

# Deep machines that know when they do not know\*

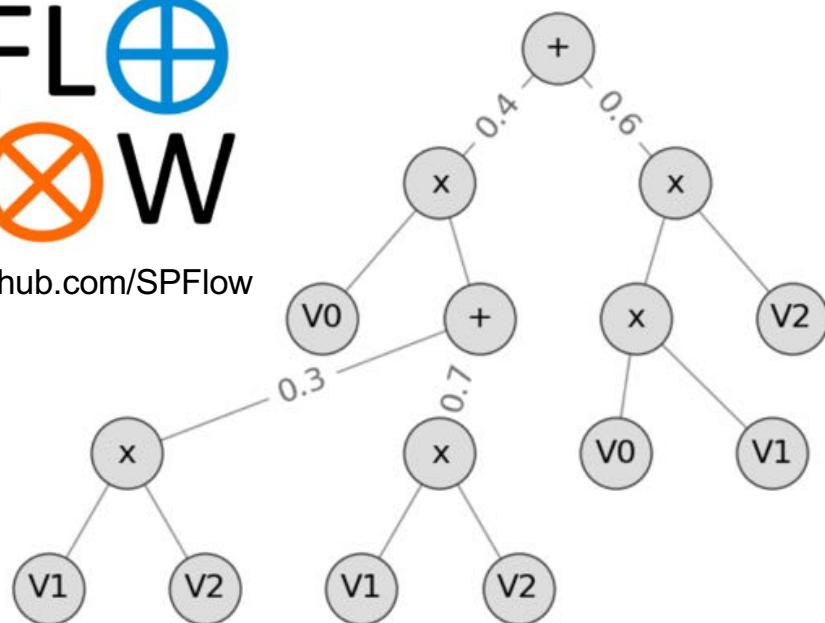
\*Thanks for Pedro Domingos for making his slides publicly available



Kristian Kersting



[github.com/SPFlow](https://github.com/SPFlow)



Alejandro Molina, Antonio Vergari, Karl Stelzner, Robert Peharz, Pranav Subramani, Nicola Di Mauro, Pascal Poupart, Kristian Kersting: **SPFlow: An Easy and Extensible Library for Deep Probabilistic Learning using Sum-Product Networks.** CoRR abs/1901.03704 (2019)

```
from spn.structure.leaves.parametric.Parametric import Categorical  
  
spn = 0.4 * (Categorical(p=[0.2, 0.8], scope=0) *  
              (0.3 * (Categorical(p=[0.3, 0.7], scope=1) *  
                      Categorical(p=[0.4, 0.6], scope=2))  
              + 0.7 * (Categorical(p=[0.5, 0.5], scope=1) *  
                      Categorical(p=[0.6, 0.4], scope=2))))  
              + 0.6 * (Categorical(p=[0.2, 0.8], scope=0) *  
              Categorical(p=[0.3, 0.7], scope=1) *  
              Categorical(p=[0.4, 0.6], scope=2)))
```

SPFLOW: AN EASY AND EXTENSIBLE LIBRARY FOR DEEP PROBABILISTIC LEARNING USING SUM-PRODUCT NETWORKS

A PREPRINT

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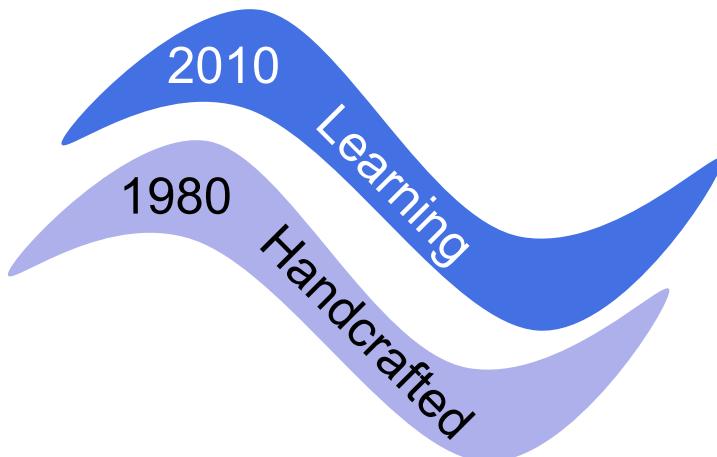
ABSTRACT

# Third wave of AI



Data are now ubiquitous; there is great value from understanding this data, building models and making predictions

However, data is not everything

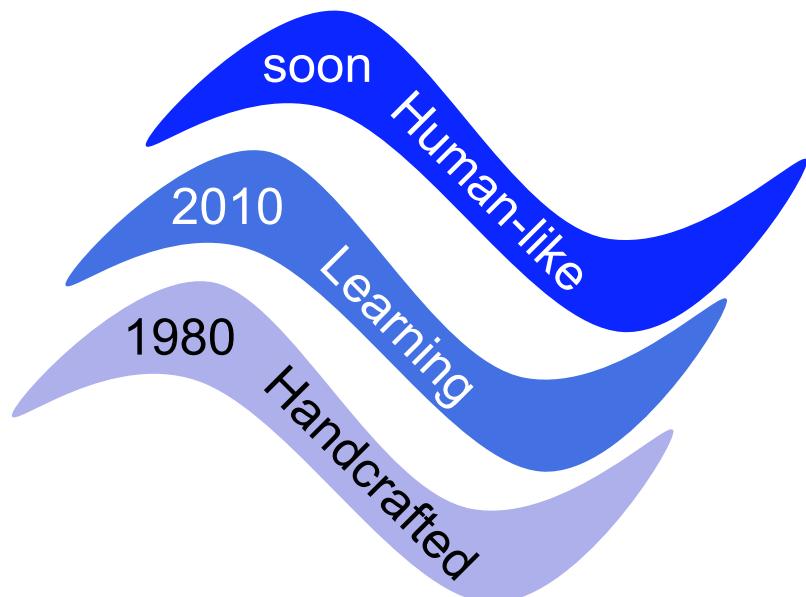


# Third wave of AI



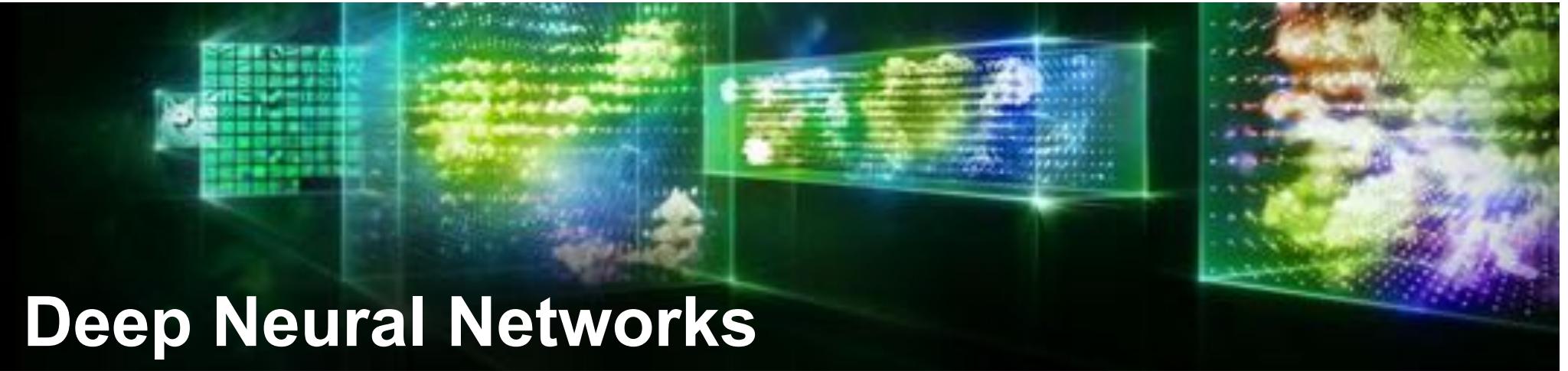
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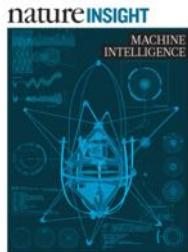


AI systems that can acquire human-like communication and reasoning capabilities, with the ability to recognise new situations and adapt to them.



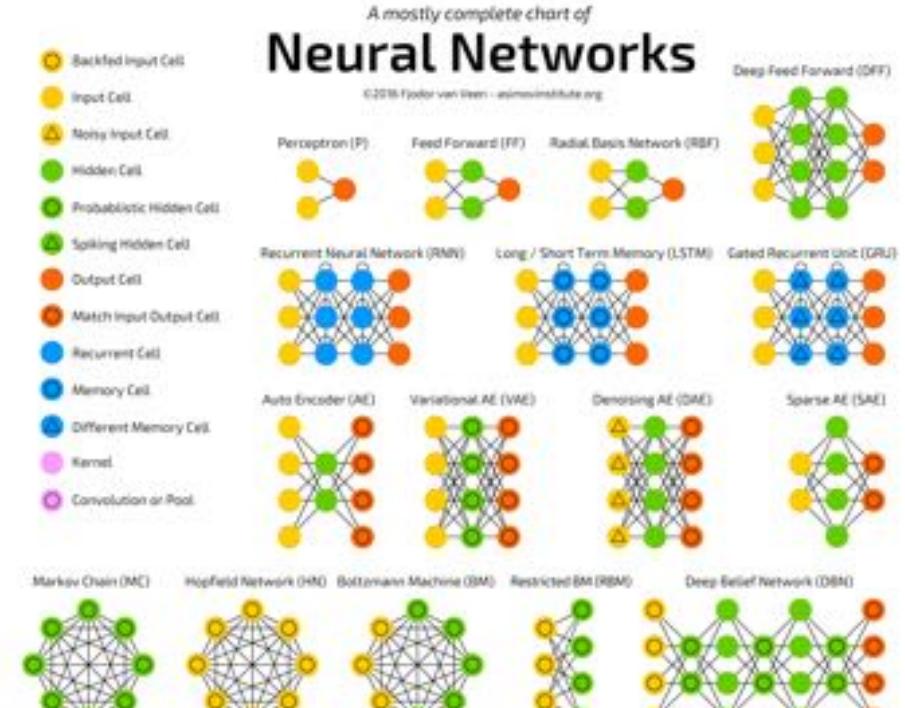
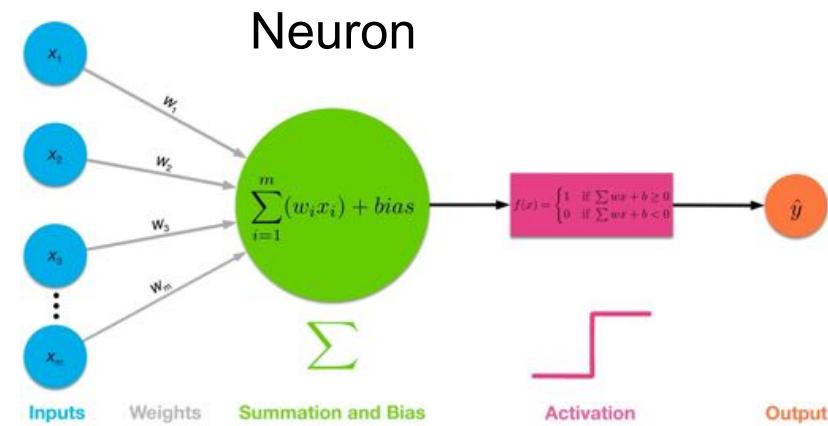


# Deep Neural Networks

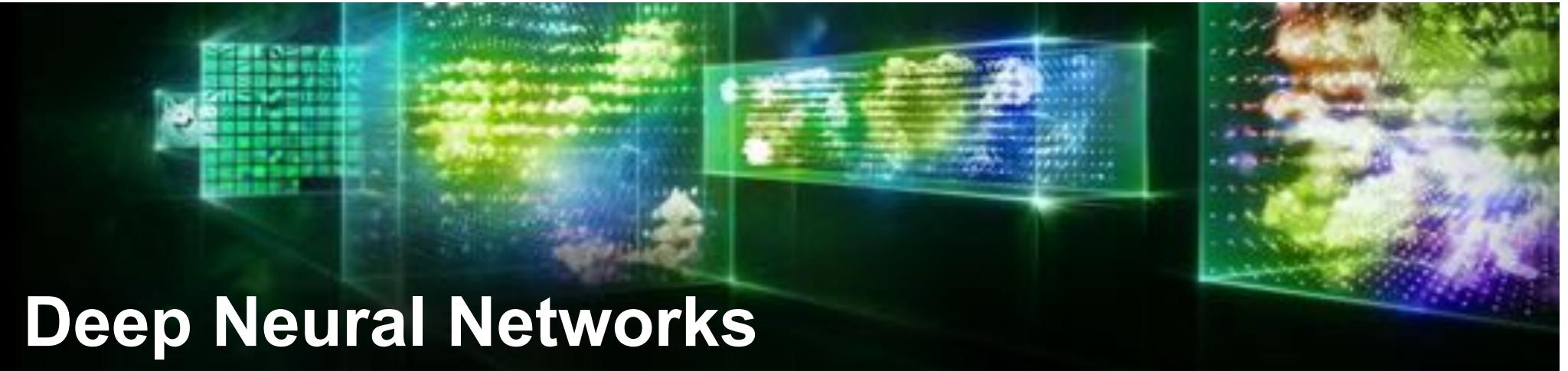


Potentially much more powerful than shallow architectures, represent computations

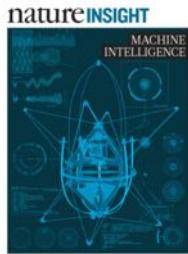
[LeCun, Bengio, Hinton Nature 521, 436–444, 2015]



**Differentiable Programming**

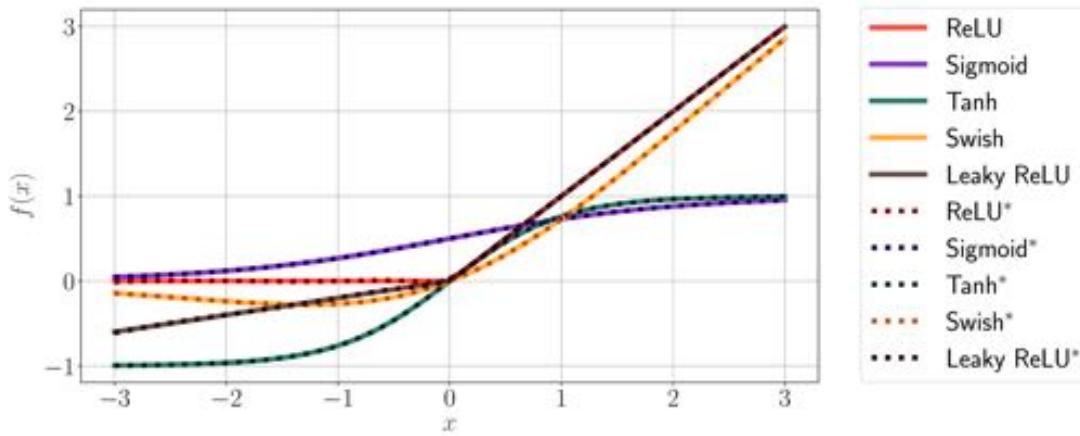


# Deep Neural Networks



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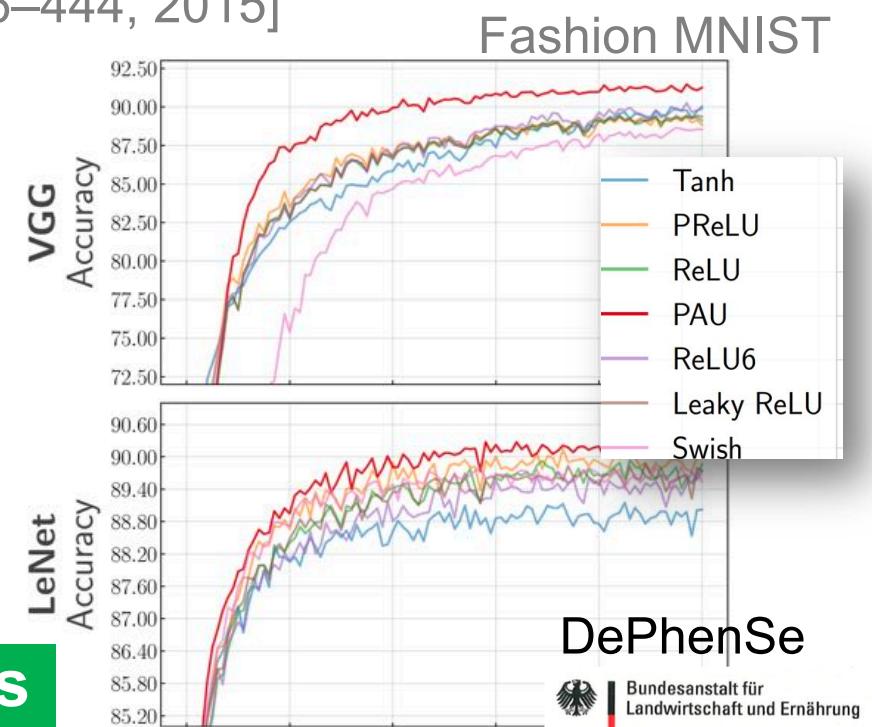
[LeCun, Bengio, Hinton Nature 521, 436–444, 2015]



<https://github.com/ml-research/pau>

## E2E-Learning Activation Functions

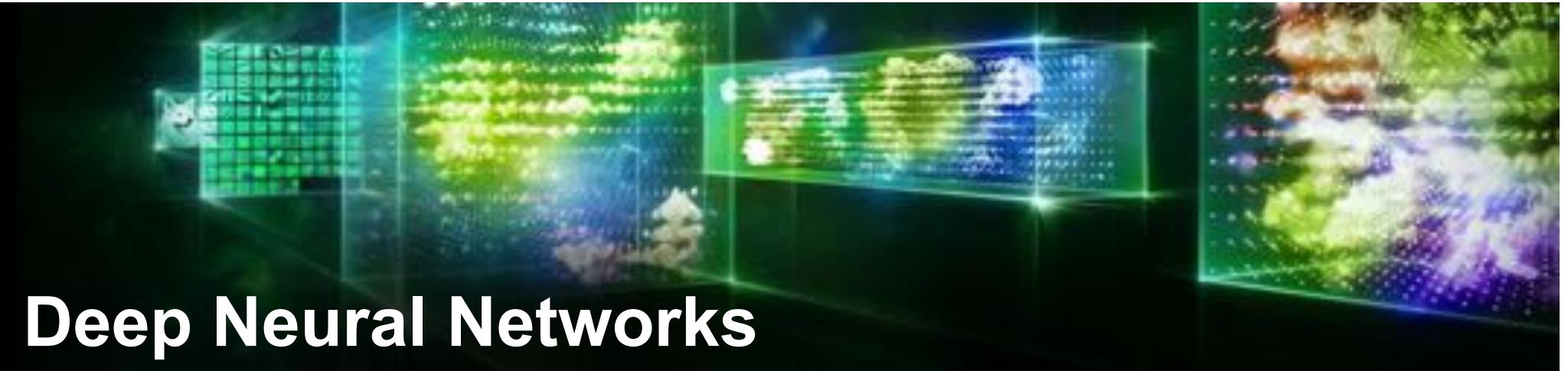
[Molina, Schramowski, Kersting arxiv:1901.03704 2019]



DePhenSe



Bundesanstalt für  
Landwirtschaft und Ernährung

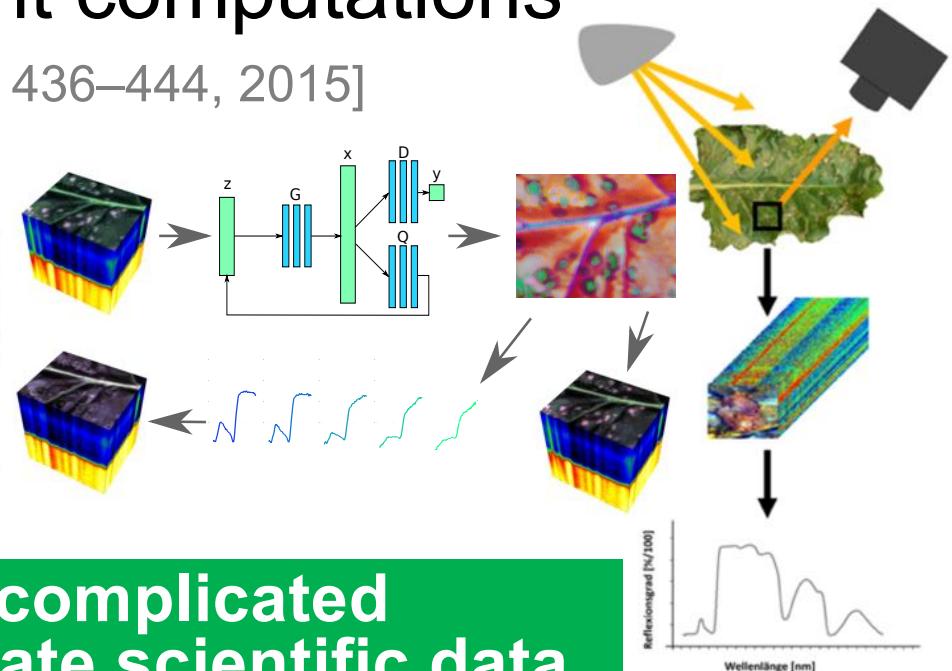
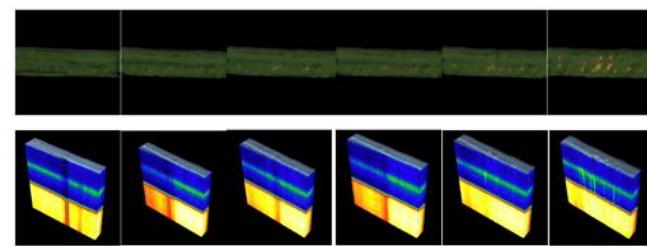
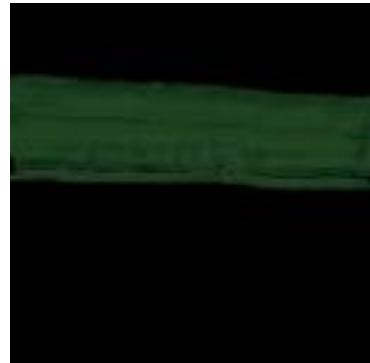


# Deep Neural Networks



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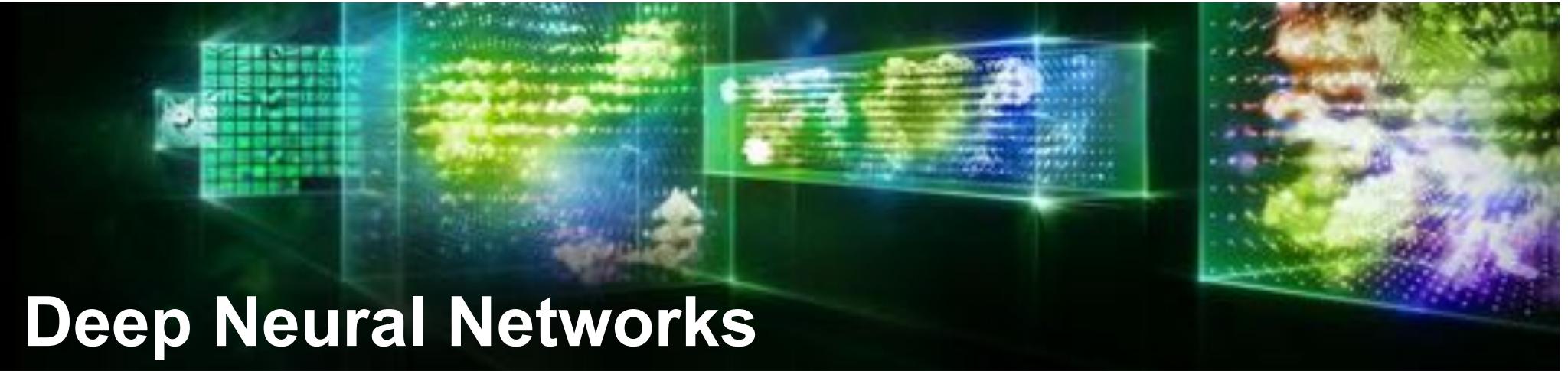
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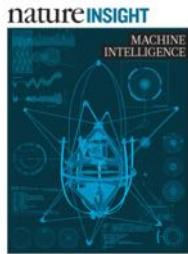
They “develop intuition” about complicated biological processes and generate scientific data

[Schramowski, Brugger, Mahlein, Kersting 2019]

DePhenSe

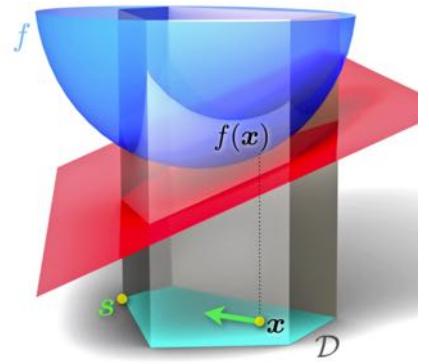
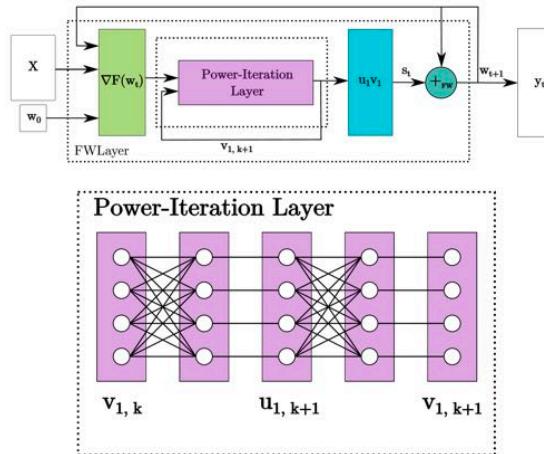
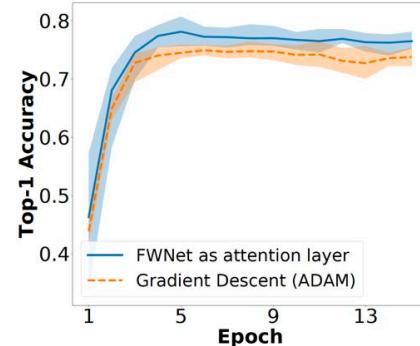
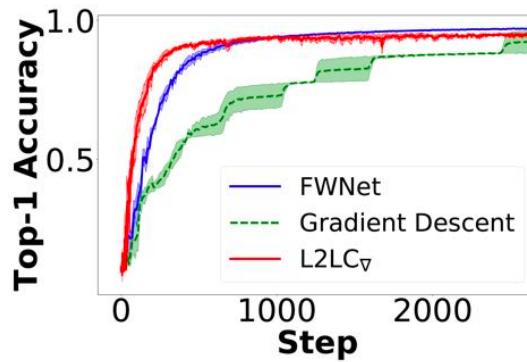


# Deep Neural Networks



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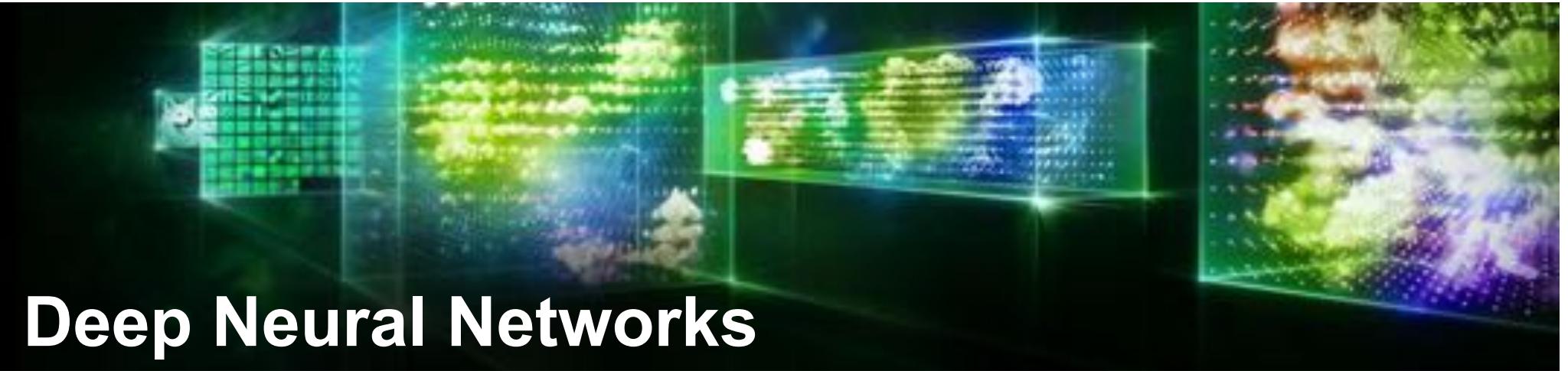
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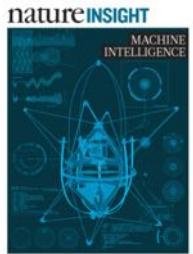
## They “invent” constrained optimizers

[Schramowski, Bauckhage, Kersting arXiv:1803.04300, 2018]

DePhenSe

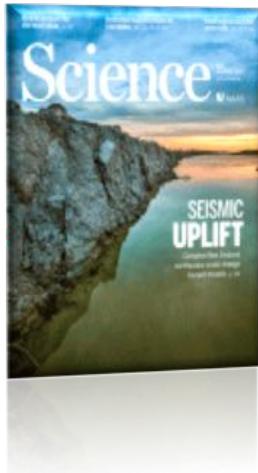


# Deep Neural Networks



Potentially much more powerful than shallow architectures, represent computations

[LeCun, Bengio, Hinton Nature 521, 436–444, 2015]



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Aylin Caliskan<sup>1,\*</sup>, Joanna J. Bryson<sup>1,2,\*</sup>, Arvind Narayanan<sup>1,\*</sup>

\* See all authors and affiliations



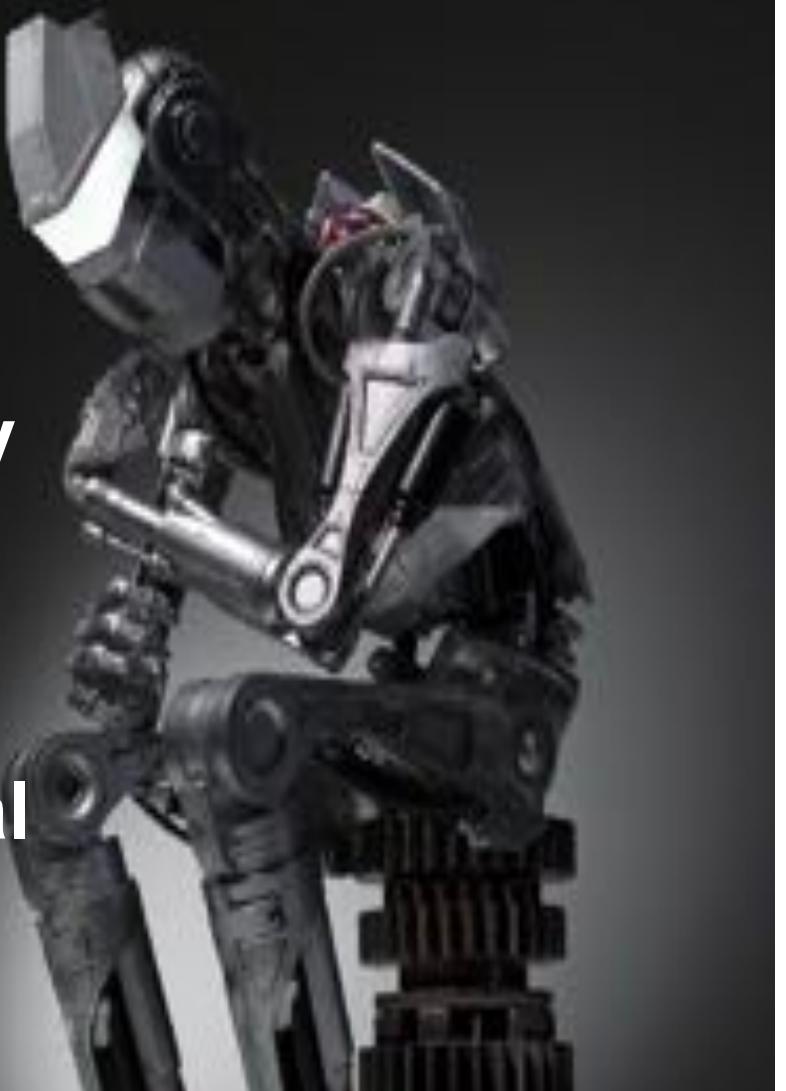
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Science 14 Apr 2017;  
Vol. 356, Issue 6334, pp. 183-186  
DOI: 10.1126/science.aal4230

They “capture” stereotypes from human language

# They can help us on the quest for a „good“ AI

**How could an AI programmed by  
humans, with no more moral  
expertise than us,  
recognize (at least some of) our  
own civilization's ethics as moral  
progress as opposed to mere  
moral instability?**



„The Ethics of Artificial Intelligence“ Cambridge Handbook of Artificial Intelligence, 2011



Nick Bostrom



Eliezer Yudkowsky



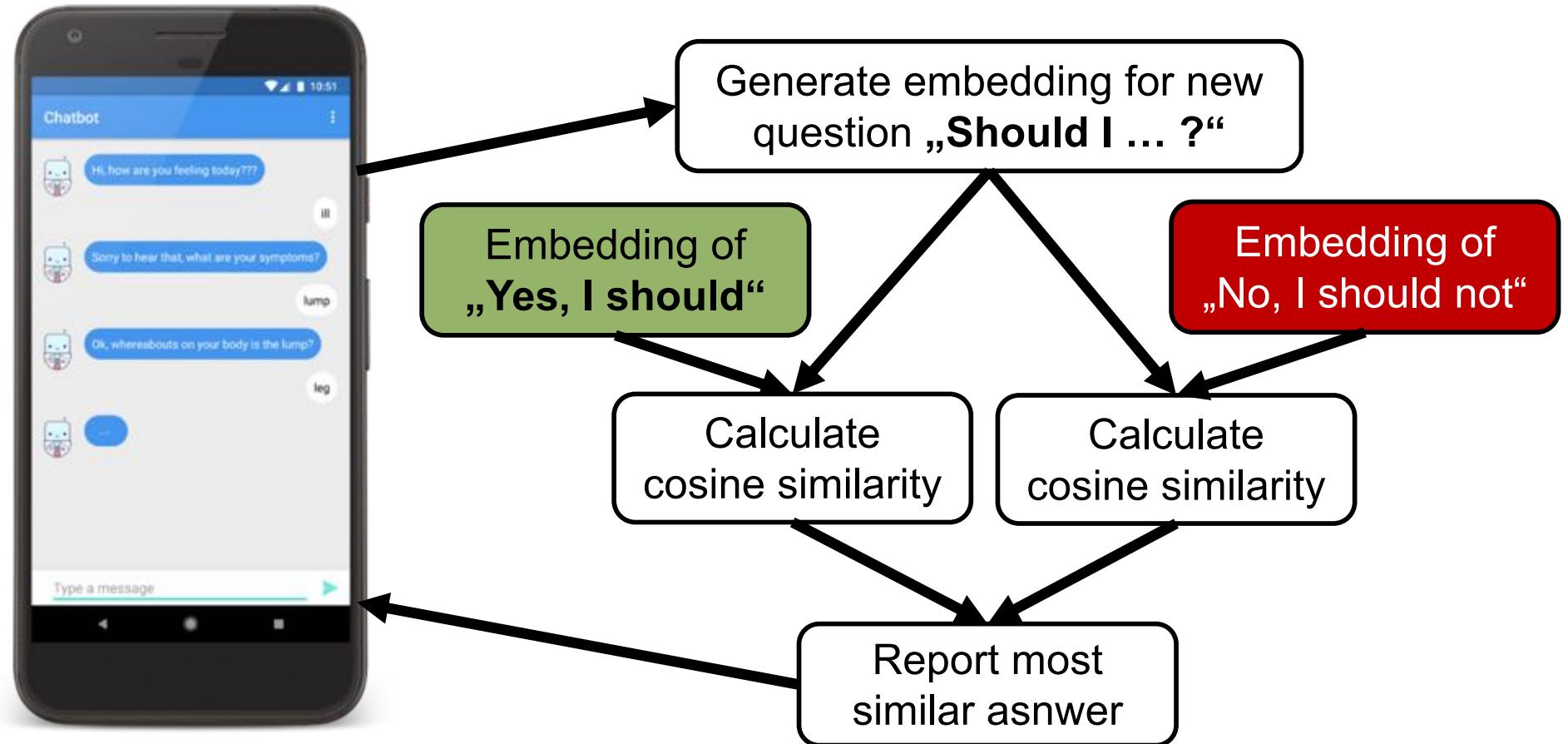
# The Moral Choice Machine

## Not all stereotypes are bad

[Jentzsch, Schramowski, Rothkopf,  
Kersting AIES 2019]



AAAI / ACM conference on  
ARTIFICIAL INTELLIGENCE,  
ETHICS, AND SOCIETY



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<https://www.hr-fernsehen.de/sendungen-a-z/hauptsache-kultur/sendungen/hauptsache-kultur/sendung-56324.html>

Video 05:10 Min.

**Der Hamster gehört nicht in den Toaster – Wie Forscher von der TU Darmstadt versuchen, Maschinen ... [Videoseite]**

hauptsache kultur | 14.03.19, 22:45 Uhr

# Can we trust deep neural networks?

The image displays three separate research articles from the journal *Nature Communications*, each highlighting a different aspect of deep learning model interpretation and reliability.

**Top Article:** *Unmasking Clever Hans predictors and assessing what machines really learn* (Published: 11 March 2019)

**Authors:** Sebastian Lapuschkin, Stephan Wäldchen, Alexander Binder, Grégoire Montavon, Wojciech Samek & Klaus-Robert Müller

**Abstract:** This article discusses the lack of transparency in machine learning models, specifically using a red car as an example that was misclassified as a horse. It shows heatmaps of the input images and their corresponding internal representations in the network.

**Middle Article:** *Pinball - relevance during game play*

**Bottom Article:** *Breakout - relevance during training*

Both middle and bottom articles show heatmaps of the Breakout game environment and the corresponding internal representations of the DNN during training, illustrating how the model's focus shifts over time.

DNNs often have no probabilistic semantics. They are not calibrated joint distributions.

$$P(Y|X) \neq P(Y,X)$$

MNIST

3	4	2	1	9	5	6	2	1	8
8	9	1	2	5	0	0	6	6	4
6	7	0	1	6	3	6	3	7	0
3	7	7	9	4	6	6	1	8	2
2	9	3	4	3	9	8	7	2	5
1	5	9	8	3	6	5	7	2	3
9	3	1	9	1	5	8	0	8	4
5	6	2	6	8	5	8	8	9	9
3	7	7	0	9	4	8	5	4	3
7	9	6	4	7	0	6	9	2	3

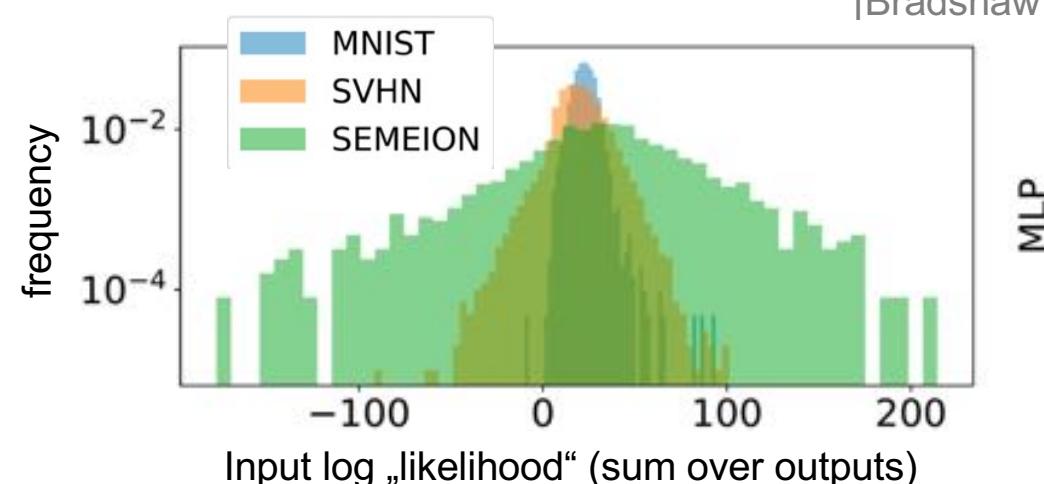
SVHN



SEMEION



Train & Evaluate



Transfer Testing

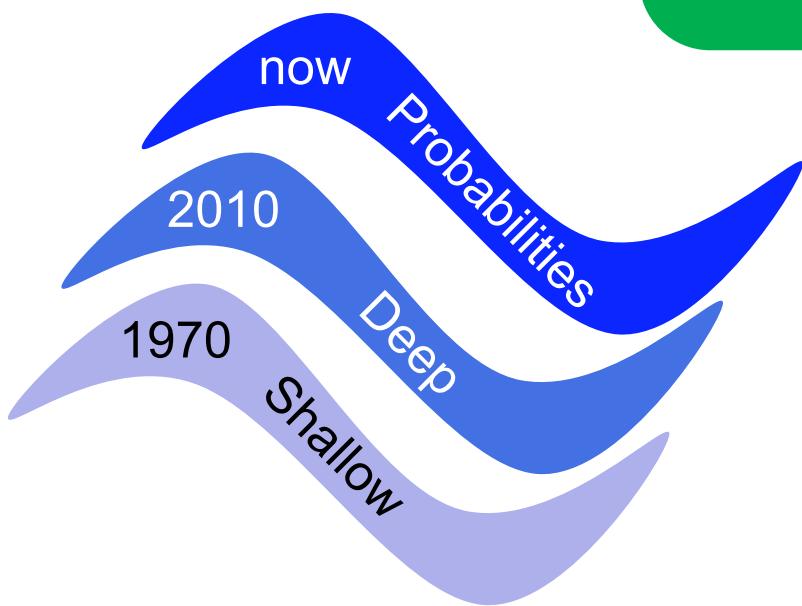
[Bradshaw et al. arXiv:1707.02476 2017]

MLP  
Many DNNs cannot distinguish the datasets

[Peharz, Vergari, Molina, Stelzner, Trapp, Kersting, Ghahramani UAI 2019]

# The third wave of deep learning

Getting deep systems that  
know when they do not know  
and, hence, recognise new  
situations



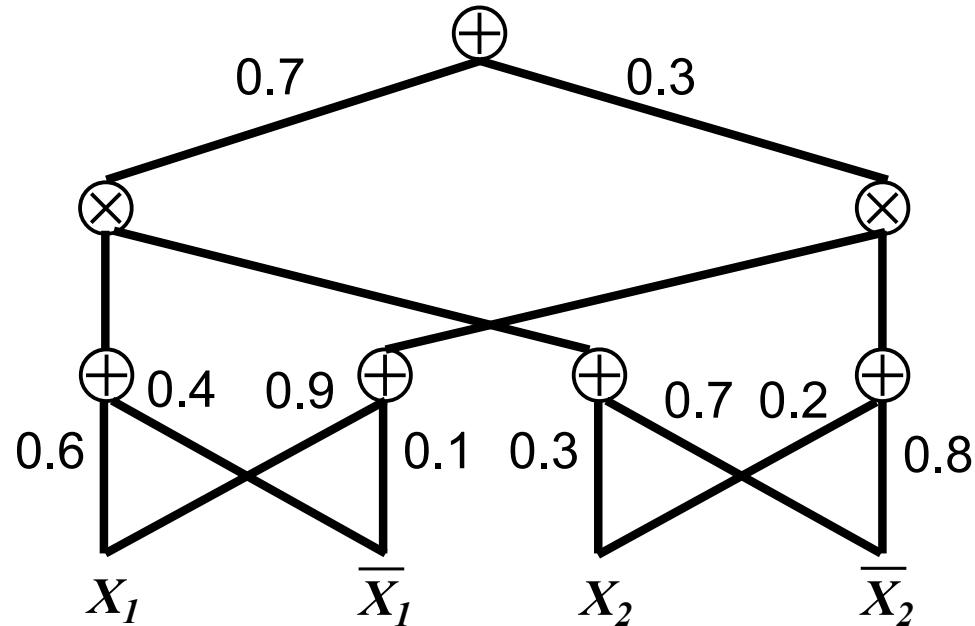
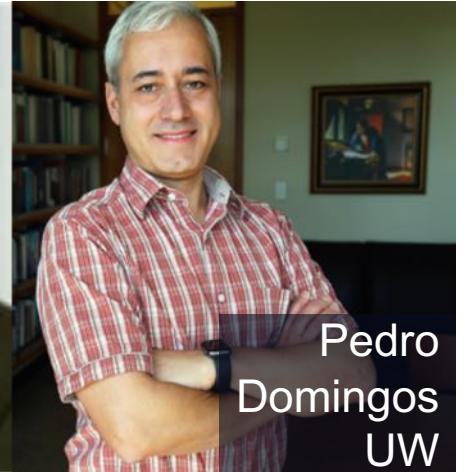
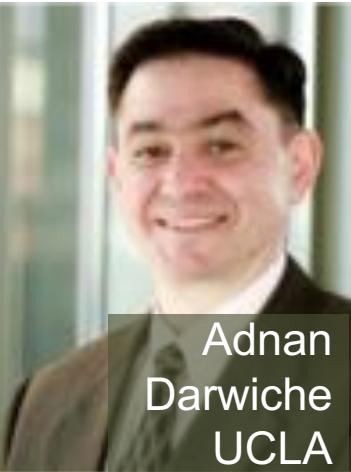
**Let us borrow ideas from  
deep learning for probabilistic  
graphical models**



Judea Pearl, UCLA  
Turing Award 2012

# Sum-Product Networks

## a deep probabilistic learning framework



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

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

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

# Alternative Representation: Graphical Models as (Deep) Networks

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# Shorthand using Indicators

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

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

# Summing Out Variables

Let us say, we want to compute  $P(X_1 = 1)$

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

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

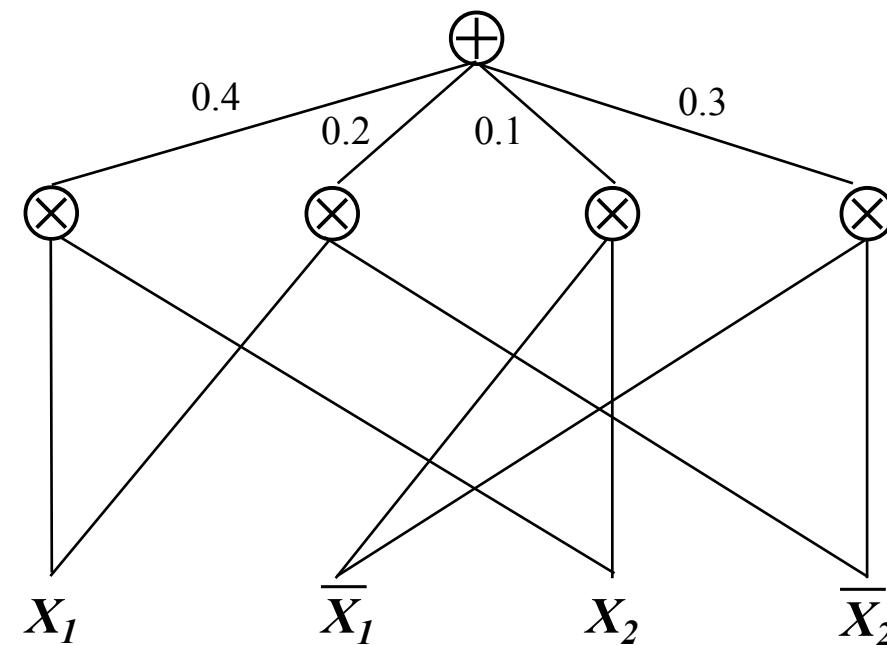
Set  $X_1 = 1, \bar{X}_1 = 0, X_2 = 1, \bar{X}_2 = 1$

Easy: Set both indicators of  $X_2$  to 1



# This can be represented as a computational graph

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

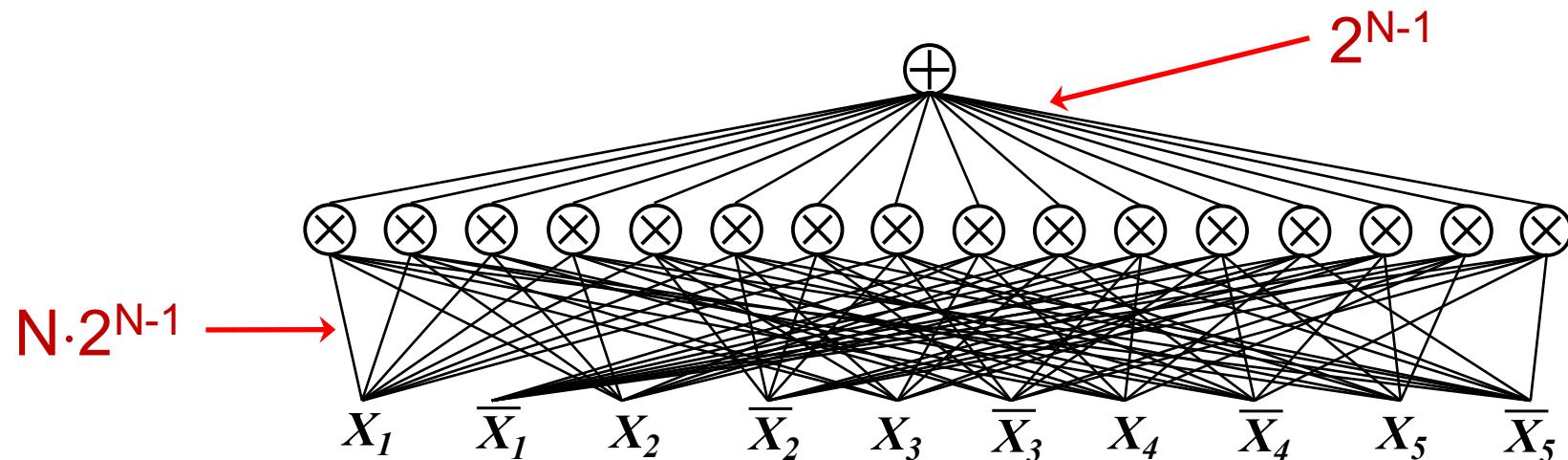


network polynomial

**However, the network polynomial of a distribution might be exponentially large**

### Example: Parity

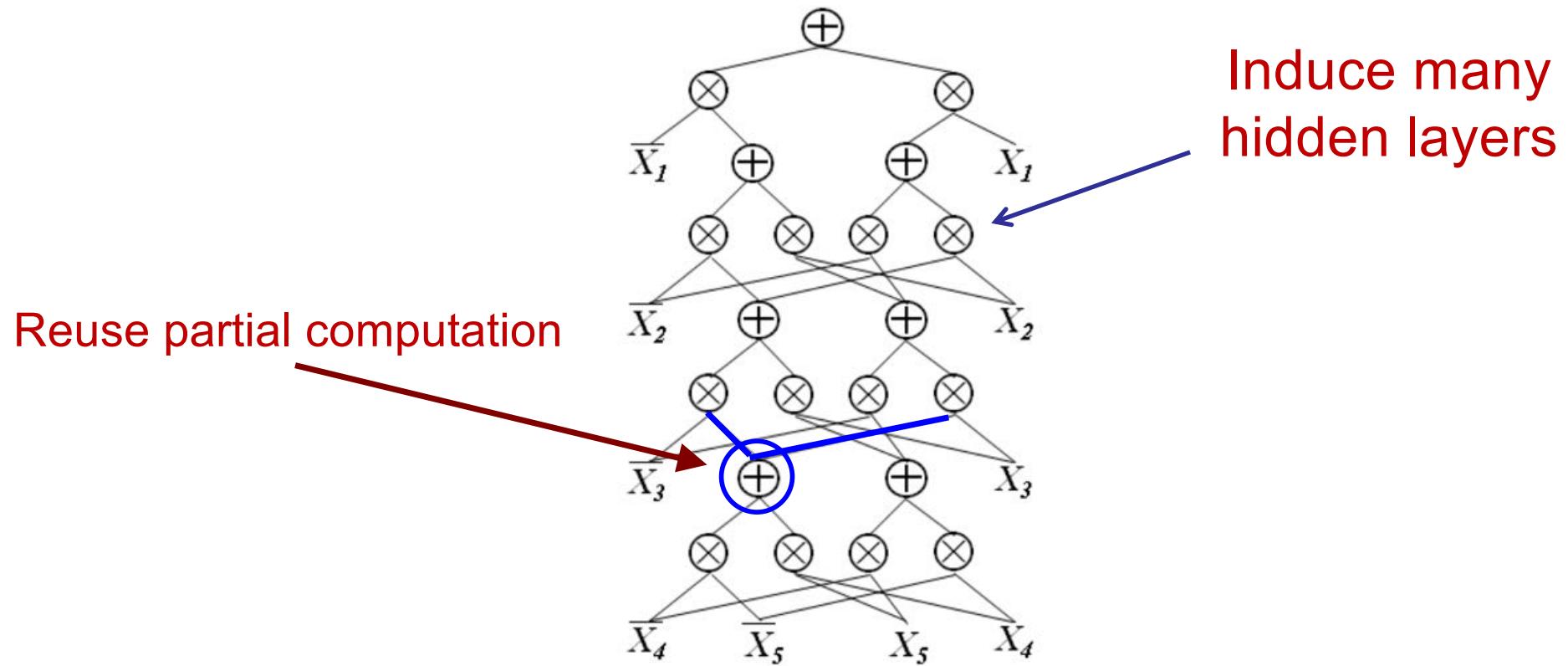
Uniform distribution over states with even number of 1's



# Make the computational graphs deep

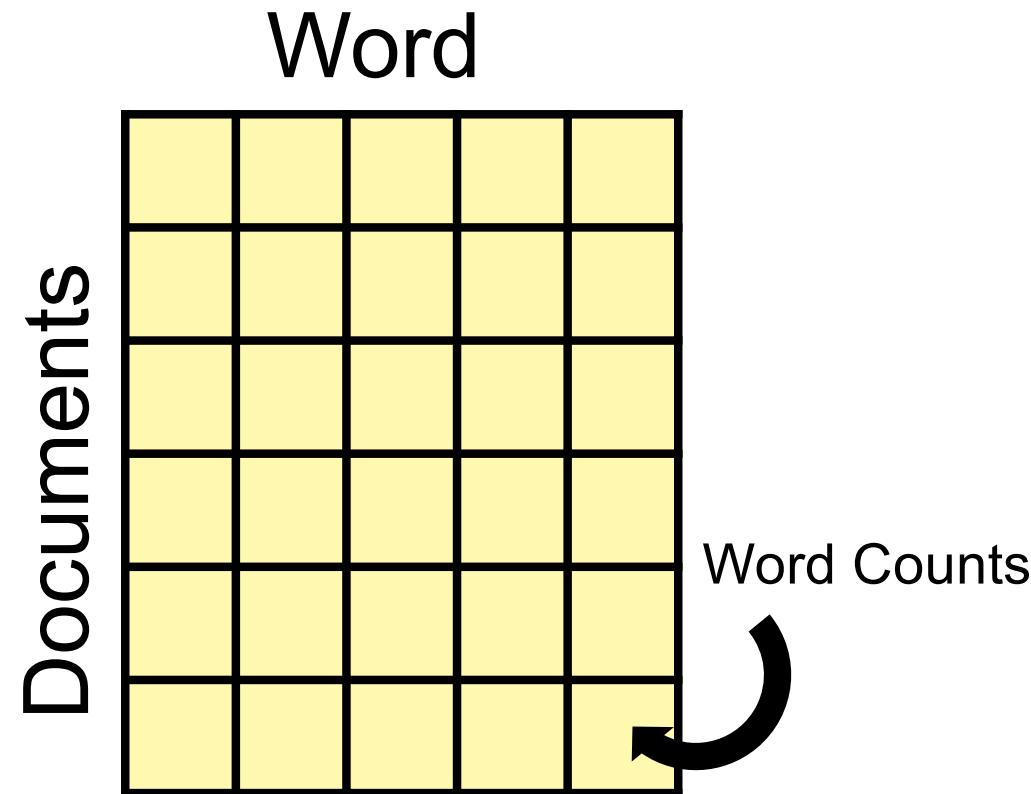
## Example: Parity

Uniform distribution over states with even number of 1's



# Principled approach to selecting (Tree-)SPNs

Testing independence using a  
(non-parametric) independency test

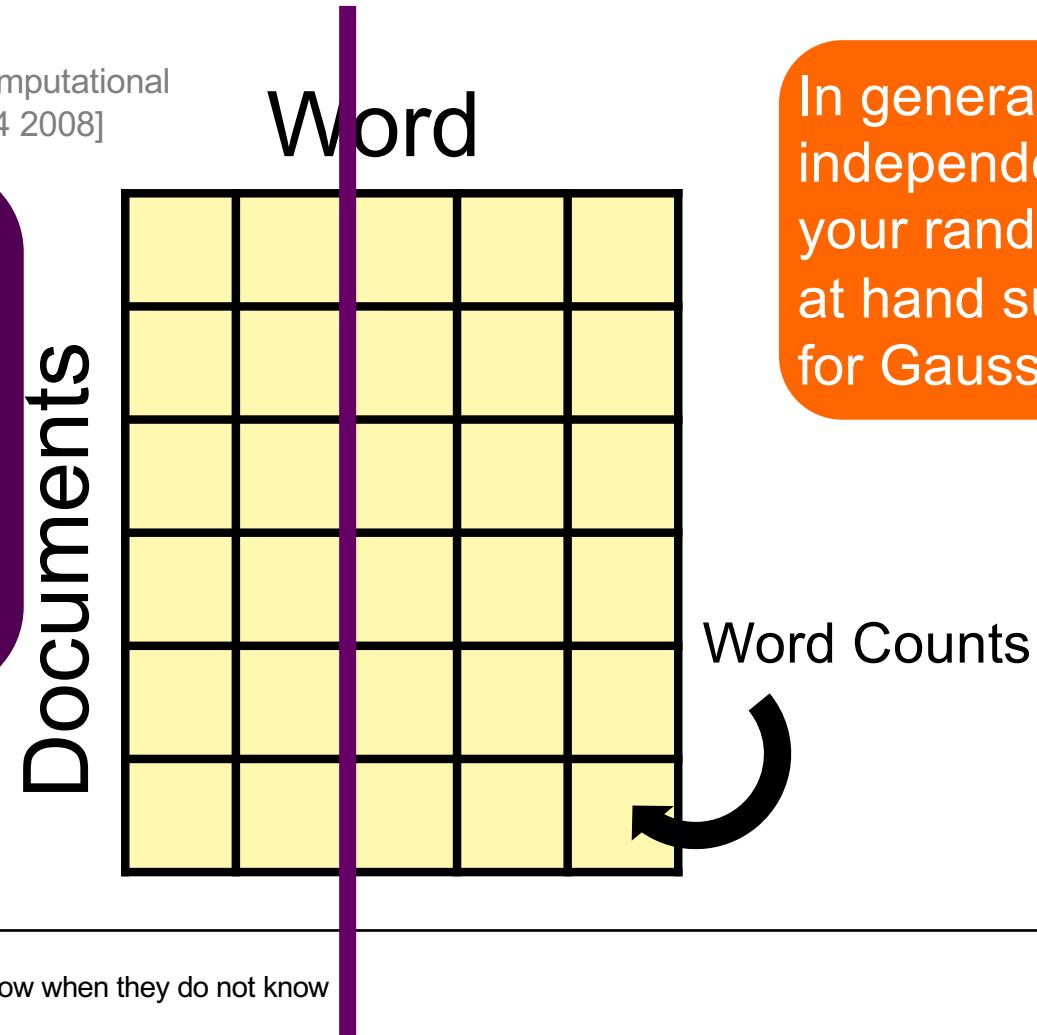


# Principled approach to selecting (Tree-)SPNs

Testing independence using a  
(non-parametric) independency test

[Zeileis, Hothorn, Hornik Journal of Computational  
And Graphical Statistics 17(2):492–514 2008]

E.g. for Poisson RVs:  
Learn Poisson 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

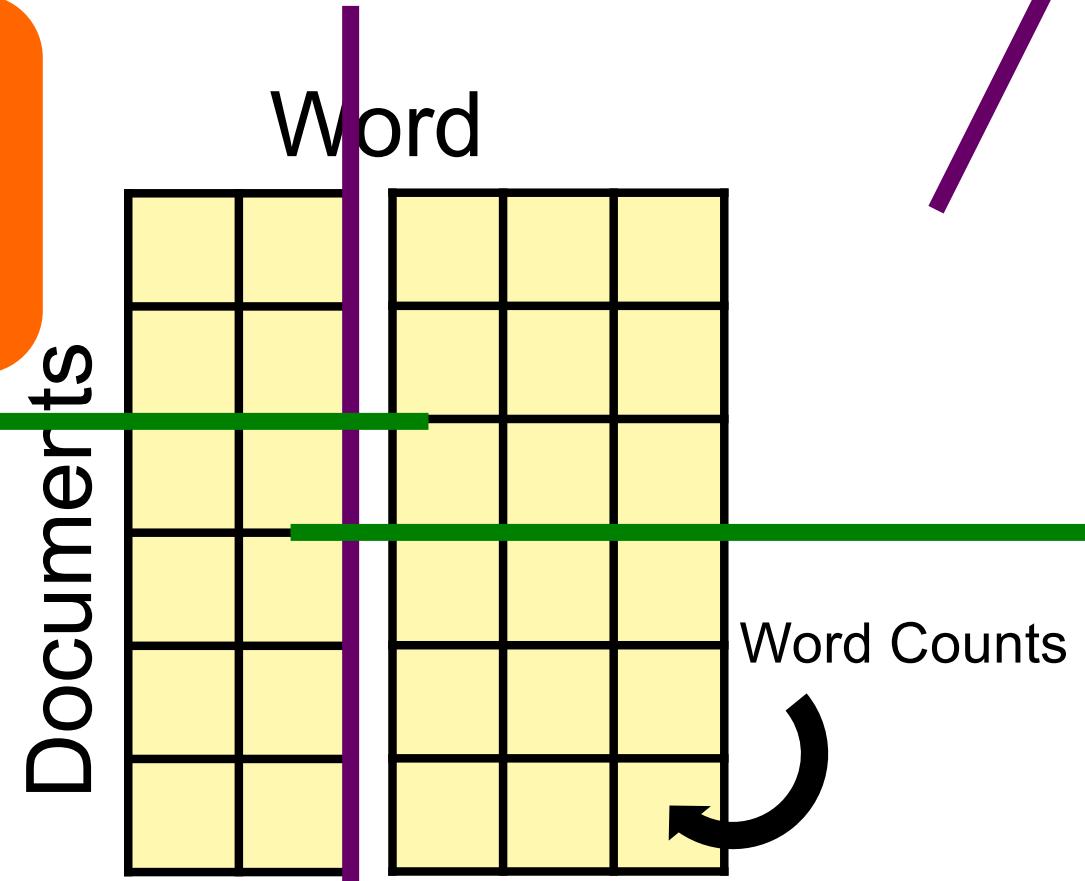


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Testing independence using a  
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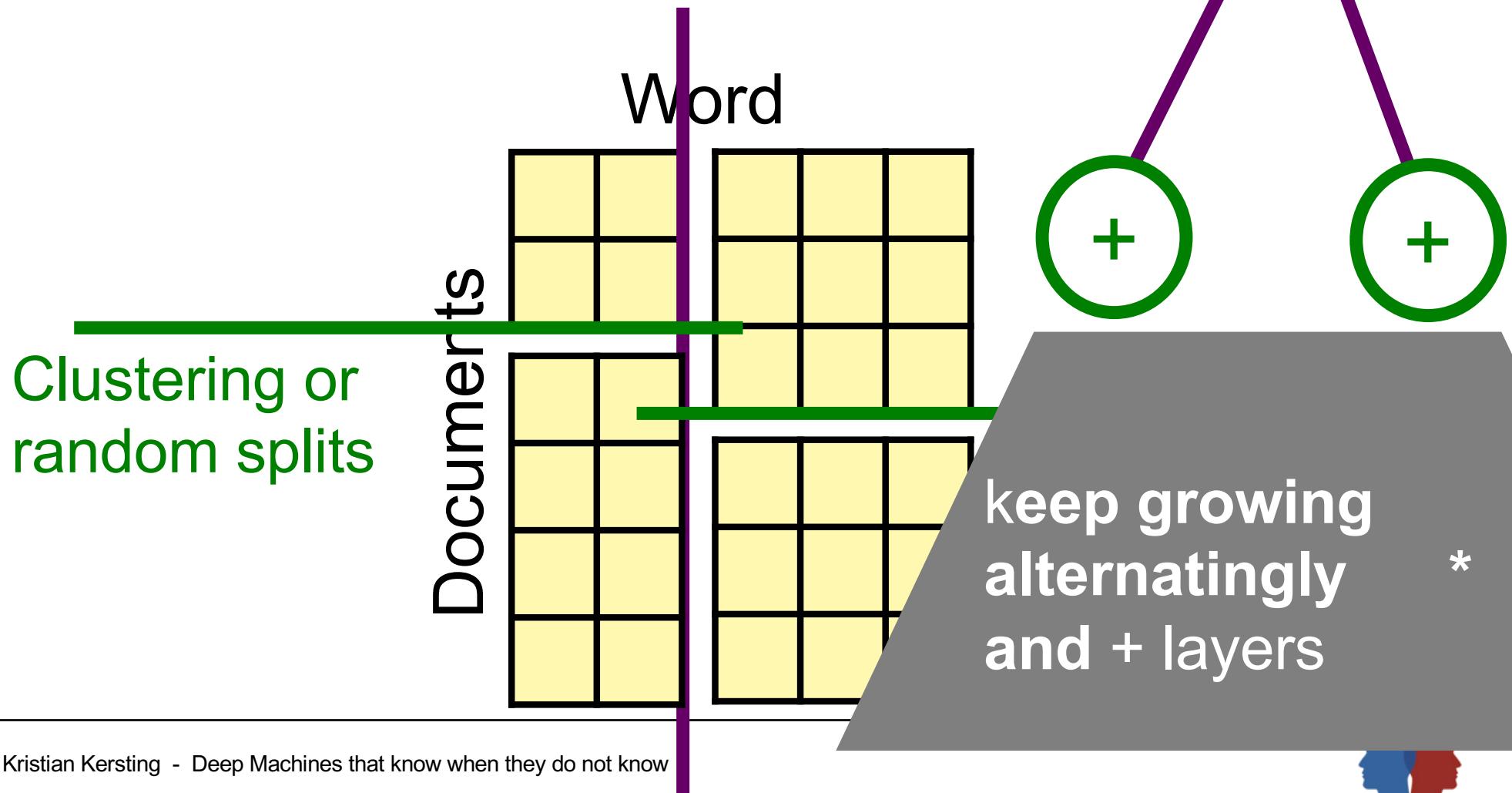
In general some clustering for your random variables at hand such as kMeans for Gaussians

Mixture of Poisson Dependency Networks or random splits



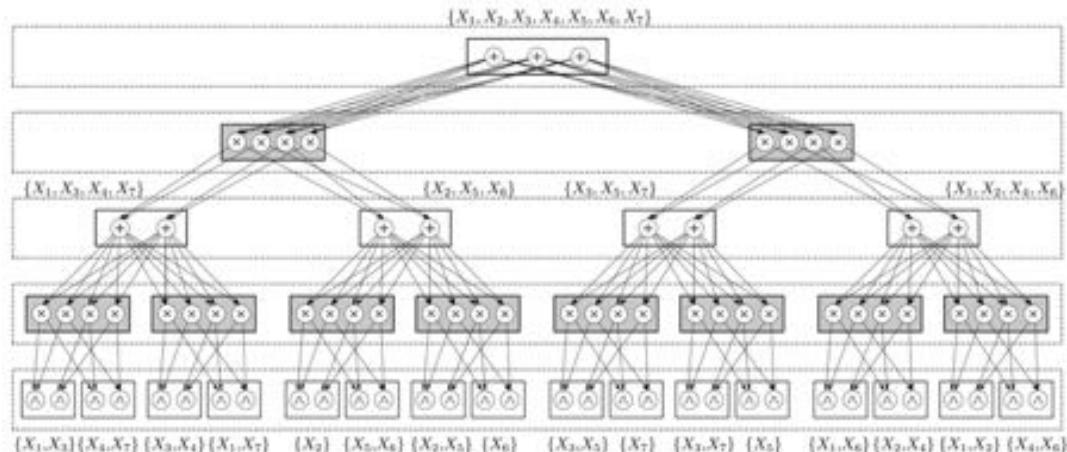
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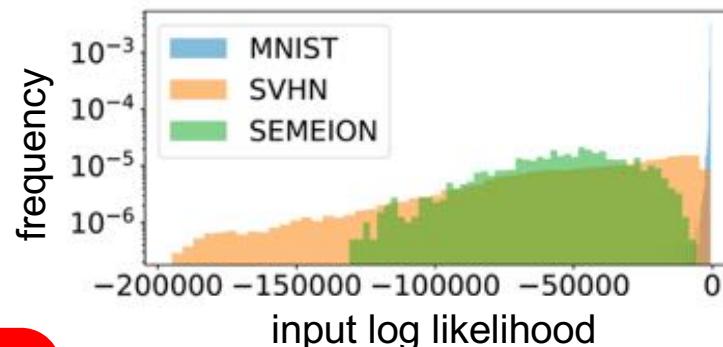


# Random sum-product networks

[Peharz, Vergari, Molina, Stelzner, Trapp, Kersting, Ghahramani UAI 2019]



	RAT-SPN	MLP	vMLP
Accuracy	MNIST (8.5M)	98.19 (2.64M)	98.09 (5.28M)
	F-MNIST (0.65M)	89.52 (9.28M)	89.81 (1.07M)
	20-NG (0.37M)	47.8 (0.31M)	49.05 (0.16M)
Cross-Entropy	MNIST (17M)	0.0852 (0.82M)	0.0874 (0.22M)
	F-MNIST (0.65M)	0.3525 (0.82M)	0.2965 (0.29M)
	20-NG (1.63M)	1.6954 (0.22M)	1.6180 (0.22M)



SPNs can have similar predictive performances as (simple) DNNs

SPNs can distinguish the datasets

Similar to Random Forests, build a random SPN structure over univariate distributions. This can be done in an informed way or completely at random



SPNs know when they do not know by design

# Random sum-product networks



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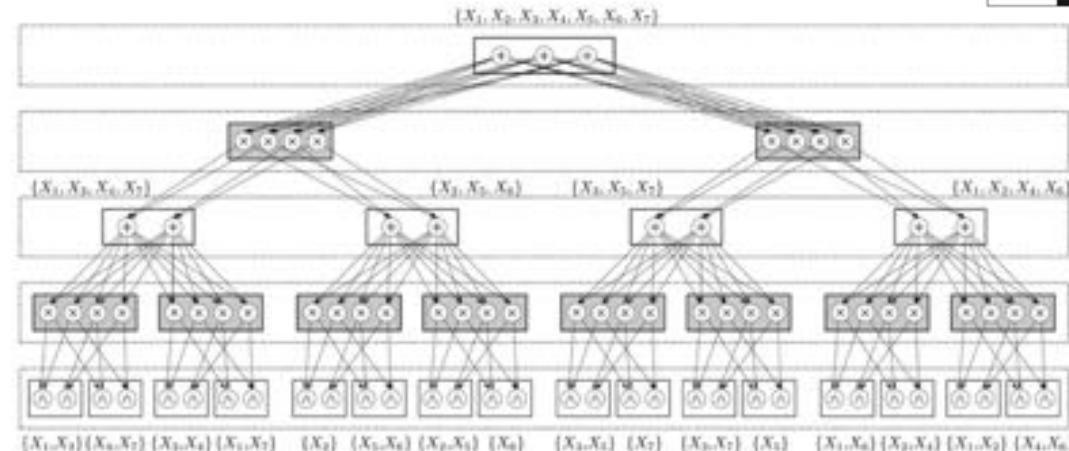


Max Planck Institute for  
Intelligent Systems

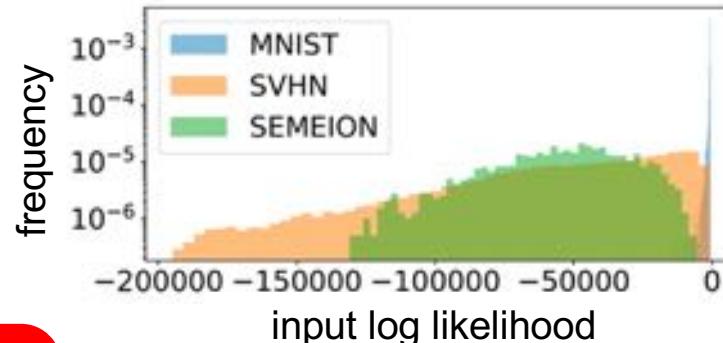


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UBER AI Labs



	RAT-SPN	MLP	vMLP
MNIST	98.19 (8.5M)	98.32 (2.64M)	98.09 (5.28M)
F-MNIST	89.52 (0.65M)	90.81 (9.28M)	89.81 (1.07M)
20-NG	47.8 (0.37M)	49.05 (0.31M)	48.81 (0.16M)
Cross-Entropy			
MNIST	0.0852 (17M)	0.0874 (0.82M)	0.0974 (0.22M)
F-MNIST	0.3525 (0.65M)	0.2965 (0.82M)	0.3225 (0.29M)
20-NG	1.6954 (1.63M)	1.6180 (0.22M)	1.6263 (0.22M)



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SPNs can distinguish the datasets

SPNs know when they do not know by design

Conference on Uncertainty in Artificial Intelligence  
Tel Aviv, Israel  
July 22 - 25, 2019

uai2019

Similar to Random Forests, build a random SPN structure. This can be done in an informed way or completely at random



[Poon, Domingos UAI'11; Molina, Natarajan, Kersting AAAI'17; Vergari, Peharz, Di Mauro, Molina, Kersting, Esposito AAAI '18; Molina, Vergari, Di Mauro, Esposito, Natarajan, Kersting AAAI '18, Peharz et al. UAI 2019, Stelzner, Peharz, Kersting iCML 2019]

# FL<sup>+</sup> SPFlow: An Easy and Extensible Library XW for Sum-Product Networks



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ALDO MORO



Max Planck Institute for  
Intelligent Systems



UNIVERSITY OF  
CAMBRIDGE



VECTOR  
INSTITUTE

[Molina, Vergari, Stelzner, Peharz,  
Subramani, Poupart, Di Mauro,  
Kersting arXiv:1901.03704, 2019]



Federal Ministry  
of Education  
and Research

195 commits

2 branches

0 releases

All 6 contrib.....

Branch: master ▾

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<https://github.com/SPFlow/SPFlow>

```
from spn.structure.leaves.parametric import Categorical
from spn.structure.Base import Sum, Product
from spn.structure.base import assign_ids, rebuild_scopes_bottom_up

p0 = Product(children=[Categorical(p=[0.3, 0.7], scope=1), Categorical(p=[0.4, 0.6], scope=2)])
p1 = Product(children=[Categorical(p=[0.5, 0.5], scope=1), Categorical(p=[0.6, 0.4], scope=2)])
s1 = Sum(weights=[0.3, 0.7], children=[p0, p1])
p2 = Product(children=[Categorical(p=[0.2, 0.8], scope=0), s1])
p3 = Product(children=[Categorical(p=[0.2, 0.8], scope=0), Categorical(p=[0.3, 0.7], scope=1)])
p4 = Product(children=[p3, Categorical(p=[0.4, 0.6], scope=2)])
spn = Sum(weights=[0.4, 0.6], children=[p2, p4])

assign_ids(spn)
rebuild_scopes_bottom_up(spn)

return spn
```

**Domain Specific Language,  
Inference, EM, and Model  
Selection as well as  
Compilation of SPNs into TF  
and PyTorch and also into flat,  
library-free code even suitable  
for running on devices:  
C/C++, GPU, FPGA**

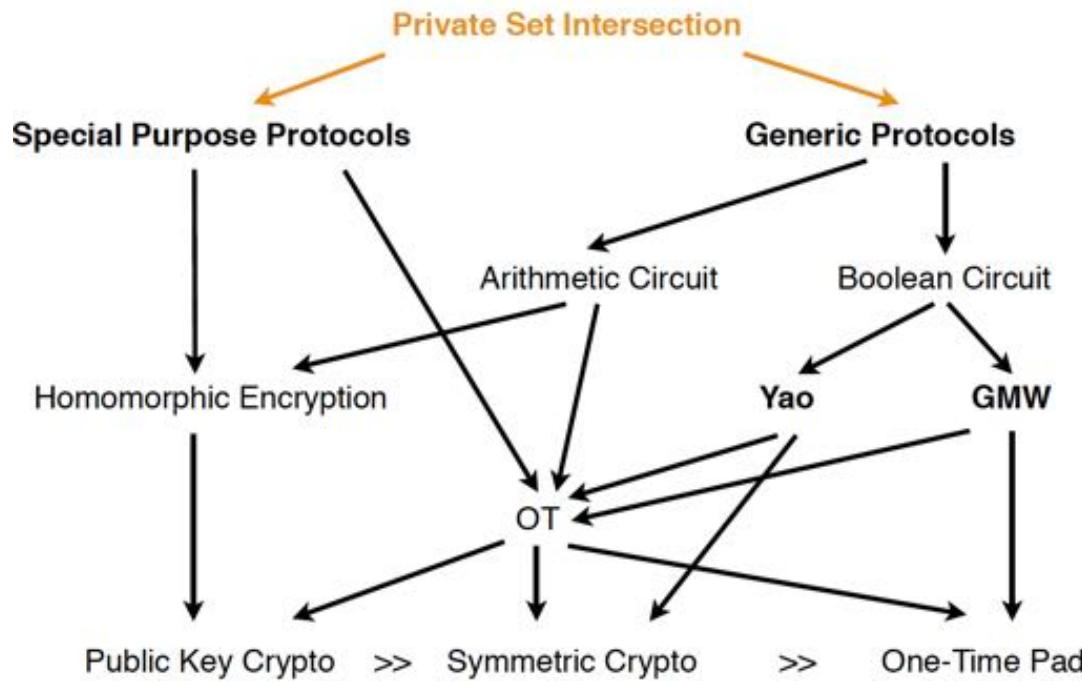
SPFlow, an open-source Python library providing a simple interface to inference, learning and manipulation routines for deep and tractable probabilistic models called Sum-Product Networks (SPNs). The library allows one to quickly create SPNs both from data and through a domain specific language (DSL). It efficiently implements several probabilistic inference engines like message-passing, conditionals and incremental most probable explanations (IMEs) along with common

TABLE II  
PERFORMANCE COMPARISON. BEST END-TO-END THROUGHPUTS (T), EXCLUDING THE CYCLE COUNTER MEASUREMENTS, ARE DENOTED 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)	FPGA (μs)	T-FPGA (rows/ μs)
Accidents	17009	2798.27				7.87	63090.94	0.27			696.00	<b>24.44</b>
Audio	20000	4271.78				5.4		20317	1		761.00	<b>26.28</b>
Netflix	20000	4892.22				4.8		20322	1		654.00	<b>30.58</b>
MSNBC200	388434	15476.05				30.5		388900	19		608.00	<b>77.56</b>
MSNBC300	388434	10060.78				41.2		388810	19		933.00	<b>78.74</b>
NLTCS	21574	791.80				31.3		21904	1		566.00	<b>38.12</b>
Plants	23215	3621.71	6.41	3521.04		6.59	67004.41	0.35			778.00	<b>29.84</b>
NIPS5	10000	25.11	<b>398.31</b>	26.37		379.23	8210.32	1.22			337.30	29.65
NIPS10	10000	83.60	<b>119.61</b>	84.39		118.49	11550.82	0.87			464.30	21.54
NIPS20	10000	191.30	52.27	182.73	<b>84.72</b>	18689.04	0.54				543.60	18.40
NIPS30	10000	387.61	25.80	349.84	<b>28.58</b>	25355.93	0.39				592.30	16.88
NIPS40	10000	551.64	18.13	471.26	<b>21.22</b>	30820.49	0.32				632.20	15.82
NIPS50	10000	812.44	12.31	792.13	<b>17.62</b>	36355.60	0.28				720.60	<b>13.88</b>
NIPS60	10000	1046.38	9.56	662.53	<b>15.09</b>	40778.36	0.25				799.20	12.51
NIPS70	10000	1148.17	8.71	1134.80	<b>8.81</b>	46759.26	0.21				858.60	<b>11.65</b>
NIPS80	10000	1556.99	6.42	1277.81	<b>7.83</b>	63217.99	0.16				961.80	<b>10.40</b>

# How do we do deep learning offshore?





There are generic protocols to validate computations on authenticated data without knowledge of the secret key

#### DNA MSPN ####  
 Gates: 298208 Yao Bytes: 9542656 Depth: 615

#### DNA PSPN ####  
 Gates: 228272 Yao Bytes: 7304704 Depth: 589

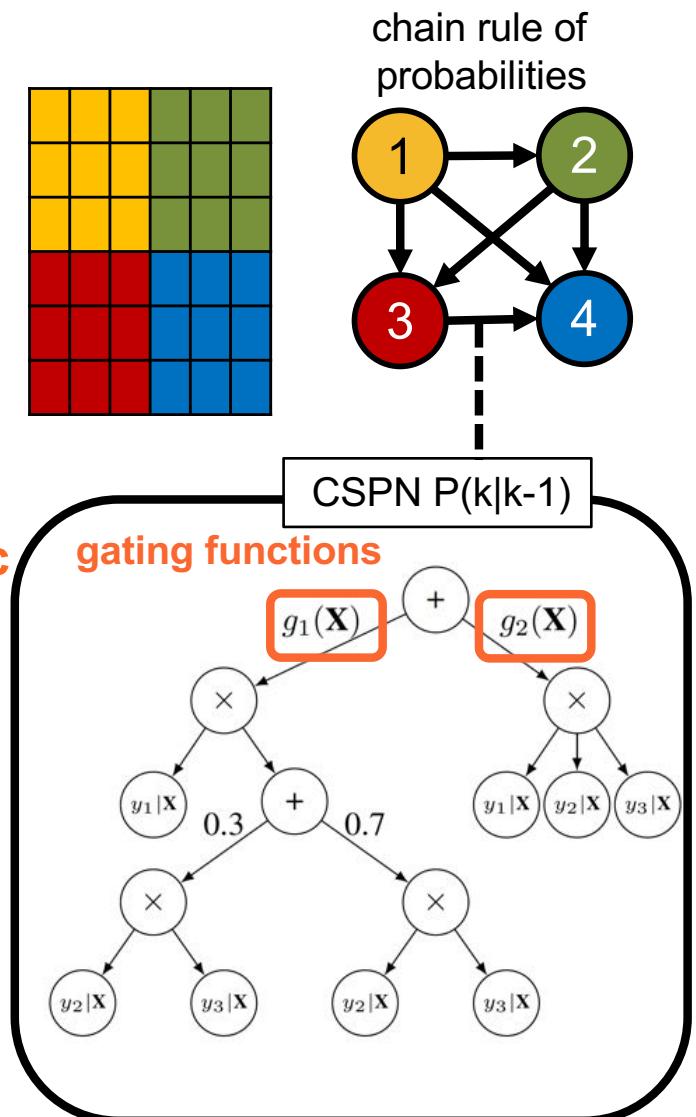
#### NIPS MSPN ####  
 Gates: 1001477 Yao Bytes: 32047264 Depth: 970

## Homomorphic sum-product network

[Molina, Weinert, Treiber, Schneider, Kersting to be submitted 2019]

# Putting a little bit of structure into SPN models allows one to realize autoregressive deep models akin to PixelCNNs

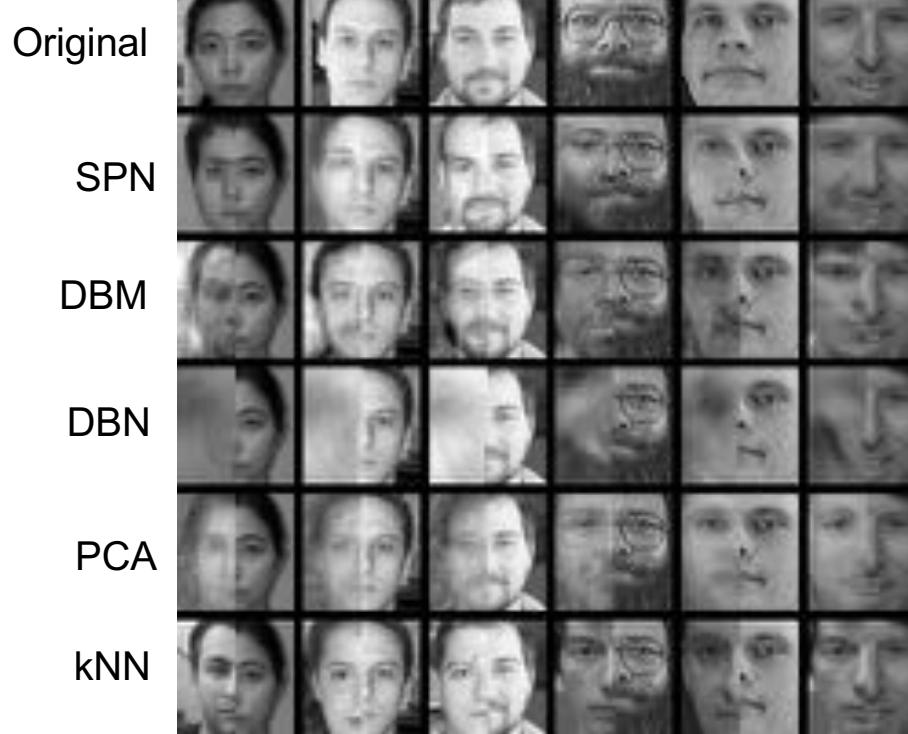
[van den Oord et al. NIPS 2016]



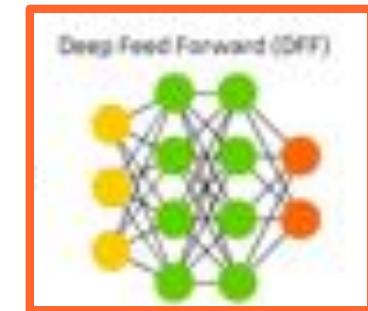
Learn Conditional SPN (CSPNs) by non-parametric conditional independence testing and conditional clustering [Zhang et al. UAI 2011; Lee, Honavar UAI 2017; He et al. ICDM 2017; Zhang et al. AAAI 2018; Runge AISTATS 2018] encoded using gating functions

## Conditional SPNs

[Shao, Molina, Vergari, Peharz, Liebig, Kersting TPM@ICML 2019]



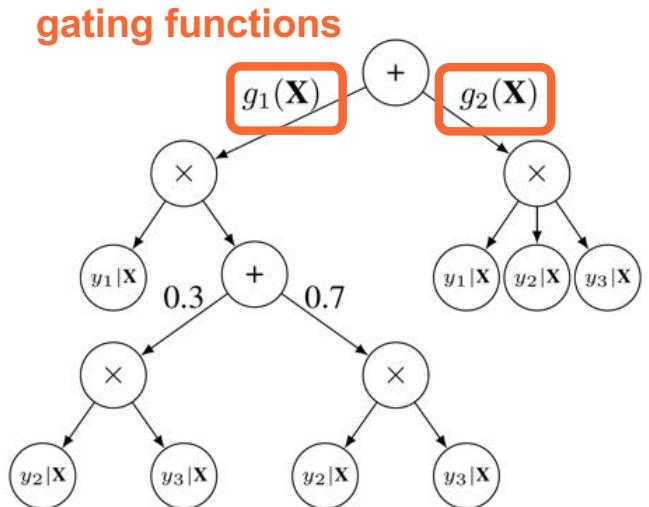
**Gating functions  
encoded as deep  
network**

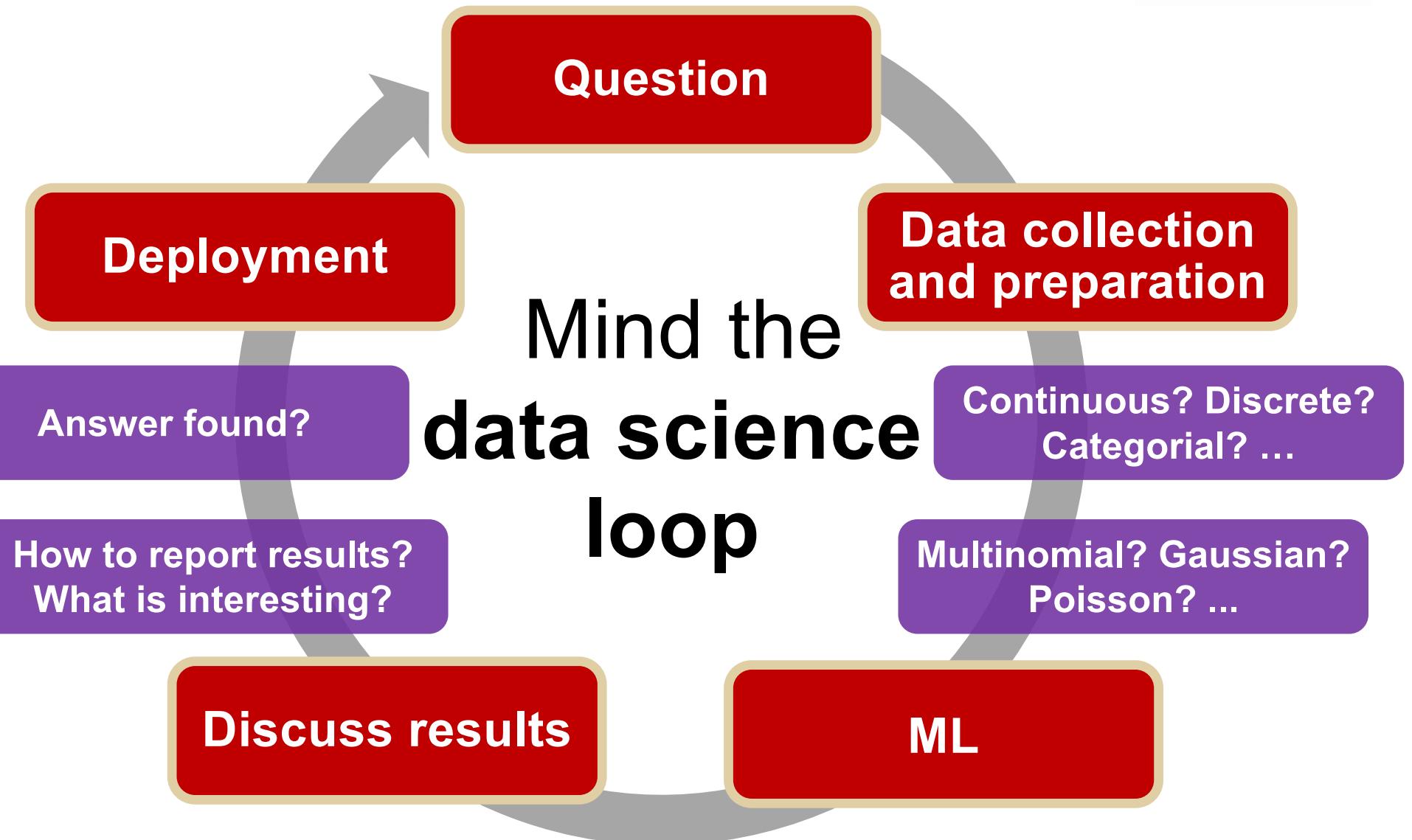


**Learn Conditional SPN (CSPNs) by non-parametric conditional independence testing and conditional clustering** [Zhang et al. UAI 2011; Lee, Honavar UAI 2017; He et al. ICDM 2017; Zhang et al. AAAI 2018; Runge AISTATS 2018]  
**encoded using softmax functions**

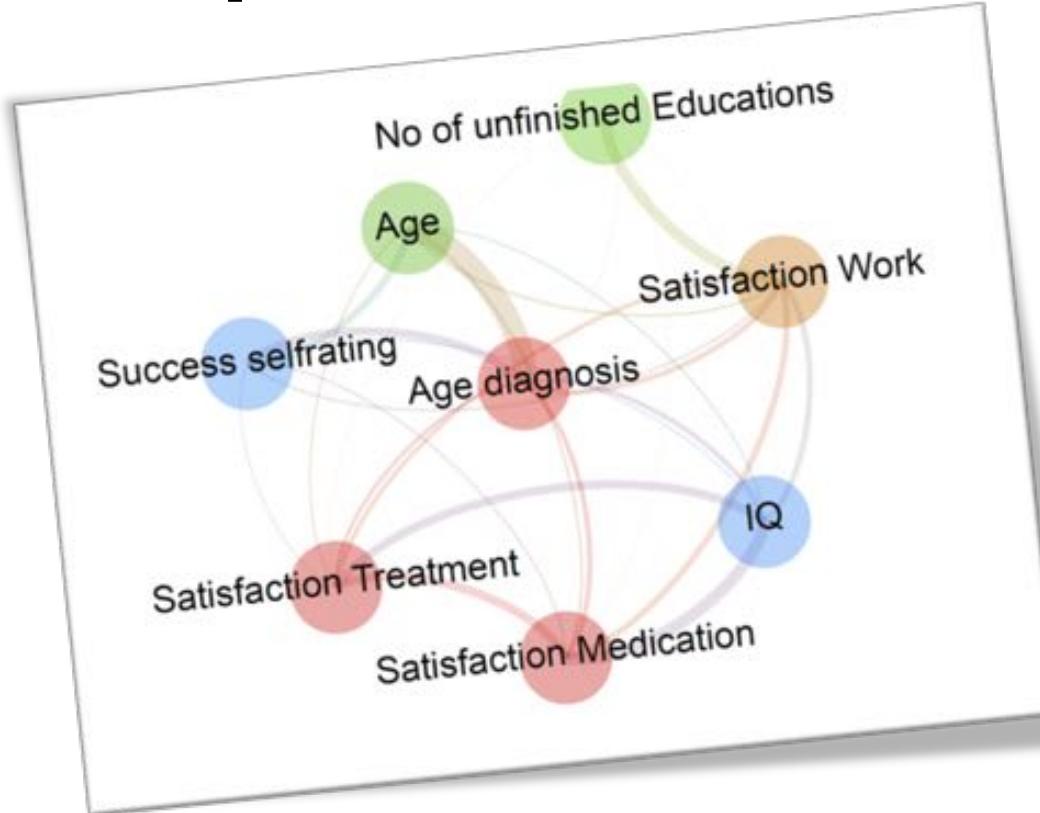
# Conditional SPNs

[Shao, Molina, Vergari, Peharz, Liebig,  
Kersting TPM@ICML 2019]

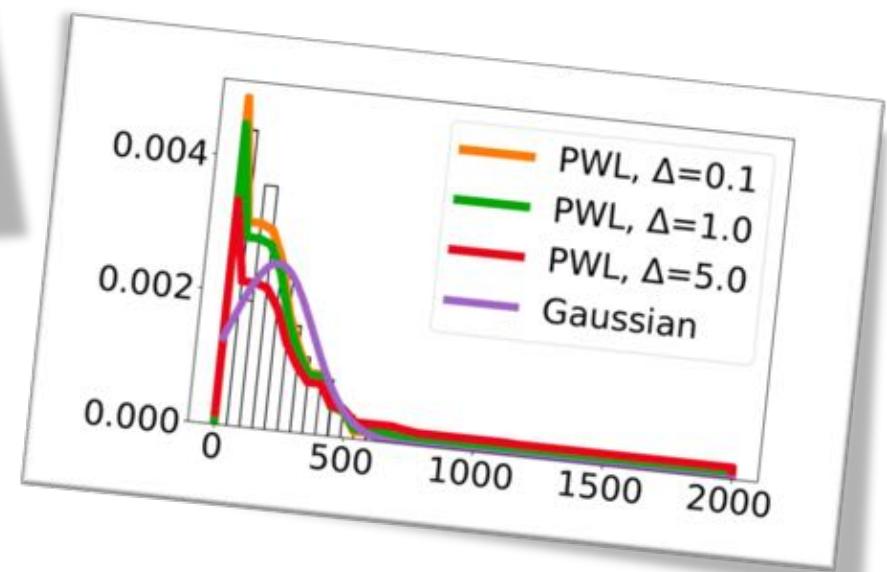




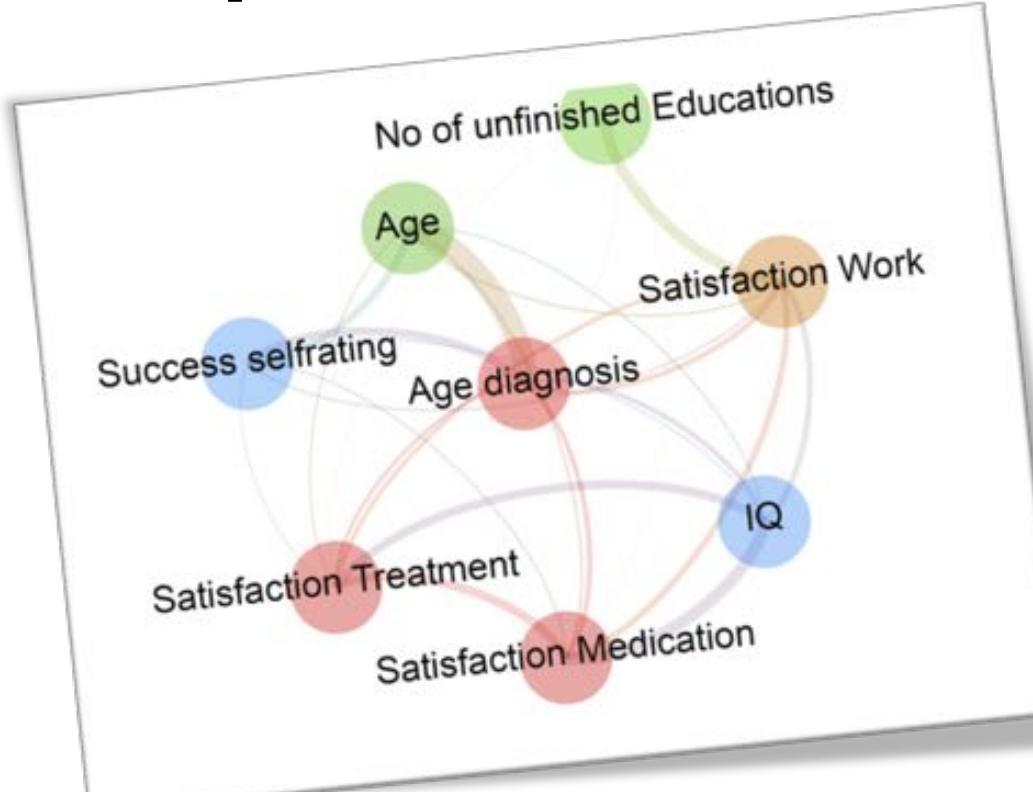
# Distribution-agnostic Deep Probabilistic Learning



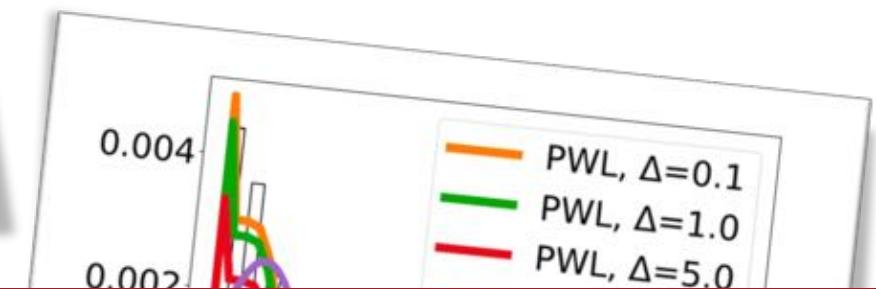
**Use nonparametric independency tests and piece-wise linear approximations**



# Distribution-agnostic Deep Probabilistic Learning



Use nonparametric  
independency tests  
and piece-wise linear  
approximations



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

# The Explorative Automatic Statistician



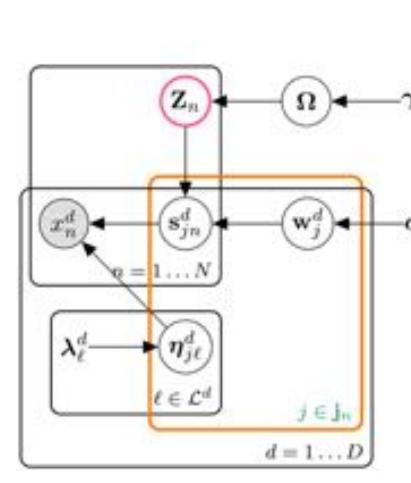
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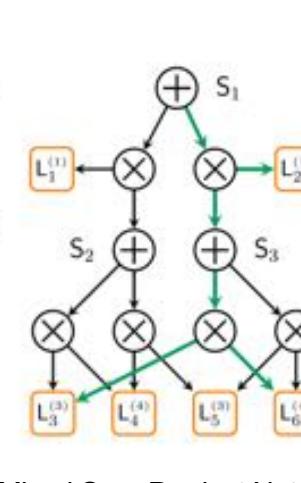
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	$X^1$	$X^2$	$X^3$	$X^4$	$X^5$
$x_8$					
$x_7$			?		
$x_6$					
missing value	$x_5$	?			
$x_4$			?		
$x_3$					
$x_2$		?			
$x_1$					

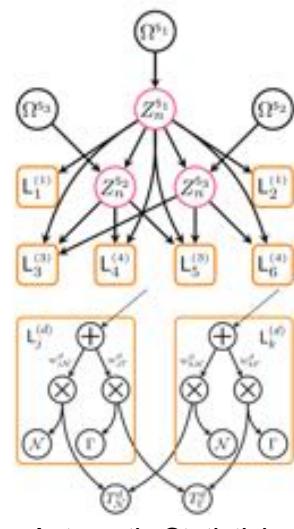
We can even automatically discovers the statistical types and parametric forms of the variables



Bayesian Type Discovery



Mixed Sum-Product Network



Automatic Statistician

# That is, the machine understands the data with few expert input ...



**Exploring the Titanic dataset**

This report describes the dataset Titanic and contains general statistical information and an analysis on the influence different features and subgroups of the data have on each other. The first part of the report contains general statistical information about the dataset and an analysis of the variables and probability distributions. The second part focusses on a subgroup analysis of the data. Different clusters identified by the network are analyzed and compared to give an insight into the structure of the data. Finally the influence different variables have on the predictive capabilities of the model are analyzed. The whole report is generated by fitting a sum product network to the data and extracting all information from this model.

Voelcker, Molina, Neumann, Westermann, Kersting (2019): DeepNotebooks: Deep Probabilistic Models Construct Python Notebooks for Reporting Datasets. In Working Notes of the ECML PKDD 2019 Workshop on Automating Data Science (ADS)

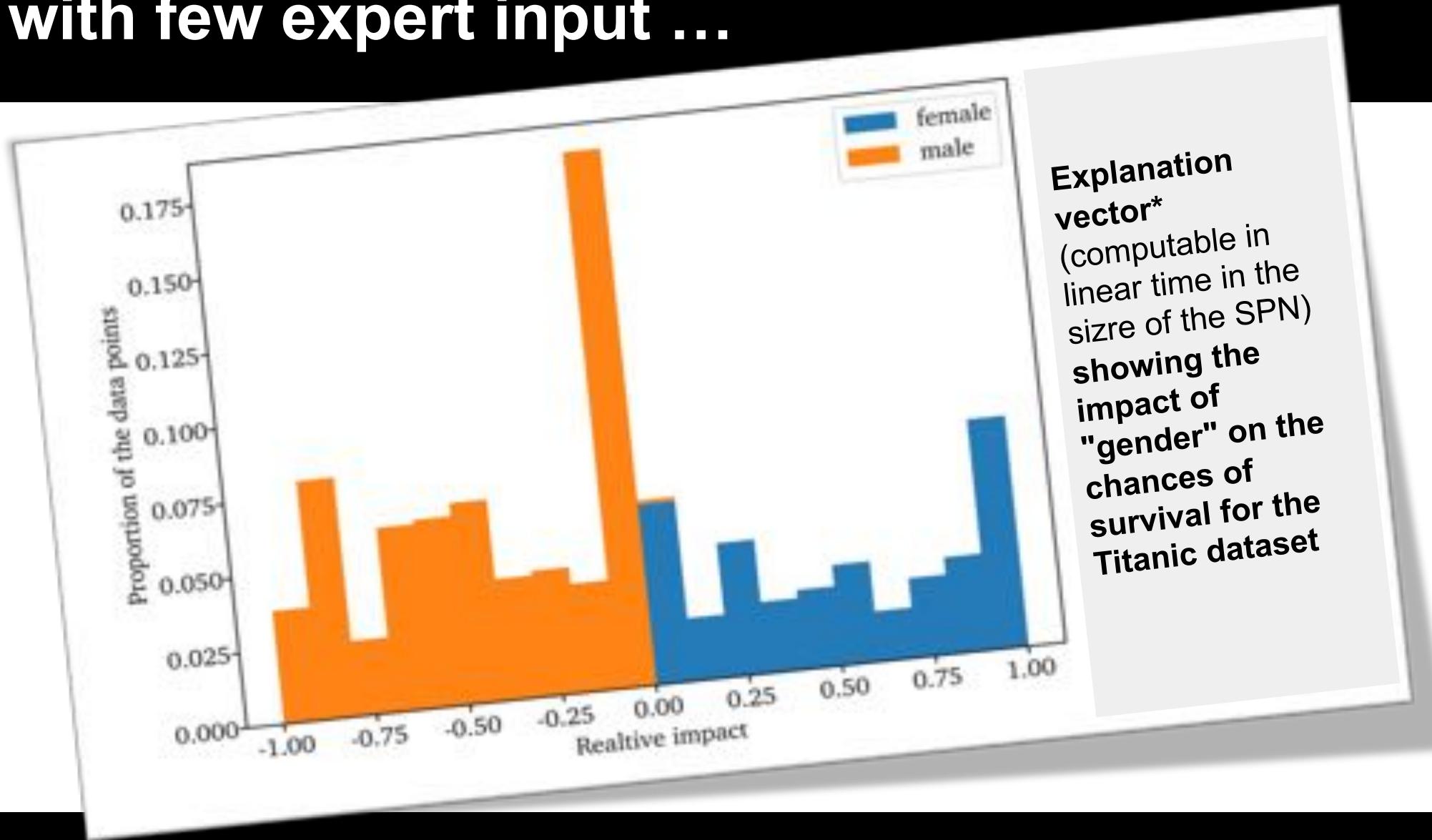


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Report framework created @ TU Darmstadt

# ...and can compile data reports automatically

# That is, the machine understands the data with few expert input ...



# ...and can compile data reports automatically

P( heart attack | )?



The New York Times

f t e ↗ 📒

Opinion

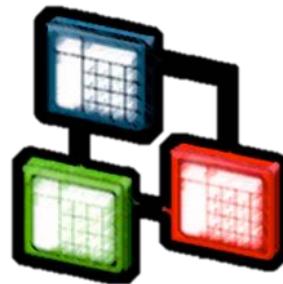
# A.I. Is Harder Than You Think and Data Science

By Gary Marcus and Ernest Davis

Mr. Marcus is a professor of psychology and neural science. Mr. Davis is a professor of computer science.

May 18, 2018

P( heart attack | )?



The New York Times

f t e ↗ 📖

Opinion

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May 18, 2018

This image shows a screenshot of a New York Times Opinion article. The article title is "A.I. Is Harder Than You Think and Data Science". It is written by Gary Marcus and Ernest Davis. The text below the title states that Mr. Marcus is a professor of psychology and neural science, and Mr. Davis is a professor of computer science. The date of the article is May 18, 2018. The image includes social media sharing icons for Facebook, Twitter, Email, and LinkedIn, as well as a magnifying glass icon for search.

P( heart  
attack | )?



The New York Times

Opinion

# A.I. Is Harder Than You Think and Data Science

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May 18, 2018

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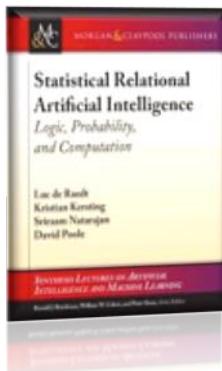
A screenshot of a New York Times Opinion article. The title is "A.I. Is Harder Than You Think and Data Science". It's written by Gary Marcus and Ernest Davis. The author bio states that Mr. Marcus is a professor of psychology and neural science, and Mr. Davis is a professor of computer science. The date of publication is May 18, 2018. The article has social sharing icons for Facebook, Twitter, Email, and a link icon. The background of the slide features a faint watermark of the three images from the top of the slide.

# P( heart attack | )?



## Crossover of ML and DS with data & programming abstractions

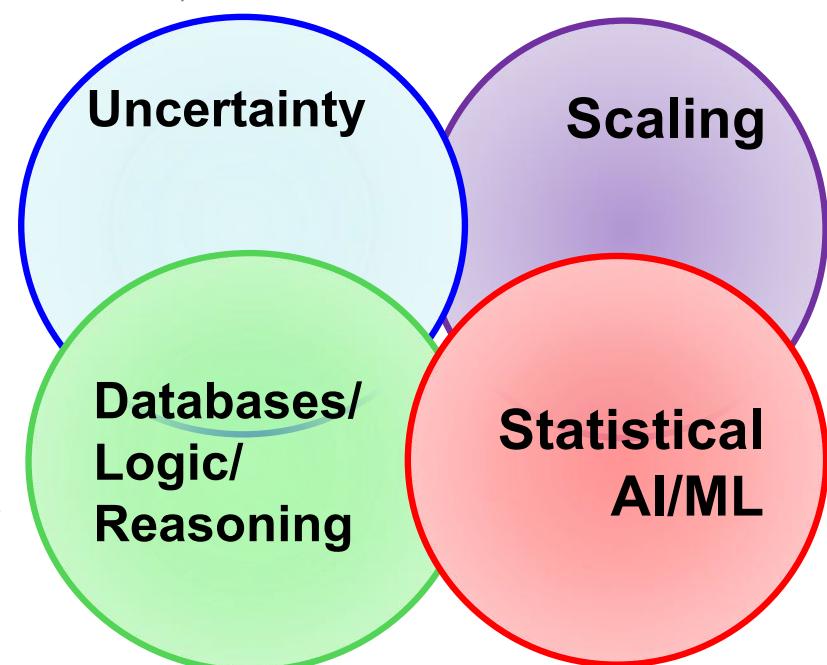
De Raedt, Kersting, Natarajan, Poole: Statistical Relational Artificial Intelligence: Logic, Probability, and Computation. Morgan and Claypool Publishers, ISBN: 9781627058414, 2016.

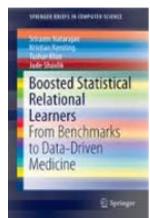


**building general-purpose  
data science and ML  
machines**

**make the ML/DS expert  
more effective**

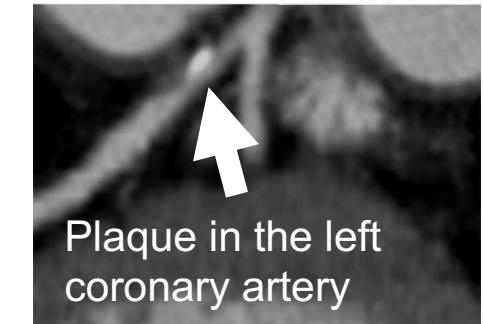
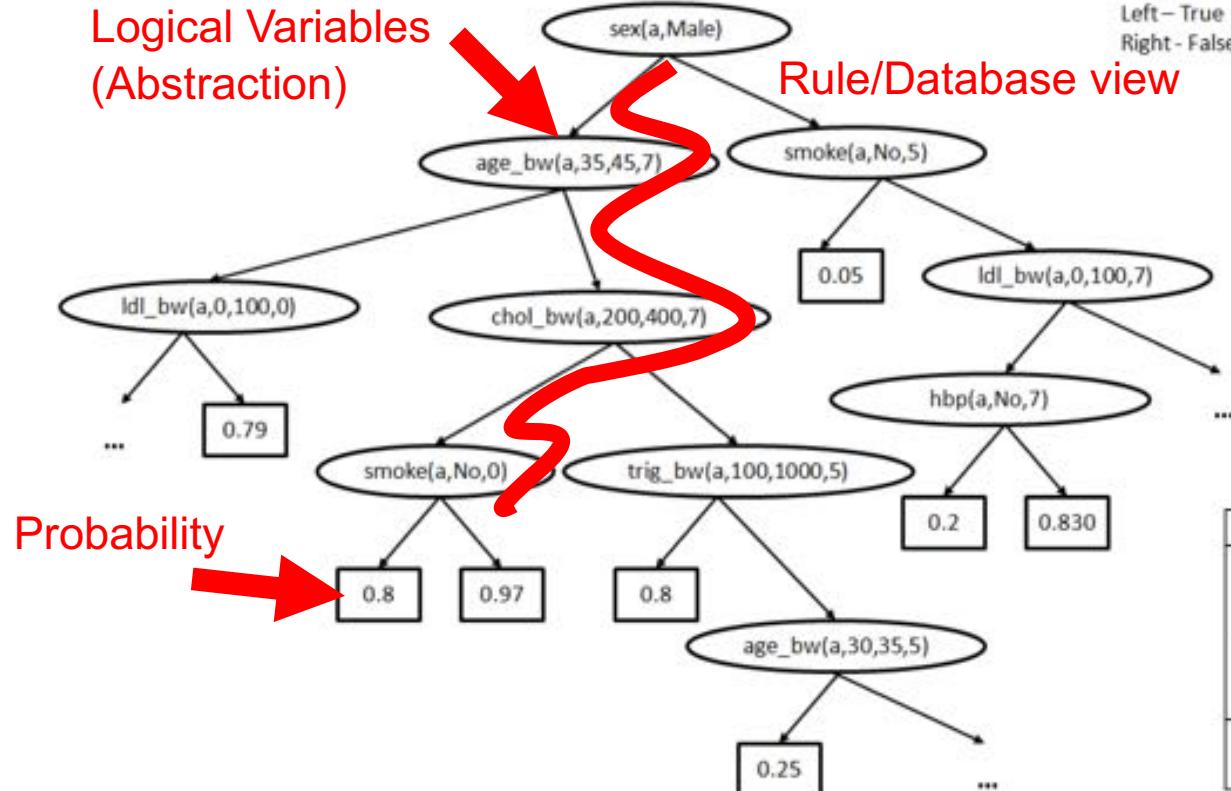
**increases the number of  
people who can  
successfully build ML/DS  
applications**





# Understanding Electronic Health Records

Atherosclerosis is the cause of the majority of Acute Myocardial Infarctions (heart attacks)



[Circulation; 92(8), 2157-62, 1995;  
JACC; 43, 842-7, 2004]

Algorithm	Accuracy	AUC-ROC	The higher, the better
J48	0.667	0.607	
SVM	0.667	0.5	
AdaBoost	0.667	0.608	
Bagging	0.677	0.613	
NB	0.75	0.653	
RPT	0.669*	0.778	
RFGB	0.667*	0.819	

25%

Algorithm for Mining Markov Logic Networks	Likelihood The higher, the better	AUC-ROC The higher, the better	AUC-PR The higher, the better	Time The lower, the better
Boosting	0.81	0.96	0.93	9s
LSM	0.73	0.54	0.62	93 hrs

37200x faster

[Kersting, Driessens ICML'08; Karwath, Kersting, Landwehr ICDM'08; Natarajan, Joshi, Tadepelli, Kersting, Shavlik. IJCAI'11; Natarajan, Kersting, Ip, Jacobs, Carr IAAI '13; Yang, Kersting, Terry, Carr, Natarajan AIME '15; Khot, Natarajan, Kersting, Shavlik ICDM'13, MLJ'12, MLJ'15, Yang, Kersting, Natarajan BIBM'17]



<https://starling.utdallas.edu/software/boostsrl/wiki/>



People

Publications

Projects

Software

Datasets

Blog



#### BOOSTSRL BASICS

Getting Started

File Structure

Basic Parameters

Advanced Parameters

Basic Modes

Advanced Modes

#### ADVANCED BOOSTSRL

Default (RDN-Boost)

MLN-Boost

Regression

One-Class Classification

Cost-Sensitive SRL

Learning with Advice

Approximate Counting

Discretization of Continuous-Valued Attributes

Lifted Relational Random Walks

Grounded Relational Random Walks

#### APPLICATIONS

Natural Language Processing

## BoostSRL Wiki

**BoostSRL** (Boosting for Statistical Relational Learning) is a gradient-boosting based approach to learning different types of SRL models. As with the standard gradient-boosting approach, our approach turns the model learning problem to learning a sequence of regression models. The key difference to the standard approaches is that we learn relational regression models i.e., regression models that operate on relational data. We assume the data in a predicate logic format and the output are essentially first-order regression trees where the inner nodes contain conjunctions of logical predicates. For more details on the models and the algorithm, we refer to our book on this topic.

Sriram Natarajan, Tushar Khot, Kristian Kersting and Jude Shavlik, Boosted Statistical Relational Learners: From Benchmarks to Data-Driven Medicine . SpringerBriefs in Computer Science, ISBN: 978-3-319-13643-1, 2015

# Human-in-the-loop learning

In general, computing the exact posterior is intractable, i.e., inverting the generative process to determine the state of latent variables corresponding to an input is time-consuming and error-prone.

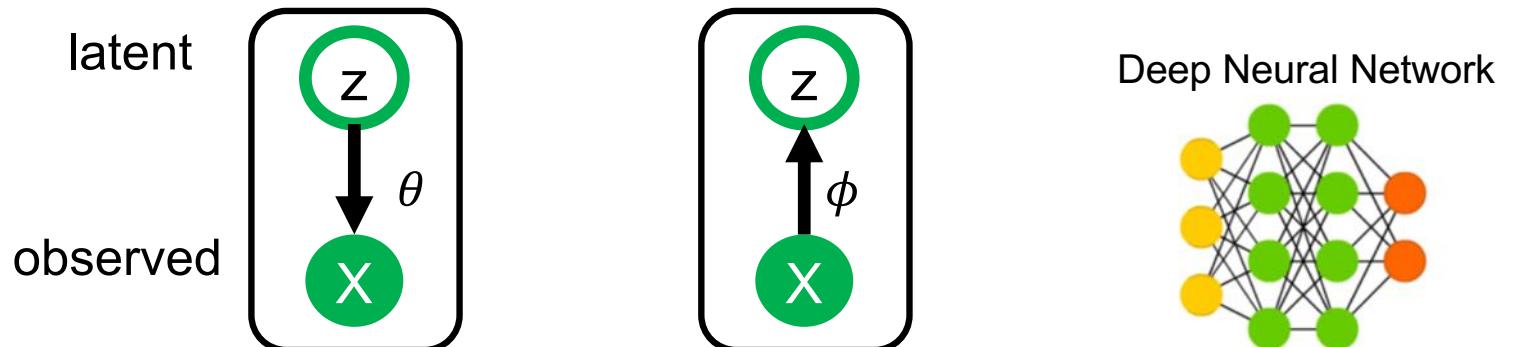
## Deep Probabilistic Programming

```
import pyro.distributions as dist

def model(data):
    # define the hyperparameters that control the beta prior
    alpha0 = torch.tensor(10.0)
    beta0 = torch.tensor(10.0)
    # sample f from the beta prior
    f = pyro.sample("latent_fairness", dist.Beta(alpha0, beta0))
    # loop over the observed data
    for i in range(len(data)):
        # observe datapoint i using the bernoulli
        # likelihood Bernoulli(f)
        pyro.sample("obs_{}".format(i), dist.Bernoulli(f), obs=data[i])
```

```
def guide(data):
    # register the two variational parameters with Pyro.
    alpha_q = pyro.param("alpha_q", torch.tensor(15.0),
                         constraint=constraints.positive)
    beta_q = pyro.param("beta_q", torch.tensor(15.0),
                         constraint=constraints.positive)
    # sample latent_fairness from the distribution Beta(alpha_q, beta_q)
    pyro.sample("latent_fairness", dist.Beta(alpha_q, beta_q))
```

### (2) Ease the implementation by some high-level, probabilistic programming language



(1) Instead of optimizing variational parameters for every new data point, use a deep network to predict the posterior given  $X$  [Kingma, Welling 2013, Rezende et al. 2014]

[Stelzner, Molina, Peharz, Vergari, Trapp, Valera, Ghahramani, Kersting ProgProb 2018]

# Sum-Product Probabilistic Programming

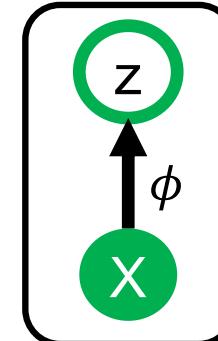
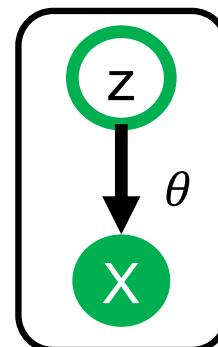
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```

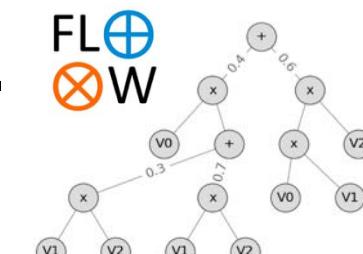
```
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    beta_q = pyro.param("beta_q", torch.tensor(15.0),
                         constraint=constraints.positive)
    # sample latent_fairness from the distribution Beta(alpha_q, beta_q)
    pyro.sample("latent_fairness", dist.Beta(alpha_q, beta_q))
```

**(2) Ease the implementation by some high-level, probabilistic programming language**

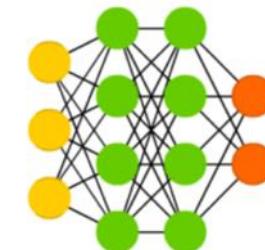
latent  
observed



Sum-Product Network



Deep Neural Network



**(1) Instead of optimizing variational parameters for every new data point, use a deep network to predict the posterior given X** [Kingma, Welling 2013, Rezende et al. 2014]

# Unsupervised scene understanding

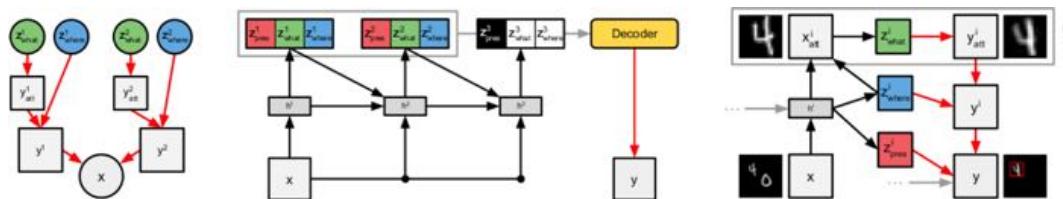
[Stelzner, Peharz, Kersting ICML 2019, Best Paper Award at TPM@ICML2019] <https://github.com/stelzner/supair>



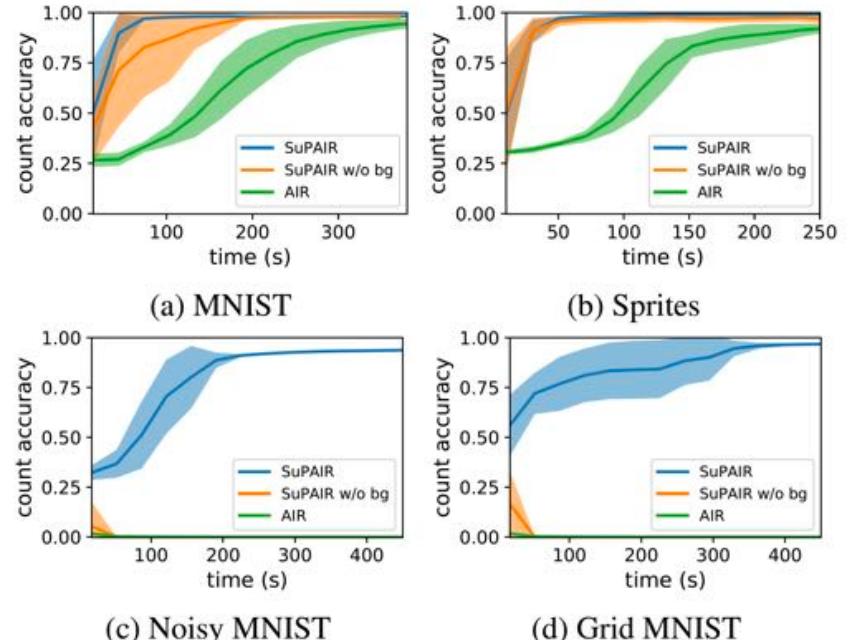
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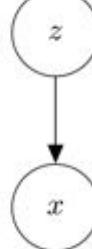
Consider e.g. unsupervised scene understanding using a generative model implemented in a neural fashion



[Attend-Infer-Repeat (AIR) model, Hinton et al. NIPS 2016]

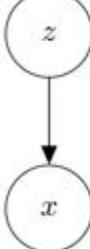


VAE

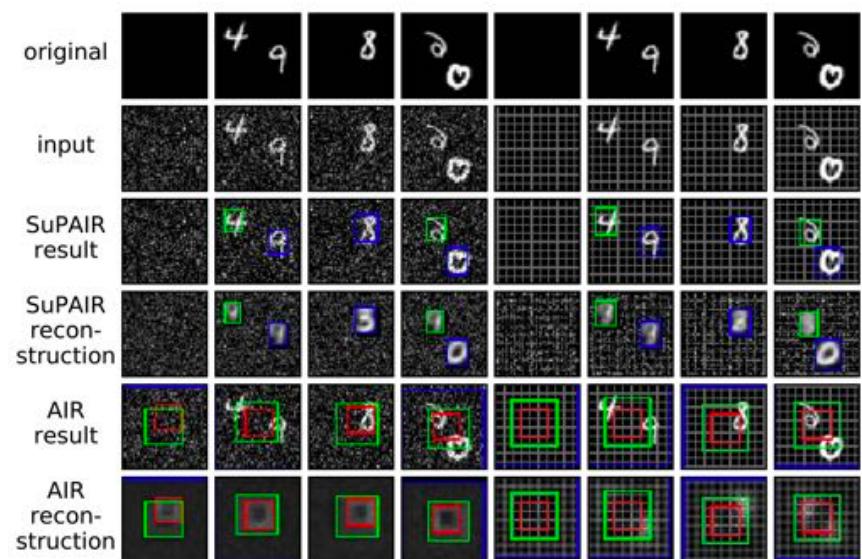


Replace VAE by SPN as object model

SPN



- infinite mixture model
  - intractable density
  - intractable posterior
- “large” but finite mixture model
  - tractable density
  - tractable marginals [Peharz et al., 2015]
  - tractable posterior [Vergari et al., 2017]



# There are strong investments into (deep) probabilistic programming



RelationalAI, Apple, Microsoft and Uber are investing hundreds of millions of US dollars



# Since we need languages for Systems AI,

the computational and mathematical modeling of complex AI systems.

[Kordjamshidi, Roth, Kersting: "Systems AI: A Declarative Learning Based Programming Perspective." IJCAI-ECAI 2018]



Eric Schmidt, Executive Chairman, Alphabet Inc.: Just Say "Yes", Stanford Graduate School of Business, May 2, 2017. <https://www.youtube.com/watch?v=vbb-AjiXyh0>.

Getting deep  
systems that reason  
and know when they  
don't know

Responsible AI  
systems that explain  
their decisions and  
co-evolve with the  
humans

Open AI systems  
that are easy to  
realize and  
understandable for  
the domain experts

„Tell the AI when it is  
right for the wrong  
reasons and it adapts  
its behavior“



Figure 4: Explaining an image classification prediction made by Google's Inception network, highlighting positive pixels. The top 3 classes predicted are "Electric Guitar" ( $p = 0.32$ ), "Acoustic guitar" ( $p = 0.24$ ) and "Labrador" ( $p = 0.21$ )

Teso, Kersting AIES 2019



AAAI / ACM conference on  
ARTIFICIAL INTELLIGENCE,  
ETHICS, AND SOCIETY

# Human algorithms teaches AI a lot

## The twin science: cognitive science

"How do we humans get so much from so little?" and by that I mean how do we acquire our understanding of the world given what is clearly by today's engineering standards so little data, so little time, and so little energy.



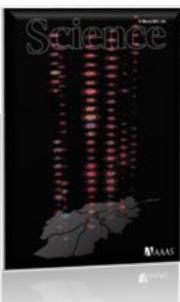
### Centre for Cognitive Science at TU Darmstadt

Establishing cognitive science at the Technische Universität Darmstadt is a long-term commitment across multiple departments (see [Members](#) to get an impression on the interdisciplinary of the supporting groups and departments). The TU offers a strong foundation including several established top engineering groups in Germany, a prominent computer science department (which is among the top four in Germany), a



Centre  
for  
Cognitive  
Science

Josh Tenenbaum, MIT



Lake, Salakhutdinov, Tenenbaum, Science 350 (6266), 1332-1338, 2015

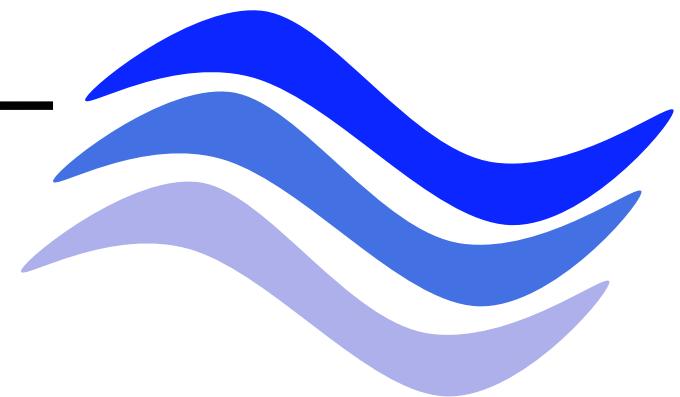
Tenenbaum, Kemp, Griffiths, Goodman, Science 331 (6022), 1279-1285, 2011

# Indeed, AI has great impact, but ...

- + **AI is more than deep neural networks.** Probabilistic and causal models are whiteboxes that provide insights into applications
- + **AI is more than a single table.** Loops, graphs, different data types, relational DBs, ... are central to ML/AI and high-level programming languages for ML/AI help to capture this complexity and makes using ML/AI simpler
- + **AI is more than just Machine Learners and Statisticians,** AI is a team sport

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= The third wave of AI requires integrative CS, from SoftEng and DBMS, over ML and AI, to computational CogSci



A lot left to be done

