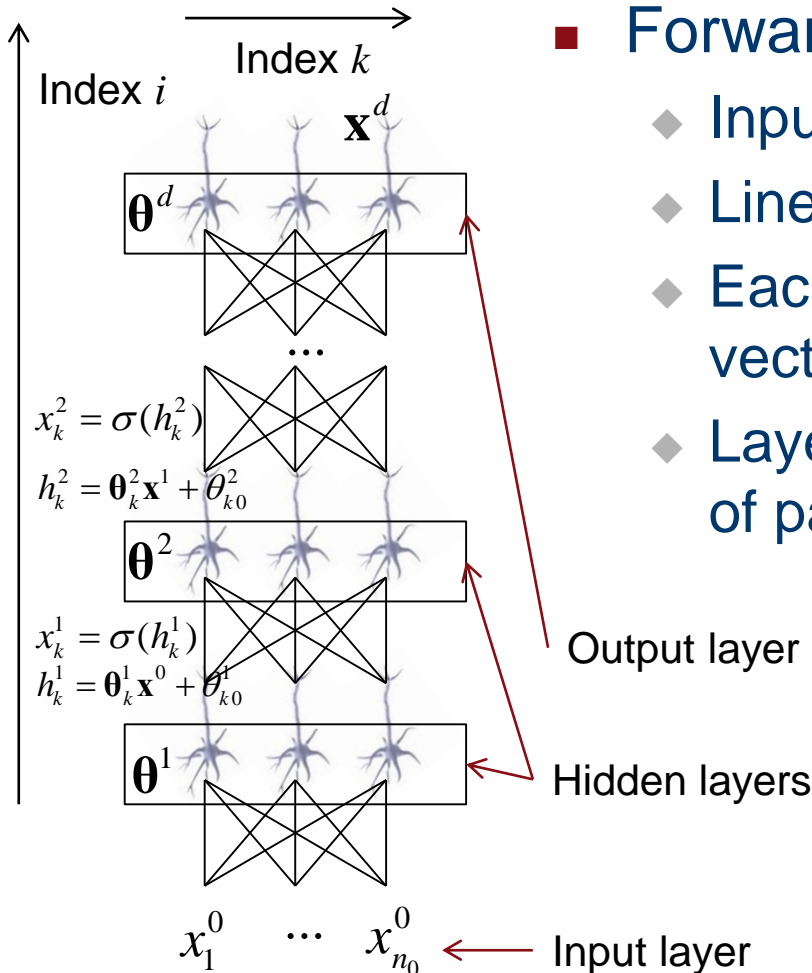
Neural Information Processing: Model



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- Training feed-forward networks: back propagation.
- Parallel inference on GPUs.
- Outlook:
 - ◆ Convolutional neural networks,
 - ◆ Recurrent neural networks.

Feed Forward Networks

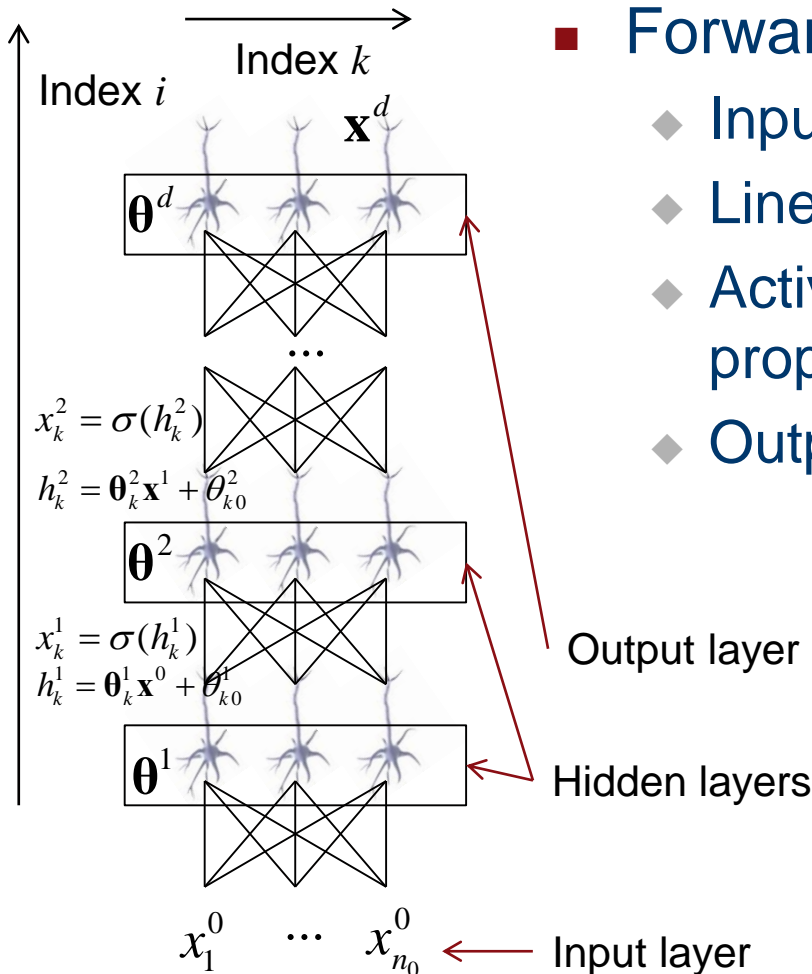


Forward propagation:

- ◆ Input vector \mathbf{x}^0
- ◆ Linear model: $h_k^i = \boldsymbol{\theta}_k^i \mathbf{x}^{i-1} + \theta_{k0}^i$
- ◆ Each unit has parameter vector $\boldsymbol{\theta}_k^i = (\theta_{k1}^i \dots \theta_{kn_{i-1}}^i)$

- ◆ Layer i has matrix of parameters $\boldsymbol{\theta}^i = \begin{pmatrix} \boldsymbol{\theta}_1^i \\ \vdots \\ \boldsymbol{\theta}_{n_i}^i \end{pmatrix} = \begin{pmatrix} \theta_{11}^i & \dots & \theta_{1n_{i-1}}^i \\ \vdots & & \vdots \\ \theta_{n_i1}^i & \dots & \theta_{n_i n_{i-1}}^i \end{pmatrix}$

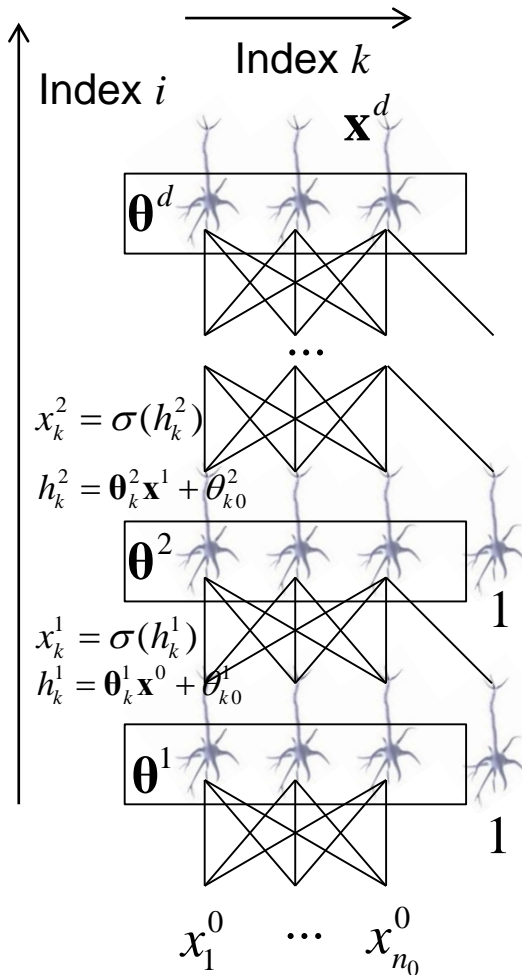
Feed Forward Networks



■ Forward propagation:

- ◆ Input vector \mathbf{x}^0
- ◆ Linear model: $h_k^i = \theta_k^i \mathbf{x}^{i-1} + \theta_{k0}^i$
- ◆ Activation function and propagation: $\mathbf{x}^i = \sigma(\mathbf{h}^i)$
- ◆ Output vector \mathbf{x}^d

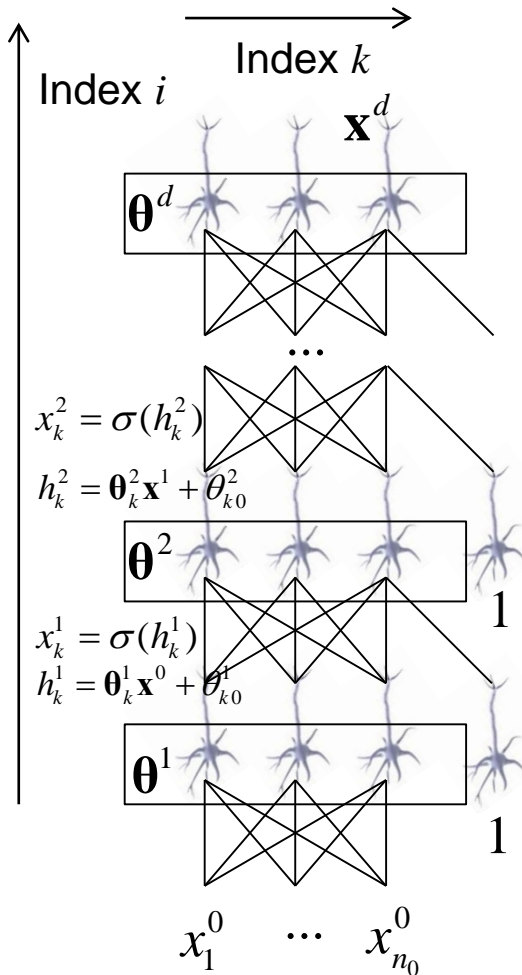
Feed Forward Networks



■ Bias unit

- ◆ Linear model $h_k^i = \theta_k^i \mathbf{x}^{i-1} + \theta_{k0}^i$
- ◆ Constant element θ_{k0}^i is replaced by additional unit with constant output 1: $h_k^i = \theta_k^i \mathbf{x}_{[1..n_k+1]}^{i-1}$

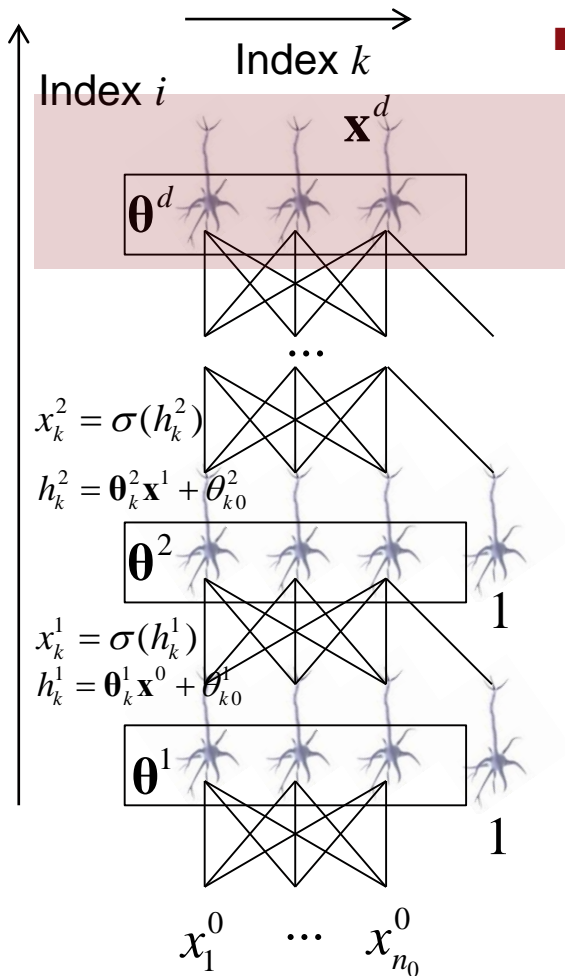
Feed Forward Networks



■ Forward propagation per layer in matrix notation:

- ◆ Linear model: $\mathbf{h}^i = \boldsymbol{\theta}^i \mathbf{x}^{i-1}$
- ◆ Activation function: $\mathbf{x}^i = \sigma(\mathbf{h}^i)$

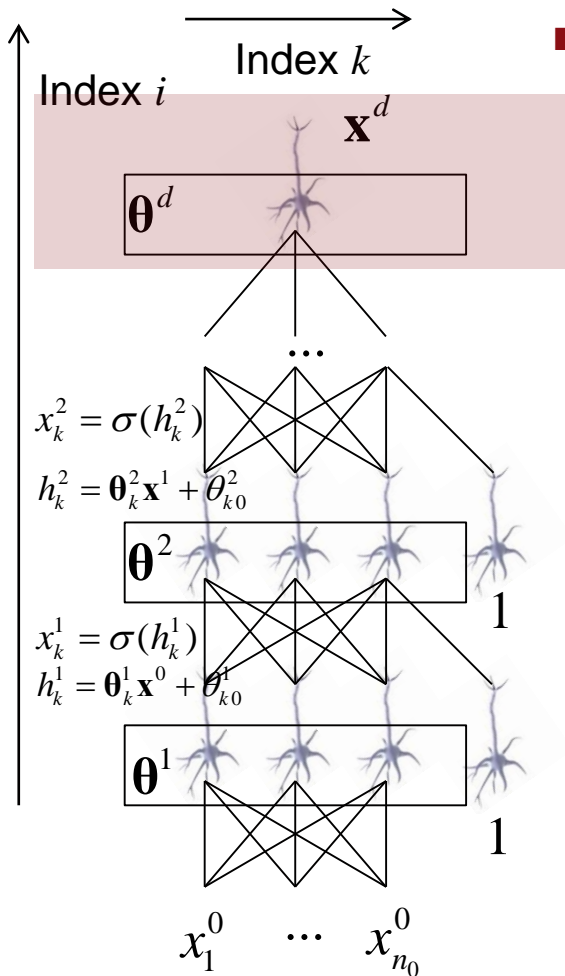
Classification: Softmax Layer



- One output unit per class:

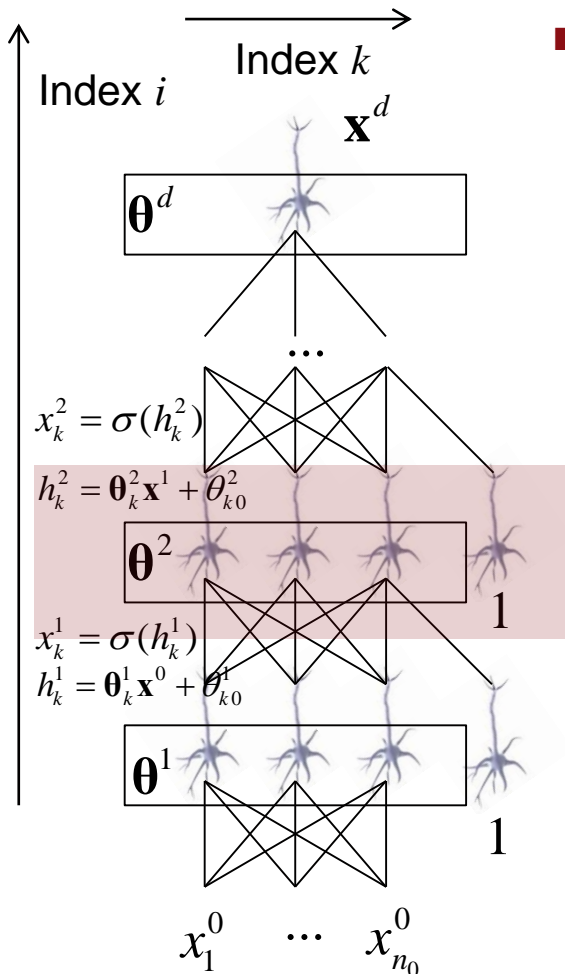
- ◆ $x_k^d = \sigma_{sm}(h_k^d) = \frac{e^{h_k^d}}{\sum_{k'} e^{h_{k'}^d}}$
- ◆ x_k^d : predicted probability for class k .

Regression: Linear Activation

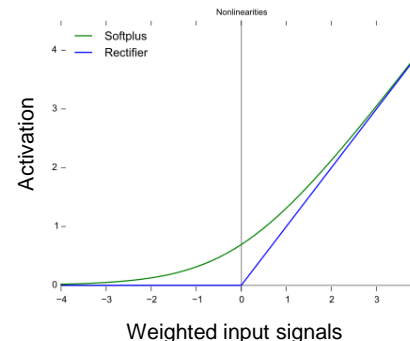


- Linear:
 - ◆ $x^d = h^d$.
 - ◆ Output unbounded.

Internal Units: Rectified Linear Units



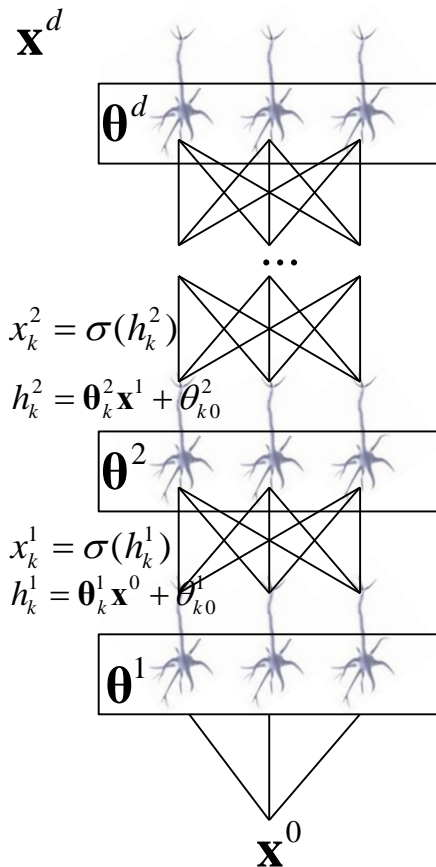
- For internal unit (i, k) :
 - ◆ $x_k^i = \sigma_{ReLU}(h_k^i) = \max(0, h_k^i)$
 - ◆ Leads to sparse activations and prevents the gradient from vanishing for deep networks.



Overview

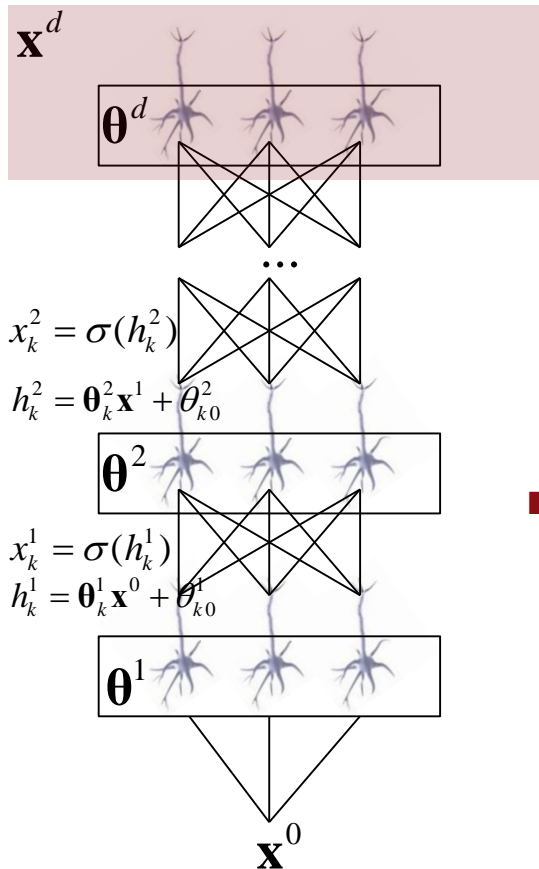
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Feed Forward Networks: Learning



- Stochastic gradient descent
- Loss function $\hat{R}(\theta) = \frac{1}{2m} \sum_{j=1}^m \ell(\mathbf{y}_j, \mathbf{x}^d)$
- Gradient descent:
 - ◆ $\theta' = \theta - \alpha \nabla \hat{R}(\theta) = \theta - \alpha \frac{\partial}{\partial \theta} \hat{R}(\theta)$
 - $$= \theta - \frac{\alpha}{2m} \sum_{j=1}^m \frac{\partial}{\partial \theta} \ell(\mathbf{y}_j, \mathbf{x}^d)$$
- Stochastic gradient for instance \mathbf{x}_j :
 - ◆ $\theta' = \theta - \alpha \nabla_{\mathbf{x}_j} \hat{R}(\theta)$
 - $$= \theta - \alpha \frac{\partial}{\partial \theta} \ell(\mathbf{y}_j, \mathbf{x}^d)$$

Learning: Back Propagation



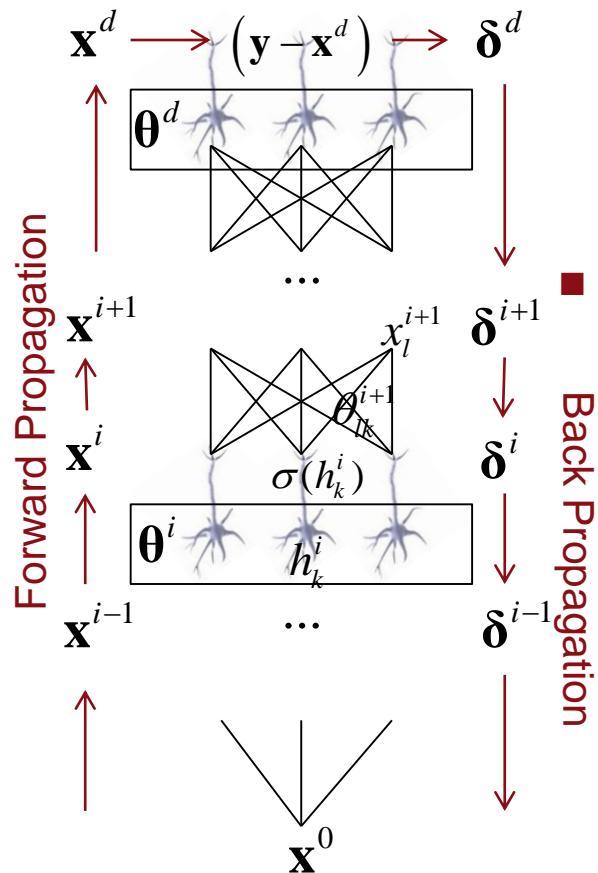
- Stochastic gradient for output units for instance \mathbf{x}_j :

$$\begin{aligned} \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \theta_k^d} &= \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \mathbf{x}^d} \frac{\partial \mathbf{x}^d}{\partial h_k^d} \frac{\partial h_k^d}{\partial \theta_k^d} \\ &= \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \mathbf{x}^d} \frac{\partial \sigma(h_k^d)}{\partial h_k^d} \mathbf{x}^{d-1} = \delta_k^d \mathbf{x}^{d-1} \end{aligned}$$

- With

$$\delta_k^d = \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \mathbf{x}^d} \frac{\partial \sigma(h_k^d)}{\partial h_k^d}$$

Learning: Back Propagation



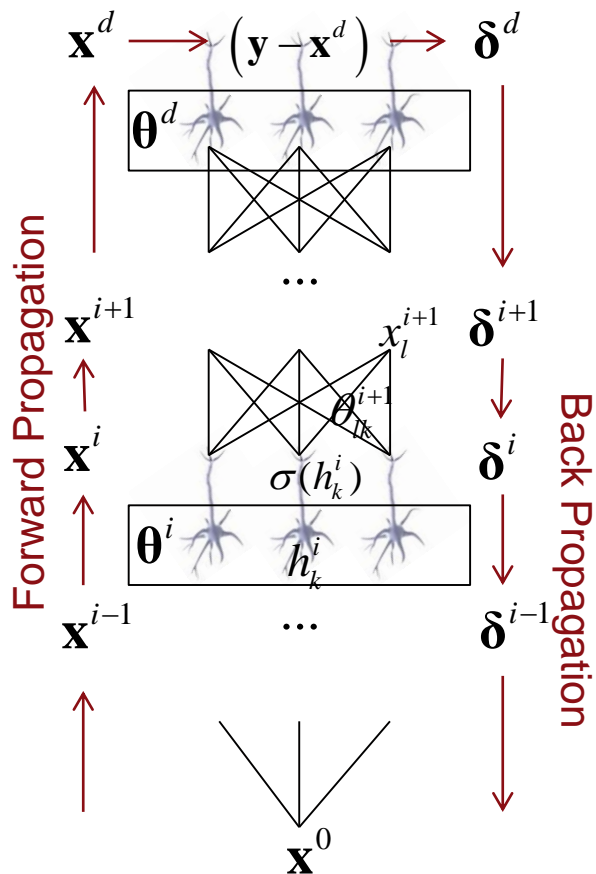
- Stochastic gradient for hidden units for instance \mathbf{x}_j :

$$\frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \theta_k^i} = \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial h_k^i} \frac{\partial h_k^i}{\partial \theta_k^i} = \delta_k^i \mathbf{x}^{i-1}$$

- With

$$\begin{aligned} \delta_k^i &= \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial h_k^i} \\ &= \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial (\mathbf{x}_1^{i+1}, \dots, \mathbf{x}_{n_{i+1}}^{i+1})} \frac{\partial (\mathbf{x}_1^{i+1}, \dots, \mathbf{x}_{n_{i+1}}^{i+1})}{\partial h_k^i} \\ &= \sum_{l=1}^{n_{i+1}} \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial h_l^{i+1}} \frac{\partial h_l^{i+1}}{\partial x_k^i} \frac{\partial x_k^i}{\partial h_k^i} \\ &= \sum_{l=1}^{n_{i+1}} \delta_l^{i+1} \theta_{lk}^{i+1} \frac{\partial \sigma(h_k^i)}{\partial h_k^i} \end{aligned}$$

Learning: Back Propagation



- Derivative of the loss function for classification.
- Softmax activation function:

$$\diamond x_k^d = \sigma_{sm}(h_k^d) = \frac{e^{h_k^d}}{\sum_{k'} e^{h_{k'}^d}}$$

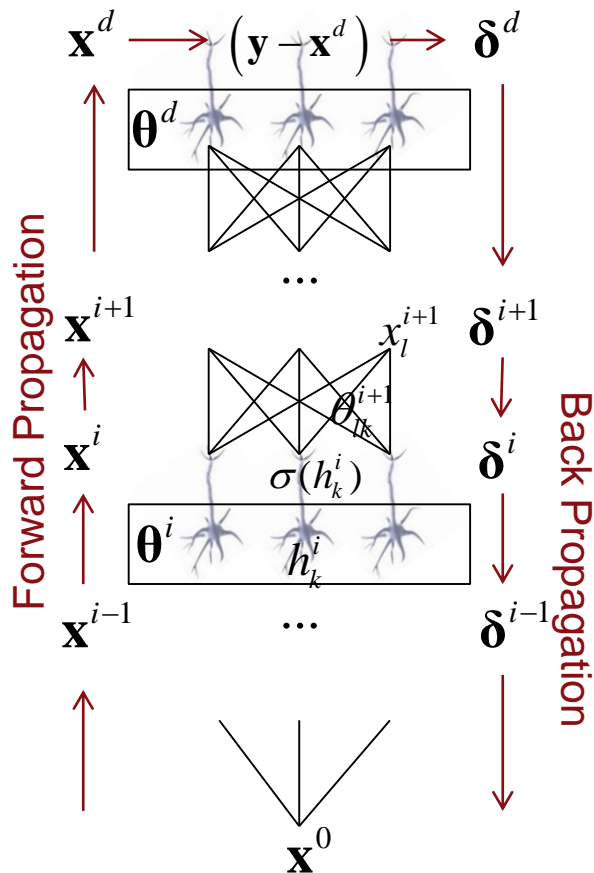
$$\diamond \frac{\partial \sigma_{sm}(h_k^d)}{\partial h_k^d} = \sigma_{sm}(h_k^d)(1 - \sigma_{sm}(h_k^d))$$

- Cost function (log loss or cross entropy):

$$\diamond \ell(\mathbf{y}, \mathbf{x}^d) = -\sum_k y_k \log x_k^d$$

$$\diamond \frac{\partial \ell(\mathbf{y}, \mathbf{x}^d)}{\partial h_k^d} = x_k^d - y_k$$

Learning: Back Propagation



- Derivative of the loss function for regression.

- Linear activation function:

- ◆ $x_k^d = \sigma_s(h_k^d) = h_k^d$

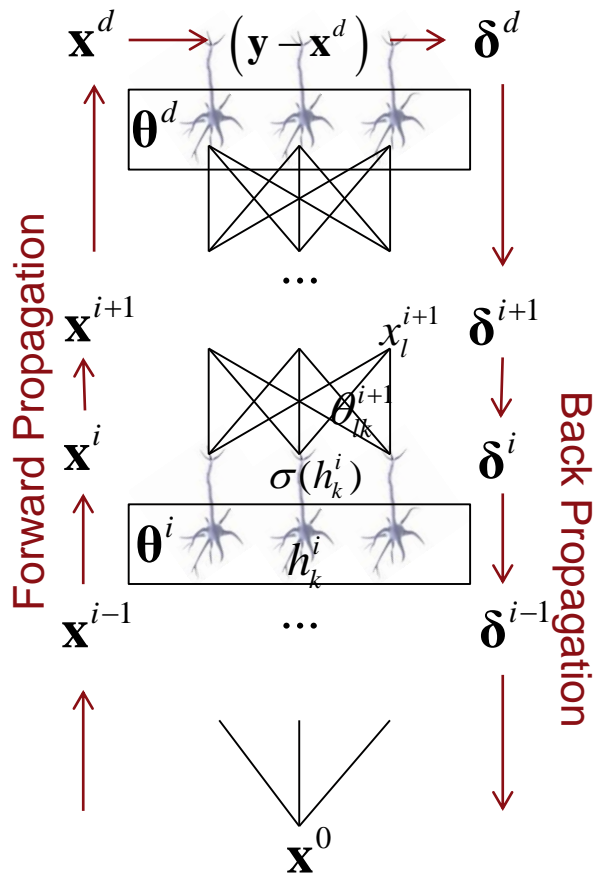
- ◆ $\frac{\partial \sigma_s(h_k^d)}{\partial h_k^d} = 1$

- Cost function:

- ◆ $\ell(\mathbf{y}, \mathbf{x}^d) = \frac{1}{2} \sum_k (x_k^d - y_k)^2$

- ◆ $\frac{\partial \ell(\mathbf{y}, \mathbf{x}^d)}{\partial x_k^d} = x_k^d - y_k$

Learning: Back Propagation



- Derivative of the activation function for internal units.
- Rectified linear activation function:
 - ◆ $x_k^i = \sigma_{ReLU}(h_k^i) = \max(0, h_k^i)$
 - ◆ $\frac{\partial \sigma_{ReLU}(h_k^i)}{\partial h_k^i} = \begin{cases} 1 & \text{if } h_k^i > 0 \\ 0 & \text{otherwise} \end{cases}$

Back Propagation: Algorithm

- Iterate over training instances (\mathbf{x}, \mathbf{y}) :

- ◆ Forward propagation: for $i=0\dots d$:

- ★ For $k=1\dots n_i$: $h_k^i = \boldsymbol{\theta}_k^i \mathbf{x}^{i-1} + \theta_{k0}^i$

- ★ $\mathbf{x}^i = \sigma(\mathbf{h}^i)$

- ◆ Back propagation:

- ★ For $k=1\dots n_i$: $\delta_k^d = \frac{\partial}{\partial h_k^d} \sigma(h_k^d) \frac{\partial}{\partial x_k^d} \ell(y_k, x_k^d)$

$$\boldsymbol{\theta}_k^{d'} = \boldsymbol{\theta}_k^d - \alpha \delta_k^d \mathbf{x}^{d-1}$$

- ★ For $i=d-1\dots 1$:

- For $k=1\dots n_i$: $\delta_k^i = \sigma'(h_k^i) \sum_l \delta_l^{i+1} \theta_{lk}^{i+1}$

$$\boldsymbol{\theta}_k^{i'} = \boldsymbol{\theta}_k^i - \alpha \delta_k^i \mathbf{x}^{i-1}$$

- Until convergence

Back Propagation

- Loss function is not convex
 - ◆ Each permutation of hidden units is a local minimum.
 - ◆ Learned features (hidden units) may be ok, but not usually globally optimal.
- But:
 - ◆ Local minima can still be arbitrarily good.
 - ◆ Many local minima can be equally good.
 - ◆ Supervised learning often works with hundreds of layers and millions of training instances.

Regularization

- L2-regularized loss
 - ◆ $\hat{R}_2(\boldsymbol{\theta}) = \frac{1}{2m} \sum_j (\mathbf{y}_j - \mathbf{x}_j^d)^2 + \frac{\eta}{2} \boldsymbol{\theta}^T \boldsymbol{\theta}$
 - ◆ Corresponds to normal prior on parameters.
- Gradient: $\nabla \hat{R}_2(\boldsymbol{\theta}^i) = \frac{1}{m} \sum_j \delta_j^i \mathbf{x}^i + \eta \boldsymbol{\theta}$
- Update: $\boldsymbol{\theta}' = \boldsymbol{\theta} - \delta_j \mathbf{x} - \eta \boldsymbol{\theta}$
- Called *weight decay*.
- Additional regularization schemes:
 - ◆ Early stopping (outdated): Stop before convergence.
 - ◆ Delete units with small weights.
 - ◆ Dropout: During training, set some units' output to zero at random.

Regularization: Dropout

- In complex networks, complex co-adaptation relationships can form between units.
 - ◆ Not robust for new data.
- Dropout: In each training set, draw a fraction of units at random and set their output to zero.
- At application time, use all units.
- Used for transitions from layers with many units to layers with few units.
- Improves overall robustness: each unit has to function within varying combinations of units.

Mini-Batches

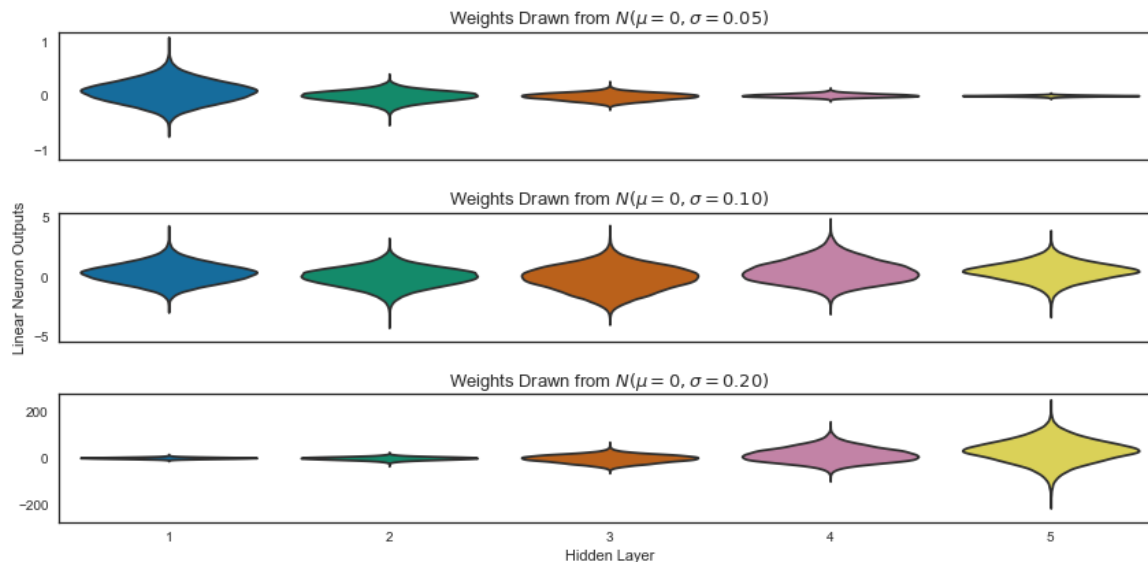
- Average stochastic gradient over batch of instances, then perform update step.
- Tends to make learning more robust than single-instance stochastic gradient descent with respect to hyper-parameters.

Input Normalization

- Large absolute value of input vectors \rightarrow large absolute value of $h_k^d \rightarrow \sigma_{sm}(h_k^d)$ tends to be close to 1 or 0 \rightarrow gradient becomes small.
- Hence, larger absolute values of inputs require larger learning rates, difficult to adjust.
- Therefore, input values are often normalized to approximately between 0 and 1.

Initialization

- Initialization with 0 often does not work.
 - ◆ Outputs become 0, derivatives become 0.
- Initialization with Gaussian distribution can increase or decrease the variance of outputs differently for different layers.
 - ◆ Example: 5 layers of 100 units.



Initialization

- It is desirable that the variance of output be similar across all network layers.

- ◆ $Var(x_k^{i+1}) = Var\left(\sum_{j=1}^{n_i} x_j^i \theta_{jk}^{i+1}\right) \approx n_i Var(x^i) Var(\theta_k^{i+1})$

- ◆ $Var(x^i) = Var(x^{i+1}) \Leftrightarrow Var(\theta_k^{i+1}) = \frac{1}{n_i}$

- Similarly, the variance of derivatives should be similar across network layers. This requires

- ◆ $Var(\theta_i) = \frac{1}{n_{i+1}}.$

- Compromise: $Var(\theta_i) = \frac{2}{n_{i+1} + n_i}.$

Initialization

- Normal initialization with $Var(\theta_i) = \frac{2}{n_{i+1}+n_i}$:
 - ◆ Draw from $N \left[0, \sqrt{\frac{2}{n_{i+1}+n_i}} \right]$.
- Uniform initialization between $-a$ and a with $Var(\theta_i) = \frac{2}{n_{i+1}+n_i}$ (Glorot initialization):
 - ◆ Draw from $U \left[-\frac{6}{n_{i+1}+n_i}, \frac{6}{n_{i+1}+n_i} \right]$.

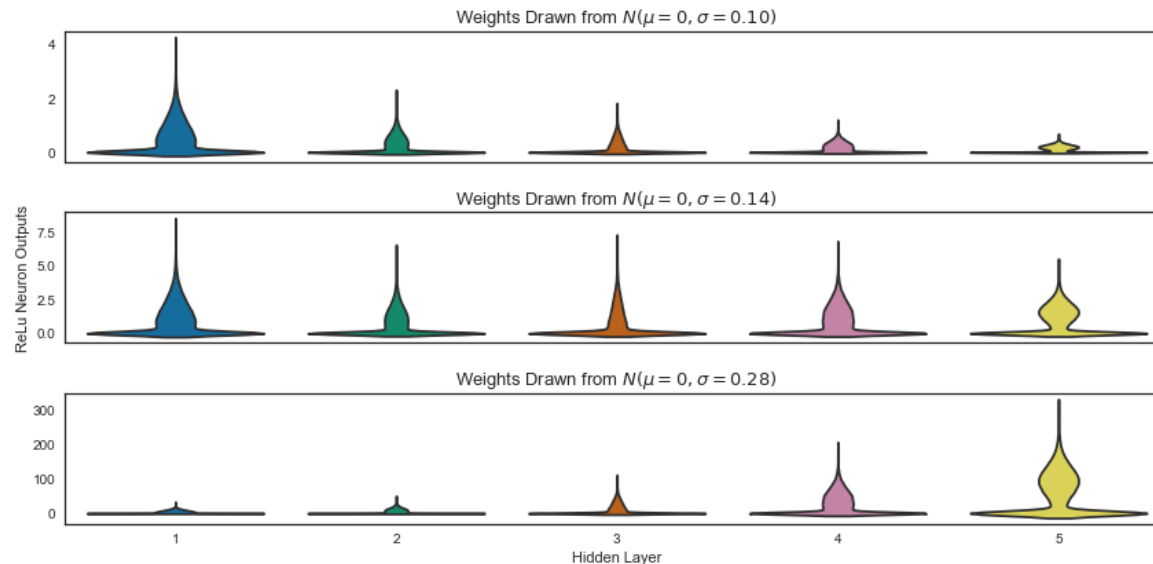
Initialization

- Normal initialization with:

- ◆ Draw from $N\left[0, \sqrt{\frac{2}{n_{i+1}+n_i}}\right]$.

- Uniform initialization (Glorot initialization):

- ◆ Draw from $U\left[-\frac{6}{n_{i+1}+n_i}, \frac{6}{n_{i+1}+n_i}\right]$.



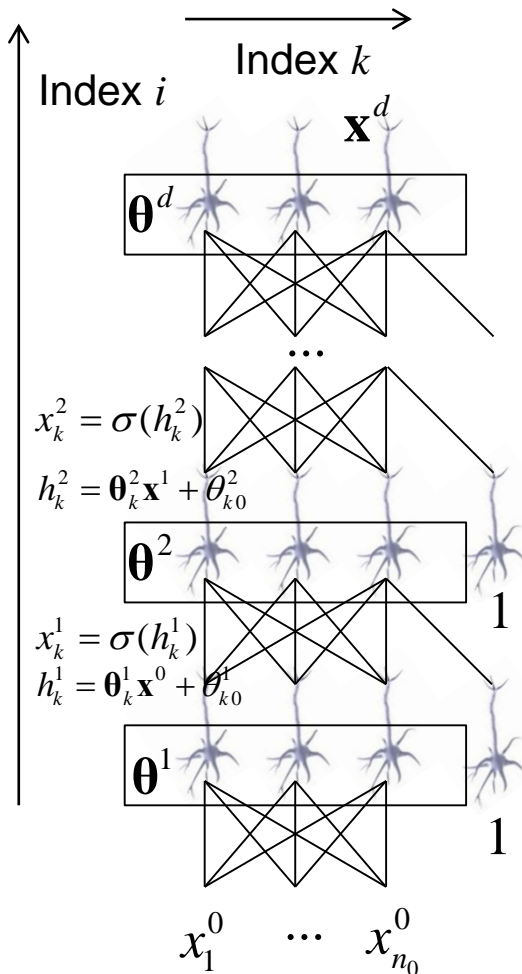
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Parallel Inference

- Both forward and backward propagation can be made much faster by parallel computation.
- GPUs are particularly suited.
- Pipelining in single-core CPU can be exploited.
- Forward- and backward-propagation can be written as matrix multiplications.
- Columns of the weight matrix can be processed in parallel.

Parallel Inference



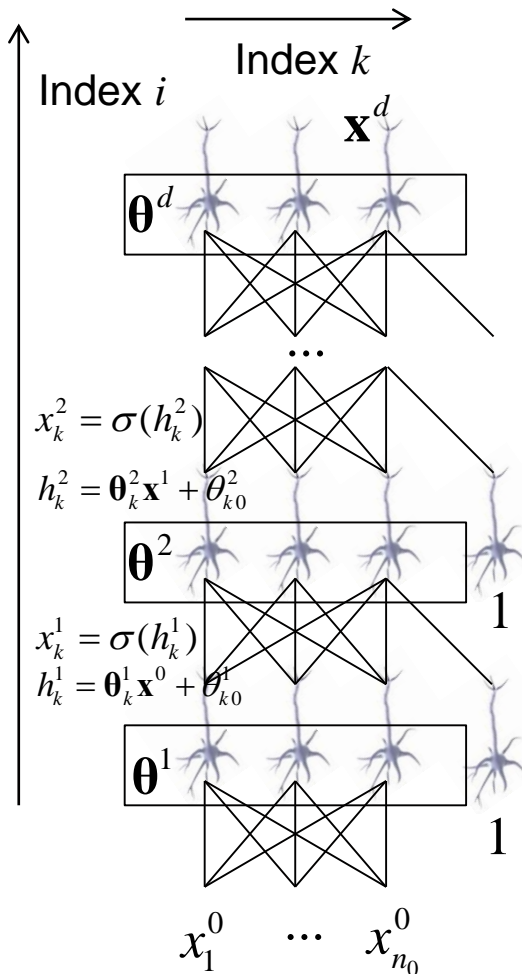
- Forward propagation per layer in matrix notation:

$$\mathbf{h}^i = \boldsymbol{\theta}^i \mathbf{x}^{i-1}$$

$$\begin{bmatrix} h_1^i \\ \vdots \\ h_{n_i}^i \end{bmatrix} = \begin{bmatrix} \theta_{11}^i & \dots & \theta_{1n_{i-1}}^i \\ \vdots & & \vdots \\ \theta_{n_i1}^i & \dots & \theta_{n_i n_{i-1}}^i \end{bmatrix} \begin{bmatrix} x_1^{i-1} \\ \vdots \\ x_{n_{i-1}}^{i-1} \end{bmatrix}$$

- Use vector coprocessor / GPU row-by-column multiplications.
- Split up rows of $\boldsymbol{\theta}$ between multiple cores.

Vectorization for Forward Inference



- Forward propagation per layer in matrix notation:

$$\mathbf{h}^i = \boldsymbol{\theta}^i \mathbf{x}^{i-1}$$

$$\begin{bmatrix} h_1^i \\ \vdots \\ h_{n_i}^i \end{bmatrix} = \begin{bmatrix} \theta_{11}^i & \dots & \theta_{1n_{i-1}}^i \\ \vdots & & \vdots \\ \theta_{n_i1}^i & \dots & \theta_{n_in_{i-1}}^i \end{bmatrix} \begin{bmatrix} x_1^{i-1} \\ \vdots \\ x_{n_{i-1}}^{i-1} \end{bmatrix}$$

- Keep $[x_1^{i-1}, \dots, x_{n_{i-1}}^{i-1}]$ in cache.
- For all rows $j = 1..n_i$ (in parallel):
 - Load $[\theta_{j1}^i, \dots, \theta_{jn_{i-1}}^i]$ into cache.
 - For all $k = 1..n_{i-1}$ (in parallel): multiply and sum $\theta_{jk}^i x_k^{i-1}$.

Software Packages

- Cafe: allows to easily apply deep learning with standard units, loss functions, learning techniques.
- Deep learning frameworks that allow development of new architectures and learning techniques.
 - ◆ TensorFlow (+Keras),
 - ◆ (Py)Torch,
 - ◆ Theano (+Lasagne),
 - ◆ CNTK.

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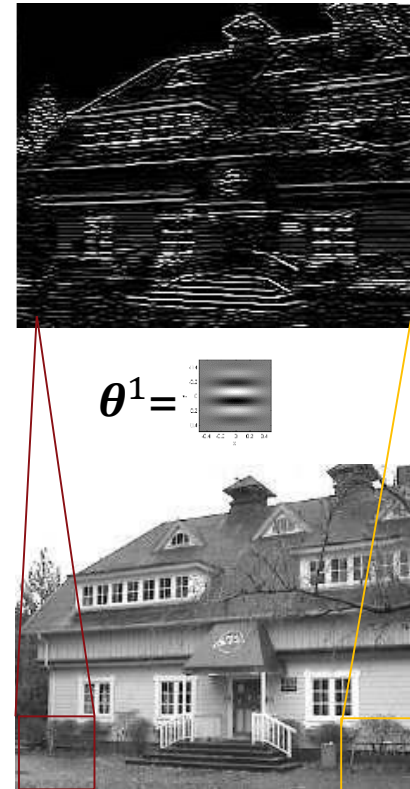
Convolutions: Motivation

- Neural network trained for digit classification trained on centered digits will not be able to recognize a digit in a different position or scale.
- Training a network to recognize digits everywhere on the input image is a more complex task, needs more training data.
- Convolutional neural networks: learn to detect patterns, apply pattern detector to all positions in input signal.



Convolution

- Filter unit takes input window, multiplies it with weight vector, produces response.
- Window slides over input signal.
- Each pixel of response image is filter result for an input window.
- Same filter is applied to all window positions of the input signal.
- Each unit produces output of same filter for different position.



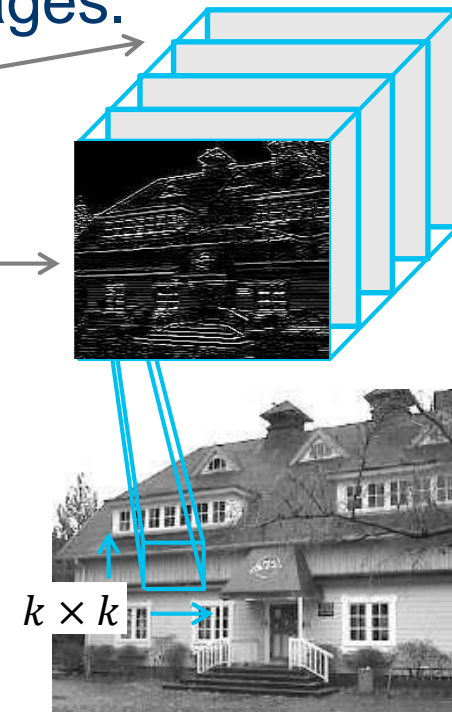
Convolutional Layer

- Applies multiple filters to all positions of input.
- Input size: $x \times y \times 1$.
- Output size: $(x - k + 1) \times (y - k + 1) \times d$.
- Creates a bank of response images.

Response image of filter d

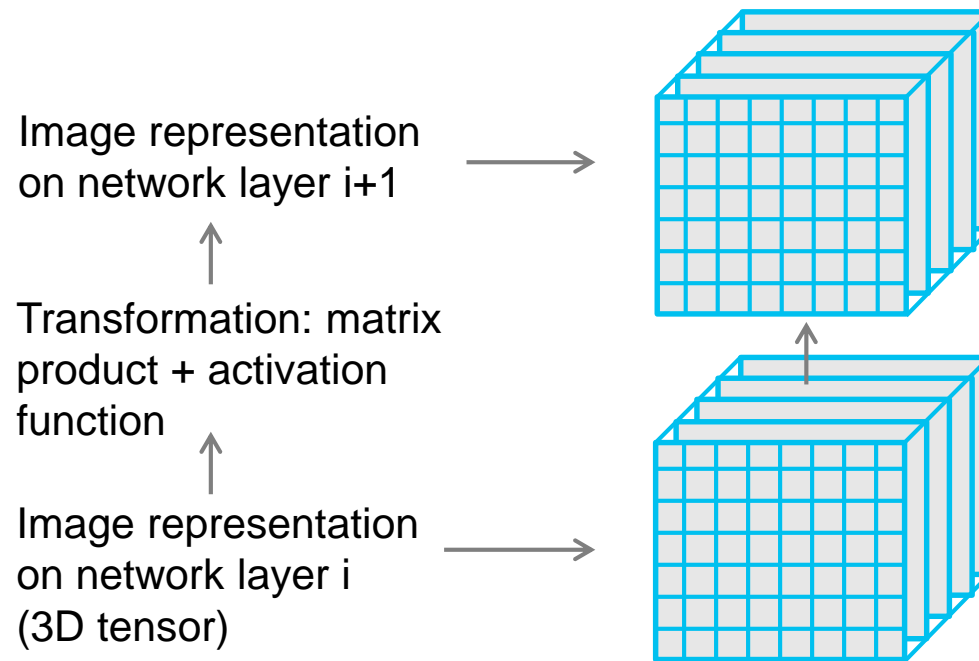
Response image of filter 1
= filter 1 applied to all
image positions

$k \times k \times d$ convolutional layer



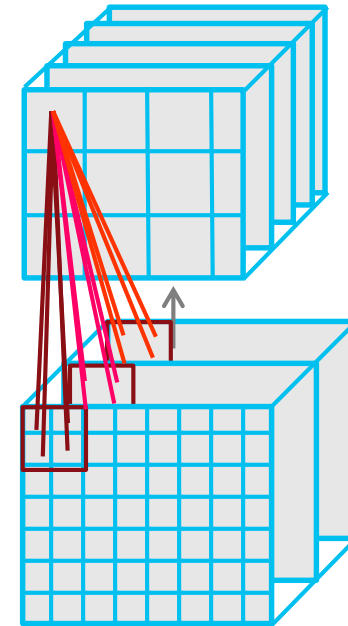
Convolutional Neural Networks

- Each network layer transforms the image into a more abstract feature representation.

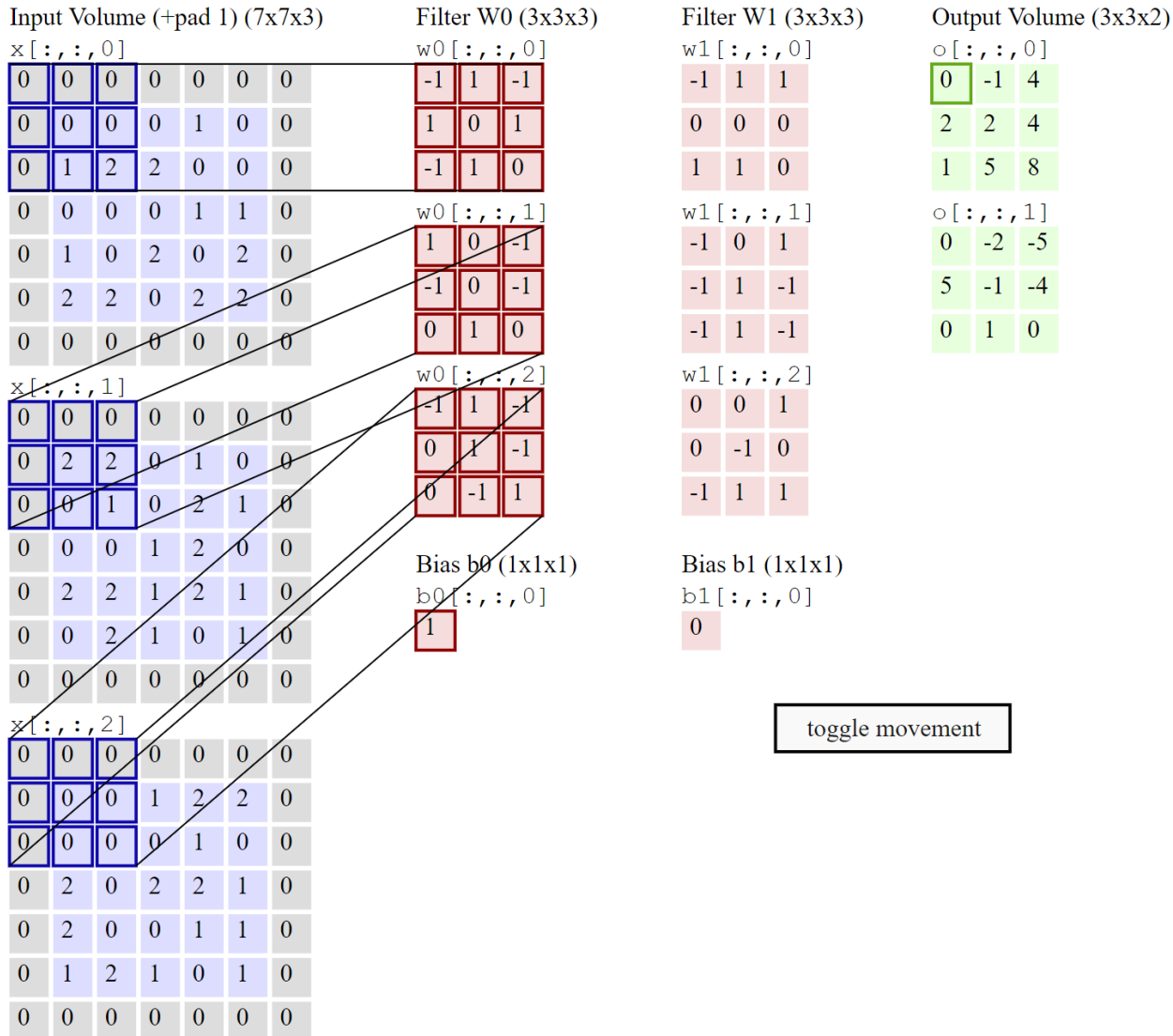


Convolutional Layers

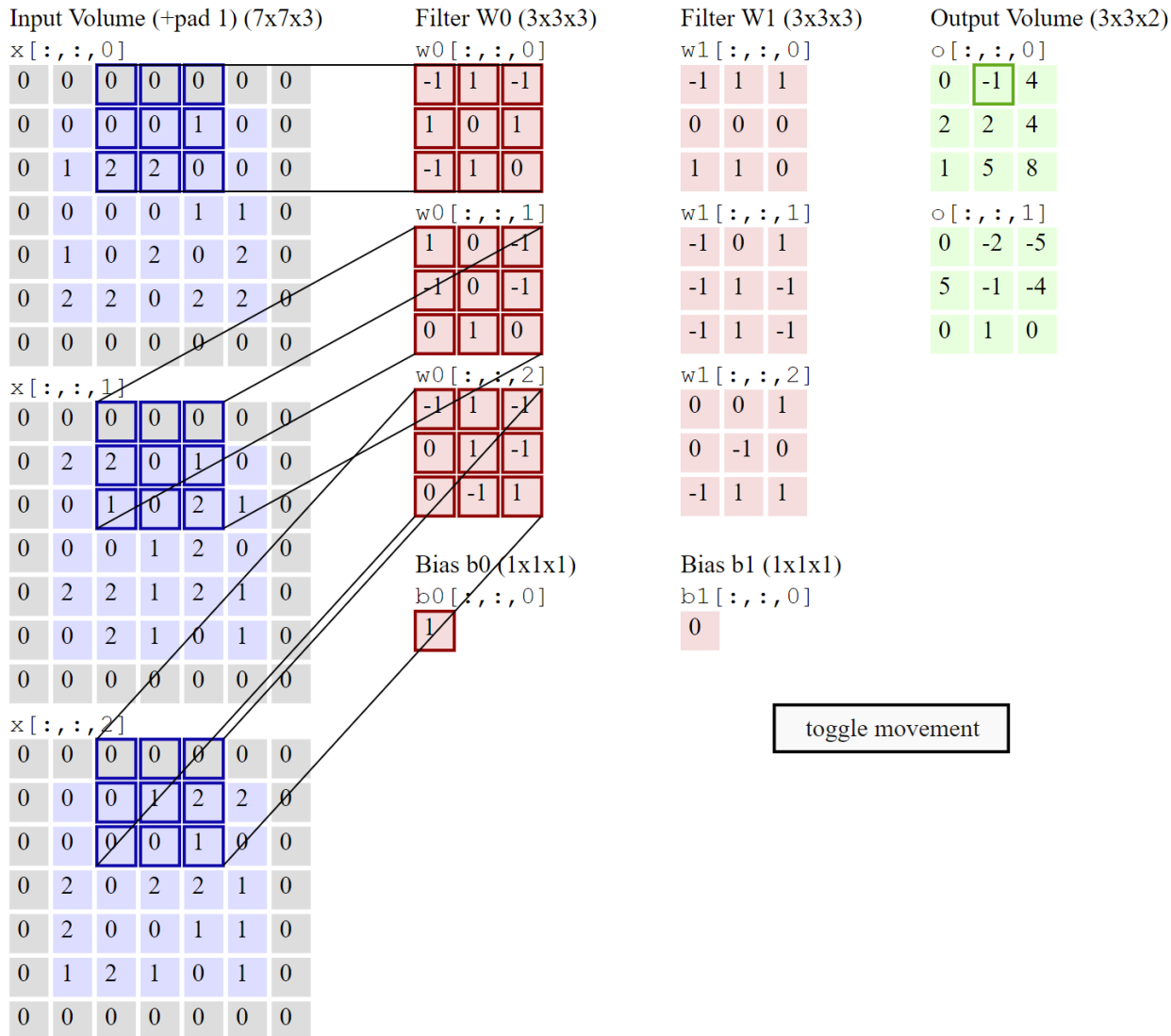
- Convolution, $k \times k \times d$, stride > 1 .
 - ◆ Input size: $x \times y \times d'$, stride s .
 - ◆ output size: $\frac{(x-k+1)}{s} \times \frac{(y-k+1)}{s} \times d$.
- Convolutional layer has
 - ◆ $k \times k \times d'$ parameters.
- Decreases the spatial resolution.



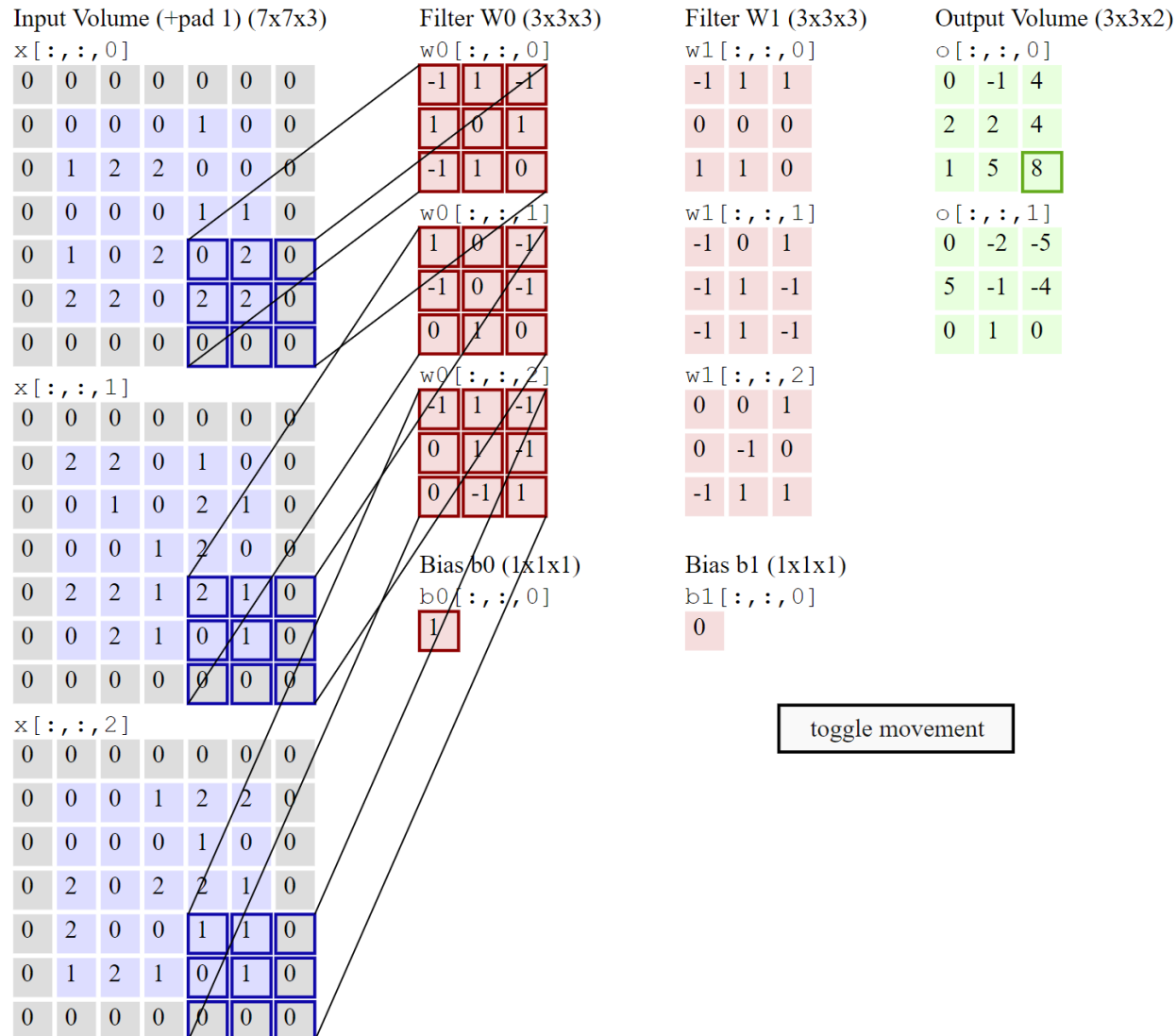
Example: Convolution 3 x 3 x 2, Stride 2



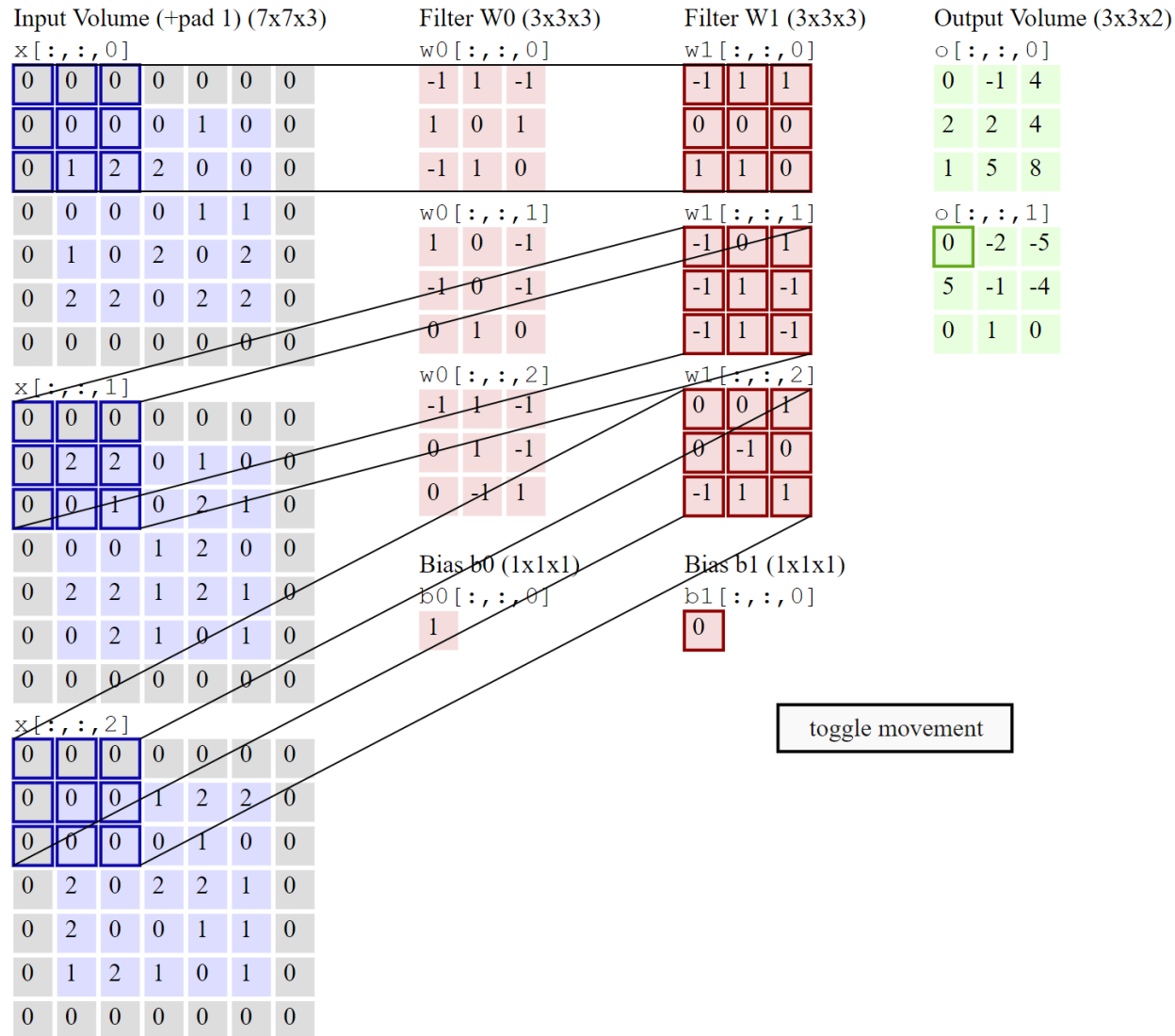
Example: Convolution 3 x 3 x 2, Stride 2



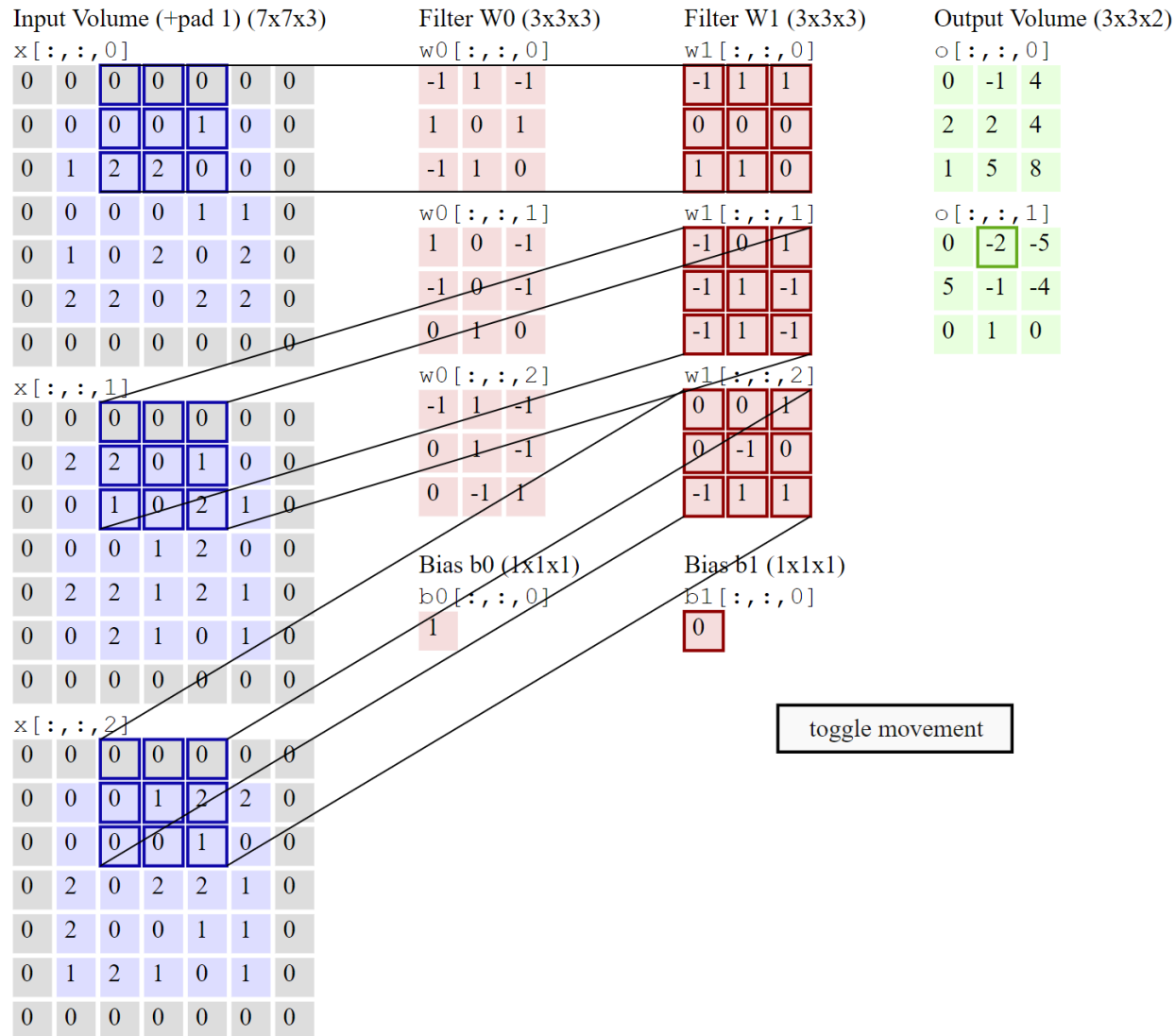
Example: Convolution 3 x 3 x 2, Stride 2



Example: Convolution 3 x 3 x 2, Stride 2



Example: Convolution 3 x 3 x 2, Stride 2

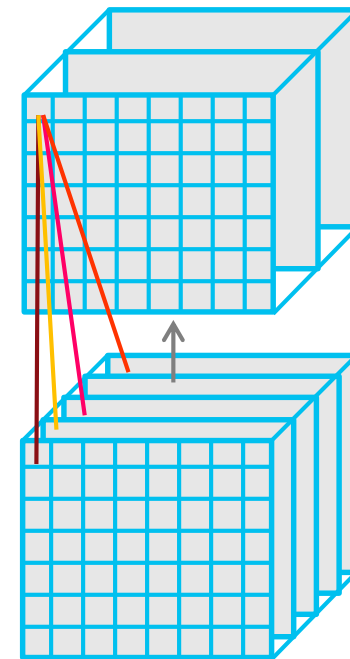


Scheffer: Intelligent Data Analysis



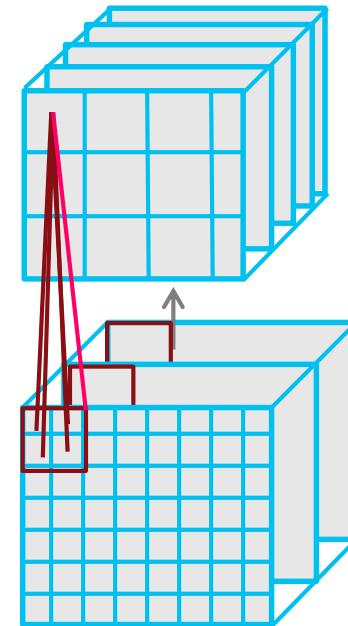
Convolutional Layers

- Convolution, $1 \times 1 \times d$, stride 1.
 - ◆ Input size: $x \times y \times d'$.
 - ◆ output size: $x \times y \times d$.
- Convolutional layer has
 - ◆ $1 \times 1 \times d'$ parameters.
- Used to decrease the resolution along the z axis (with $d < d'$).



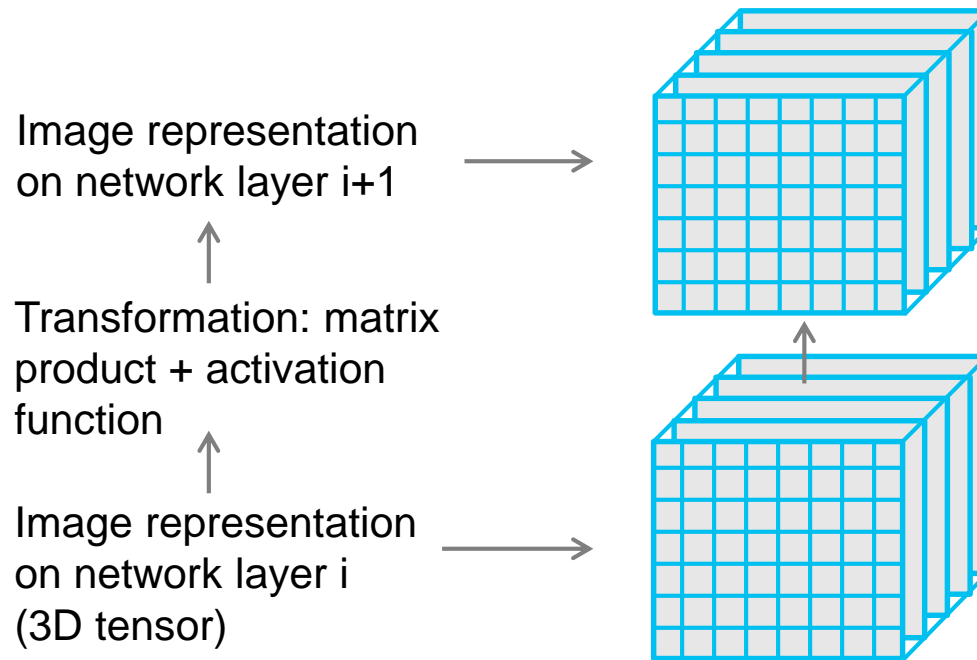
Max-Pooling Layers

- Max pooling:
 - ◆ Input size: $x \times y \times d$, stride s .
 - ◆ output size: $\frac{x}{s} \times \frac{y}{s} \times d$.
- Output for each pixel is maximum over input window.
- Applied to each filter bank separately.
- Used to decrease the spatial resolution.



Convolutional Neural Networks

- Widely used in image processing; e.g.,
 - ◆ Image classification (e.g., ImageNet),
 - ◆ Face identification (e.g., DeepFace, FaceNet).



Training Convolutional Layers

- Some weights are fixed to zero: depending on kernel size and stride, some pairs of input and output units are not connected.
- Some weights are coupled: the same kernel is applied to all input windows.

Training step for convolutional layer:

1. Calculate gradient using back-propagation.
2. Average the gradient for all coupled weights, perform joint update step for each coupled set.
3. Set weights to zero for connections that do not exist.

Overview

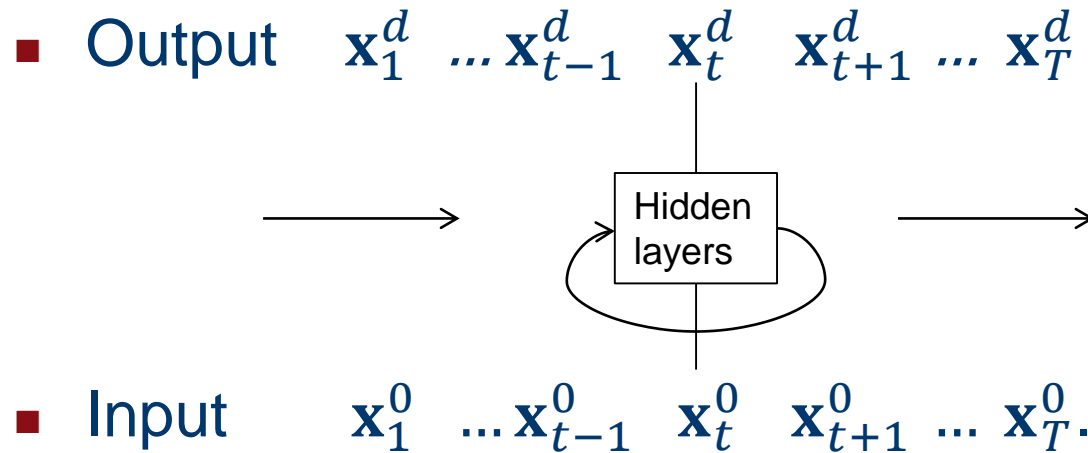
- Neural information processing.
- Deep learning.
- Feed-forward networks.
- Training feed-forward networks: back propagation.
- Parallel inference on GPUs.
- Convolutional neural networks,
- **Recurrent neural networks.**

Recurrent Neural Networks

- Input: time series $\mathbf{x}_1^0, \dots, \mathbf{x}_T^0$.
- Output can be:
 - ◆ One output (vector) for entire time series: \mathbf{x}^d .
 - ◆ One output at each time step: $\mathbf{x}_1^d, \dots, \mathbf{x}_T^d$.

Recurrent Neural Networks

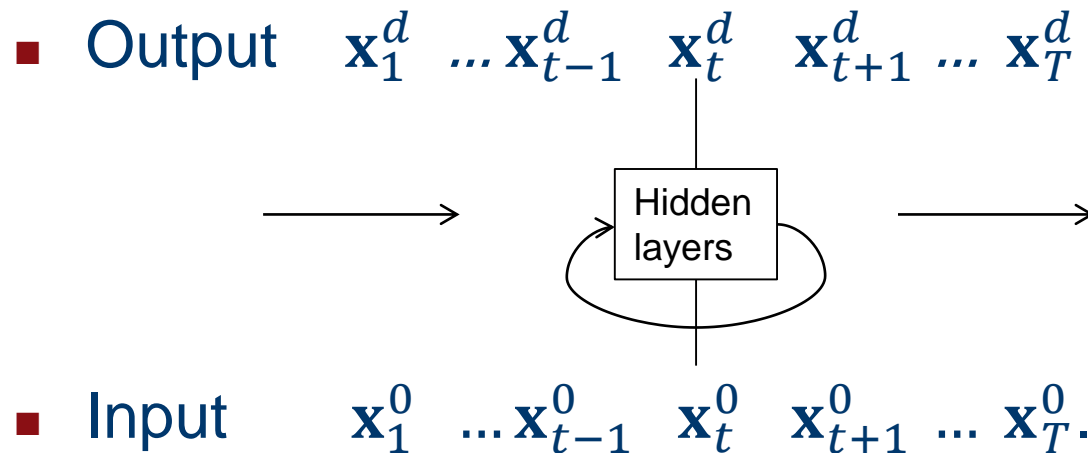
- Hidden layer propagates information to itself.
- Hidden layer activation stores context information.



Recurrent Neural Networks

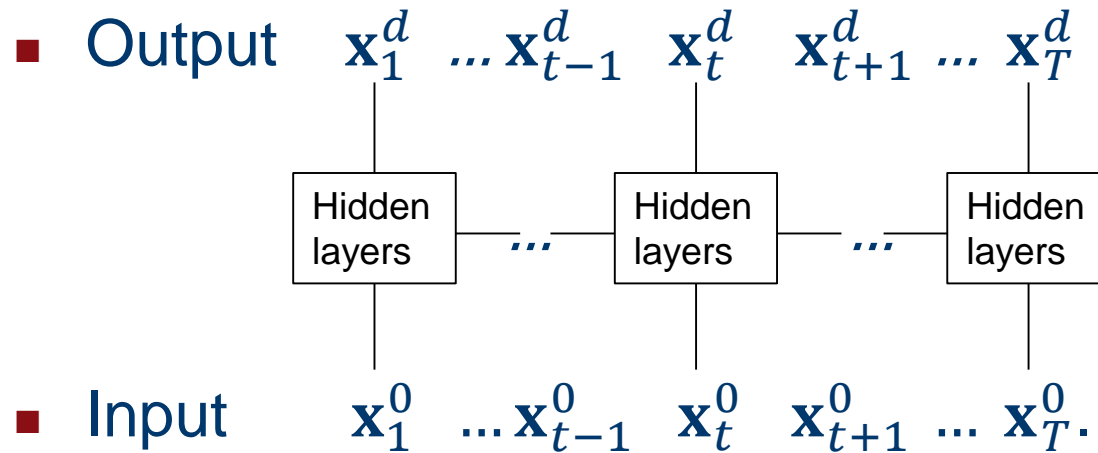
- Propagation:

- ◆ $\mathbf{h}_t^1 = \theta^1 \begin{pmatrix} \mathbf{x}_t^0 \\ \mathbf{x}_{t-1}^1 \end{pmatrix}; \mathbf{x}_t^1 = \sigma(\mathbf{h}_t^1)$



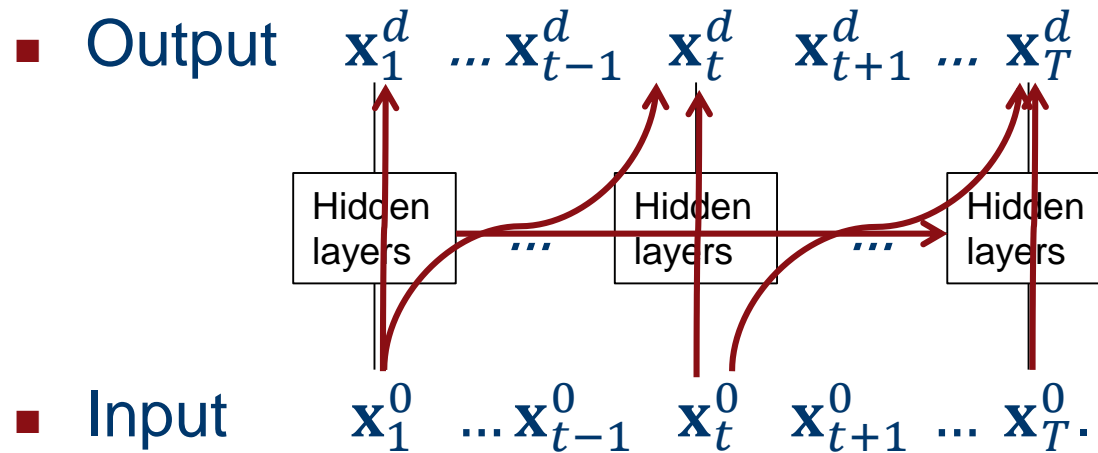
Recurrent Neural Networks

- Identical network “unfolded” in time.
- Units on hidden layer propagate to the right.
- Hidden layer activation stores context information.



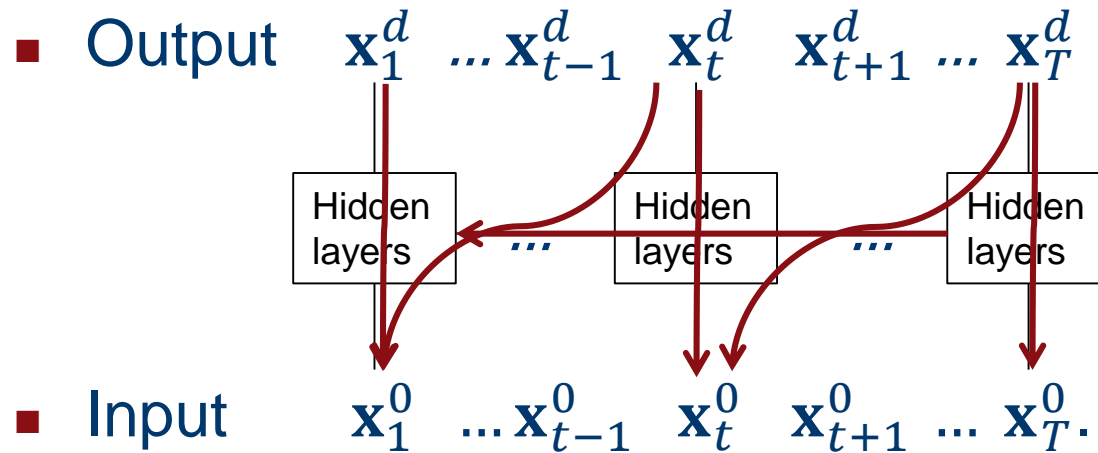
Recurrent Neural Networks

- Forward propagation



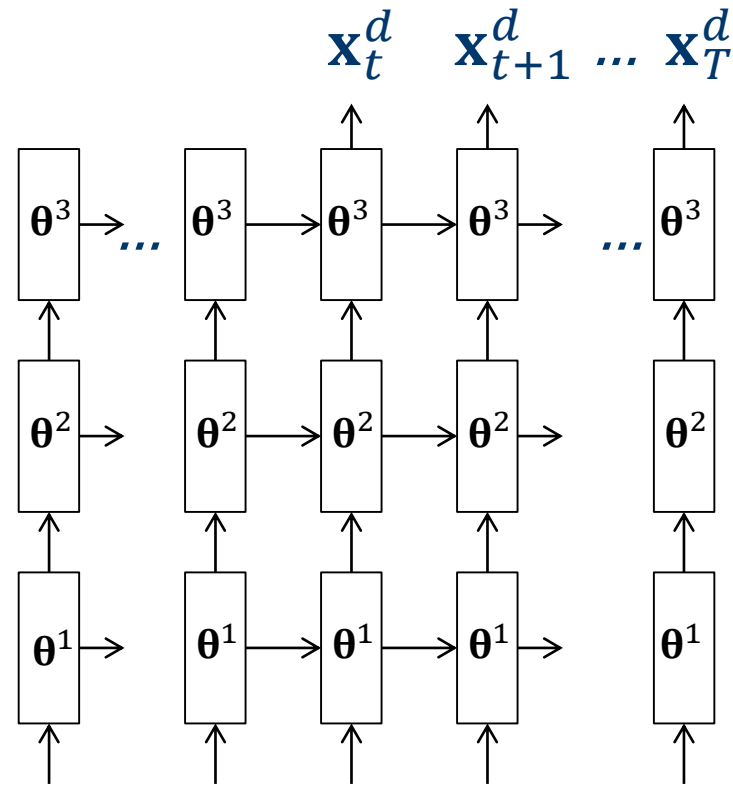
Recurrent Neural Networks

- Back propagation through time.



Deep Recurrent Neural Networks

■ Output



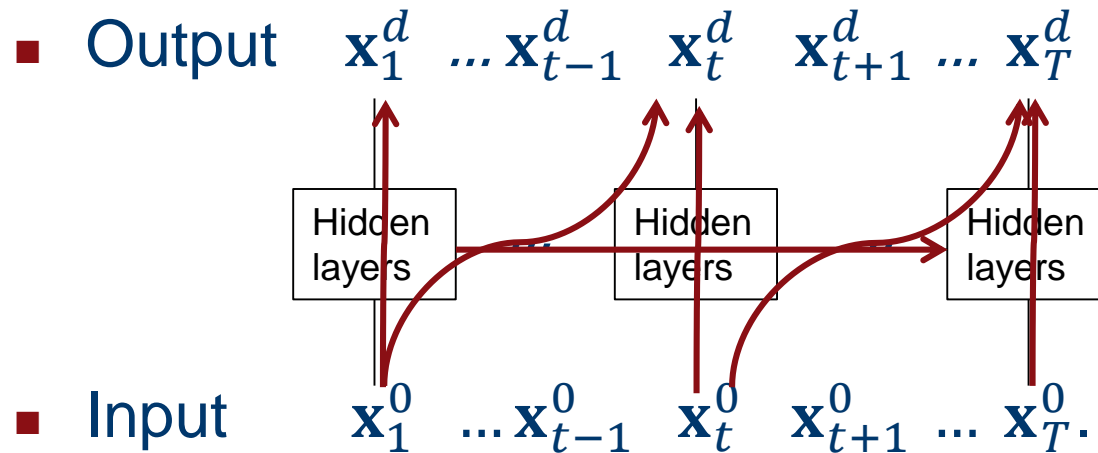
Many paths through which long-term dependencies can be propagated through the network

■ Input

$x_1^0 \dots x_{t-1}^0 x_t^0 x_{t+1}^0 \dots x_T^0$

Recurrent Neural Networks

- Widely used in language processing:
 - ◆ Speech recognition,
 - ◆ Machine translation,



Summary

- Computational model of neural information processing.
- Feed-forward networks: layer-wise matrix multiplication + activation function.
- Back propagation: stochastic gradient descent. Gradient computation by layer-wise matrix multiplication + derivative of activation function.
- Convolutional neural networks: layer-wise application of local filters.
- Recurrent neural networks: state information passed on to next time step.