Deep Neural and Probabilistic Learning

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Centre for Cognitive Science

Fachbereich Informatik

Thanks to Pedro Domingos, Fie-Fei Li, Geoff Hinton, Viktoriia Sharmanska and many others for making their slides publically available. Thanks to Zoubin Ghahramani, Sriraam Natarajan, Antonio Vergari, Isabel Valera, Robert Peharz, Alejandro Molina, Karl Stelzner, Carsten Binnig, Nicola Di Mauro, Floriana Esposito, Martin Trapp and many others for the amazing collaborations

Kristian Kersting

Arms race to deeply understand data

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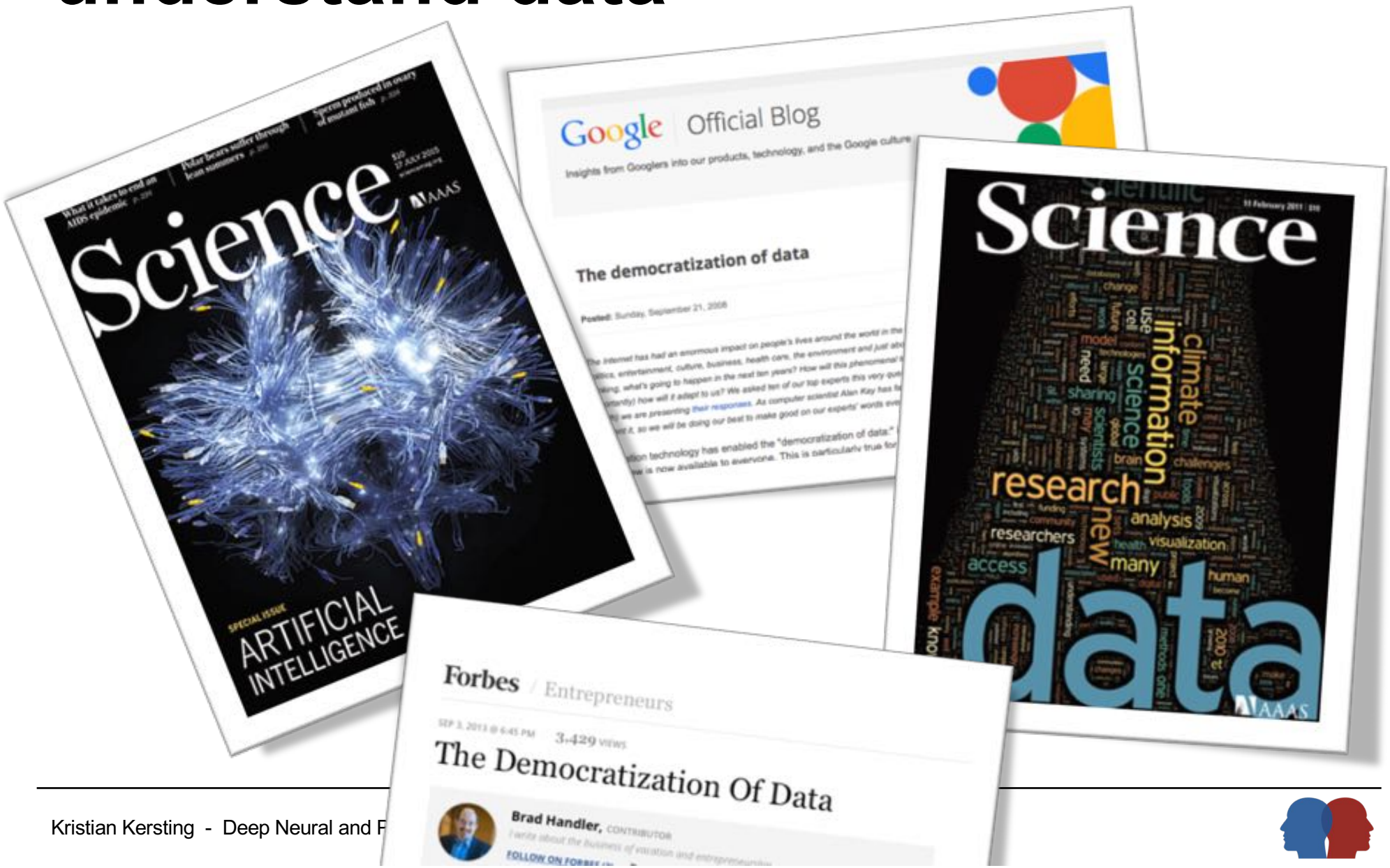
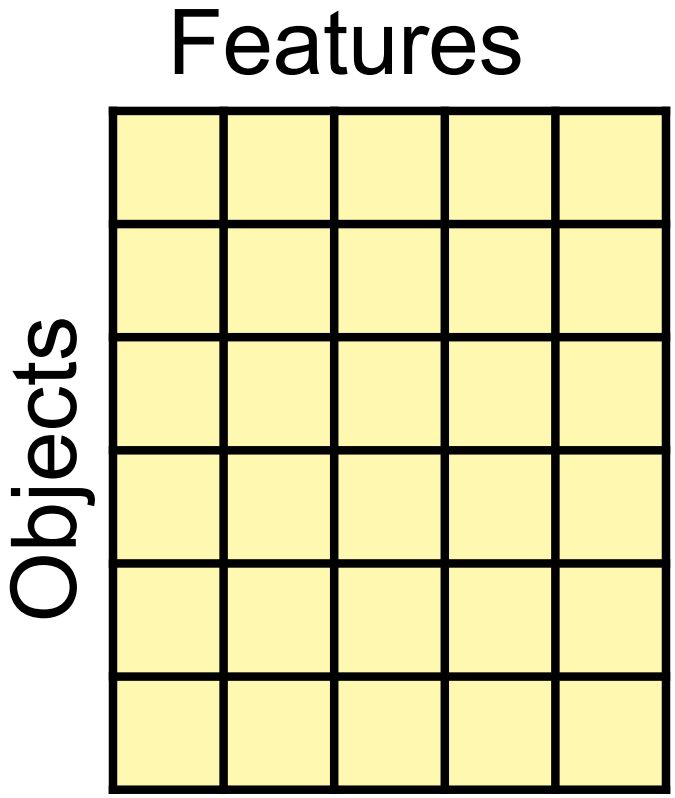
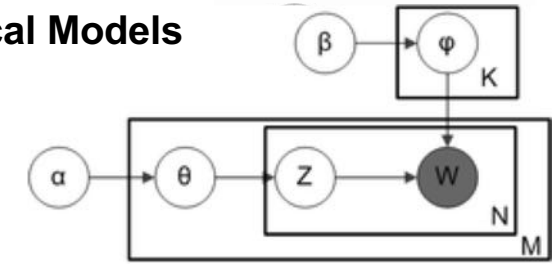


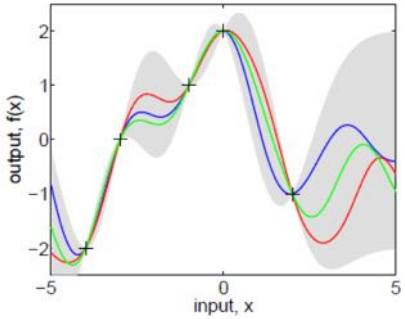
Bottom line:
Take your data spreadsheet …



… and apply Machine Learning

Probabilistic Graphical Models
Arithmetic Circuits





Gaussian Processes

Features

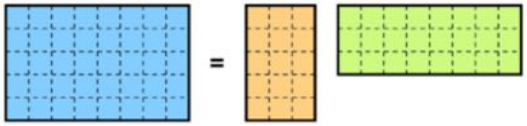
Objects

Is it really that simple?

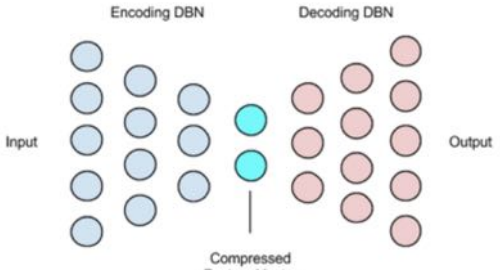
Big Model

Small Model

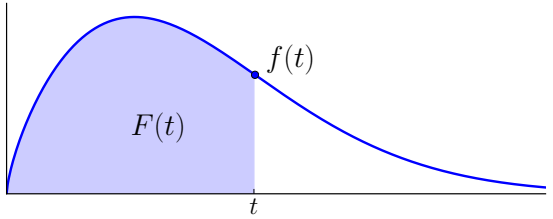
Distillation/LUPI



Big Data Matrix Factorization

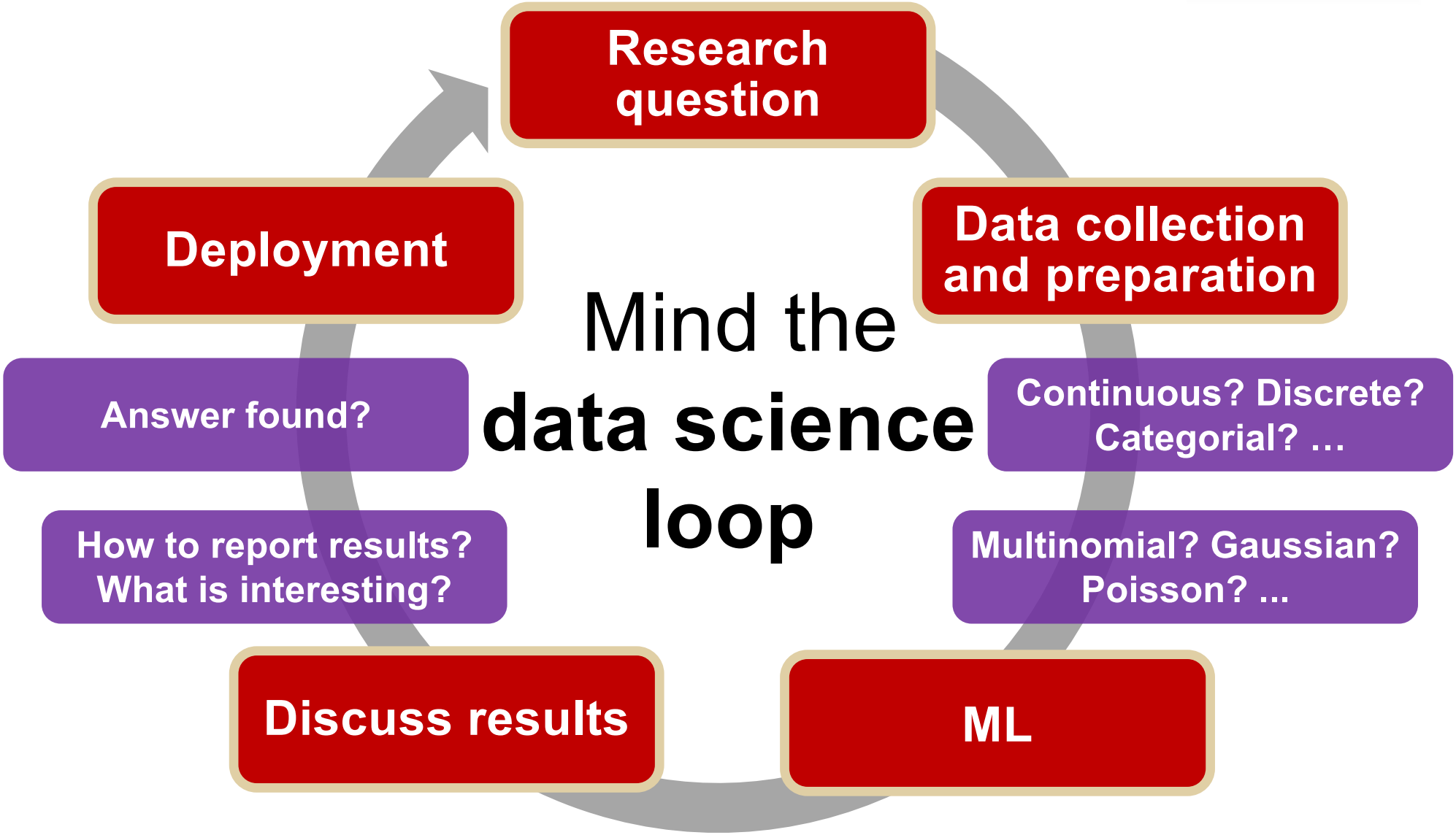


Autoencoder,
Deep Learning

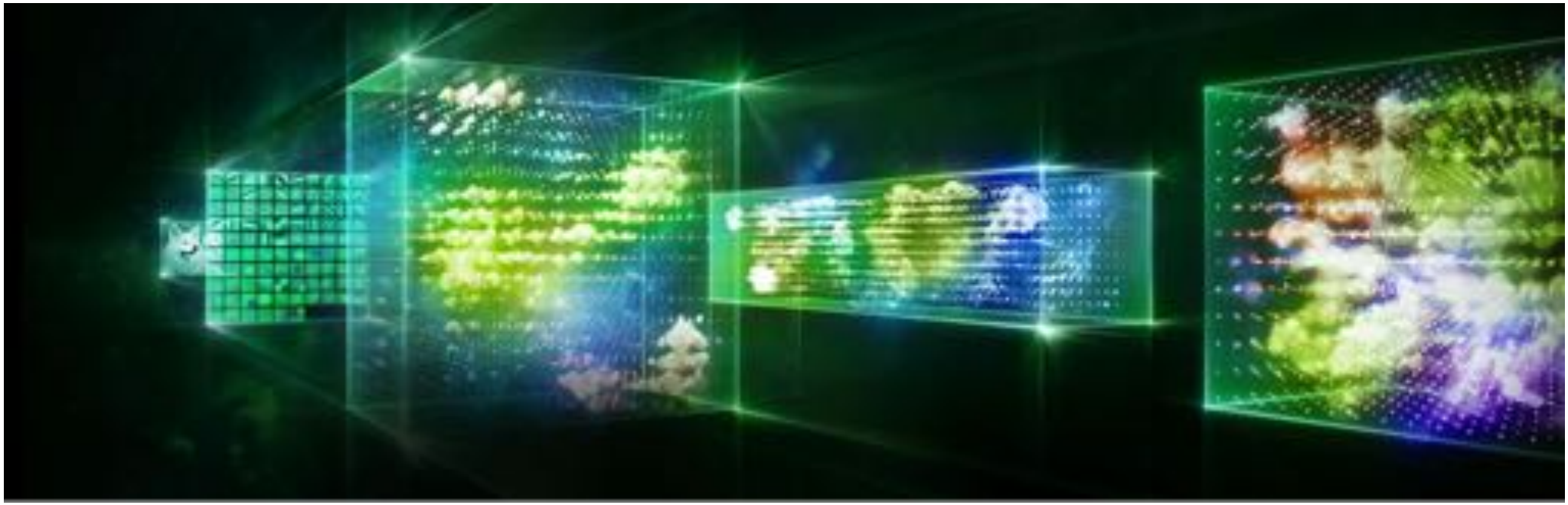


Diffusion Models

and many more …

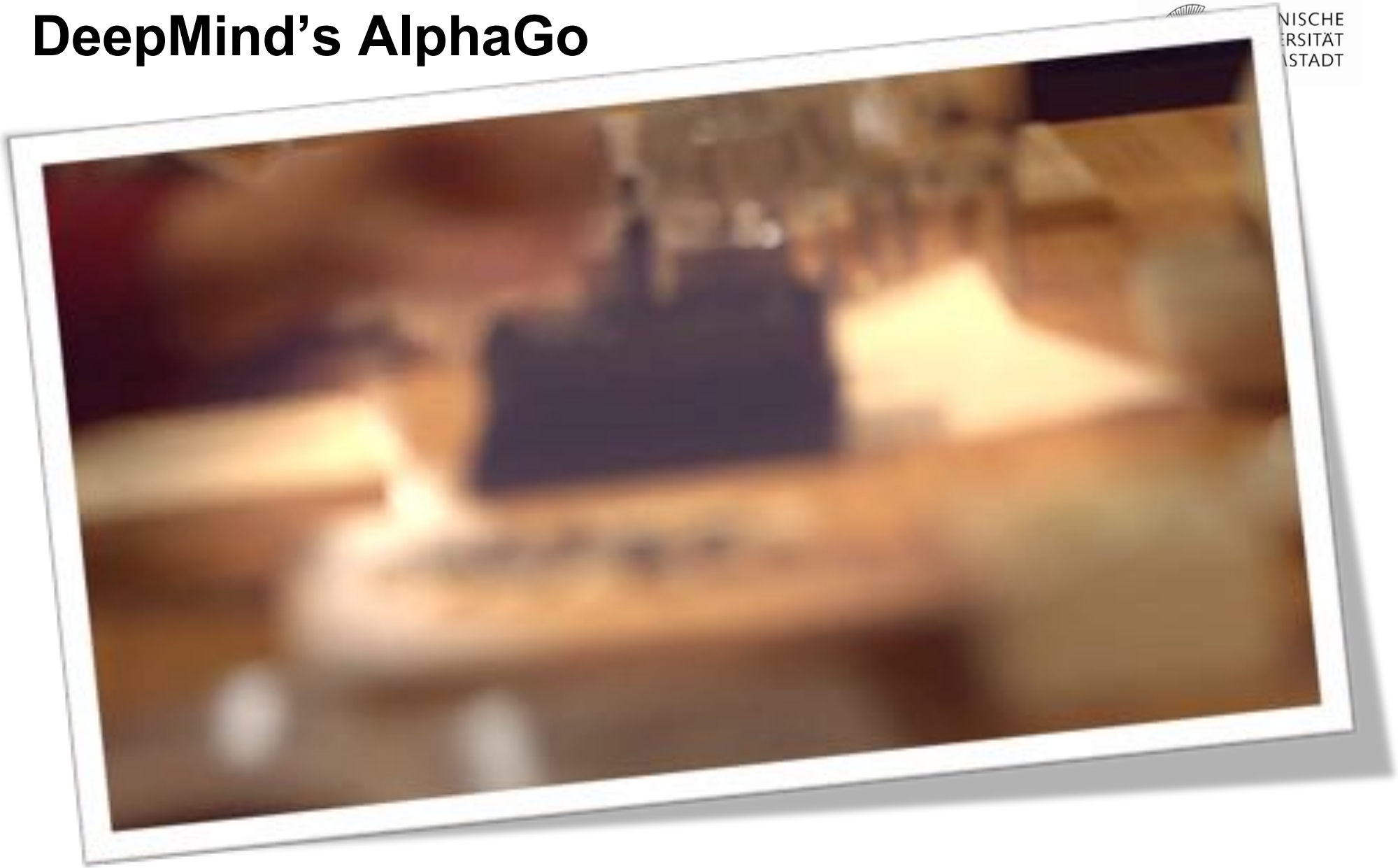

Research question
Data collection and preparation
Continuous? Discrete? Categorial? …
Multinomial? Gaussian? Poisson? ...
ML
Discuss results
How to report results? What is interesting?
Answer found?
Deployment
Mind the data science loop

What if the machine can help to find the right representation?



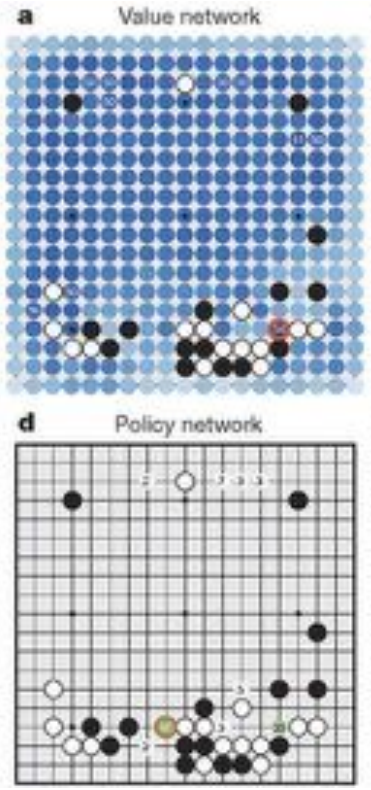
Deep Neural Learning

DeepMind's AlphaGo



Watch NATURE video at https://www.youtube.com/watch?v=g-dKXOlsf98

DeepMind's AlphaGo



Deep policy network is trained to produce probability map of promising moves. The deep value network is used to prune the search tree (monte-carlo tree search); so there is a lot of classical AI machinery around the deep (p)art.

And yes, the machine may also learn to play other games

Goal of Deep Architectures

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High-level semenatical representations

To this aim most approaches use (stacked) neural networks

Edges, local shapes, object parts

Low level representation

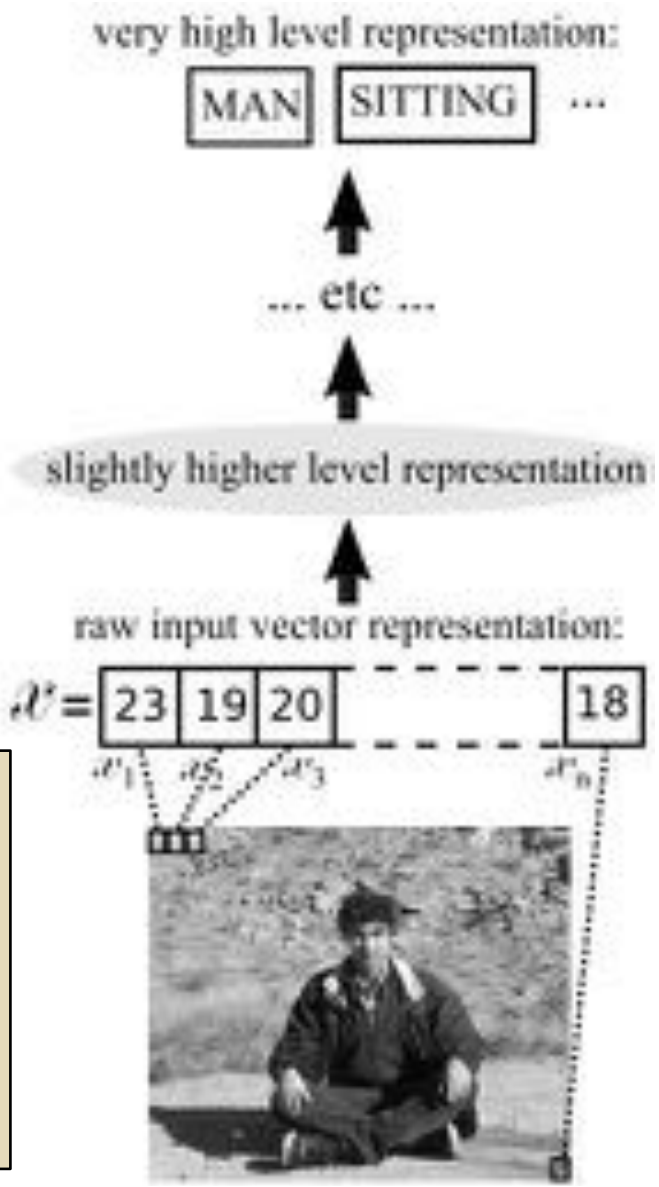

Figure is from Yoshua Bengio

Deep learning methods aim at

- **learning feature hierarchies**
- where features from higher levels of the hierarchy are formed by lower level features.

Deep Architectures

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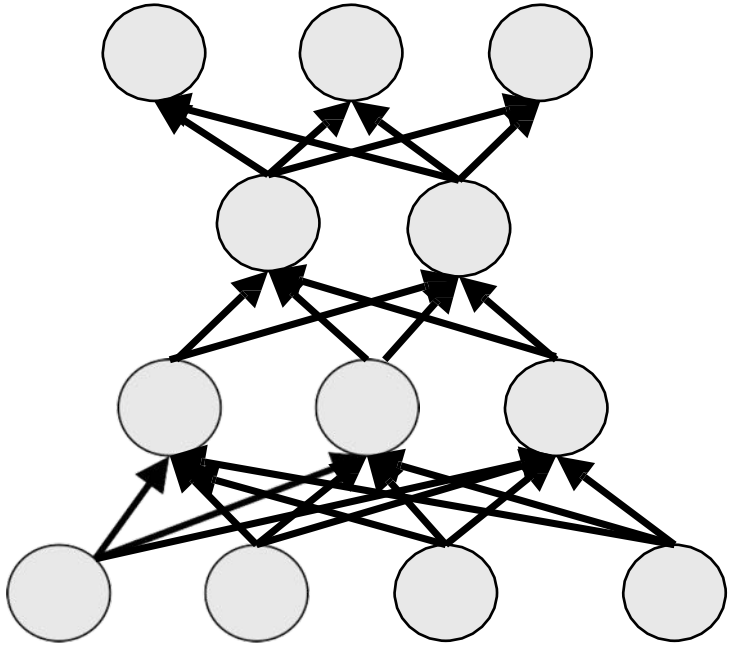
Deep architectures are composed of multiple levels of non-linear operations, such as neural nets with many hidden layers.

Output layer

Hidden layers

Input layer



Examples of non-linear activations:

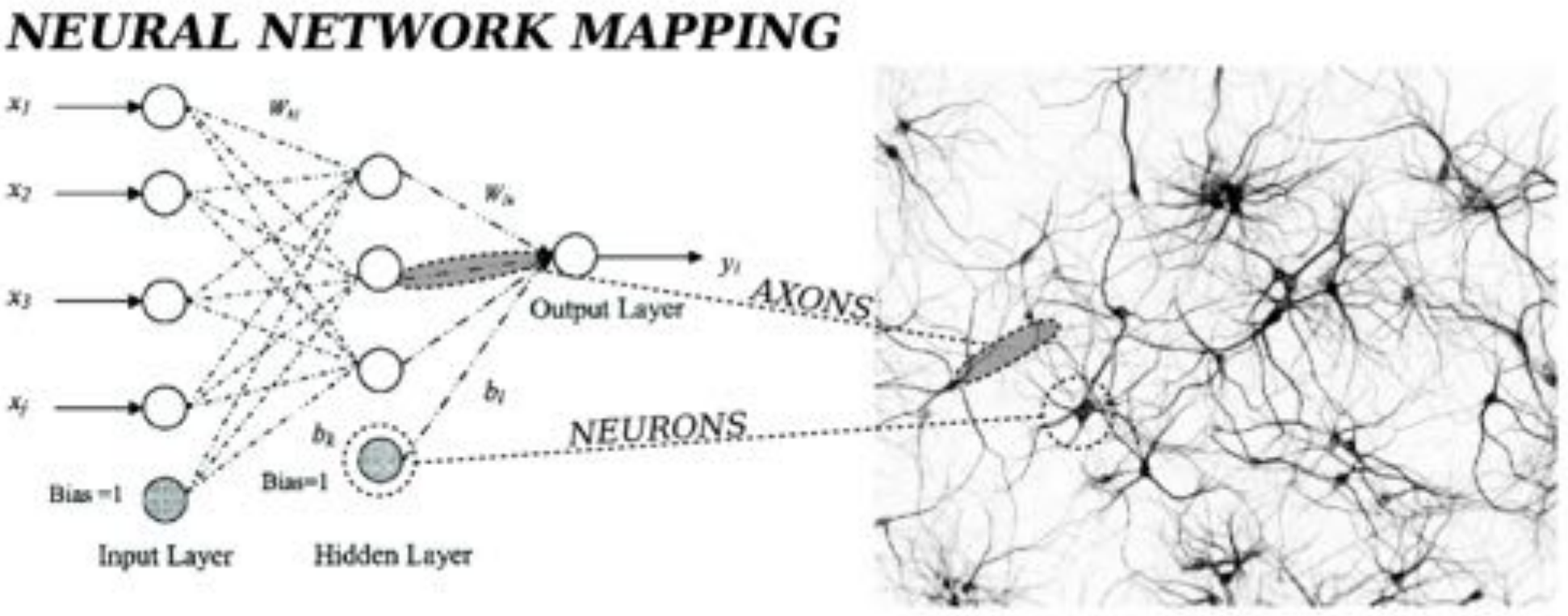
$$\tanh(x)$$

$$\sigma(x) = (1 + e^{-x})^{-1}$$

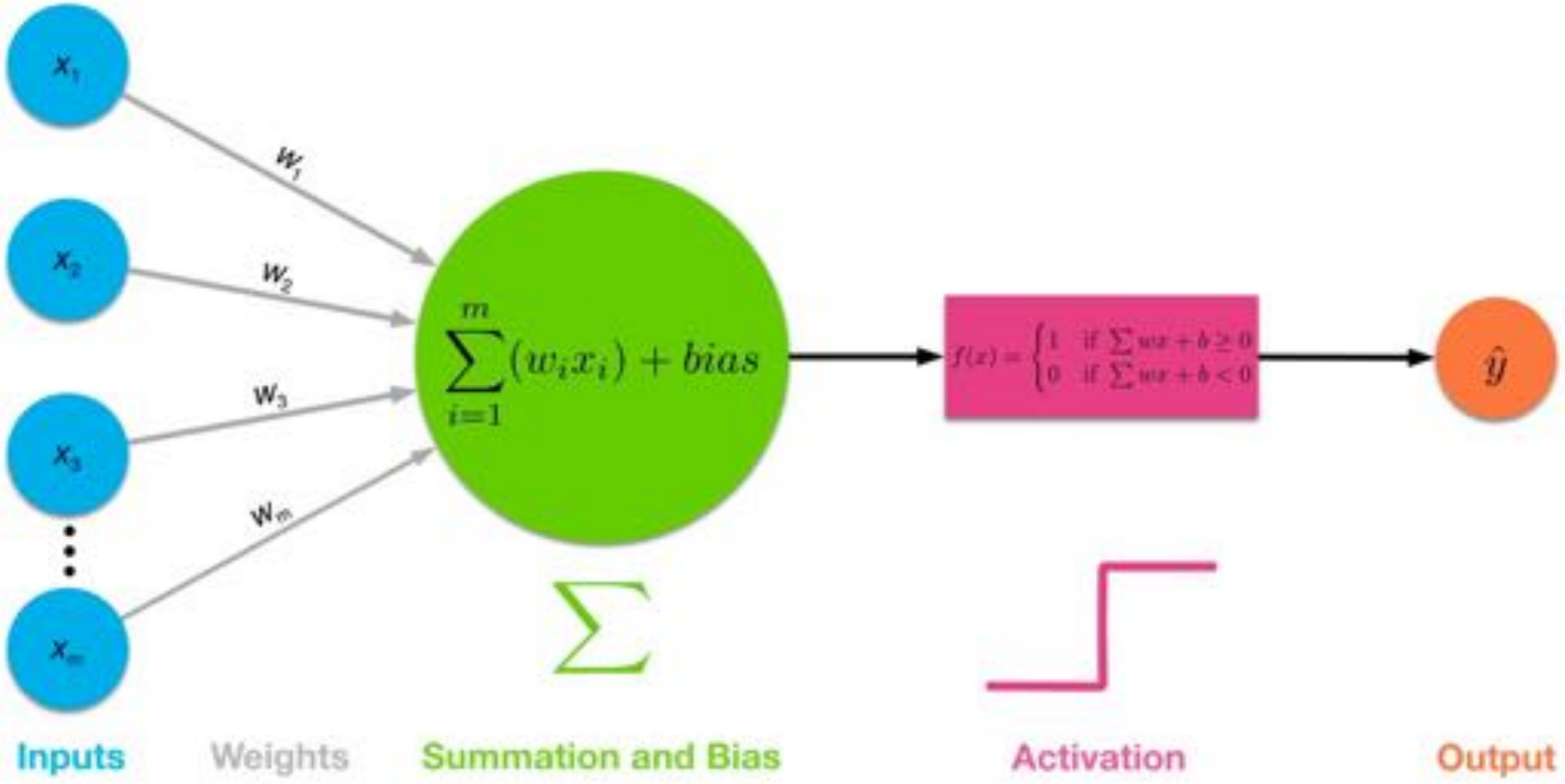
$$\max(0, x)$$

In practice, NN with multiple hidden layers work better than with a single hidden layer.

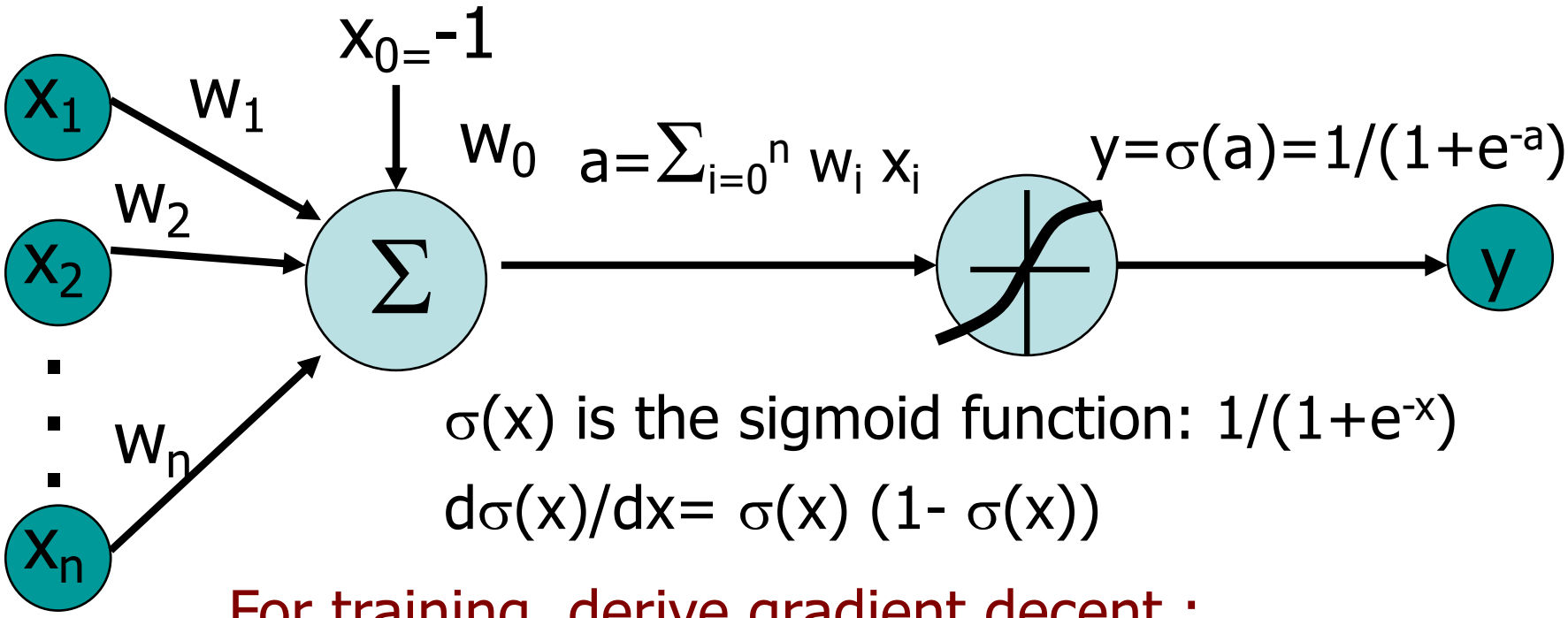
Artificial Neural Networks are inspired by neural networks



Abstract Neural Unit



Commonly, neurons are encoded as **Sigmoid Unit (but other units are possible)**



$\sigma(x)$ is the sigmoid function: $1/(1+e^{-x})$

$d\sigma(x)/dx = \sigma(x)\,(1-\sigma(x))$

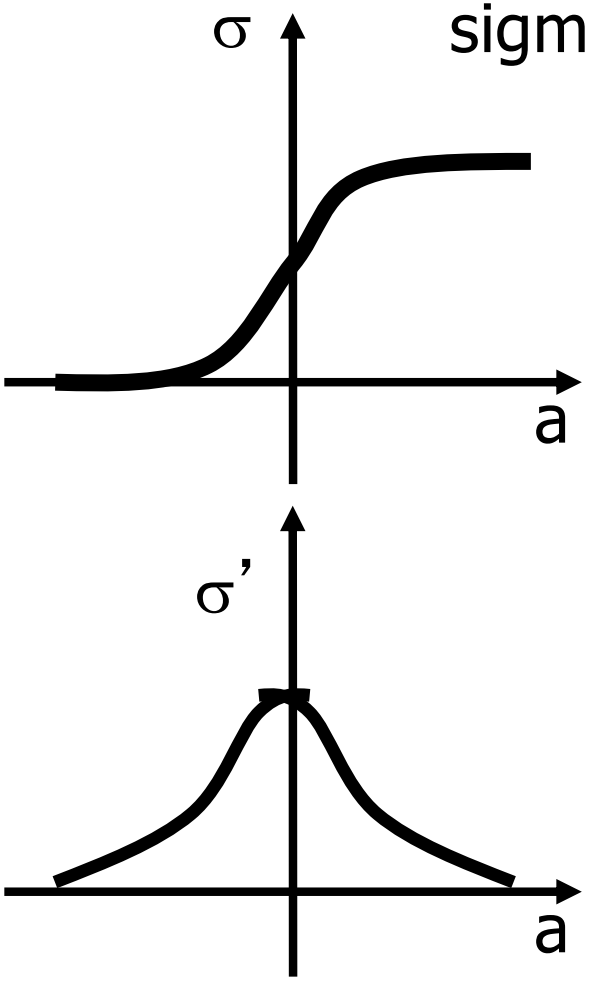
For training, derive gradient decent :

- one sigmoid function

  $\partial E/\partial w_i = -\sum_p (t^p - y^p)\, y^p\, (1-y^p)\, x_i^p$

- Multilayer networks of sigmoid units use **backpropagation**

Gradient Descent Rule for Sigmoid Output Function



sigmoid

$$E^p[w_1,\ldots,w_n] = \tfrac{1}{2}\,(t^p-y^p)^2$$

$$\partial E^p/\partial w_i = \partial/\partial w_i\ \tfrac{1}{2}\,(t^p-y^p)^2$$

$$= \partial/\partial w_i\ \tfrac{1}{2}\,(t^p-\sigma(\textstyle\sum_i w_i\, x_i^p))^2$$

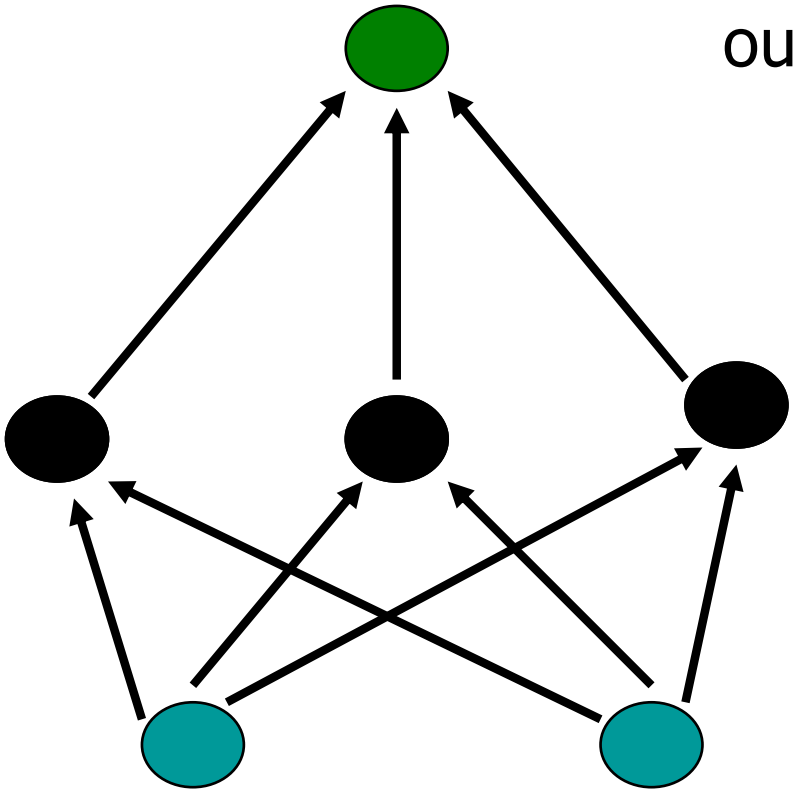
$$= (t^p-y^p)\ \sigma'(\textstyle\sum_i w_i\, x_i^p)\ (-x_i^p)$$

for $y=\sigma(a) = 1/(1+e^{-a})$

$\sigma'(a)= e^{-a}/(1+e^{-a})^2=\sigma(a)\,(1-\sigma(a))$

$$w'_i= w_i + \alpha\ y^p\,(1-y^p)(t^p-y^p)\ x_i^p$$

Build (feedforward) Multi-Layer Networks by sticking together units

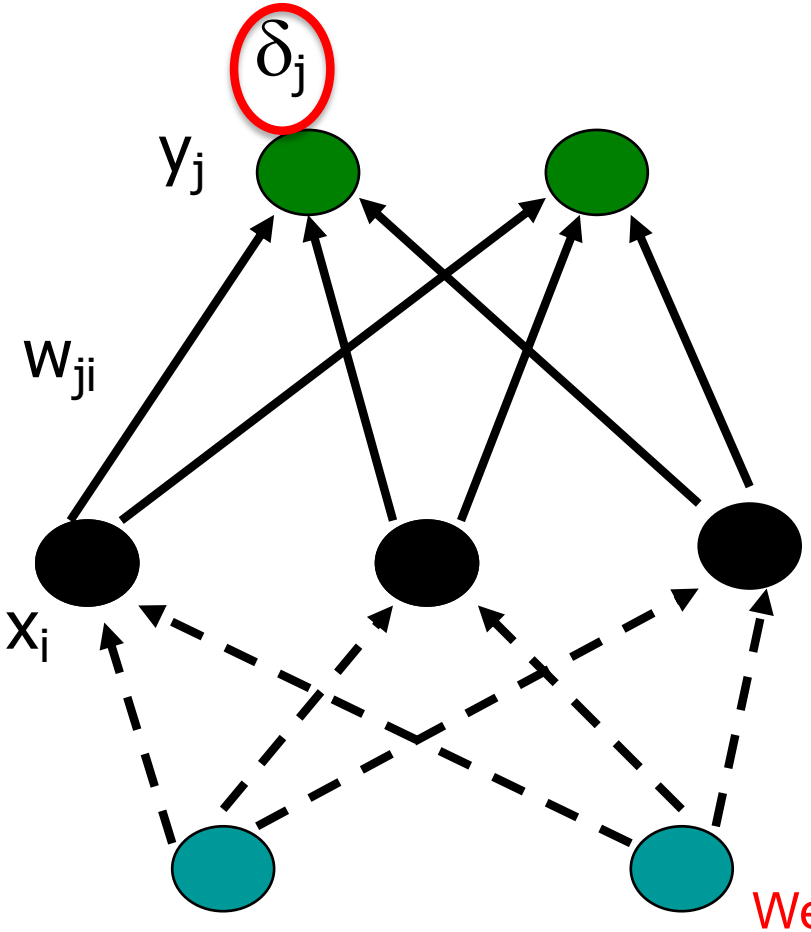


output layer

hidden layer

input layer

Training-Rule for Weights to the Output Layer



$$E^p[w_{ij}] = \tfrac{1}{2} \Sigma_j (t_j^p - y_j^p)^2$$

$$\partial E^p/\partial w_{ji} = \partial/\partial w_{ji} \tfrac{1}{2} \Sigma_j (t_j^p - y_j^p)^2$$
$$= \ldots$$
$$= - y_j^p(1-y^p_j)(t^p_j - y^p_j)\ x_i^p$$

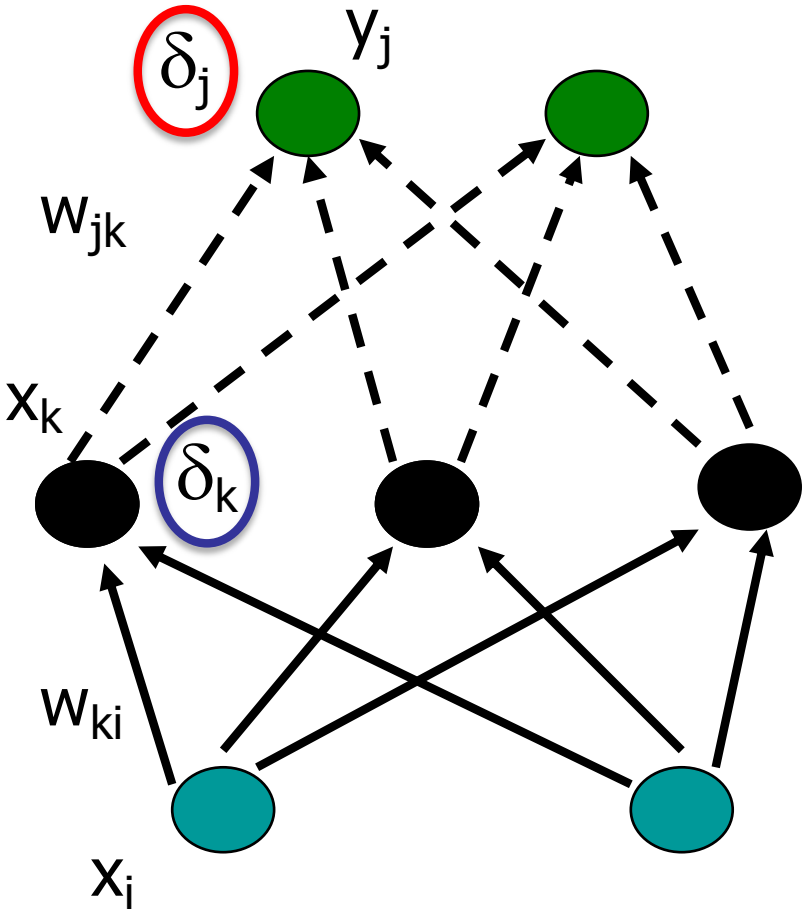
$$\Delta w_{ji} = \alpha\ y_j^p(1-y_j^p)\ (t^p_j - y_j^p)\ x_i^p$$
$$= \alpha\ \delta_j^p\ x_i^p$$

activation

We just want to rewrite in terms of input-output only

with $\delta_j^p := y_j^p(1-y_j^p)\ (t^p_j - y_j^p)$

Training-Rule for Weights to the Output Layer



Credit assignment problem:
No target values t for hidden layer units.

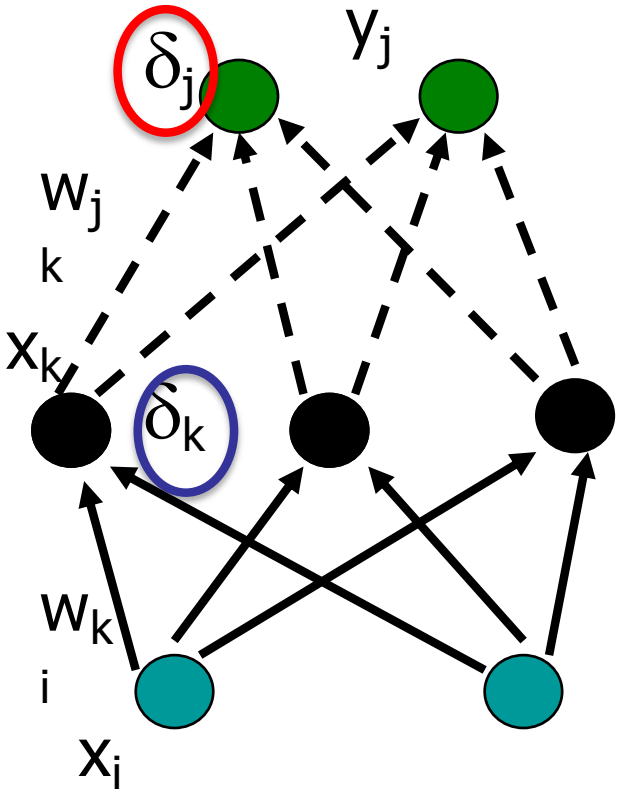
Error for hidden units?

$$\delta_k = \Sigma_j \, w_{jk} \, \delta_j \, y_j \, (1-y_j)$$

$$\Delta w_{ki} = \alpha \; x_k^p(1-x_k^p) \; \delta_k^p \; x_i^p$$

activation — $x_k^p(1-x_k^p)$: View x_k as intermediate output — δ_k^p — x_i^p: activation

Training-Rule for Weights to the Output Layer

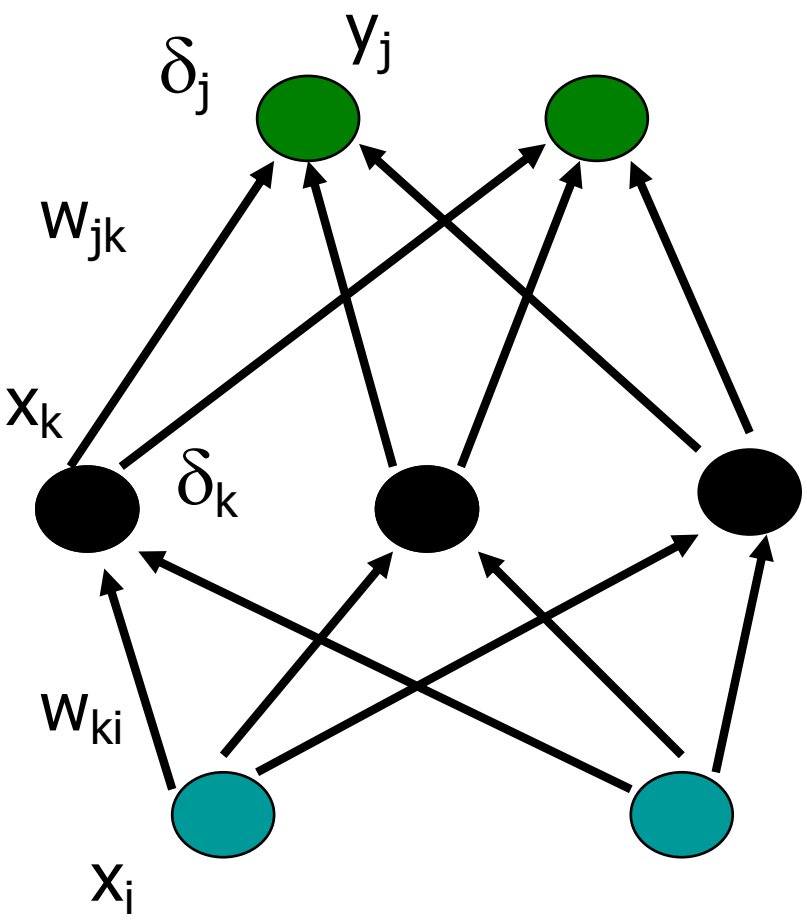


$$E^p[w_{ki}] = \tfrac{1}{2} \Sigma_j (t_j^p - y_j^p)^2$$

$$\partial E^p/\partial w_{ki} = \partial/\partial w_{ki}\ \tfrac{1}{2} \Sigma_j (t_j^p - y_j^p)^2$$
$$= \partial/\partial w_{ki}\ \tfrac{1}{2} \Sigma_j (t_j^p - \sigma(\Sigma_k w_{jk}\ x_k^p))^2$$
$$= \partial/\partial w_{ki}\ \tfrac{1}{2} \Sigma_j (t_j^p - \sigma(\Sigma_k w_{jk}\ \sigma(\Sigma_i w_{ki}\ x_i^p)))^2$$
$$= -\Sigma_j (t_j^p - y_j^p)\ \sigma'_j(a)\ w_{jk}\ \sigma'_k(a)\ x_i^p$$
$$= -\Sigma_j\ \delta_j\ w_{jk}\ \sigma'_k(a)\ x_i^p$$
$$= -\Sigma_j\ \delta_j\ w_{jk}\ x_k\ (1-x_k)\ x_i^p$$

$$\Delta w_{ki} = \alpha\ \delta_k\ x_i^p \quad \text{with } \delta_k = \Sigma_j\ \delta_j\ w_{jk}\ x_k(1-x_k)$$

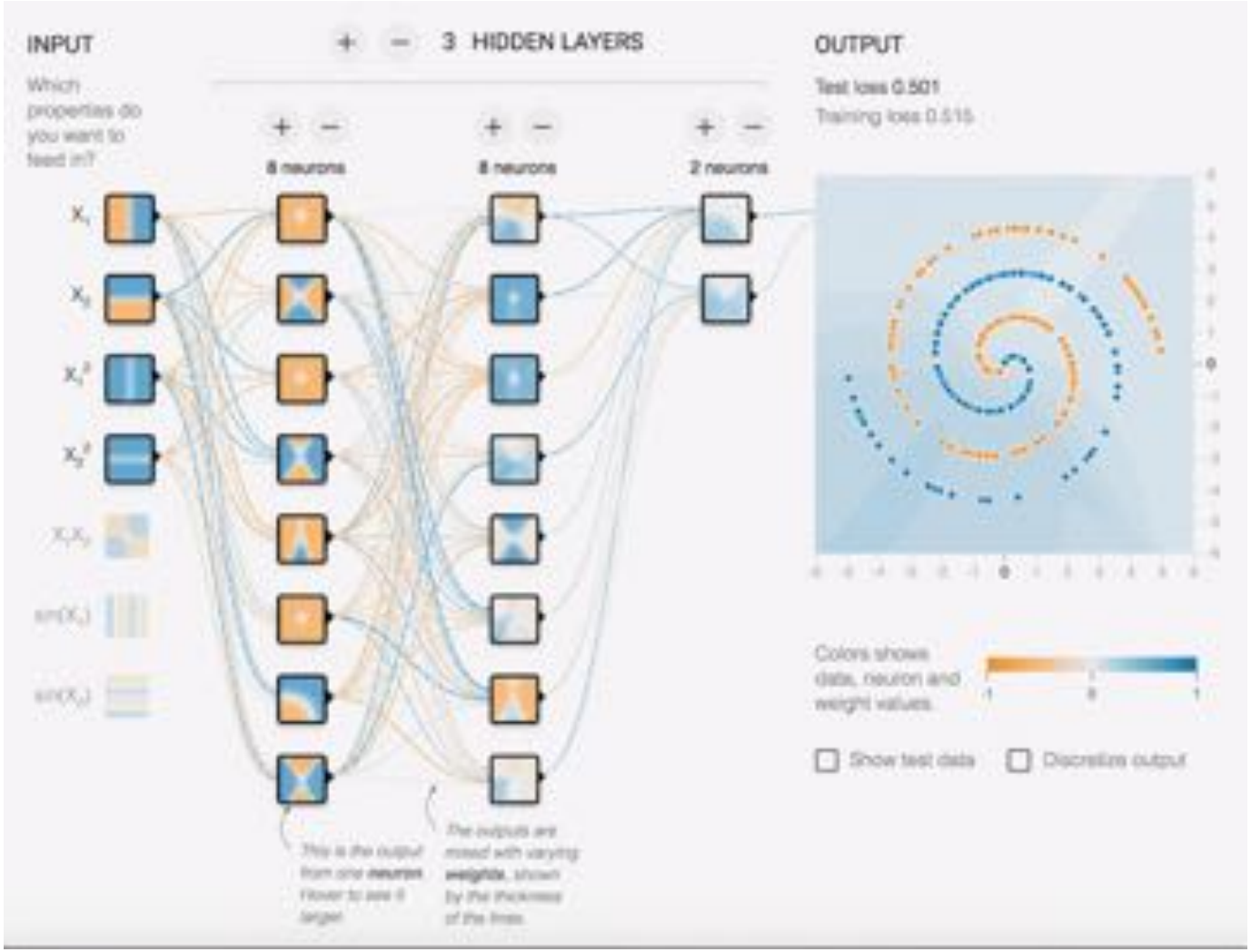
Backpropagation



Backward step:
propagate errors from output to hidden layer

Forward step:
Propagate activation from input to output layer

Tinker with a neural network at http://playground.tensorflow.org/



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The first breakthrough of (D)NNs was on image classification

Deep Convolutional Networks

- Convolutional layer
- Non-linear activation function ReLU
- Max pooling layer
- Fully connected layer

Deep Convolutional Networks CNNs

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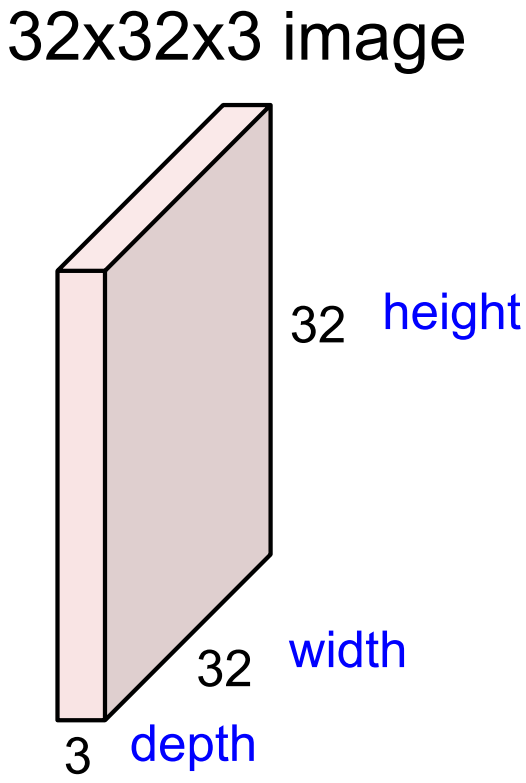
Compared to standard neural networks with similarly-sized layers,

- CNNs have much fewer connections and parameters
- and so they are easier to train
- and typically have more than five layers (a number of layers which makes fully-connected neural networks almost impossible to train properly when initialized randomly)
- and they are tailored towards computer vision

LeNet, 1998 LeCun Y, Bottou L, Bengio Y, Haffner P: Gradient-Based Learning Applied to Document Recognition, Proceedings of the IEEE

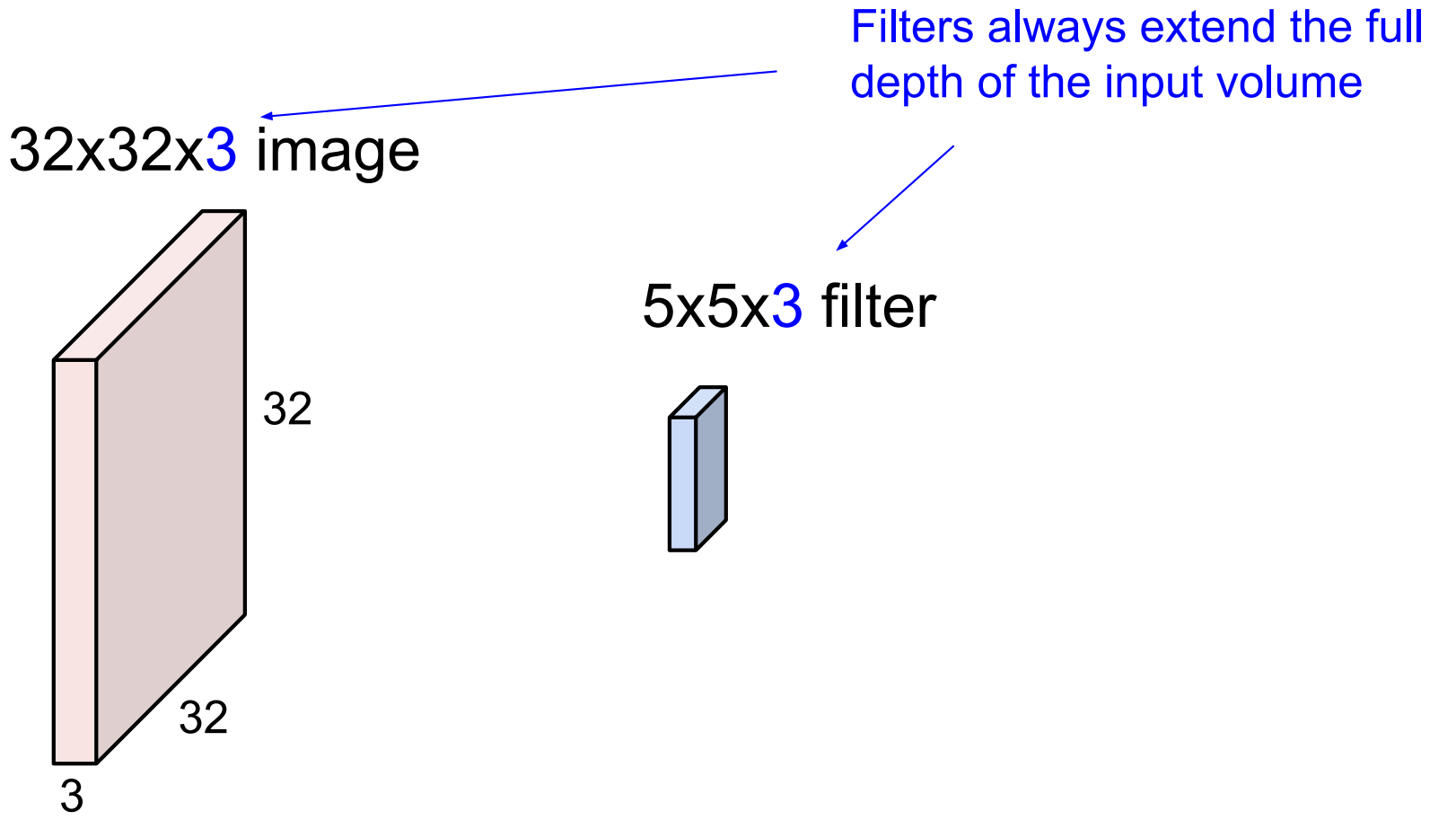
AlexNet, 2012 Krizhevsky A, Sutskever I, Hinton G: ImageNet Classification with Deep Convolutional Neural Networks, NIPS 2012

Convolutional layer



Filter try to detect local patterns such as color, edges, …

Convolutional layer

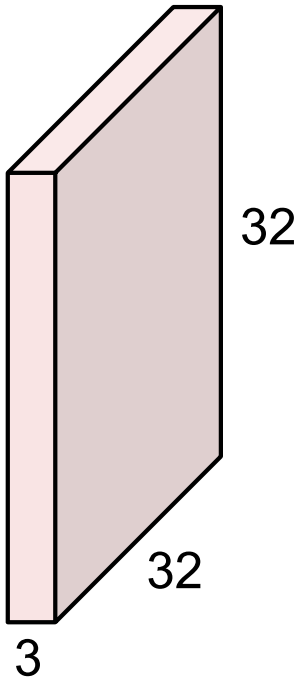


Filter try to detect local patterns such as color, edges, …

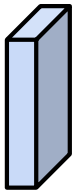
Convolutional layer

Filters always extend the full depth of the input volume

32x32x3 image



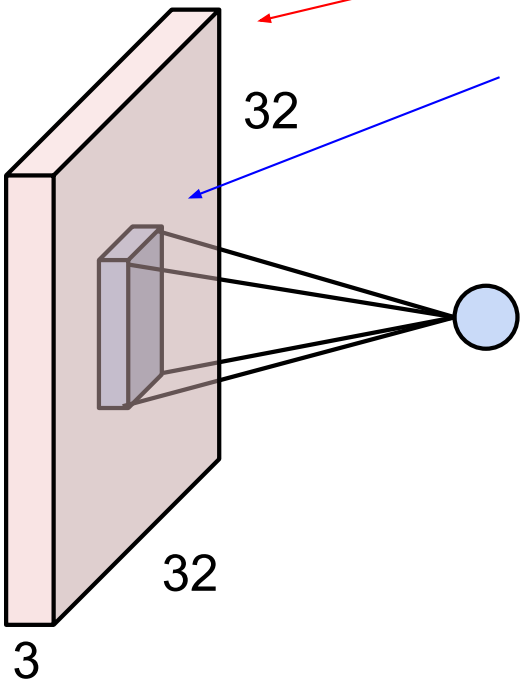
5x5x3 filter



Convolve the filter with the image i.e. “slide over the image spatially, computing dot products”

Filter try to detect local patterns such as color, edges, …

Convolutional layer

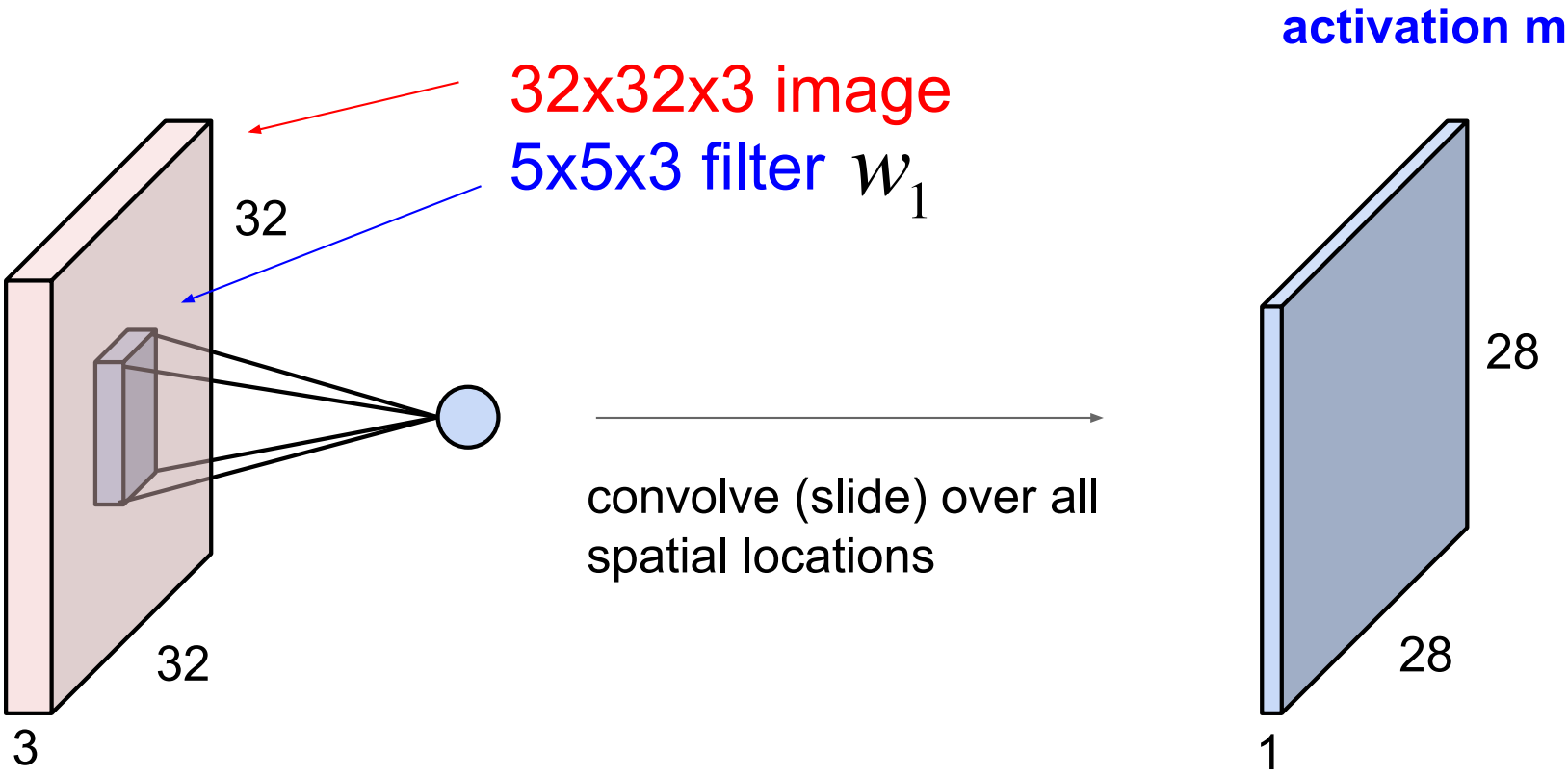


1 number:
the result of taking a dot product between the filter and a small 5x5x3 chunk of the image x

$w^T x$ (in general, $w^T x$ + bias)

Filter try to detect local patterns such as color, edges, …

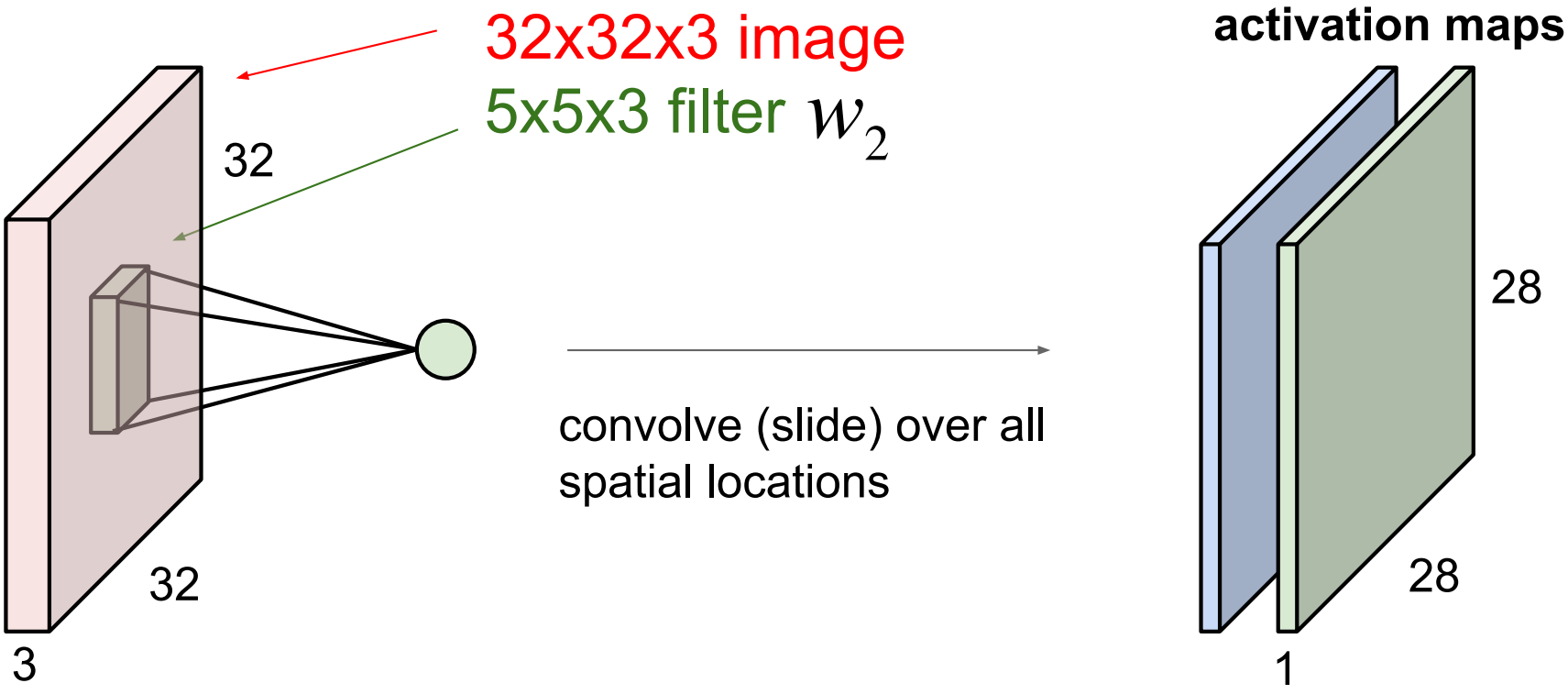
Convolutional layer



Filter try to detect local patterns such as color, edges, …

Convolutional layer

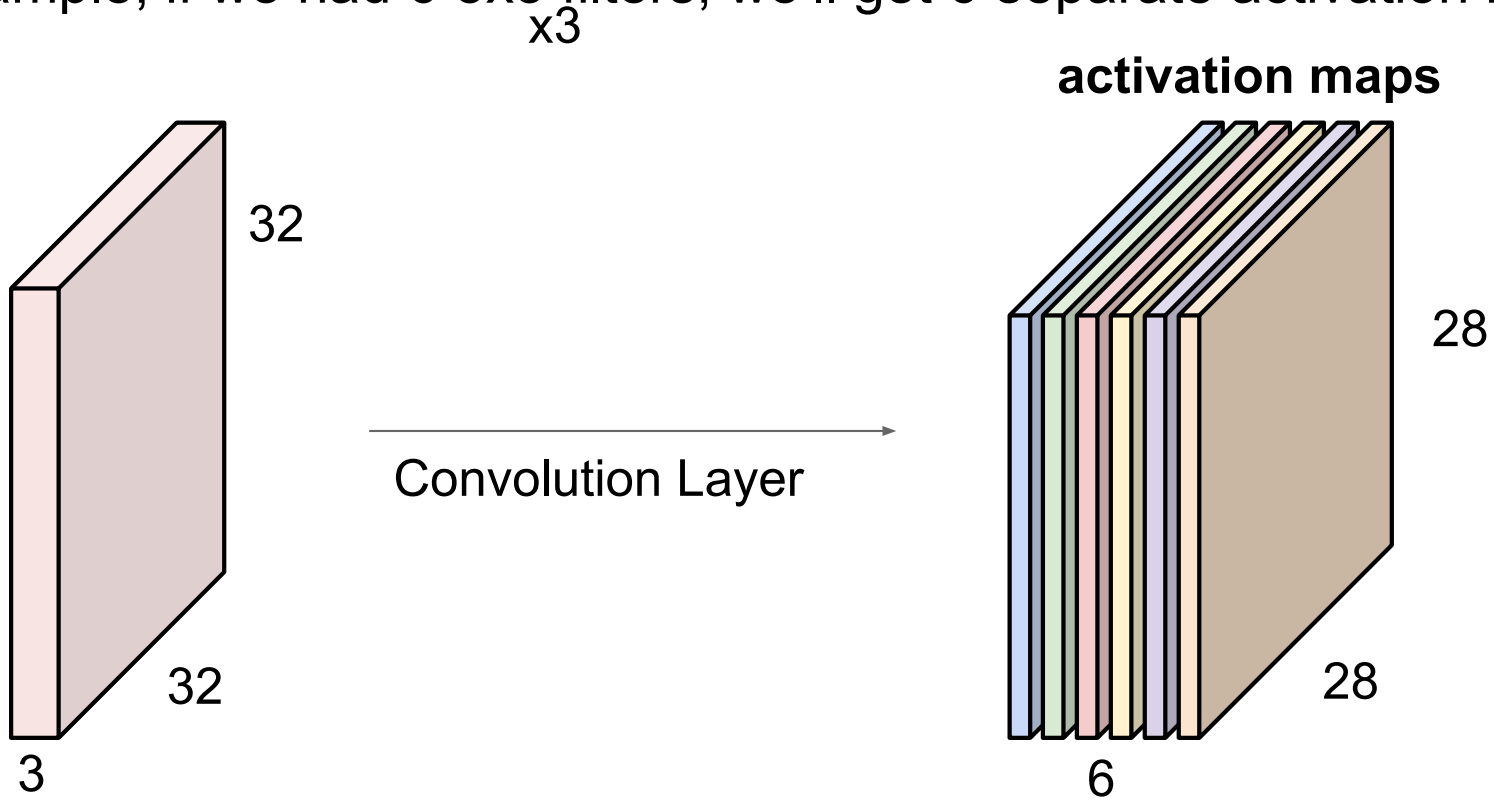
consider a second, green filter



Filter try to detect local patterns such as color, edges, …

Convolutional layer

For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:

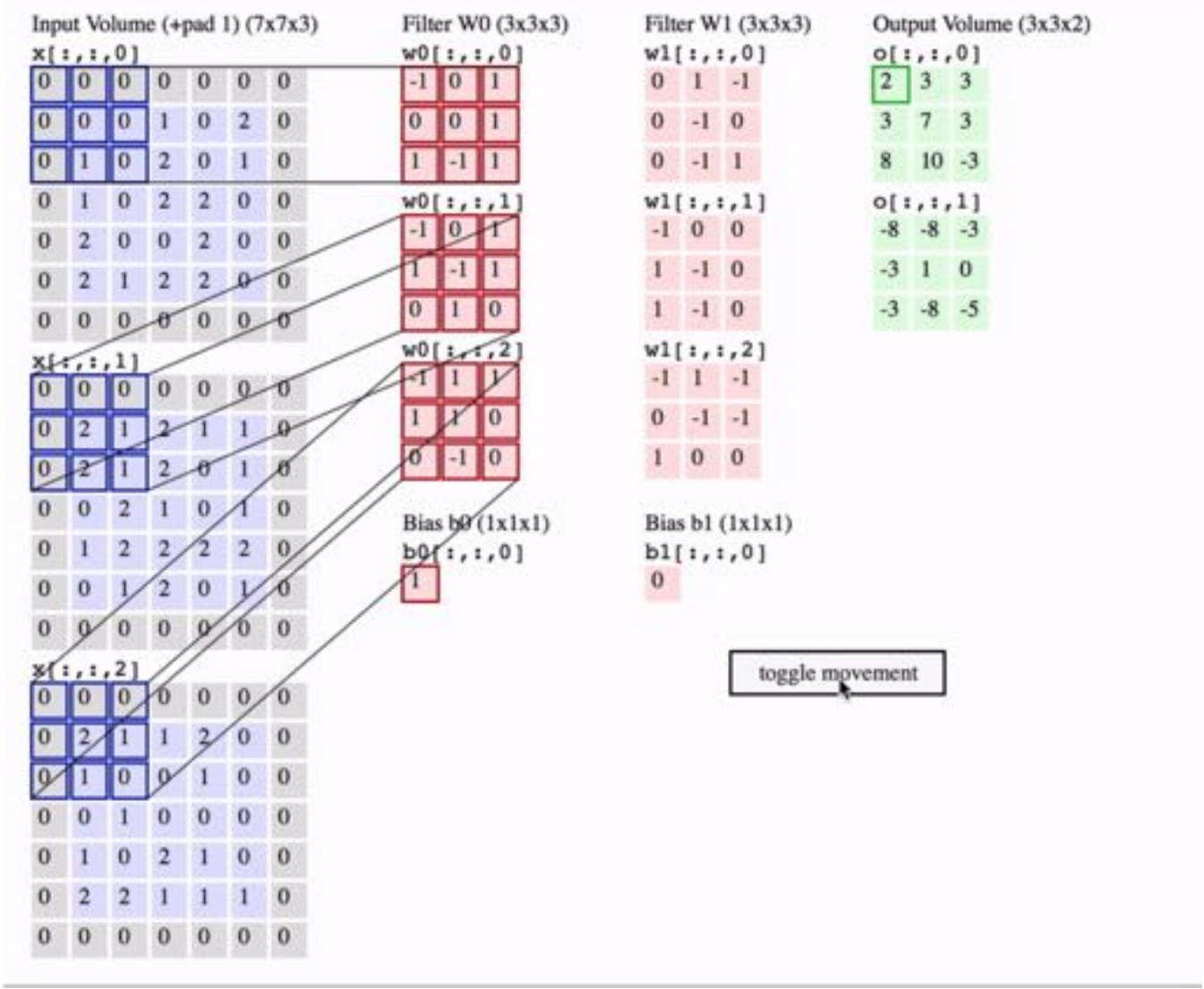


We stack these up to get a "new image" of size 28x28x6!

Filter try to detect local patterns such as color, edges, …

Convolutional layer demo

To see this in action: http://cs231n.github.io/assets/conv-demo/index.html



Why is it called convolutional layer?

Because it is related to convolution of two signals:

$$f[x,y] * g[x,y] = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} f[n_1,n_2] \cdot g[x-n_1, y-n_2]$$

elementwise multiplication and sum of a filter and the signal (image)

E.g. convolution by a bump function is a kind of "blurring", i.e., its effect on images is similar to what a short-sighted person experiences when taking off his or her glasses.

… or edges

Input image

Convolution Kernel

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

Feature map

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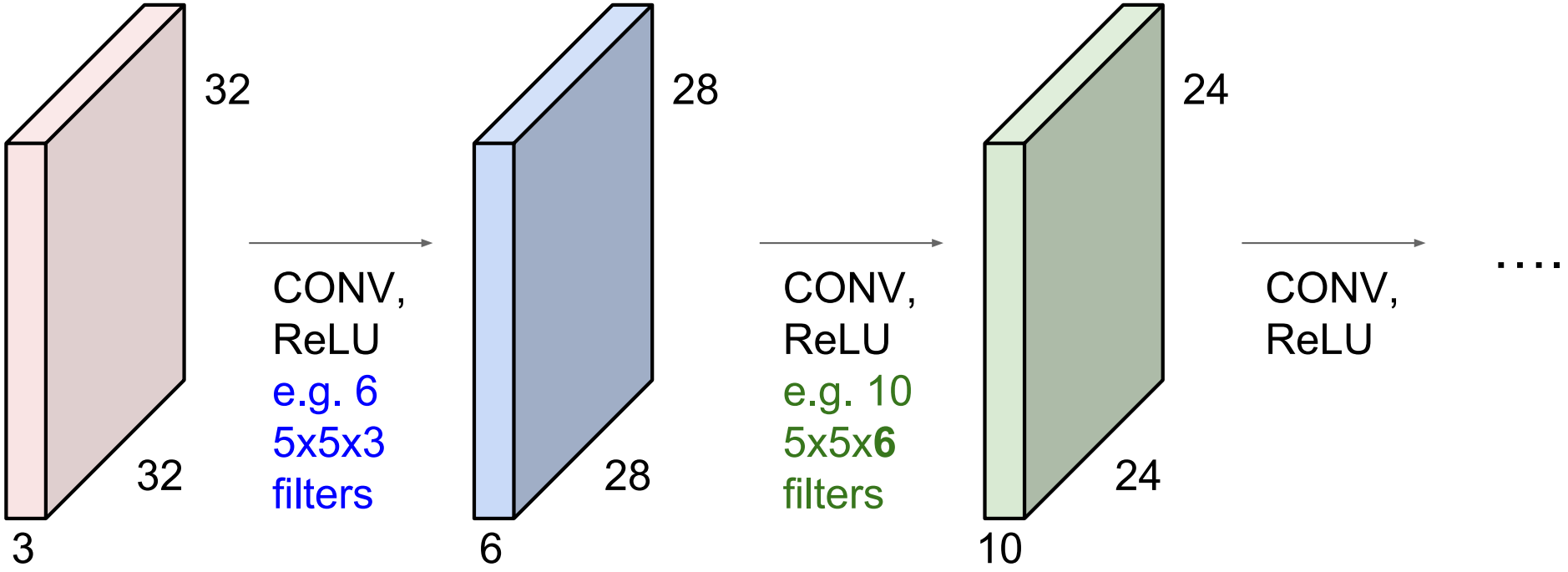
Deep Convolutional Networks

- Convolutional layer
- Non-linear activation function ReLU
- Max pooling layer
- Fully connected layer

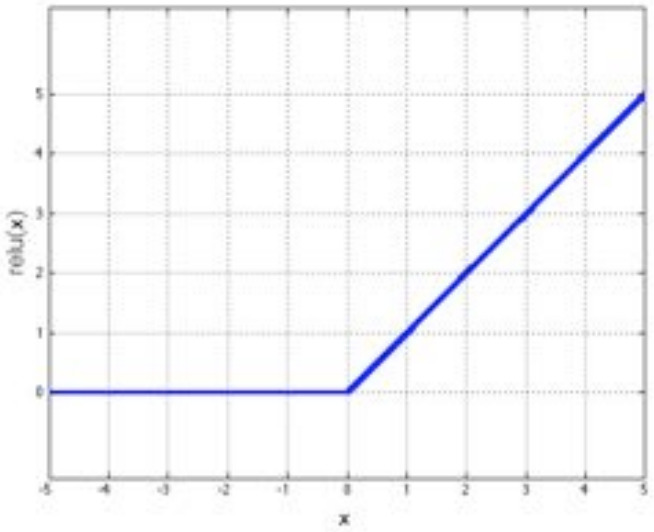
Where is ReLU?

Preview: ConvNet is a sequence of Convolutional Layers, interspersed with activation functions



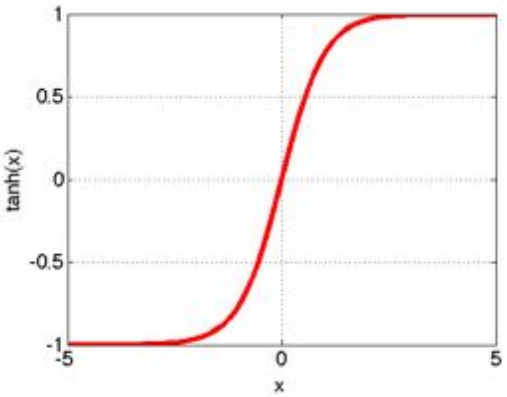
Rectified Linear Unit, ReLU

- Non-linear activation function are applied per-element
- Rectified linear unit (ReLU):
  - max(0,x)
  - makes learning faster (in practice x6)
  - avoids saturation issues (unlike sigmoid, tanh)
  - simplifies training with backpropagation
  - preferred option (works well)

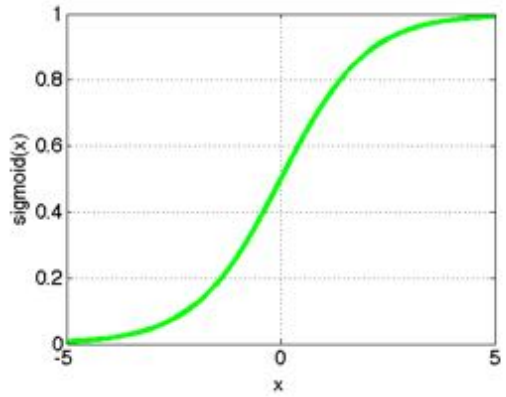


Other examples:

tanh(x)



$\text{sigmoid}(x)=(1+e^{-x})^{-1}$



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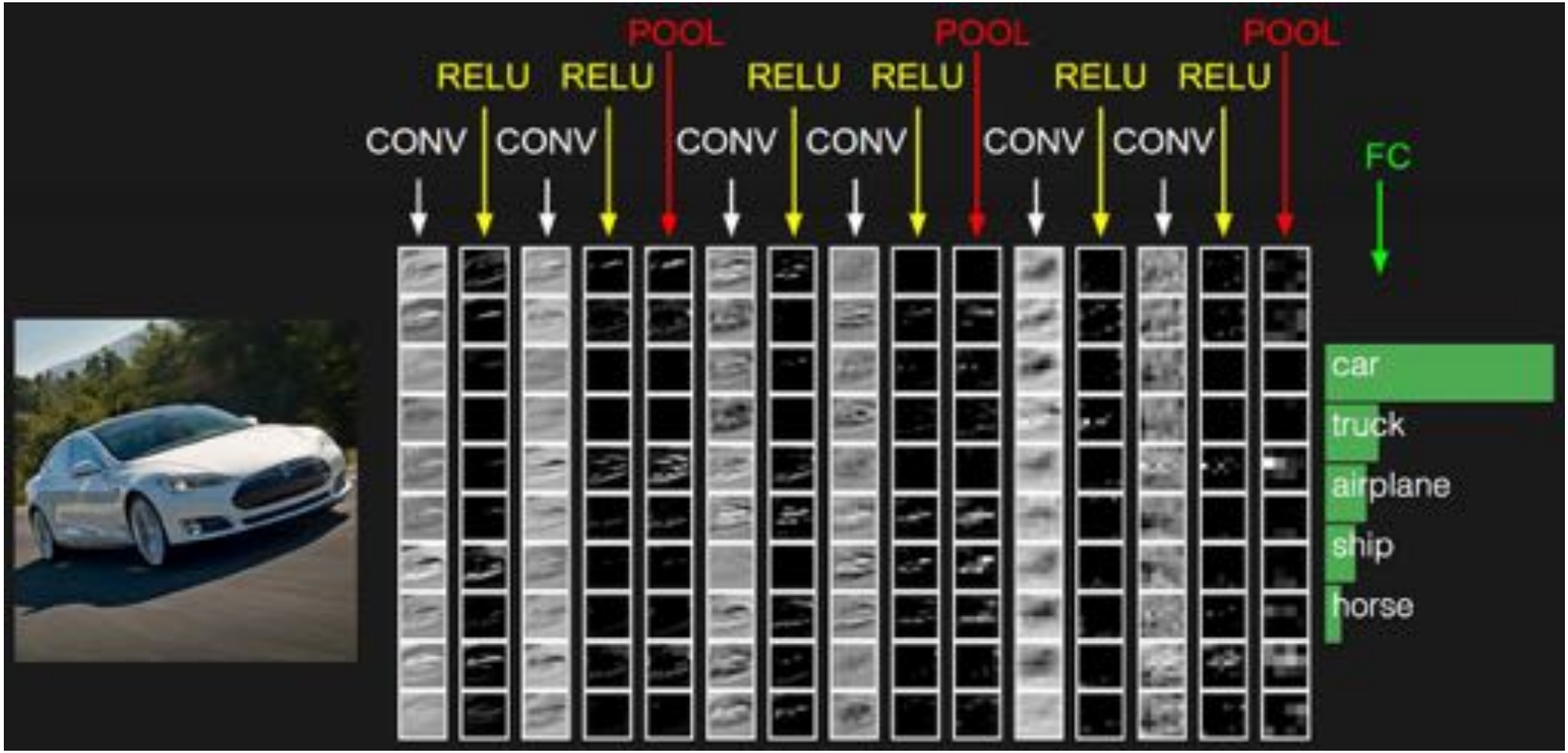
Deep Convolutional Networks

- ❑ Convolutional layer
- ❑ Non-linear activation function ReLU
- ❑ Max pooling layer
- ❑ Fully connected layer

Where is pooling?

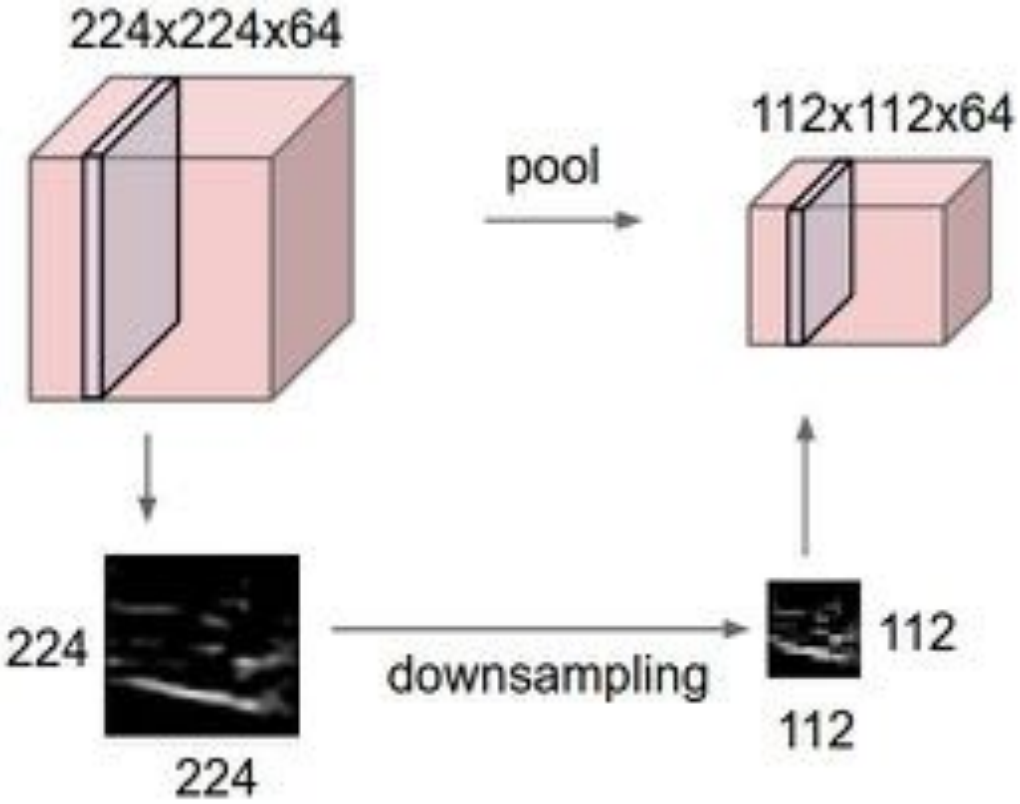


Two more layers to go: pooling and fully connected layers ☺

Spatial pooling

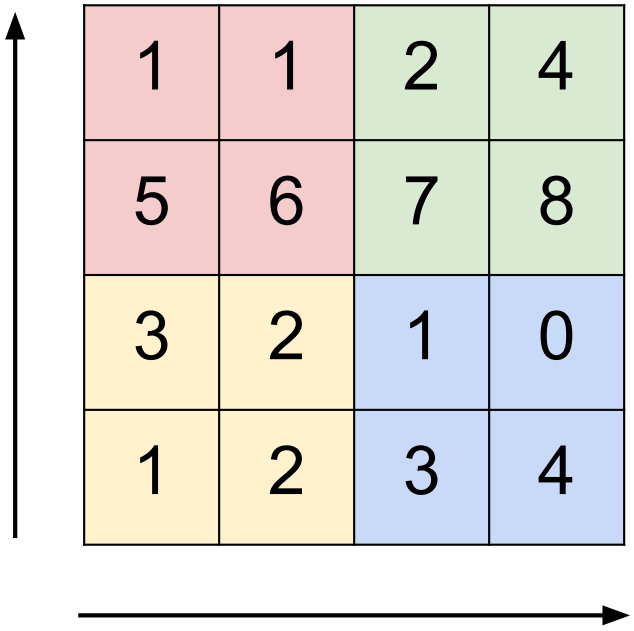
Pooling layer

- **Makes the representations smaller (downsampling)**
- Operates over each activation map independently
- Role: invariance to small transformation

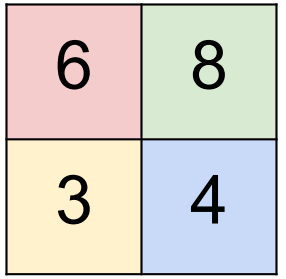


Max pooling

Single activation map



max pool with 2x2 filters
and stride 2



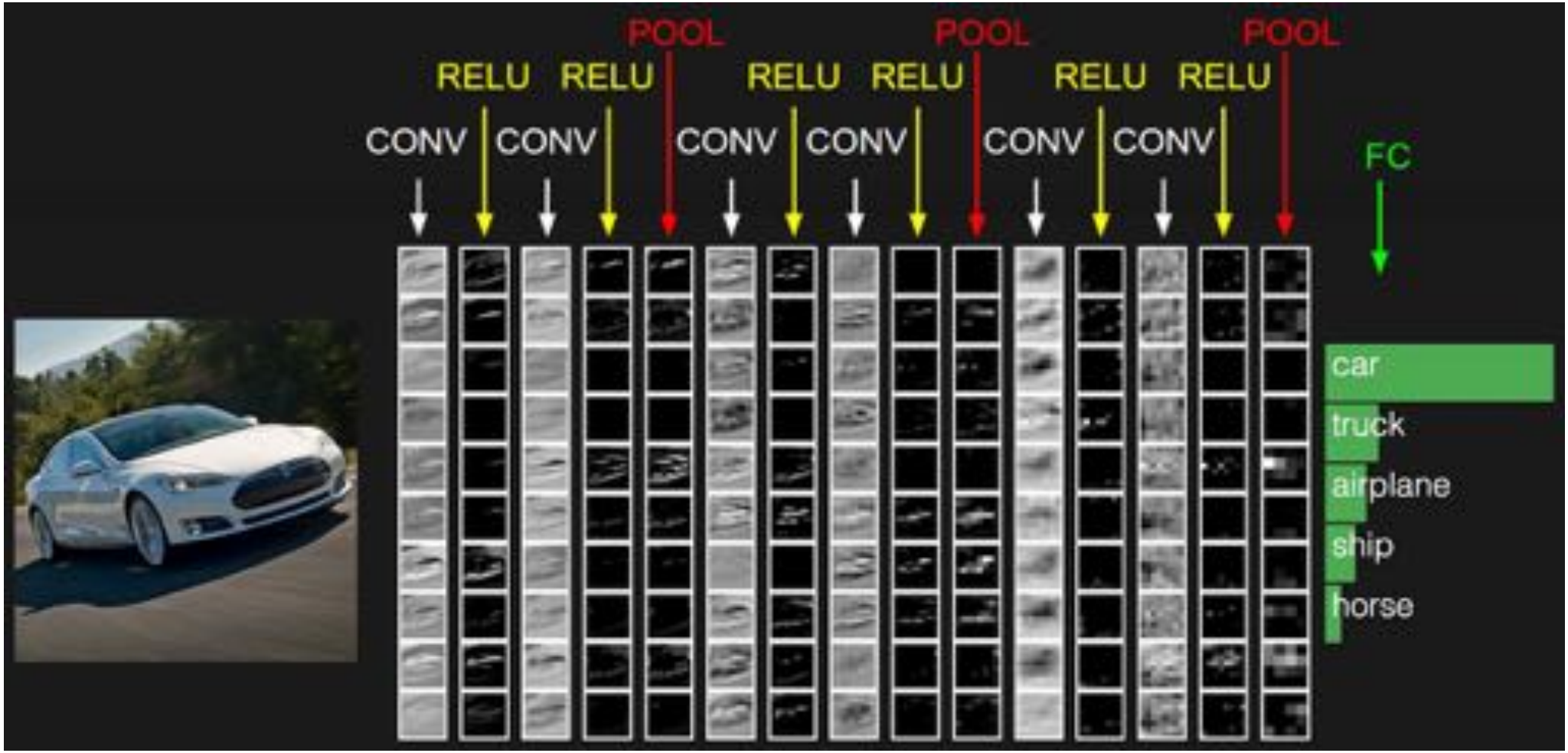
Alternatives:

- sum pooling
- overlapping pooling

Deep Convolutional Networks

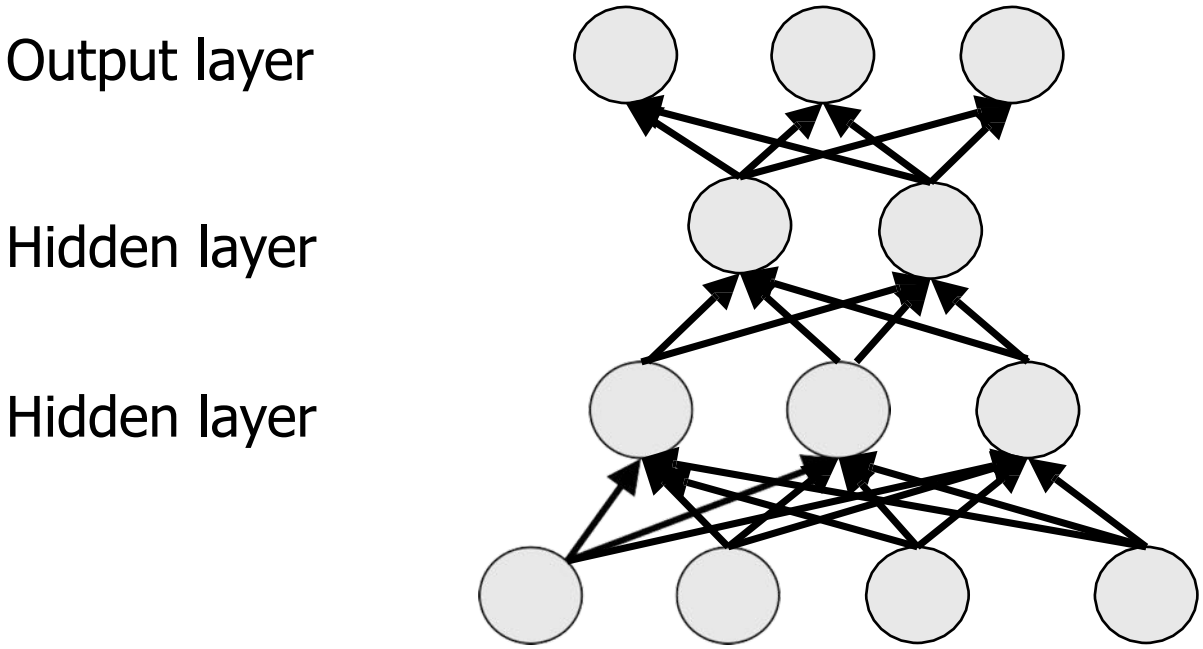
- Convolutional layer
- Non-linear activation function ReLU
- Max pooling layer
- Fully connected layer

Where is a fully connected layer (FC)?



Fully connected (last) layer

Contains neurons that connect to the entire input volume, as in ordinary Neural Networks:

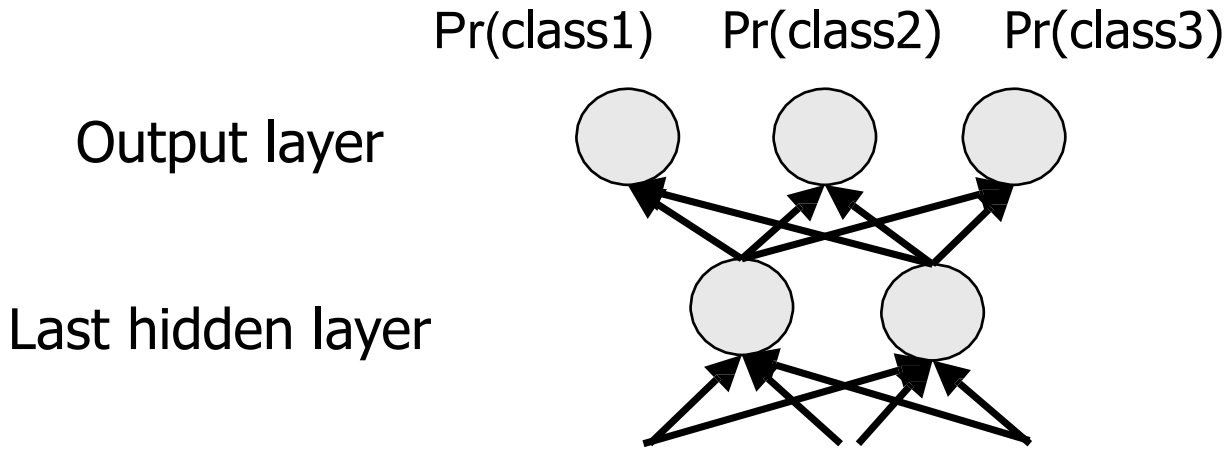


neurons between two adjacent layers are fully pairwise connected, but neurons within a single layer share no connections

Output layer

In classification:

- the output layer is fully connected with number of neurons equal to number of classes
- followed by softmax non-linear activation



Running CNNs demo

To see this in action, check

http://cs.stanford.edu/people/karpathy/convnetjs/demo/cifar10.html

https://www.tensorflow.org/tutorials/deep_cnn

http://scienceai.github.io/neocortex/cifar10_cnn/

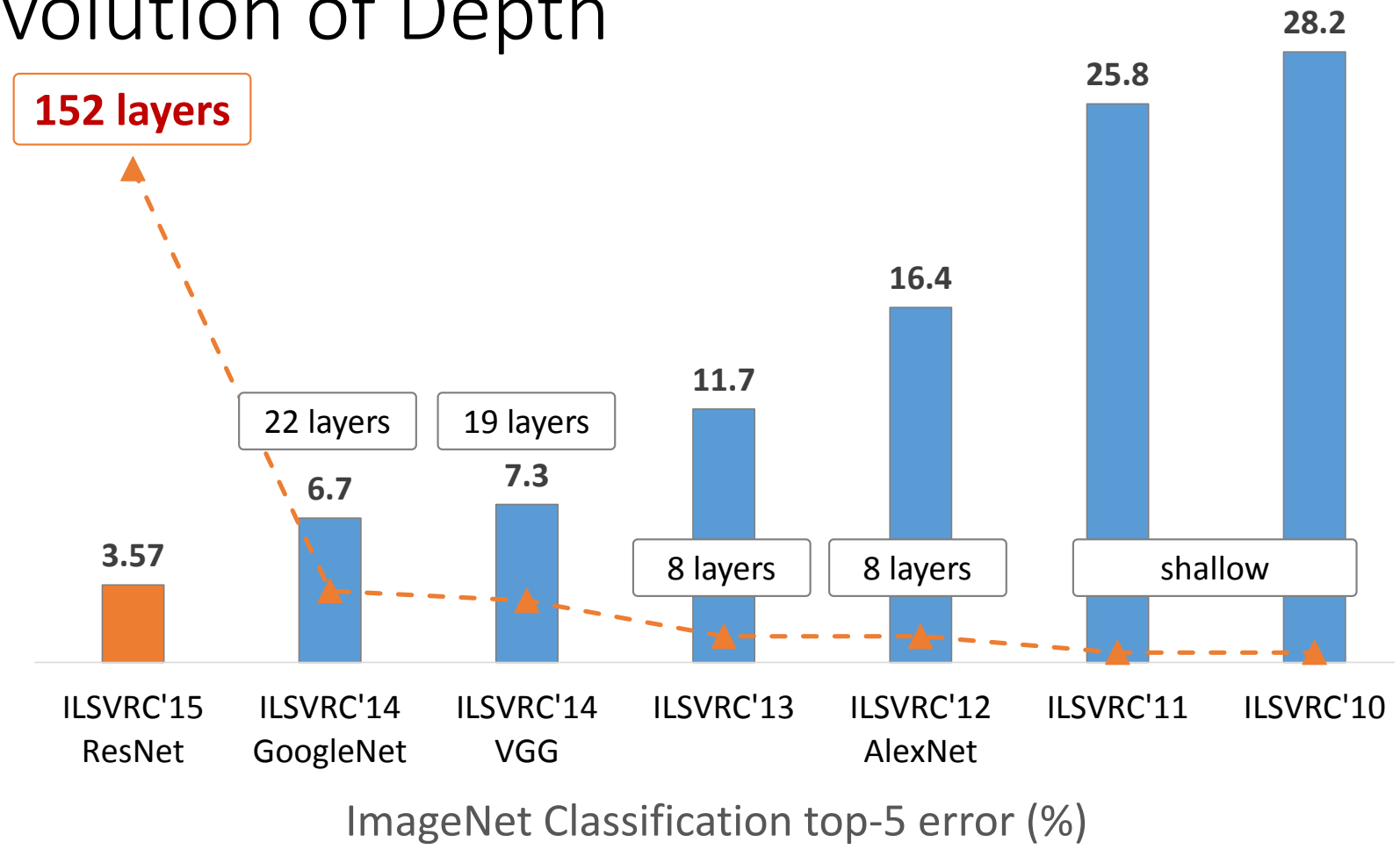
- Deep Networks are composed of multiple levels of non-linear operations, such as neural nets with many hidden layers
- We went through the architecture of a standard deep network and have seen all major ingredients.

Deep Convolutional Networks

- Convolutional layer
- Non-linear activation function ReLU
- Max pooling layer
- Fully connected layer

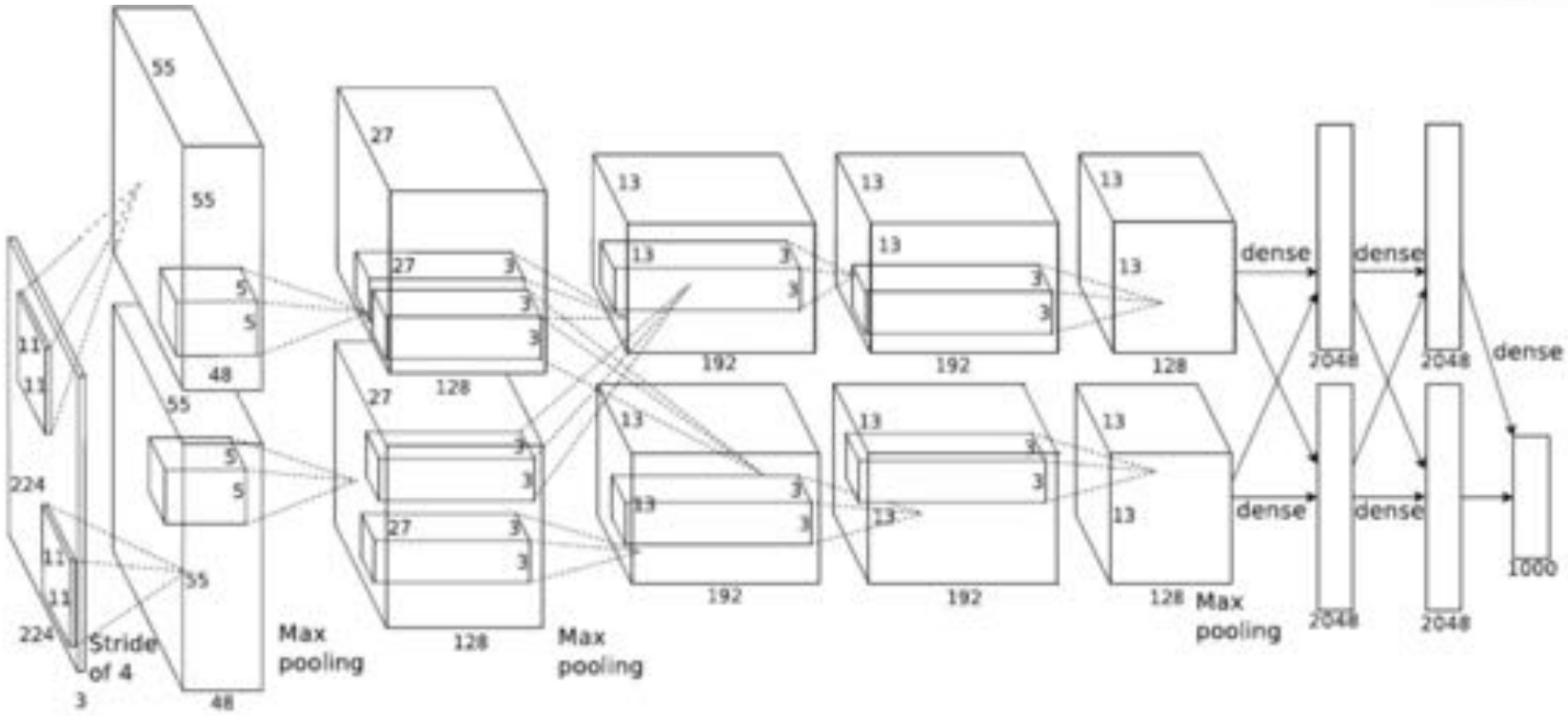
Fast-forward to today

Revolution of Depth



Kaiming He, et al. Deep residual learning for Image Recognition, 2015

A “deeper” example: AlexNet



- Input: RGB image
- Output: class label (out of 1000 classes)
- 5 convolutional layers + 3 fully connected layers (with ReLU, max pooling)
- trained using 2 streams (2 GPU). In this lecture, we will present the architecture as 1 stream for simplicity and clarity.

AlexNet was trained on ImageNet

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- 15M images
- 22K categories
- Images collected from Web
- Human labelers (Amazon's Mechanical Turk crowd-sourcing)
- ImageNet Large Scale Visual Recognition Challenge (ILSVRC-2010)
    - 1K categories
    - 1.2M training images (~1000 per category)
    - 50,000 validation images
    - 150,000 testing images
- RGB images; mean normalization
- Variable-resolution, but this architecture scales them to 256x256 size

ImageNet Tasks

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Classification goals:

- Make 1 guess about the label (Top-1 error)
- make 5 guesses about the label (Top-5 error)

Results of AlexNet on ImageNet

What have we learnt so far?

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- Deep Neural Networks aim at learning feature hierachies
- We have understood the structure of convolutional neural networks, one of the central DNN architectures

  Convolutional layer, ReLU,Max pooling layer, fully connected layer
- DNNs are rather large but result in state-of-the-art performance on many tasks

Let's now consider training in more details

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- Training Deep Convolutional Neural Networks
  - Stochastic gradient descent
  - Backpropagation
  - Initialization
- Preventing overfitting
  - Dropout regularization
  - Data augmentation
- Fine-tuning

Stochastic gradient descent (SGD)

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(Mini-batch) SGD

Initialize the parameters randomly but smart

Loop over the whole training data (multiple times):

- **Sample** a datapoint (a batch of data)
- **Forward** propagate the data through the network, compute the classification loss. $E = \frac{1}{2}(y_{predicted} - y_{true})^2$
- **Backpropagate** the gradient of the loss w.r.t. parameters through the network
- **Update** the parameters using the gradient $w^{t+1} = w^t - \alpha \cdot \frac{dE}{dw}(w^t)$

Recall Backpropagation

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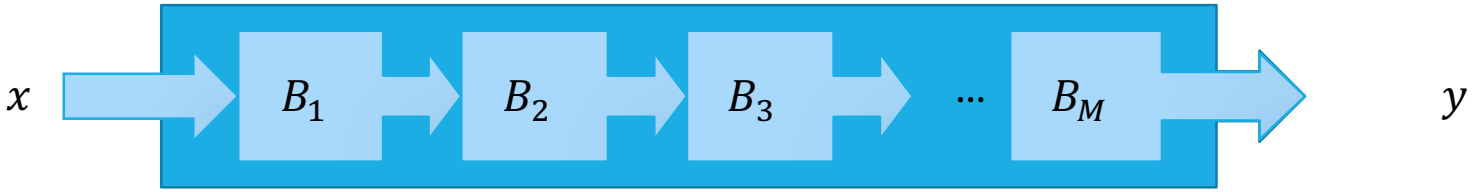
Implementations typically maintain a modular structure, where the nodes/bricks implement the forward and backward procedures

Sequential brick



Propagation

- Apply propagation rule to $B_1, B_2, B_3, \dots, B_M$.

Back-propagation

- Apply back-propagation rule to $B_M, \dots, B_3, B_2, B_1$.

Recall Backpropagation

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Last layer used for classification

Square loss brick

Propagation

$$E = y = \frac{1}{2}(x - d)^2$$

Back-propagation

$$\frac{\partial E}{\partial x} = (x - d)^T \frac{\partial E}{\partial y} = (x - d)^T$$

Recall Backpropagation

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Typical choices

Loss bricks

		Propagation	Back-propagation
Square		$y = \frac{1}{2}(x-d)^2$	$\frac{\partial E}{\partial x} = (x-d)^T \frac{\partial E}{\partial y}$
Log	$c = \pm 1$	$y = \log(1+e^{-cx})$	$\frac{\partial E}{\partial x} = \frac{-c}{1+e^{cx}} \frac{\partial E}{\partial y}$
Hinge	$c = \pm 1$	$y = \max(0, m-cx)$	$\frac{\partial E}{\partial x} = -c \ \mathbb{I}\{cx < m\} \frac{\partial E}{\partial y}$
LogSoftMax	$c = 1 \dots k$	$y = \log(\sum_k e^{x_k}) - x_c$	$\left[\frac{\partial E}{\partial x}\right]_s = (e^{x_s}/\sum_k e^{x_k} - \delta_{sc}) \frac{\partial E}{\partial y}$
MaxMargin	$c = 1 \dots k$	$y = \left[\max_{k \neq c}\{x_k + m\} - x_c\right]_+$	$\left[\frac{\partial E}{\partial x}\right]_s = (\delta_{sk^*} - \delta_{sc}) \ \mathbb{I}\{E > 0\} \frac{\partial E}{\partial y}$

Recall Backpropagation

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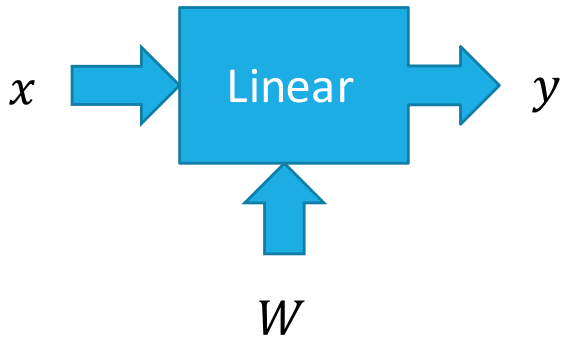
Fully connected layers, convolutional layers (dot product)

Linear brick



Propagation

$$y = Wx$$

Back-propagation

$$\frac{\partial E}{\partial x} = \frac{\partial E}{\partial y} W$$

$$\frac{\partial E}{\partial W} = x \frac{\partial E}{\partial v}$$

Recall Backpropagation

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Non-linear activations

Activation function brick

Propagation

$$y_s = f(x_s)$$

Back-propagation

$$\left[\frac{\partial E}{\partial x}\right]_s = \left[\frac{\partial E}{\partial y}\right]_s f'(x_s)$$

Recall Backpropagation

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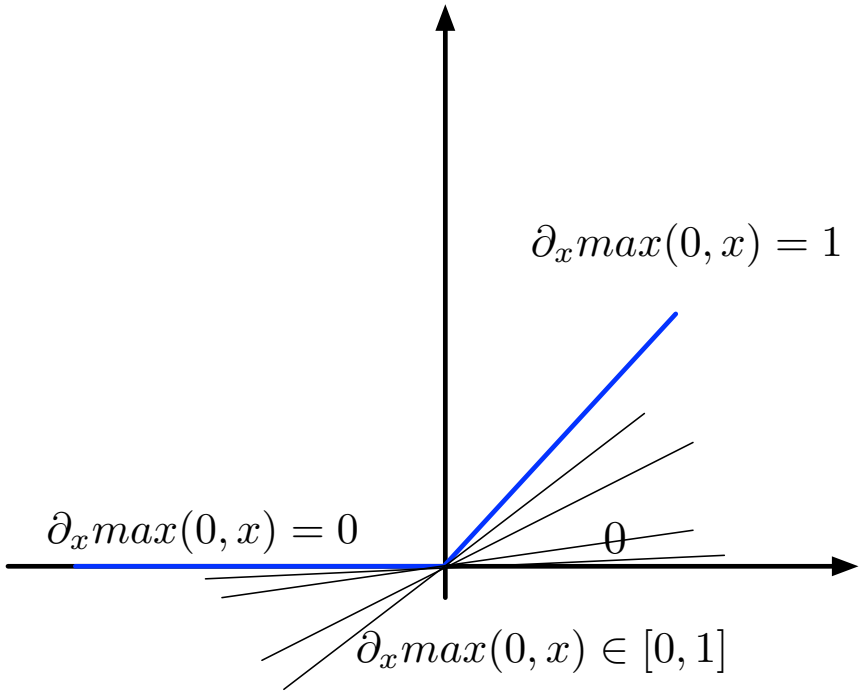
Typical non-linear activations

Activation functions

	Propagation	Back-propagation
Sigmoid	$y_s = \frac{1}{1+e^{-x_s}}$	$\left[\frac{\partial E}{\partial x}\right]_s = \left[\frac{\partial E}{\partial y}\right]_s \frac{1}{(1+e^{x_s})(1+e^{-x_s})}$
Tanh	$y_s = \tanh(x_s)$	$\left[\frac{\partial E}{\partial x}\right]_s = \left[\frac{\partial E}{\partial y}\right]_s \frac{1}{\cosh^2 x_s}$
ReLu	$y_s = \max(0, x_s)$	$\left[\frac{\partial E}{\partial x}\right]_s = \left[\frac{\partial E}{\partial y}\right]_s \mathbb{I}\{x_s > 0\}$
Ramp	$y_s = \min(-1, \max(1, x_s))$	$\left[\frac{\partial E}{\partial x}\right]_s = \left[\frac{\partial E}{\partial y}\right]_s \mathbb{I}\{-1 < x_s < 1\}$

Subgradients

ReLU gradient is not defined at x=0, use a subgradient instead



Practice note: during training, when a 'kink' point was crossed, the numerical gradient will not be exact.

Some SGD guidelines

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Initialization of the (filter) weights

- don't initialize with zero
- don't initialize with the same value
- sample from uniform distribution U[-b,b] around zero or from Normal distribution

Decay of the learning rate α

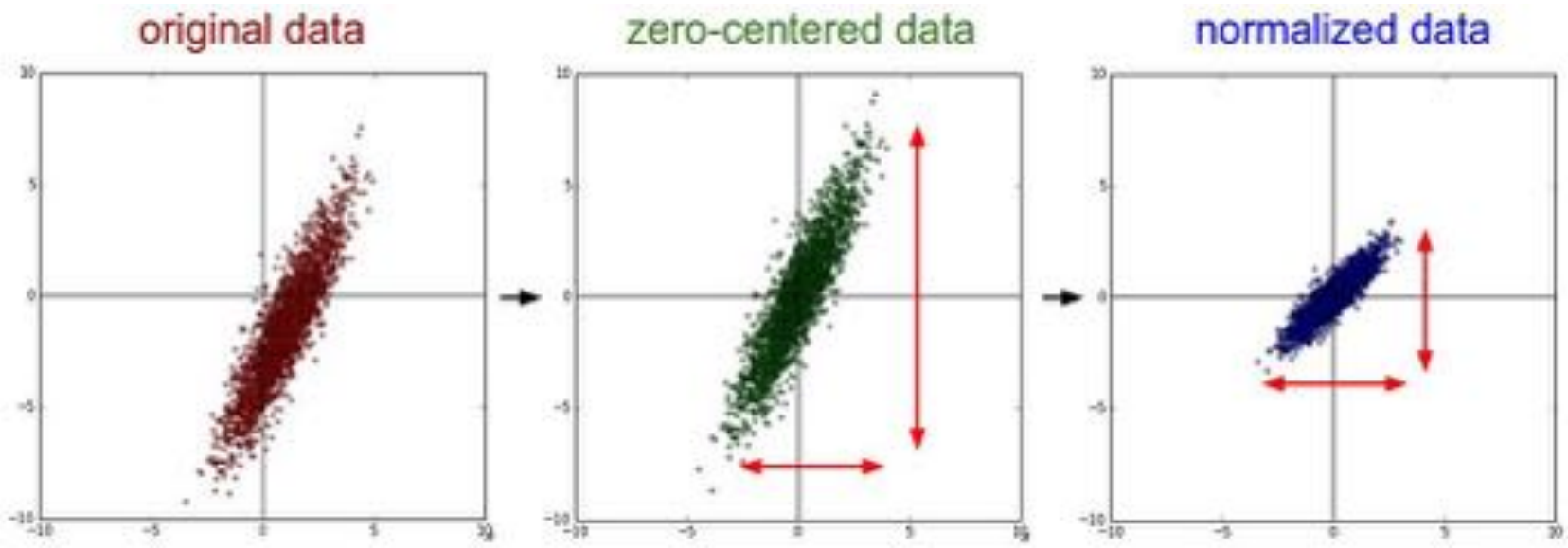
$$w^{t+1} = w^t - \alpha \cdot \frac{dE}{dw}(w^t)$$

as we get closer to the optimum, take smaller update steps

- start with large learning rate (e.g. 0.1)
- maintain until validation error stops improving
- divide learning rate by 2 and go back to previous step

Normalization is important

Data preprocessing: normalization (recall e.g. clustering)



In images: subtract the mean of RGB intensities of the whole dataset from each pixel

Also regularization

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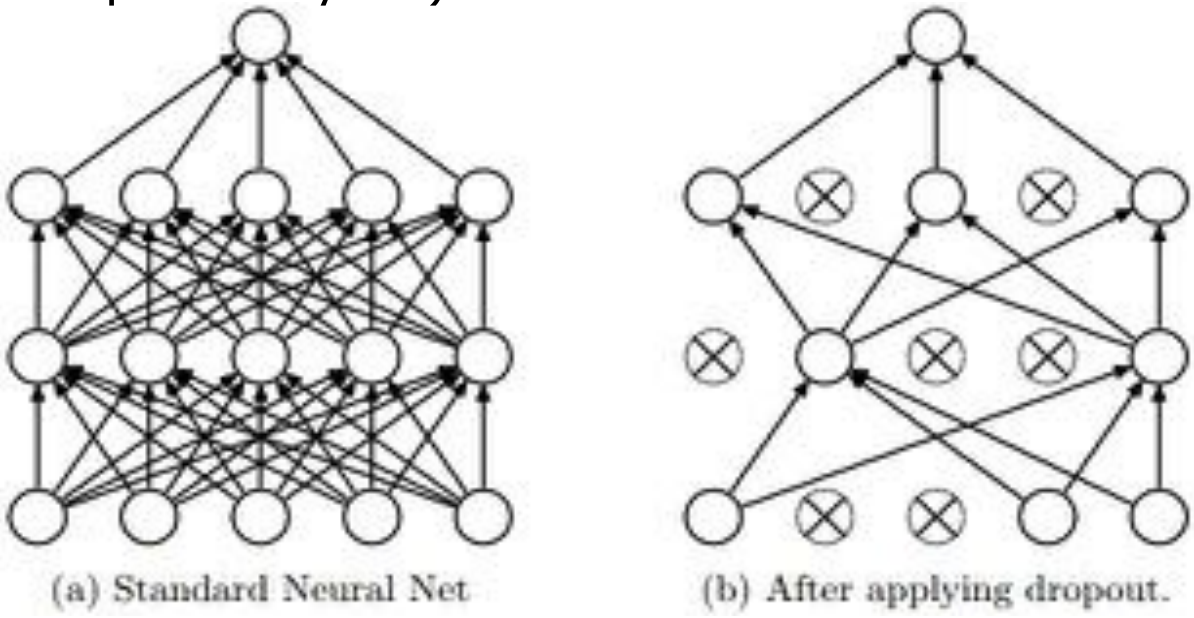
Regularization: **Dropout**

"randomly set some neurons to zero in the forward pass"

(with probability 0.5)



(a) Standard Neural Net

(b) After applying dropout.

[Srivastava et al., 2014]

The neurons which are "dropped out" do not contribute to the forward pass and do not participate in backpropagation.

So every time an input is presented, the neural network samples different architecture, but all these architectures share weights.

Also regularization

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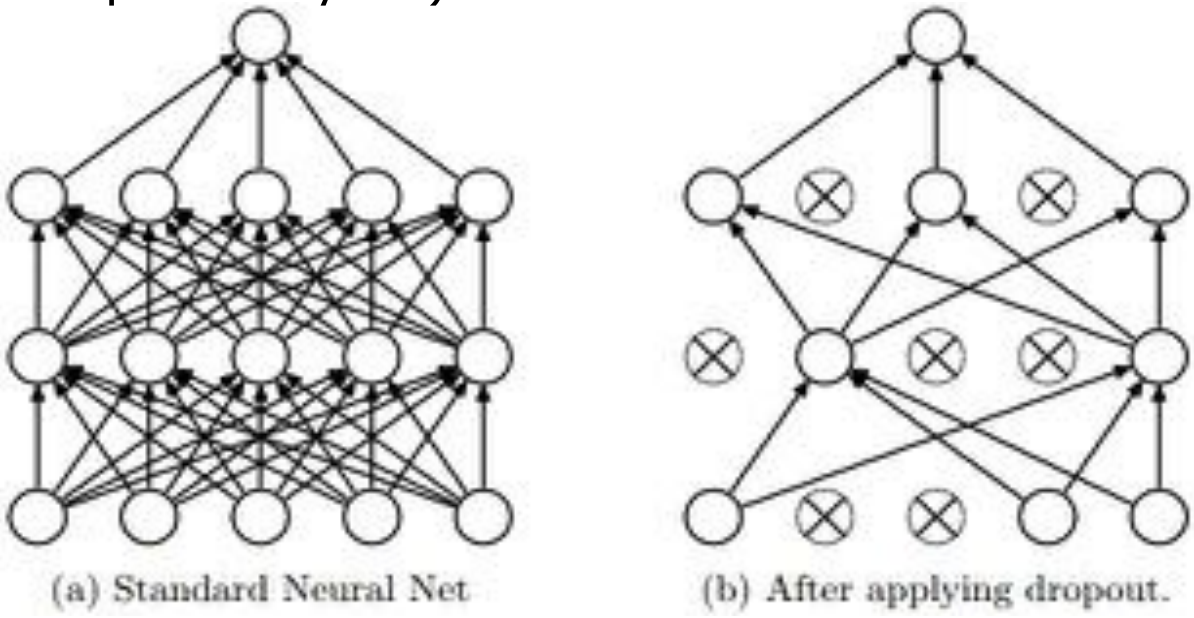
Regularization: **Dropout**

"randomly set some neurons to zero in the forward pass"

(with probability 0.5)



(a) Standard Neural Net

(b) After applying dropout.

[Srivastava et al., 2014]

At test time, use average predictions over all the ensemble of models

(weighted with 0.5)

And data augmentation

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The easiest and most common method to **reduce overfitting** on image data is to artificially **enlarge the dataset** using label-preserving transformations.

Forms of data augmentation (for images):

- horizontal reflections
- random crop
- changing RGB intensities
- image translation

As well as fine-tuning

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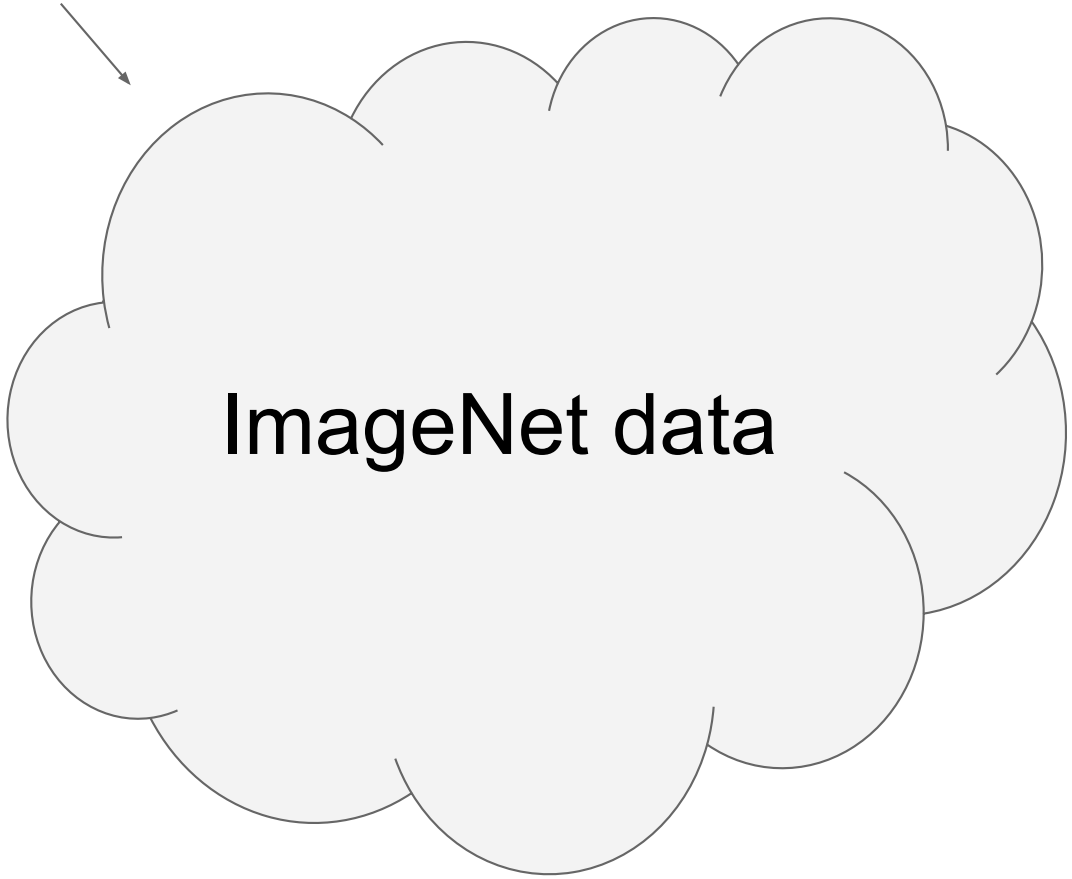
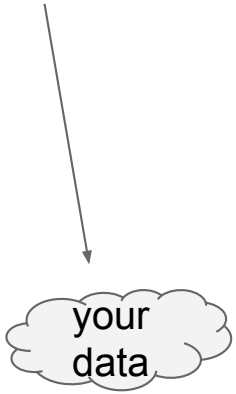
1. Train on ImageNet



2. Finetune network on your own data



Fine-tuning

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Transfer Learning with CNNs

1. Train on ImageNet

2. If small dataset: fix all weights (treat CNN as fixed feature extractor), retrain only the classifier

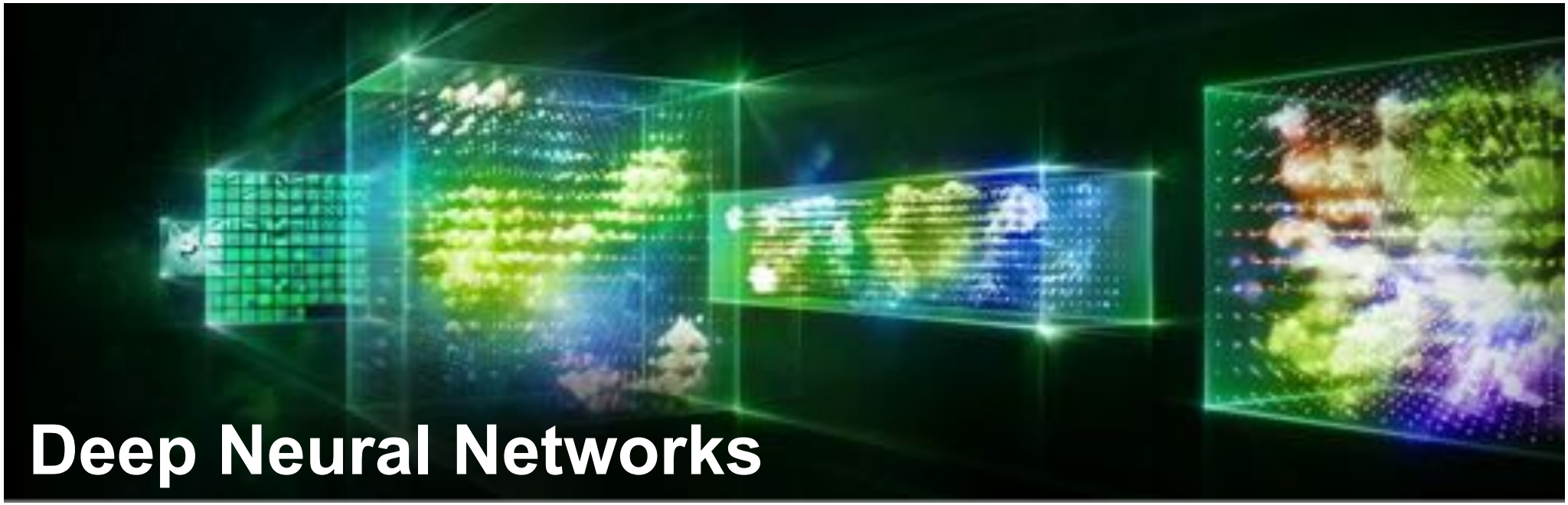
i.e. swap the Softmax layer at the end

3. If you have medium sized dataset, **"finetune"** instead: use the old weights as initialization, train the full network or only some of the higher layers

retrain bigger portion of the network, or even all of it.

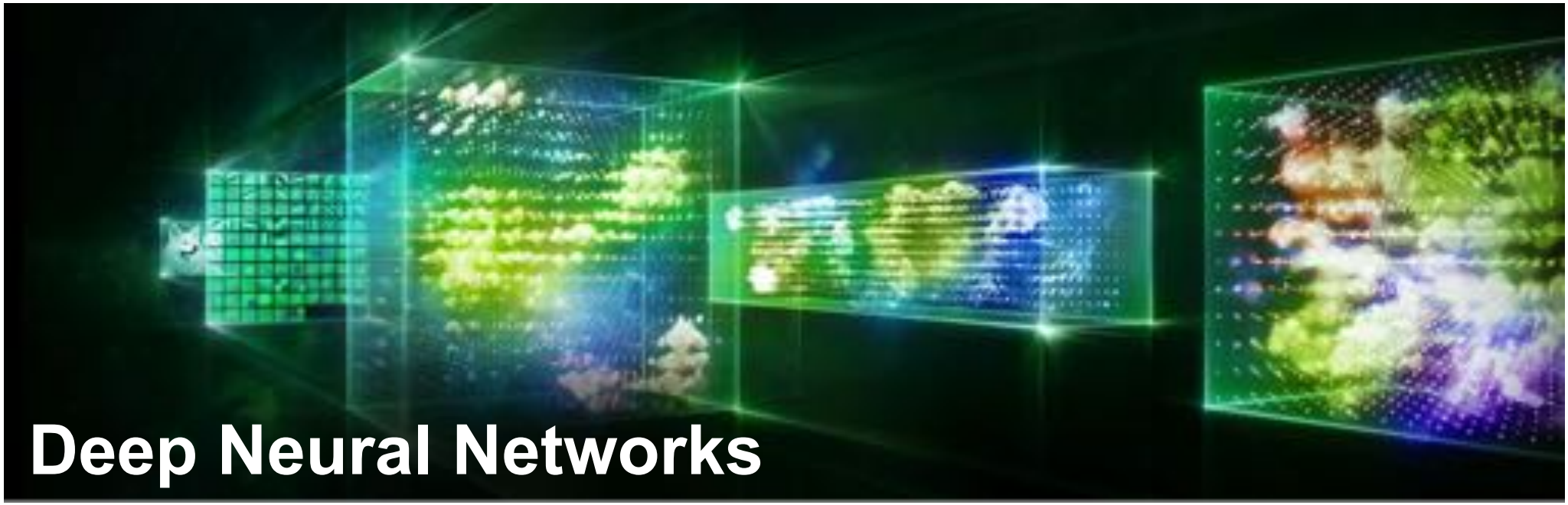
A lot of pre-trained models in Caffe Model Zoo

https://github.com/BVLC/caffe/wiki/Model-Zoo



Deep Neural Networks

- Aim at learning feature hierachies
- Typical architectures: Convolutional layer, ReLU,Max pooling layer, fully connected layer
- Rather large networks but SOTA performance on many tasks
- Training done via SGD together with normalization, regularization, and data augmention
- Large networks often used in a pre-trained fashion

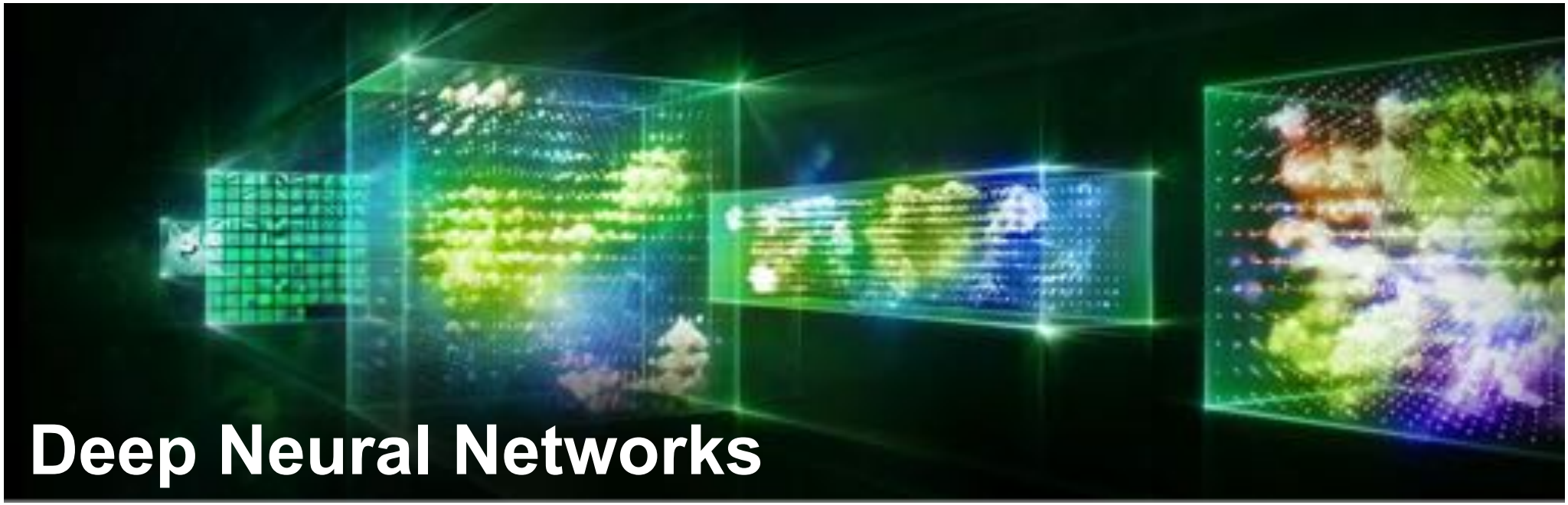


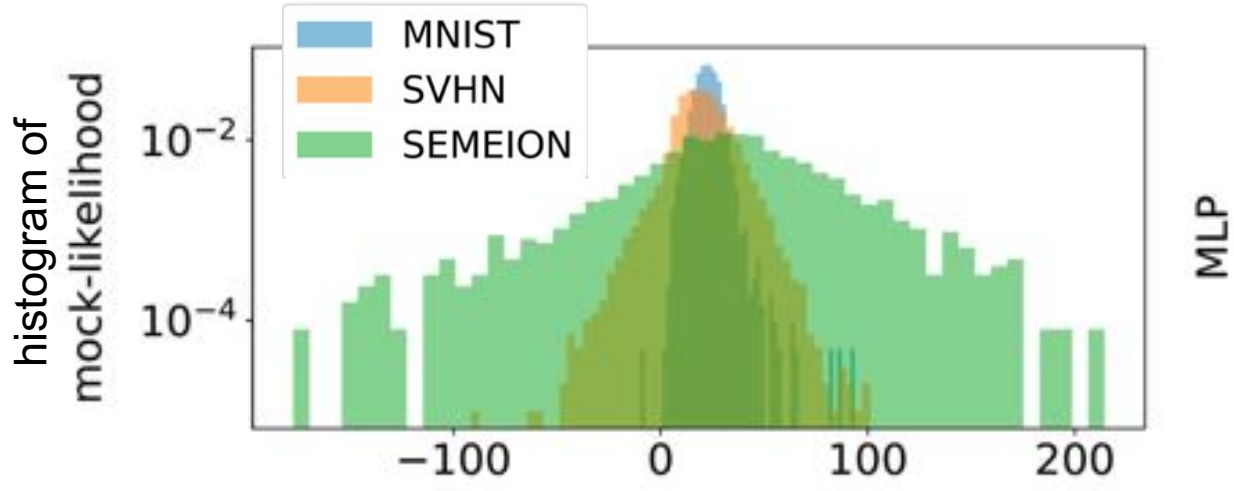
Deep Neural Networks

Potentially much more powerful than shallow architectures, represent computations [Bengio, 2009]

But …

- **Learning requires extensive efforts**
- **Often no probabilistic semantics**



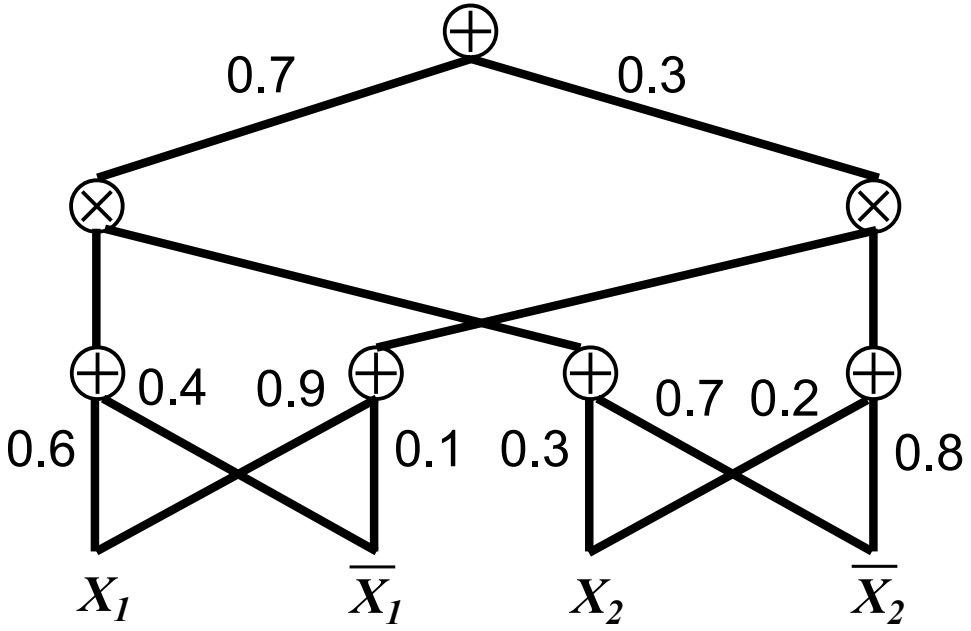


Deep neural networks may not be faithful probabilistic models

Can we borrow ideas from deep learning for probabilistic graphical models?

Judea Pearl, UCLA
Turing Award 2012

Deep Probabilistic Modelling using Sum-Product Networks



Computational graph (kind of TensorFlow graphs) that encodes how to compute probabilities

Inference is Linear in Size of Network

Alternative Representation: Graphical Models as Deep Networks

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X_1	X_2	$P(X)$
1	1	0.4
1	0	0.2
0	1	0.1
0	0	0.3

$$P(X) = 0.4 \cdot \mathrm{I}[X_1{=}1] \cdot \mathrm{I}[X_2{=}1] + 0.2 \cdot \mathrm{I}[X_1{=}1] \cdot \mathrm{I}[X_2{=}0] + 0.1 \cdot \mathrm{I}[X_1{=}0] \cdot \mathrm{I}[X_2{=}1] + 0.3 \cdot \mathrm{I}[X_1{=}0] \cdot \mathrm{I}[X_2{=}0]$$

Alternative Representation: Graphical Models as Deep Networks

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X_1	X_2	$P(X)$
1	**1**	**0.4**
1	0	0.2
0	1	0.1
0	0	0.3

$$P(X) = \mathbf{0.4 \cdot I[X_1{=}1] \cdot I[X_2{=}1]} + 0.2 \cdot \mathrm{I}[X_1{=}1] \cdot \mathrm{I}[X_2{=}0] + 0.1 \cdot \mathrm{I}[X_1{=}0] \cdot \mathrm{I}[X_2{=}1] + 0.3 \cdot \mathrm{I}[X_1{=}0] \cdot \mathrm{I}[X_2{=}0]$$

Shorthand for Indicators

X_1	X_2	$P(X)$
1	1	0.4
1	0	0.2
0	1	0.1
0	0	0.3

$$
\begin{aligned}
P(X) = 0.4 \cdot X_1 \cdot X_2 \\
+ 0.2 \cdot X_1 \cdot \overline{X}_2 \\
+ 0.1 \cdot \overline{X}_1 \cdot X_2 \\
+ 0.3 \cdot \overline{X}_1 \cdot \overline{X}_2
\end{aligned}
$$

Sum Out Variables

X_1	X_2	$P(X)$
1	1	0.4
1	0	0.2
0	1	0.1
0	0	0.3

$$e: X_1 = 1$$

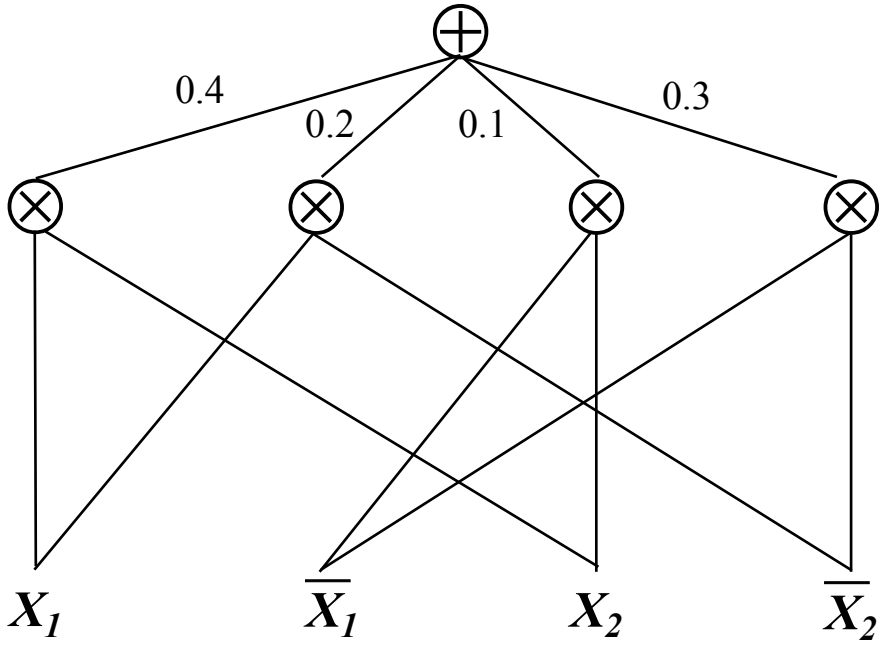
$$P(e) = \mathbf{0.4 \cdot X_1 \cdot X_2} + \mathbf{0.2 \cdot X_1 \cdot \overline{X}_2} + 0.1 \cdot \overline{X}_1 \cdot X_2 + 0.3 \cdot \overline{X}_1 \cdot \overline{X}_2$$

Set $X_1 = 1, \overline{X}_1 = 0, X_2 = 1, \overline{X}_2 = 1$

Easy: Set both indicators of X2 to 1

Idea: Deeper Network Representation of a Graphical Model that encodes how to compute probabilities

X_1	X_2	$P(X)$
1	1	0.4
1	0	0.2
0	1	0.1
0	0	0.3



Sum-Product Networks* (SPNs)

[Poon, Domingos UAI 2011]

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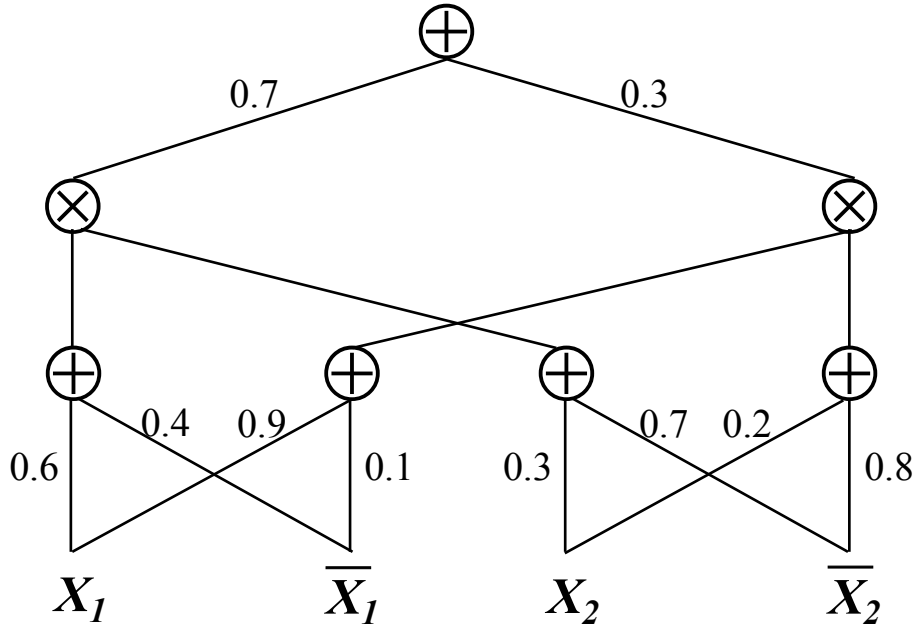
A SPN S is a rooted DAG where:
Nodes: Sum, product, input indicator
Weights on edges from sum to children



*SPNs are an instance of Arithmetic Circuits (ACs). ACs have been introduced into the AI literature more than15 years ago as a tractable representation of probability distributions

[Darwiche CACM 48(4):608-647 2001]

SPFlow: An Easy and Extensible Library for Sum-Product Networks

[Molina, Vergari, Stelzner, Peharz, Kersting 2018]

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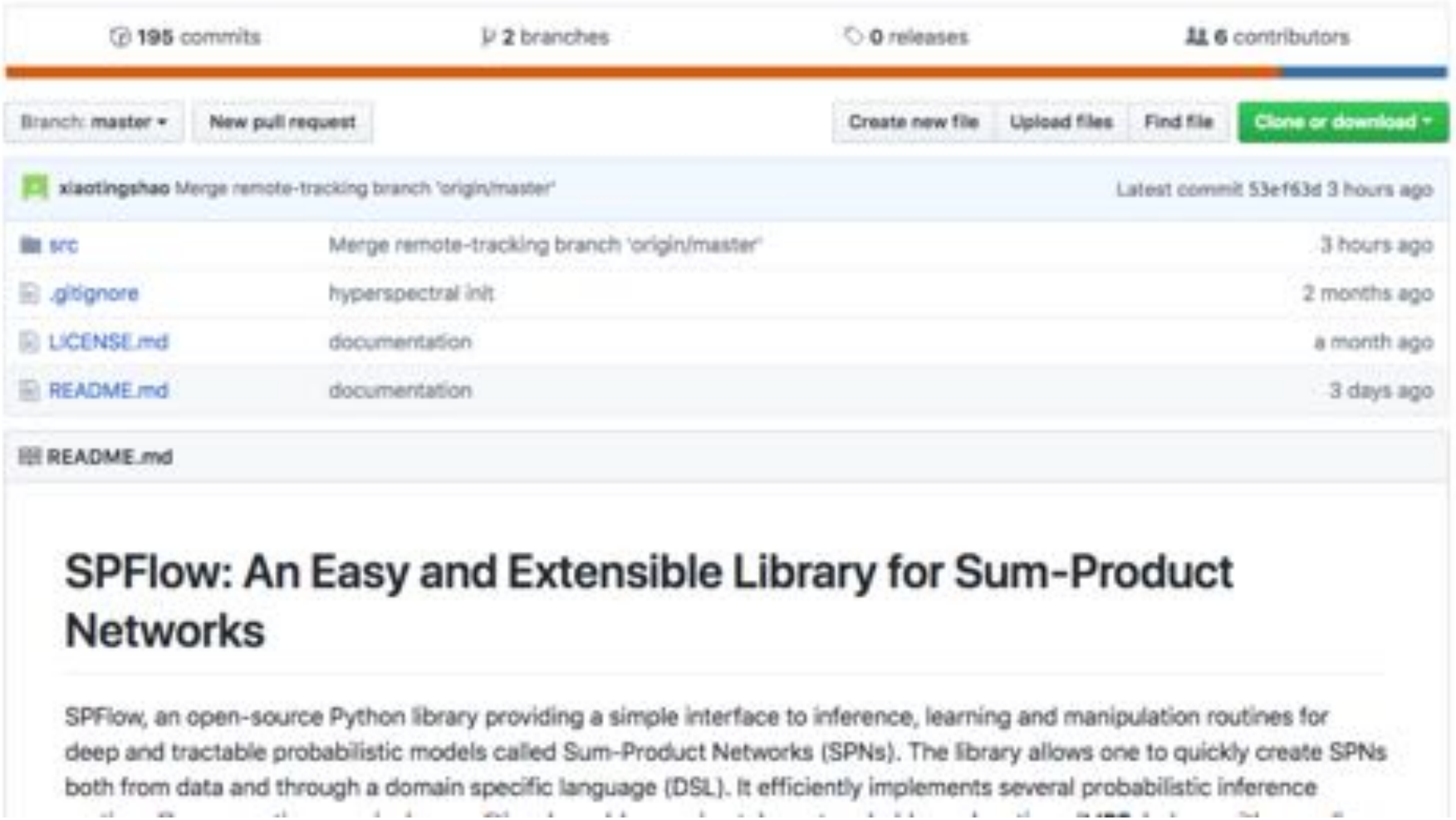
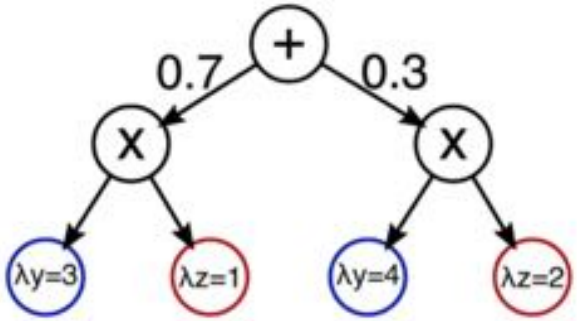
https://github.com/alejandromolinaml/SPFlow



Deep Probabilistic Inference Units



SPNs can be compiled into flat, library-free code suitable for embedding in real-time applications and devices

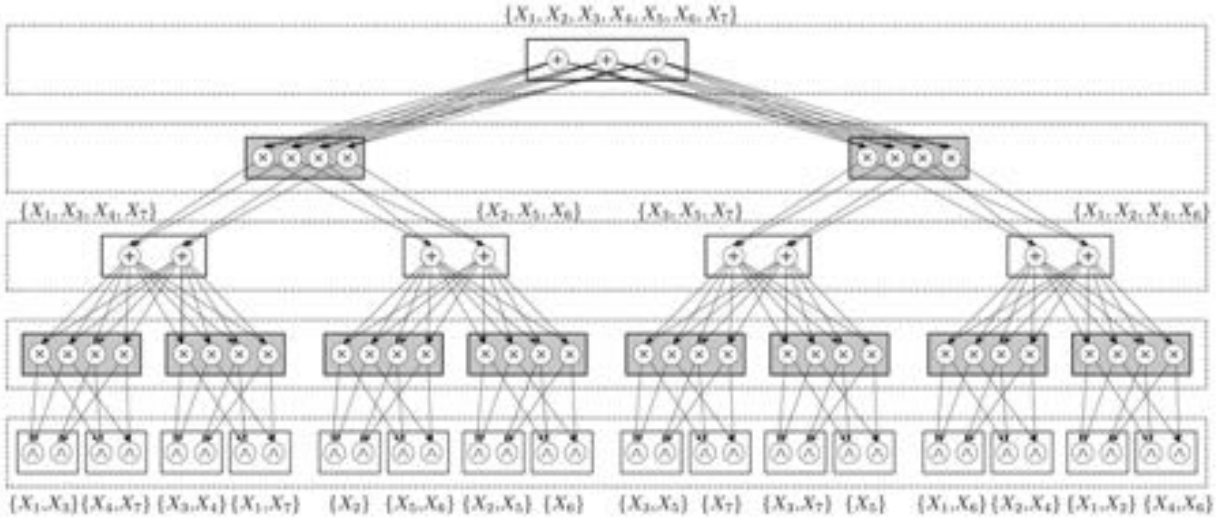
TABLE II
PERFORMANCE COMPARISON. BEST END-TO-END THROUGHPUTS (T), EXCLUDING THE CYCLE COUNTER MEASUREMENTS, ARE [illegible]TED BOLD.

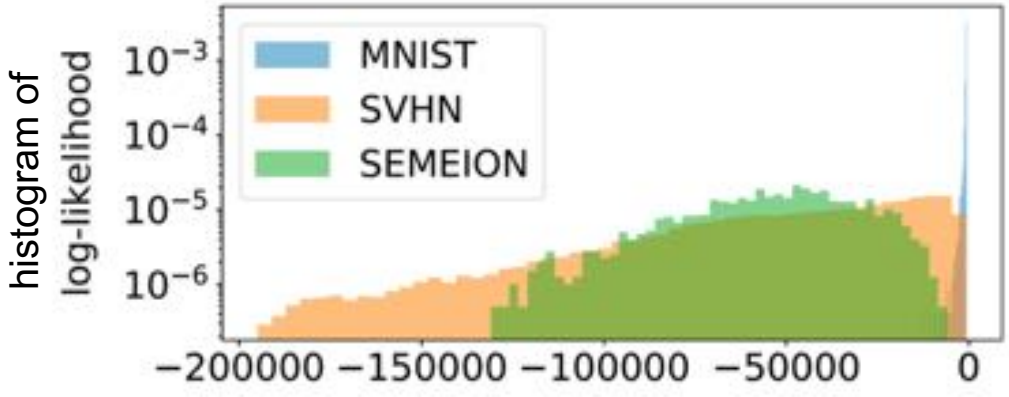
Dataset	Rows	CPU (µs)	T-CPU (rows/µs)	CPUF (µs)	T-CPUF (rows/µs)	GPU (µs)	T-GPU (rows/µs)	FPGA Cycle Counter	FPGAC (µs)	T-FPGAC (rows/µs)	FPG[illegible] (µs)	[illegible]FPGA (rows/µs)
Accidents	17009	2798.27	[illegible]	[illegible]	7.87	63090.94	0.27	17249	[illegible]	[illegible]	696.00	**24.44**
Audio	20000	4271.78	[illegible]	[illegible]	5.4[illegible]	[illegible]	[illegible]	20317	[illegible]	[illegible]	761.00	**26.28**
Netflix	20000	4892.22	[illegible]	[illegible]	4.8[illegible]	[illegible]	[illegible]	20322	[illegible]	[illegible]	654.00	**30.58**
MSNBC200	388434	15476.05	[illegible]	[illegible]	30.5[illegible]	[illegible]	[illegible]	388900	19[illegible]	[illegible]	008.00	**77.56**
MSNBC300	388434	10060.78	[illegible]	[illegible]	41.2[illegible]	[illegible]	[illegible]	388810	19[illegible]	[illegible]	933.00	**78.74**
NLTCS	21574	791.80	[illegible]	[illegible]	31.3[illegible]	[illegible]	[illegible]	21904	[illegible]	[illegible]	566.00	**38.12**
Plants	23215	3621.71	[illegible]	3521.04	6.59	67004.41	0.35	23592	117.96	196.80	778.00	**29.84**
NIPS5	10000	25.11	**398.31**	26.37	379.23	8210.32	1.22	10236	51.18	195.39	337.30	[illegible]
NIPS10	10000	83.60	**119.61**	84.39	118.49	11550.82	0.87	10279	51.40	194.57	464.30	21.54
NIPS20	10000	191.30	52.27	182.73	**54.72**	18689.04	0.54	10285	51.43	194.46	543.60	18.40
NIPS30	10000	387.61	25.80	349.84	**28.58**	25355.93	0.39	10308	51.80	193.06	592.30	16.88
NIPS40	10000	551.64	18.13	471.26	**21.22**	30820.49	0.32	10306	51.53	194.06	632.20	15.82
NIPS50	10000	812.44	12.31	792.13	12.62	36355.60	0.28	10559	52.80	189.41	720.60	**13.88**
NIPS60	10000	1046.38	9.56	662.53	**15.09**	40778.36	0.25	12271	61.36	162.99	799.20	12.51
NIPS70	10000	1148.17	8.71	1134.80	8.81	46759.26	0.21	14022	70.11	142.63	858.60	**11.65**
NIPS80	10000	1556.99	6.42	1277.81	7.83	63217.99	0.16	14275	78.51	127.37	961.80	**10.40**

And also learning is conceptually easy

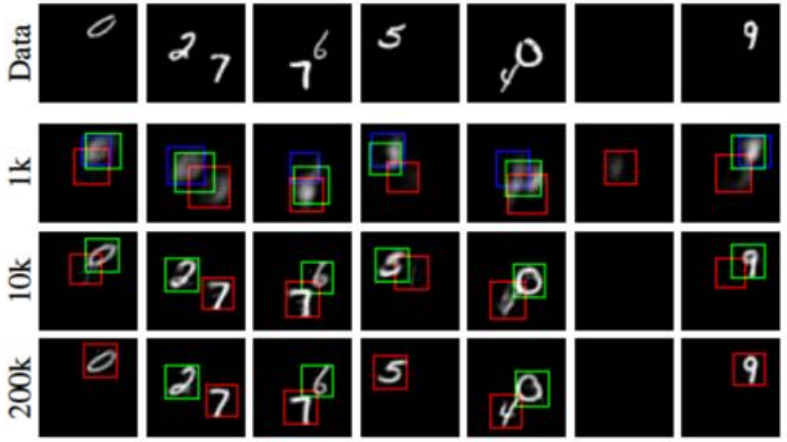
[Peharz, Vergari, Molina, Stelzner, Trapp, Kersting, Ghahramani UDL@UAI 2018]

Random sum-product networks



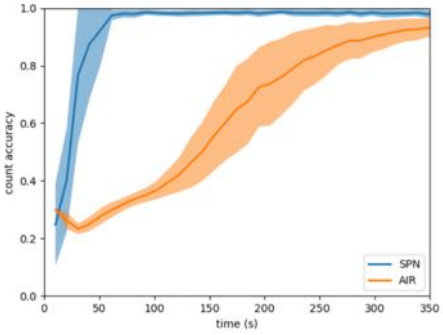


And also learning is conceptually easy

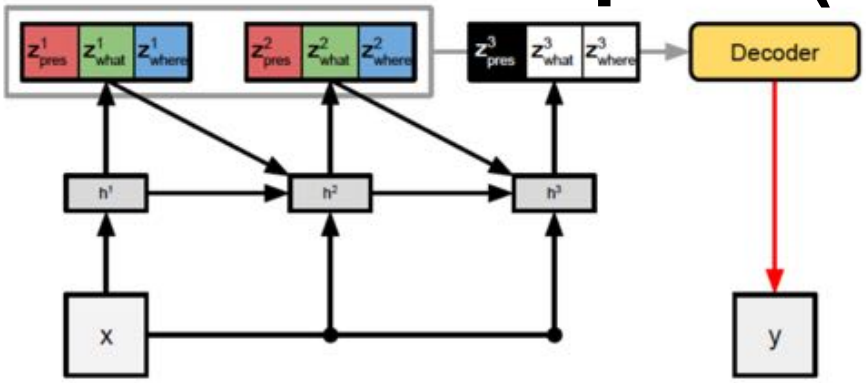


Explicit AIR

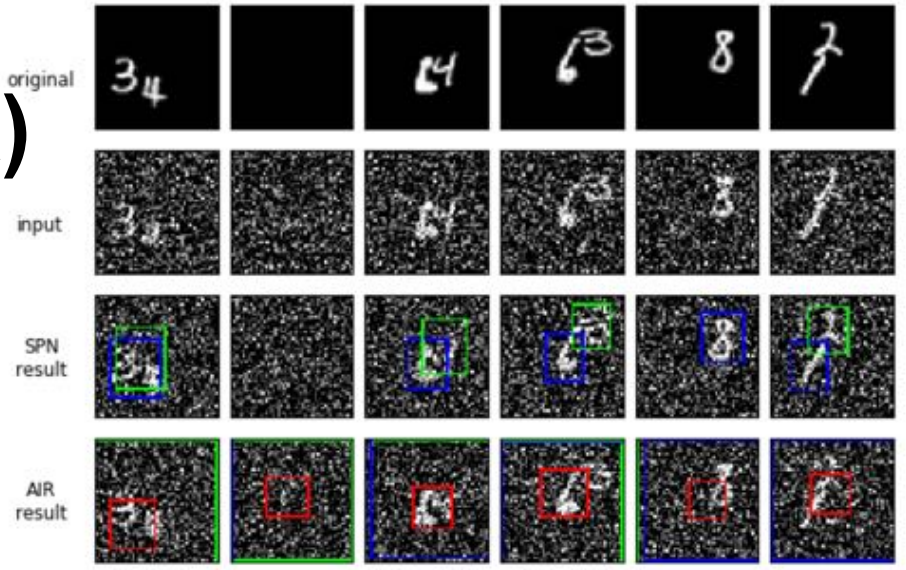
[Stelzner, Peharz, Kersting 2018]



Attend Infer Repeat (AIR)



[Eslami et al. NIPS 2016]



Or you do greedy learning

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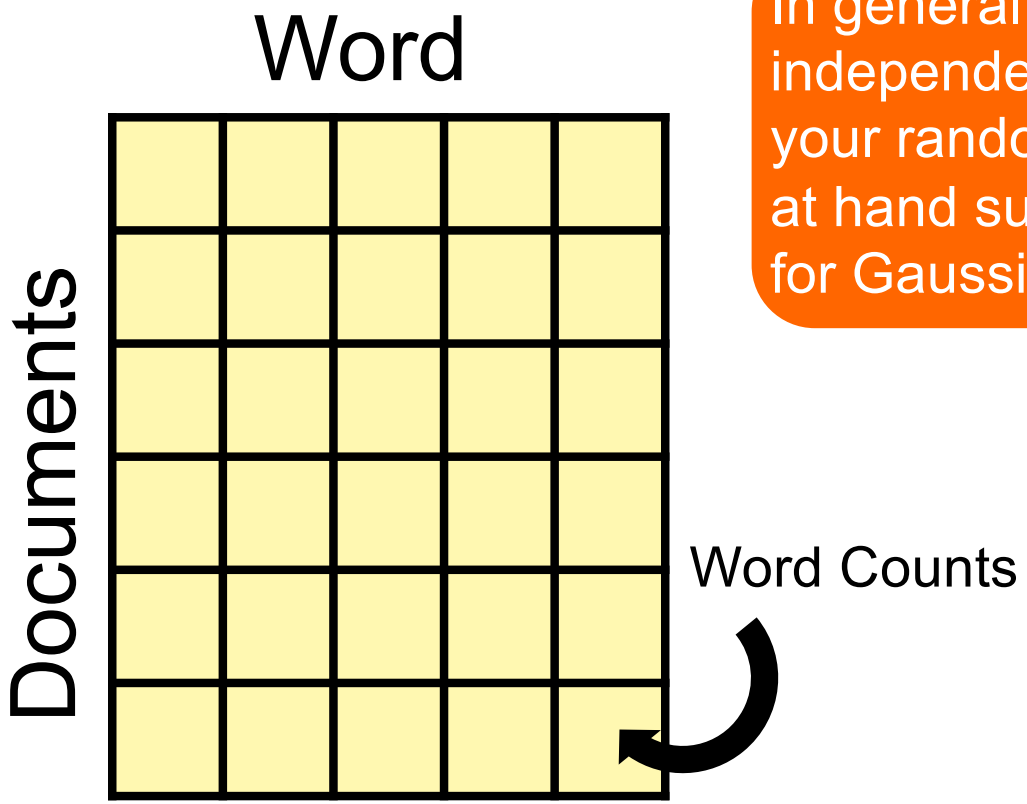
Testing independence of random variables using e.g. nonparametric tests



In general use the independency test for your random variables at hand such as g-test for Gaussians

[Poon, Domingos UAI'11; Molina, Natarajan, Kersting AAAI´17, Molina et al AAAI ,18]

Or you do greedy learning

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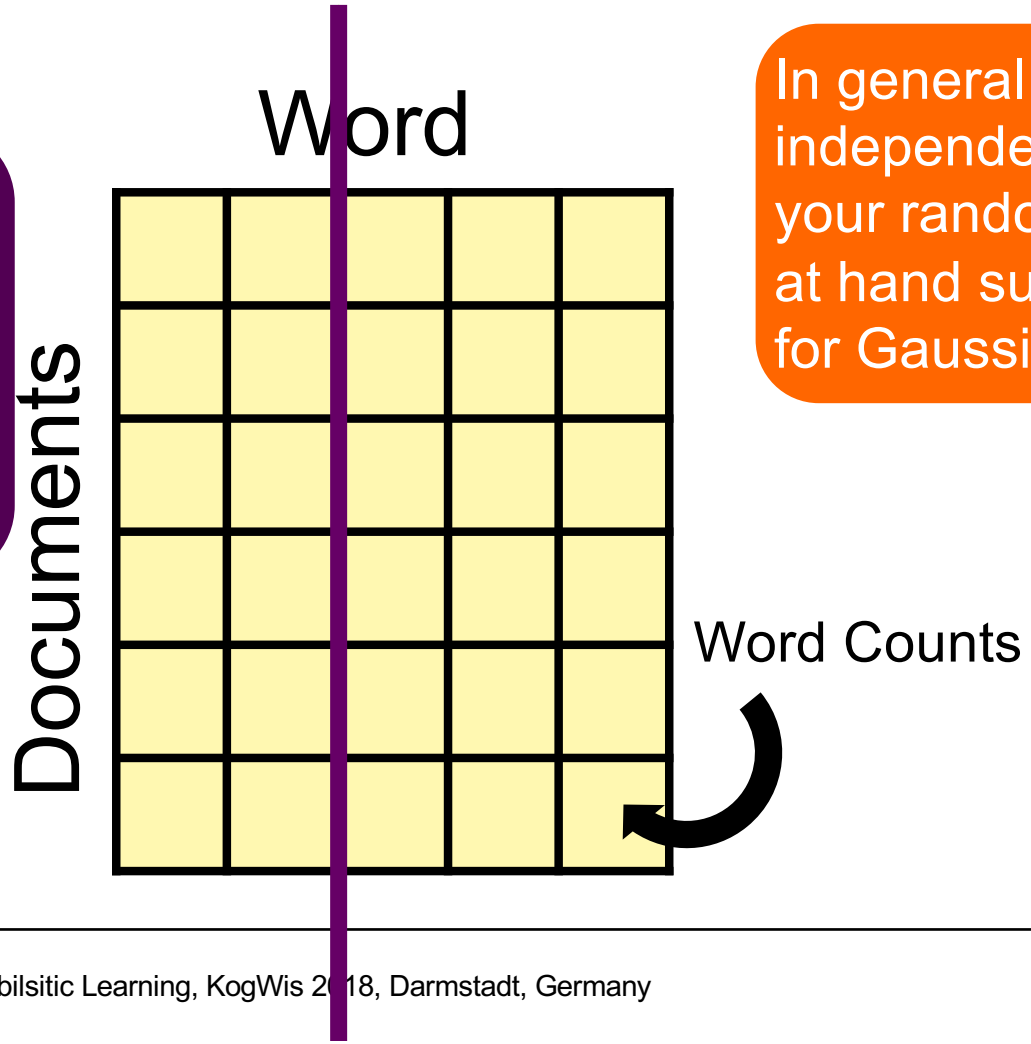
Testing independence of random variables using e.g. nonparametric tests

Learn GLM model trees for P(x|V-x) and P(y|V-y). Check whether X resp. Y is significant in P(y|V-x) resp. P(x|V-y)



In general use the independency test for your random variables at hand such as g-test for Gaussians

Or you do greedy learning

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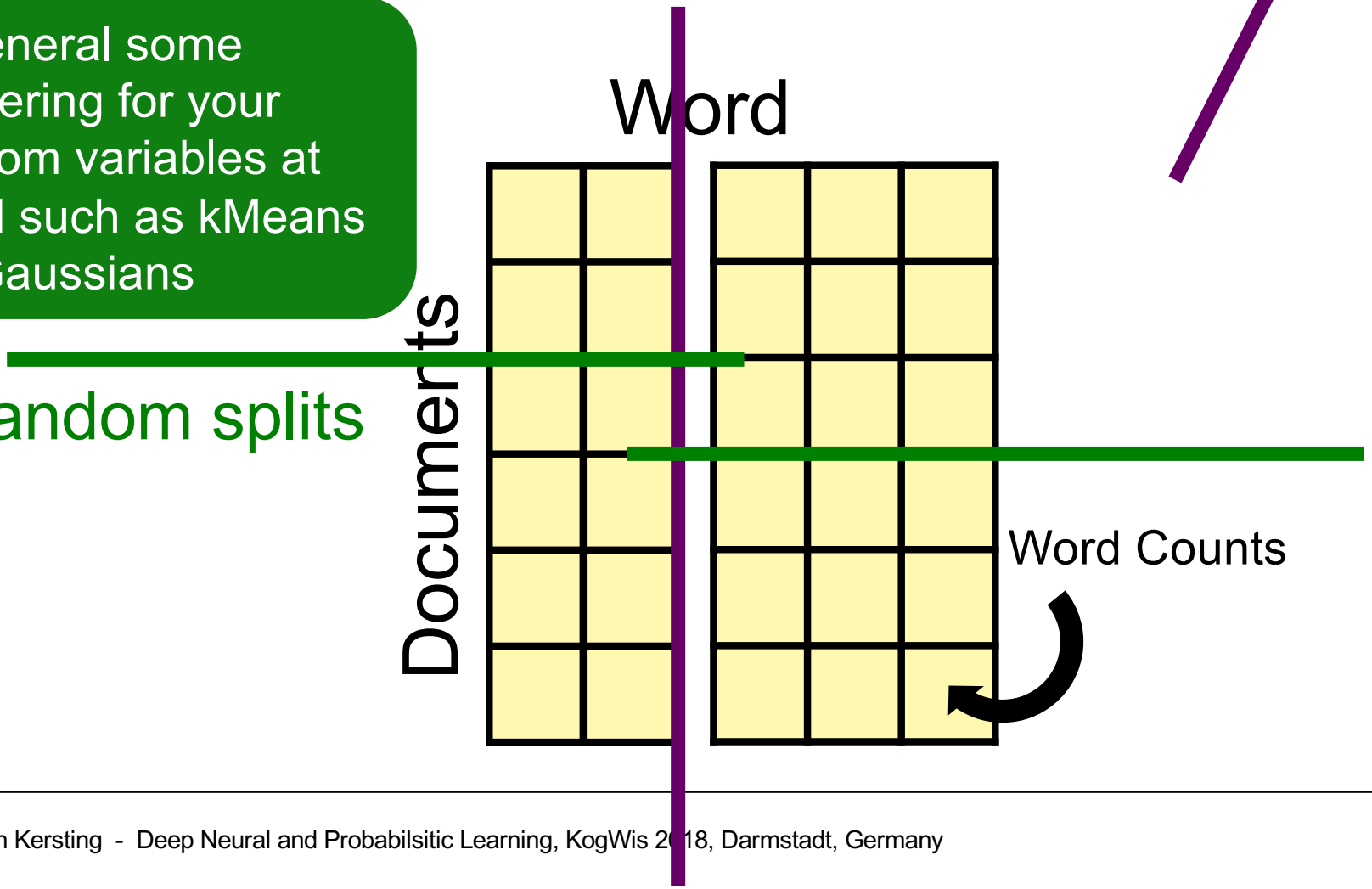
Testing independence of random variables using e.g. nonparametric tests

In general some clustering for your random variables at hand such as kMeans for Gaussians



[Poon, Domingos UAI'11; Molina, Natarajan, Kersting AAAI`17, Molina et al AAAI ,18]

Or you do greedy learning

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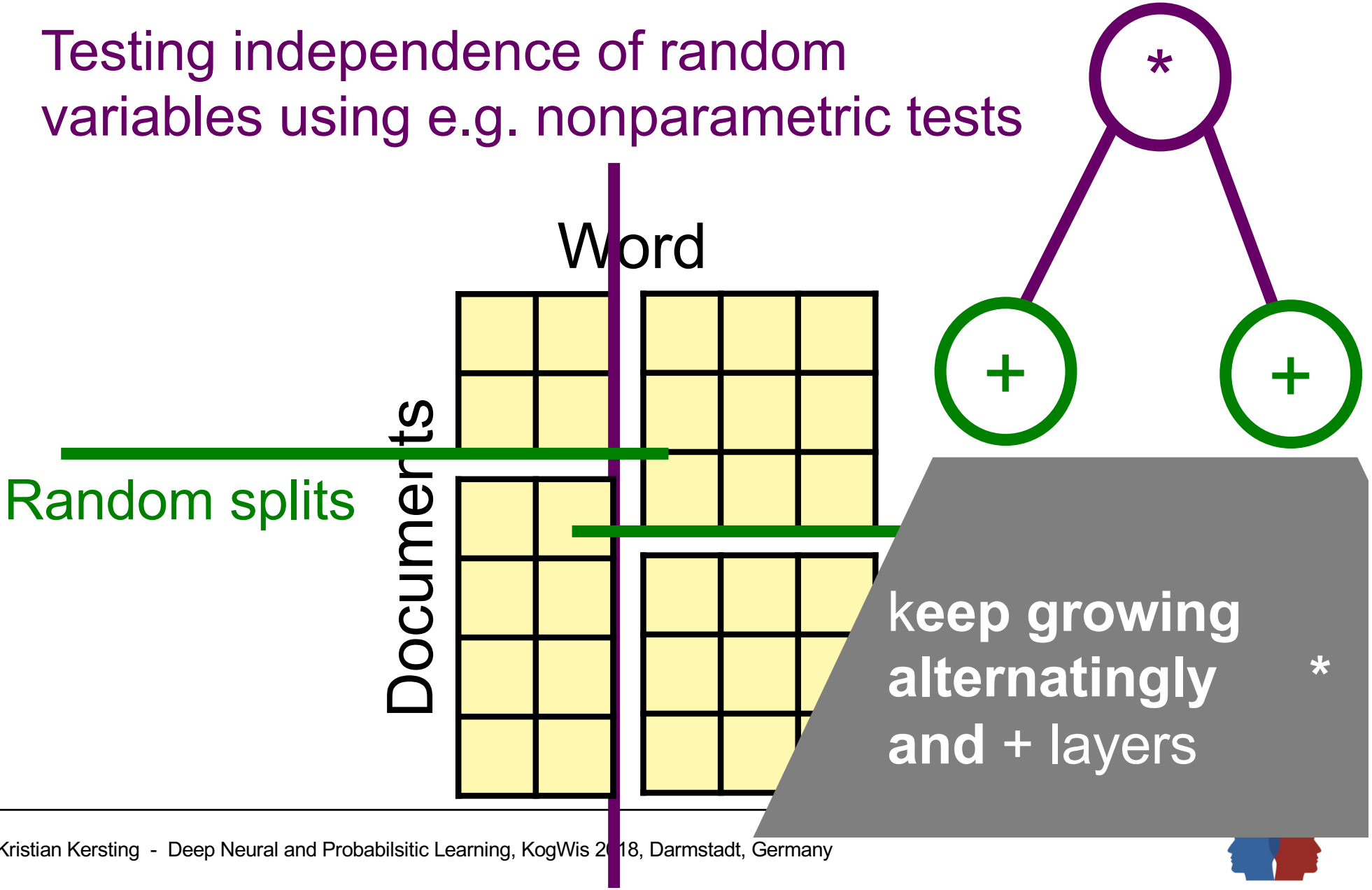
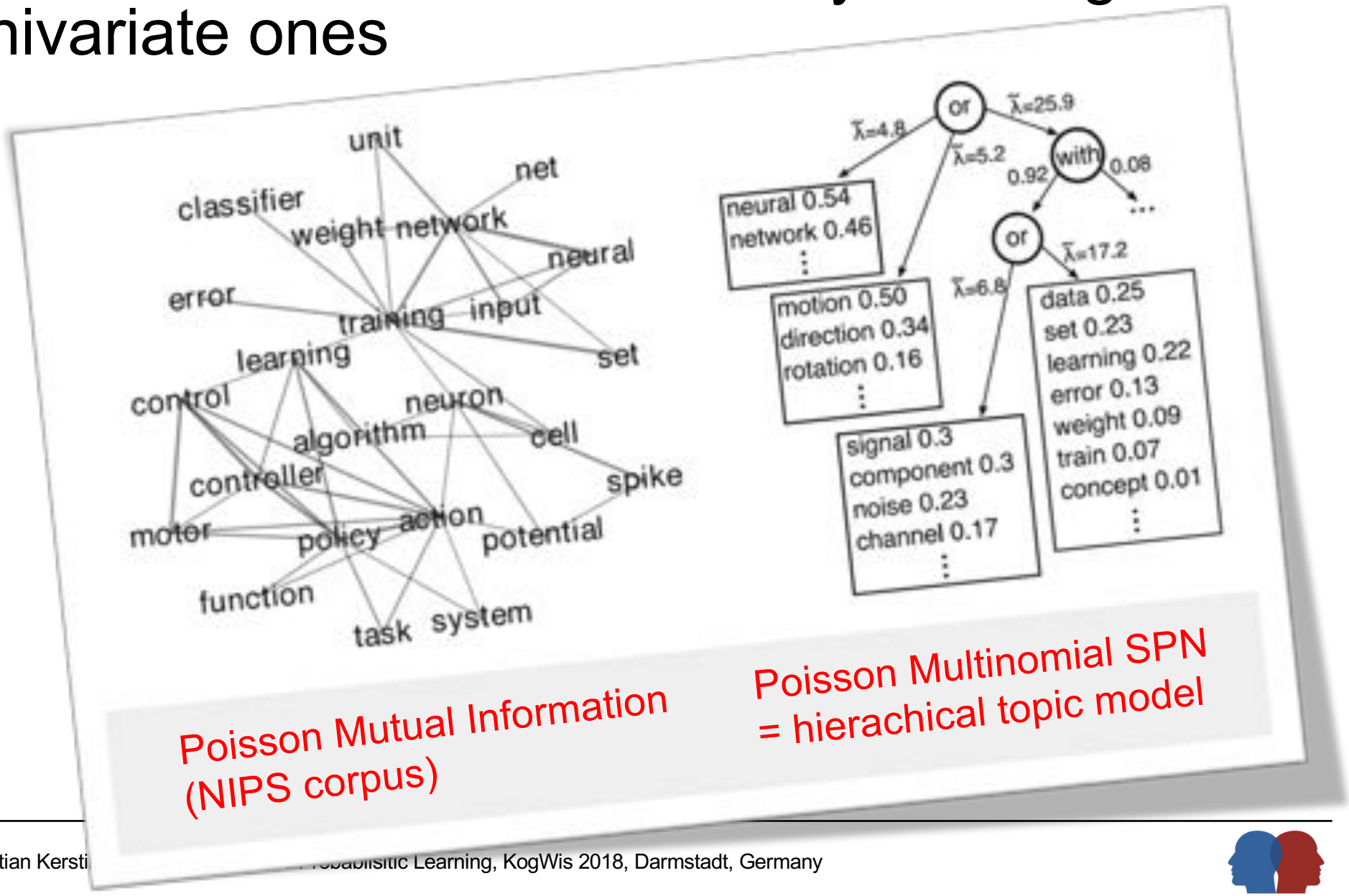
Testing independence of random variables using e.g. nonparametric tests

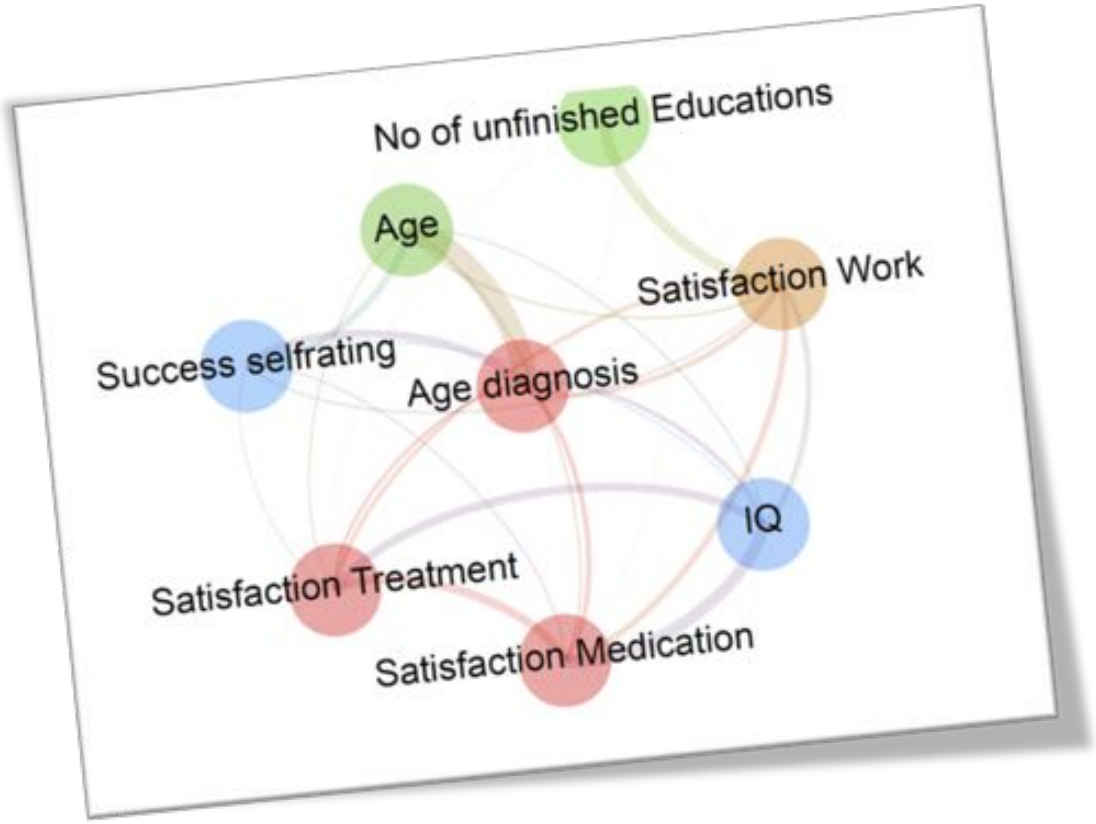


[Molina, Natarajan, Kersting AAAI 2017]

Probabilistic modelling made easy:
Build multivariate distribution by stacking univariate ones

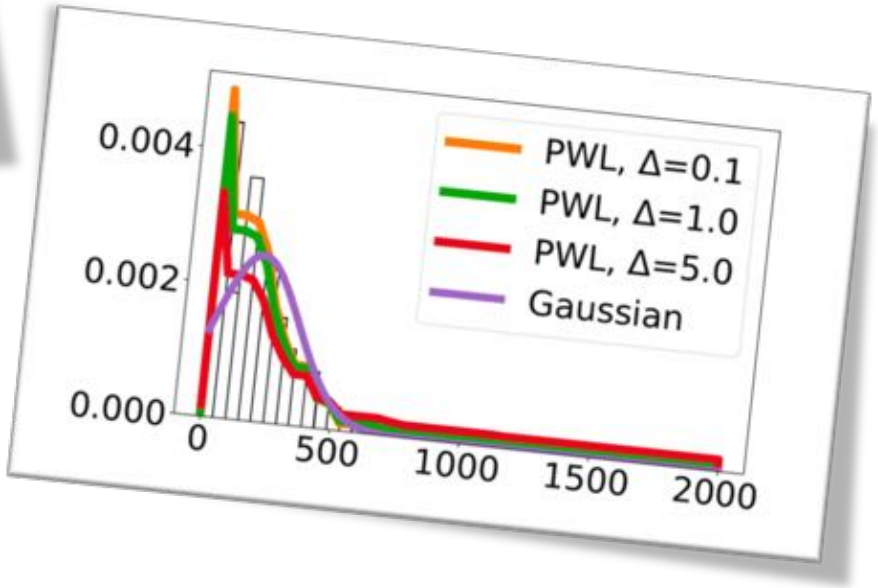


… even in a distribution-agnostic way



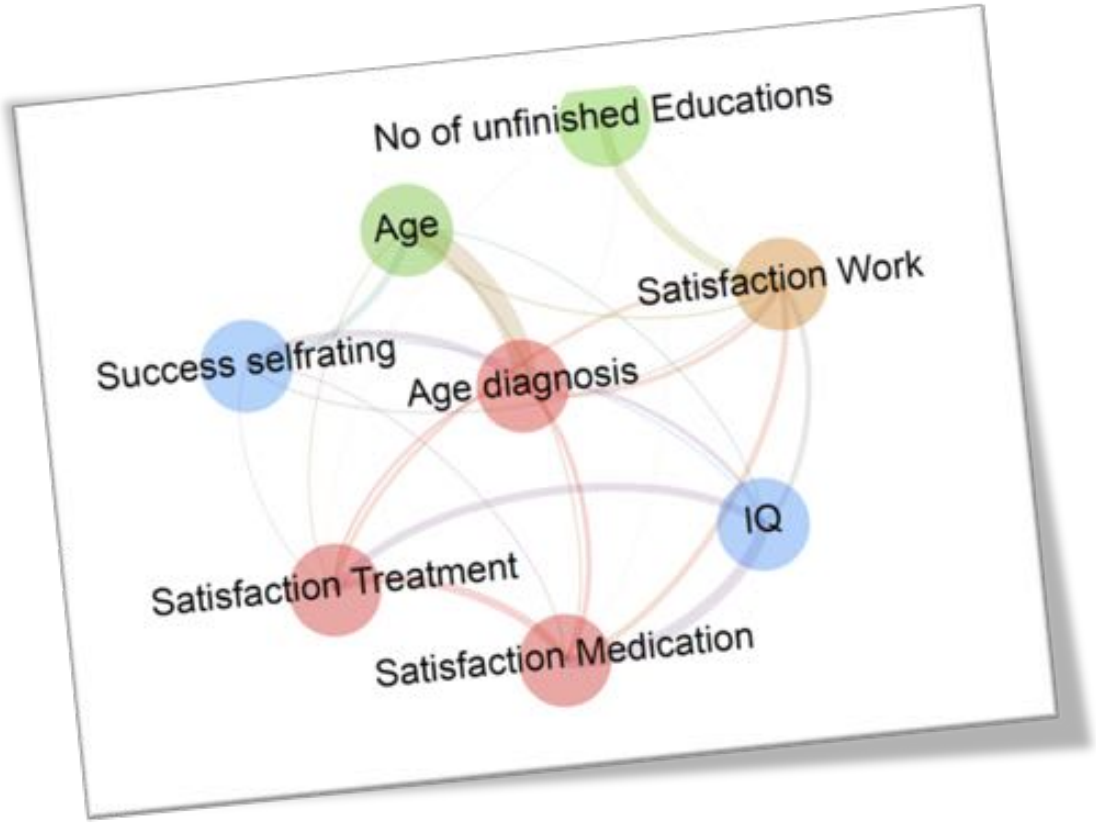
Visualization the gist of a Mixed SPN (learned on the hybrid Autism dataset) using normalized mutual info (the thicker, the higher). **The machine does not know anything about the data types.**

Use nonparametric independency tests and piece-wise linear approximations



[Molina, Natarajan, Vergari, Di Mauro, Esposito, Kersting AAAI 2018]

… even in a distribution-agnostic way

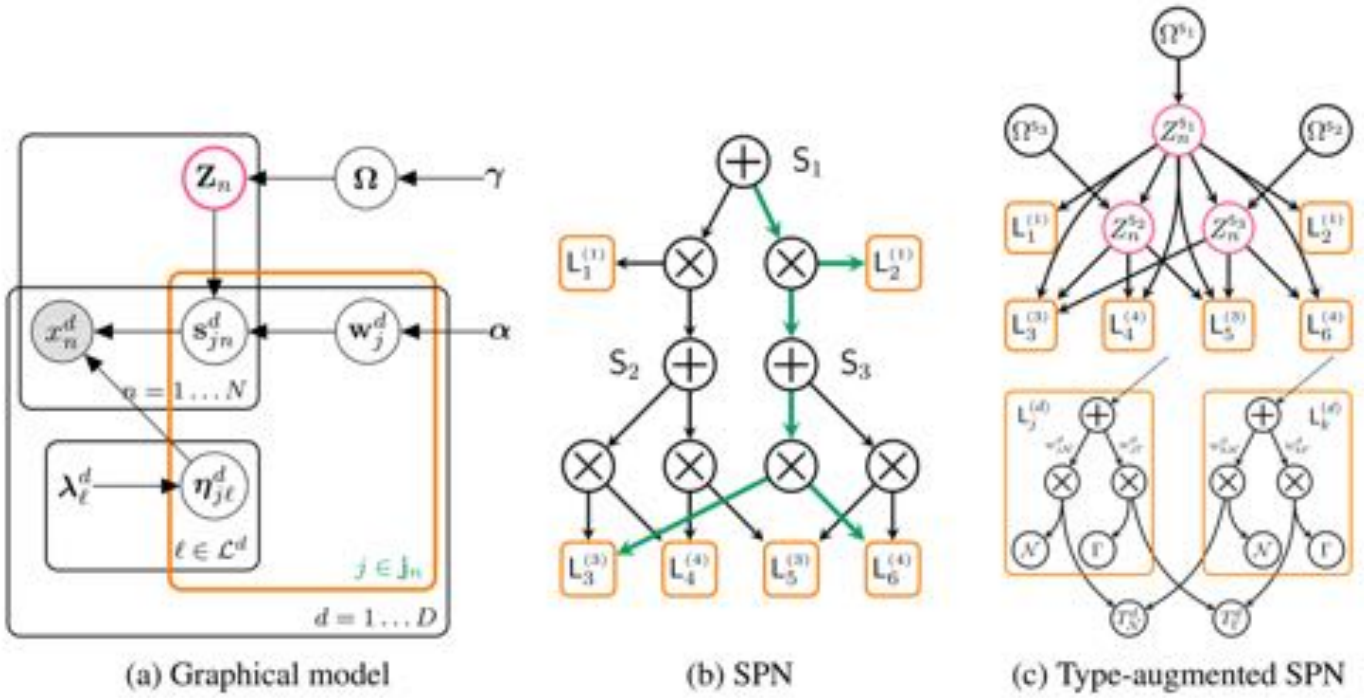


Visualization the gist of a Mixed SPN (learned on the hybrid Autism dataset) using normalized mutual info (the thicker, the higher). **The machine does not know anything about the data types.**

Use nonparametric

However, we have to provide the statistical types and do not gain insights into the parametric forms of the variables. **Are they Gaussians? Gammas? …**

Automatic Bayesian Density Analysis



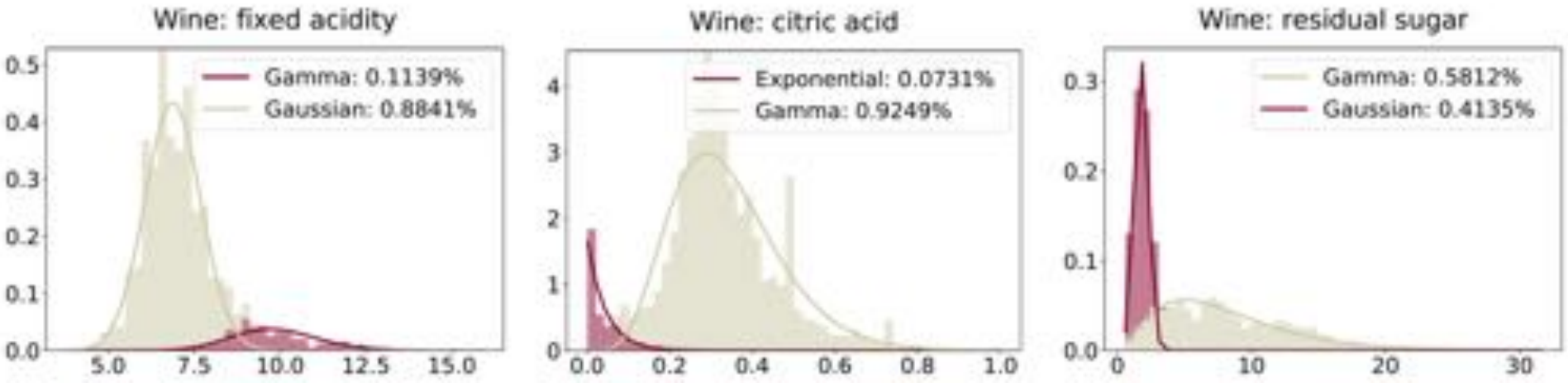
(a) Graphical model (b) SPN (c) Type-augmented SPN

Bayesian discovery of statistical types and parametric forms of variables

+

Type-agnostic deep probabilistic learning

Automatic Bayesian Density Analysis



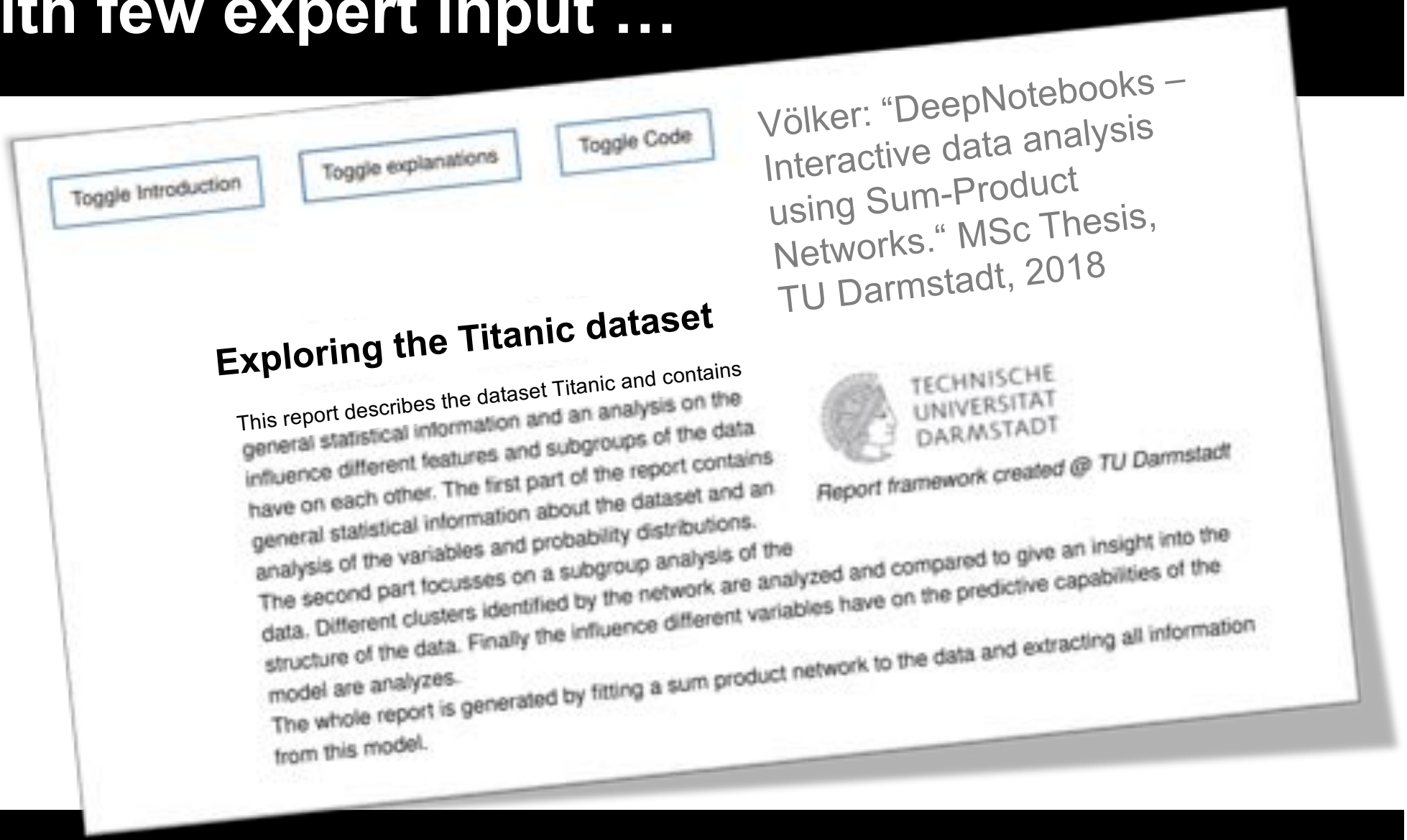
… can automatically discovers the statistical types and parametric forms of the variables

Automatic Bayesian Density Analysis

	transductive setting						*inductive setting*	
	10%			50%			70%-10%-20%	
	ISLV	**ABDA**	**MSPN**	**ISLV**	**ABDA**	**MSPN**	**ABDA**	**MSPN**
Abalone	-1.15±0.12	-0.02±0.03	**0.20**	-0.89±0.36	-0.05±0.03	**0.14**	2.22±0.03	**9.73**
Adult	-	**-0.60**±0.02	-3.46	-	**-0.69**±0.01	-5.83	**-5.91**±0.01	-44.07
Australian	-7.92±0.96	**-1.74**±0.19	-3.85	-9.37±0.69	**-1.63**±0.04	-3.76	**-16.44**±0.04	-36.14
Autism	-2.22±0.06	**-1.23**±0.02	-1.54	-2.67±0.16	**-1.24**±0.01	-1.57	**-27.93**±0.02	-39.20
Breast	-3.84±0.05	-2.78±0.07	**-2.69**	-4.29±0.17	**-2.85**±0.01	-3.06	**-25.48**±0.05	-28.01
Chess	-2.49±0.04	**-1.87**±0.01	-3.94	-2.58±0.04	**-1.87**±0.01	-3.92	**-12.30**±0.00	-13.01
Crx	-12.17±1.41	**-1.19**±0.12	-3.28	-11.96±1.01	**-1.20**±0.04	-3.51	**-12.82**±0.07	-36.26
Dermatology	-2.44±0.23	**-0.96**±0.02	-1.00	-3.57±0.32	**-0.99**±0.01	-1.01	**-24.98**±0.19	-27.71
Diabetes	-10.53±1.51	**-2.21**±0.09	-3.88	-12.52±0.52	**-2.37**±0.09	-4.01	**-17.48**±0.05	-31.22
German	-3.49±0.21	**-1.54**±0.01	-1.58	-4.06±0.28	**-1.55**±0.01	-1.60	**-25.83**±0.05	-26.05
Student	-2.83±0.27	**-1.56**±0.03	-1.57	-3.80±0.29	**-1.57**±0.01	-1.58	**-28.73**±0.10	-30.18
Wine	-1.19±0.02	-0.90±0.02	**-0.13**	-1.34±0.01	-0.92±0.01	**-0.41**	-10.12±0.01	**-0.13**
wins	0	9	3	0	10	2	10	2

… but also models its uncertainty about the statistical types and parametric forms, which can lead to better models

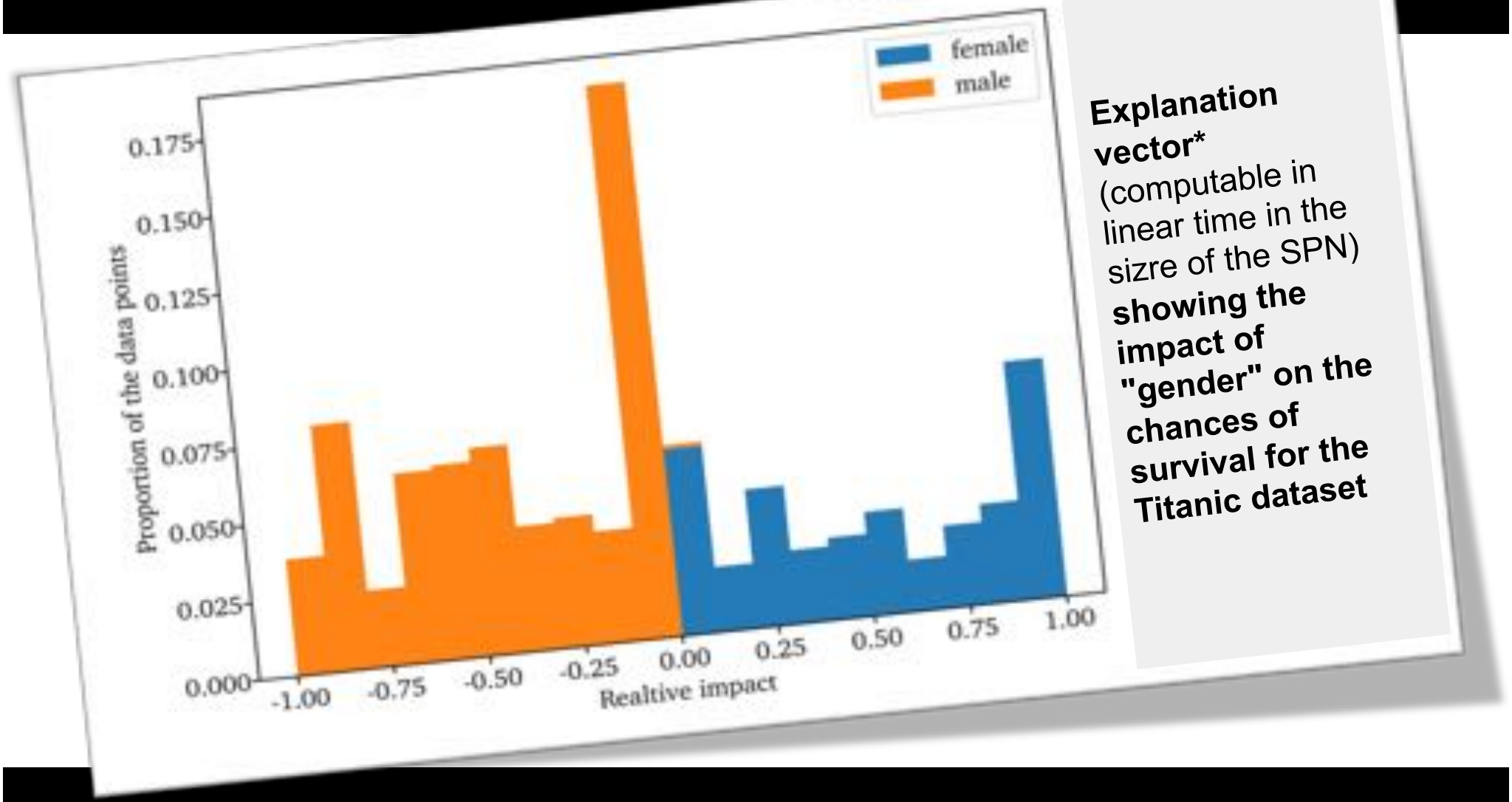
The machine understands the data with few expert input …



…and can compile data reports automatically

*[Baehrens, Schroeter, Harmeling, Kawanabe, Hansen, Müller JMLR 11:1803-1831, 2010]

The machine understands the data with no expert input …



Explanation vector* (computable in linear time in the sizre of the SPN) **showing the impact of "gender" on the chances of survival for the Titanic dataset**

…and can compile data reports automatically

What have we learnt about SPNs?

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Sum-product networks (SPNs)

- DAG of sums and products
- They are instances of Arithmetic Circuits (ACs)
- Compactly represent partition function
- Learn many layers of hidden variables

Efficient marginal inference

Easy learning

Can outperform well-known alternatives

Deep Neural and Probabilistic Learning

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Centre for Cognitive Science

Fachbereich Informatik

- Artificial Intelligence is currently receiving a lot of attention due to the recent successes of deep learning
- Deep Learning aims at finding automatically good representations
- Deep networks should be seen as trainable computational graphs, i.e., they are (skeletons of) algorithms/computation
- Deep architectures can be neural and probabilistic

Kristian Kersting