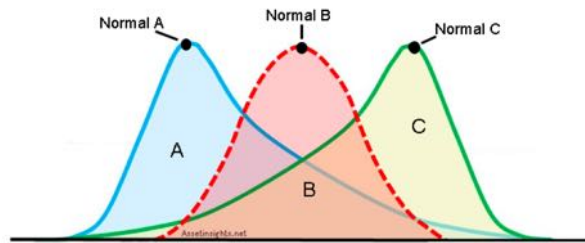# Deep Probabilistic Programming (for Healthcare)*

*Thanks for Sriraam Natarajan (UT Dallas) and many others for all the great collaborations

Kristian Kersting

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

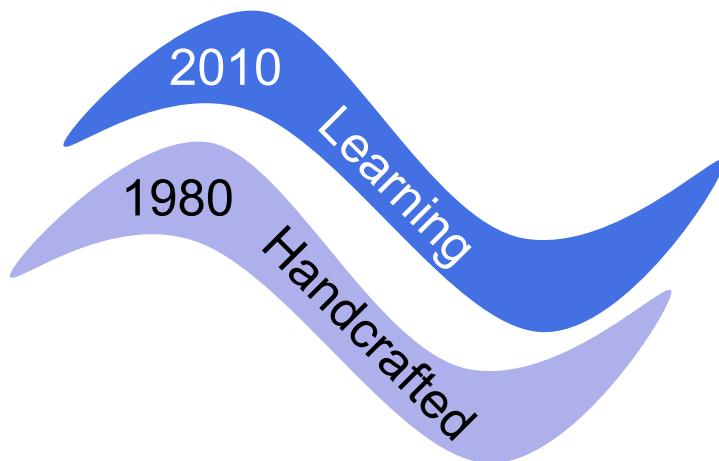**Responsible AI systems that explain their decisions and co-evolve with the humans**

Open AI systems that are easy to realize and deal with complex data and knowledge

AI has impact

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

However, there are not enough data scientists, statisticians, machine learning and AI experts.

2010
Learning

1980
Handcrafted

The third wave of AI

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

However, there are not enough data scientists, statisticians, machine learning and AI experts.
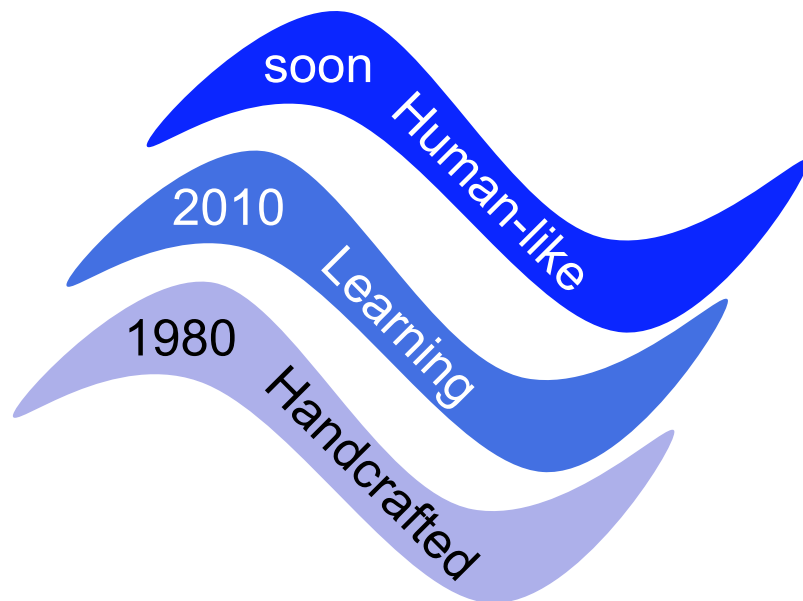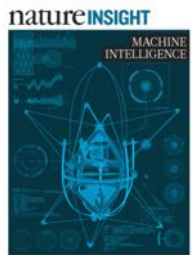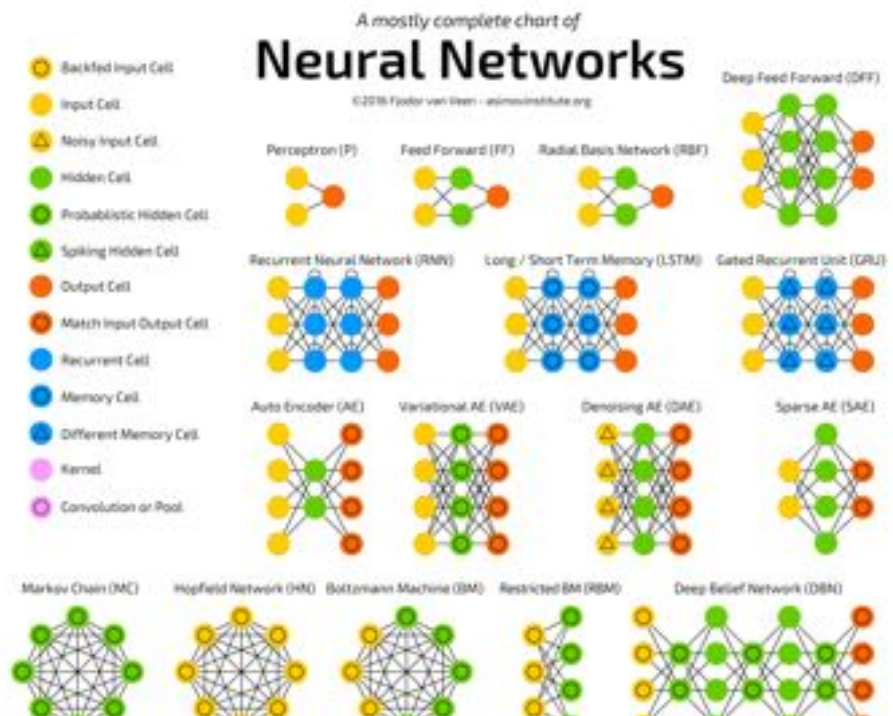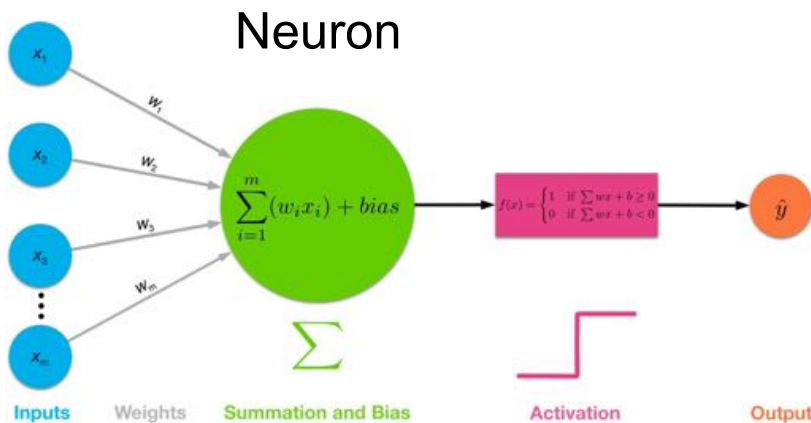
soon — Human-like

2010 — Learning

1980 — Handcrafted

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

Potentially much more powerful than shallow architectures, represent computations

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

They "develop intuition" about complicated biological processes and generate scientific data

[Schramowski, Brugger, Mahlein, Kersting 2019]

DePhenSe

Bundesanstalt für
Landwirtschaft und Ernährung
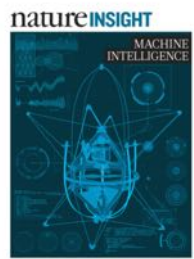
Deep Neural Networks

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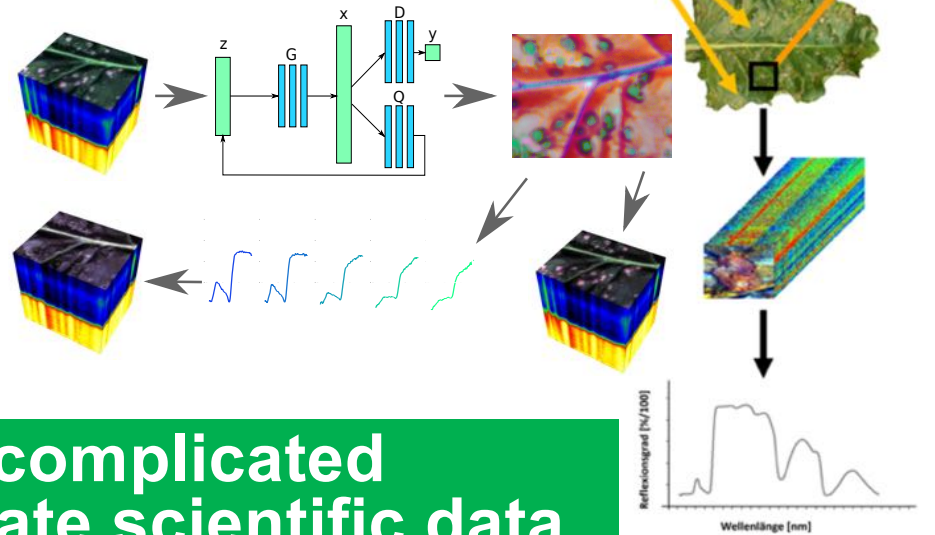[LeCun, Bengio, Hinton Nature 521, 436–444, 2015]

SHARE   REPORTS | PSYCHOLOGY

Semantics derived automatically from language corpora contain human-like biases

Aylin Caliskan[1,*], Joanna J. Bryson[1,2,*], Arvind Narayanan[1,*]

+ See all authors and affiliations

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

They "capture" stereotypes from human language

Deep Neural Networks

Potentially much more powerful than shallow architectures, represent computations
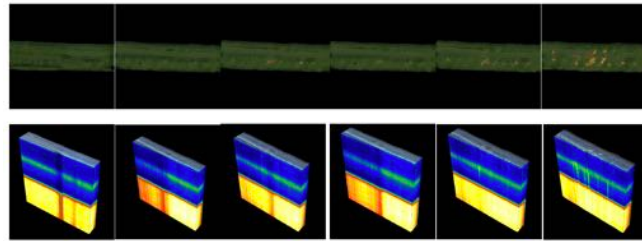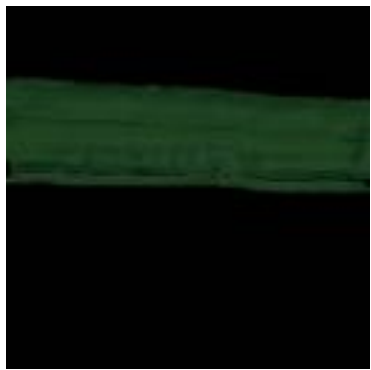
[LeCun, Bengio, Hinton Nature 521, 436–444, 2015]
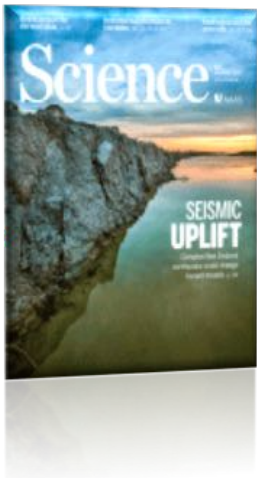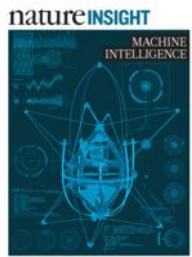
The Moral Choice Machine

Dos	WEAT	Bias		Don'ts	WEAT	Bias
smile	0.116	0.348		rot	-0.099	-1.118
sightsee	0.090	0.281		negative	-0.101	-0.763
cheer	0.094	0.277		harm	-0.110	-0.730
celebrate	0.114	0.264		damage	-0.105	-0.664
picnic	0.093	0.260		slander	-0.108	-0.600
snuggle	0.108	0.238		slur	-0.109	-0.569

But lucky they also "capture" our moral choices

[Jentzsch, Schramowski, Rothkopf, Kersting AIES 2019]

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

hr

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

The Moral Choice Machine

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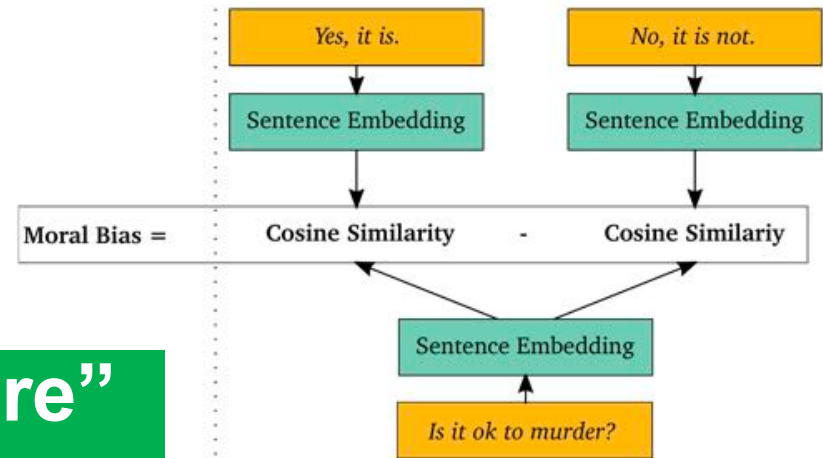**ARTIFICIAL INTELLIGENCE, ETHICS, AND SOCIETY**

Can we trust deep neural networks?

DNNs do not quantify all of the uncertainty. They are not calibrated joint distributions.

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

MNIST **SVHN** **SEMEION**

Train & Evaluate   **Transfer Testing**

[Bradshaw et al. arXiv:1707.02476 2017]

Input log „likelihood" (sum over outputs)

DNNs cannot distinguish the datasets

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

Getting deep systems that know when they don't know.

Sum-Product Networks:
A deep probabilistic learning framework

Adnan Darwiche UCLA

Pedro Domingos UW

$\oplus$ ... convex sum

$\otimes$ ... product

$\wedge$ ... distribution

completeness
sum children: same scope

decomposability
product children:
non-overlapping scope

$\{X_1, X_2, X_3\}$

$\{X_1, X_2\}$

$\{X_3\}$

$X_1 \quad X_2 \quad X_3$

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

Inference is linear in size of network

And there is a principled approach to select SPNs from data

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

Random Variables

Examples

Conditoning, e.g., via clustering

*

\+ \+

keep growing alternatingly
* and + layers

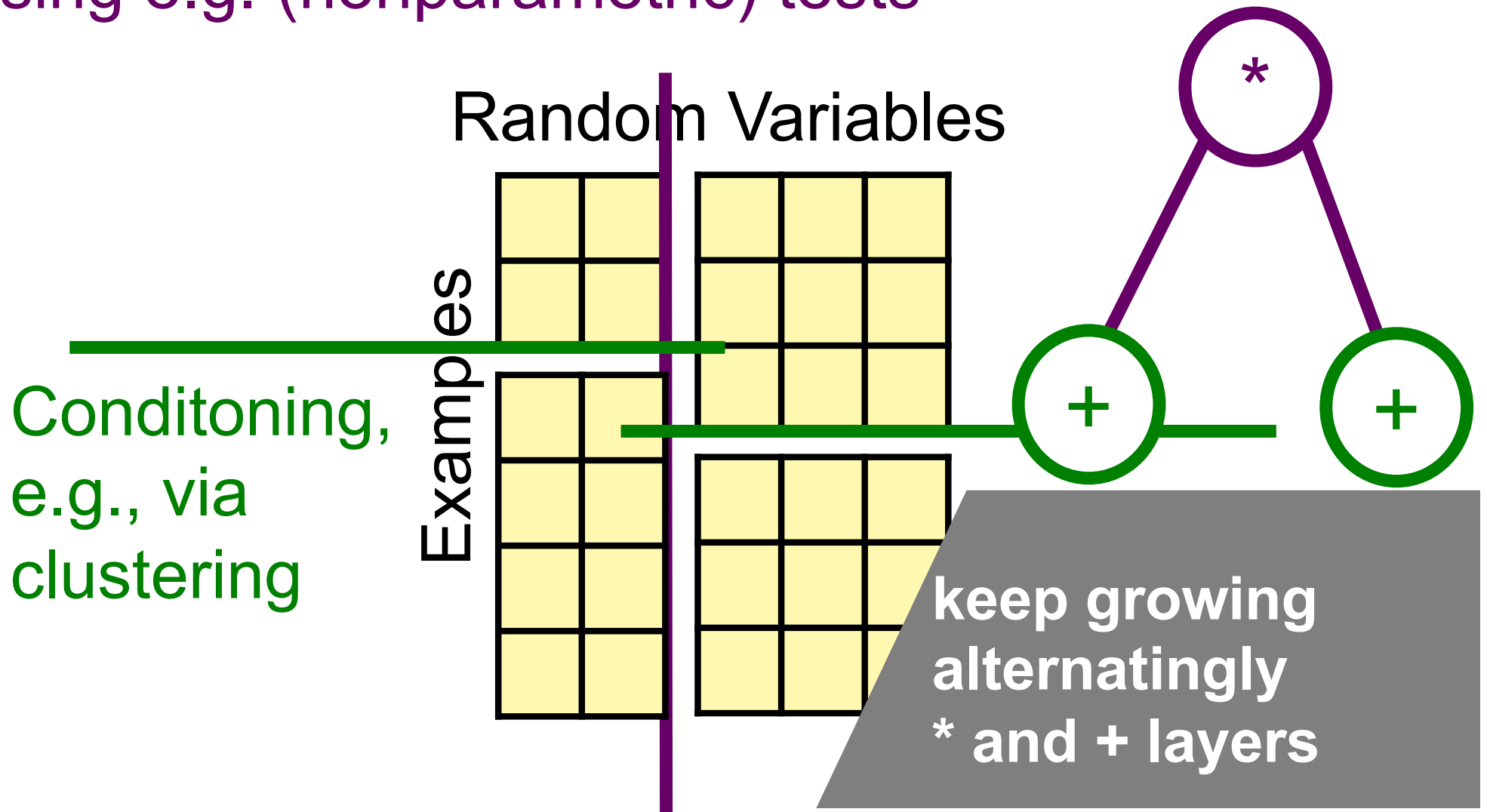[Poon, Domingos UAI'11; Molina, Natarajan, Kersting AAAI'17; Vergari, Peharz, Di Mauro, Molina, Kersting, Esposito AAAI '18; Molina, Vergari, Di Mauro, Esposito, Natarajan, Kersting AAAI '18]

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

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

TECHNISCHE UNIVERSITÄT DARMSTADT · UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO · UNIVERSITY OF WATERLOO · CAML · MADESI · Max Planck Institute for Intelligent Systems · UNIVERSITY OF CAMBRIDGE · VECTOR INSTITUTE · DFG · Federal Ministry of Education and Research

195 commits   2 branches   0 releases   6 contrib___

Branch: master ▾   New pull request   Create new file   Upload files   Find file   Clone or download ▾

https://github.com/SPFlow/SPFlow

```python
from spn.structure.leaves.parametric.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
```
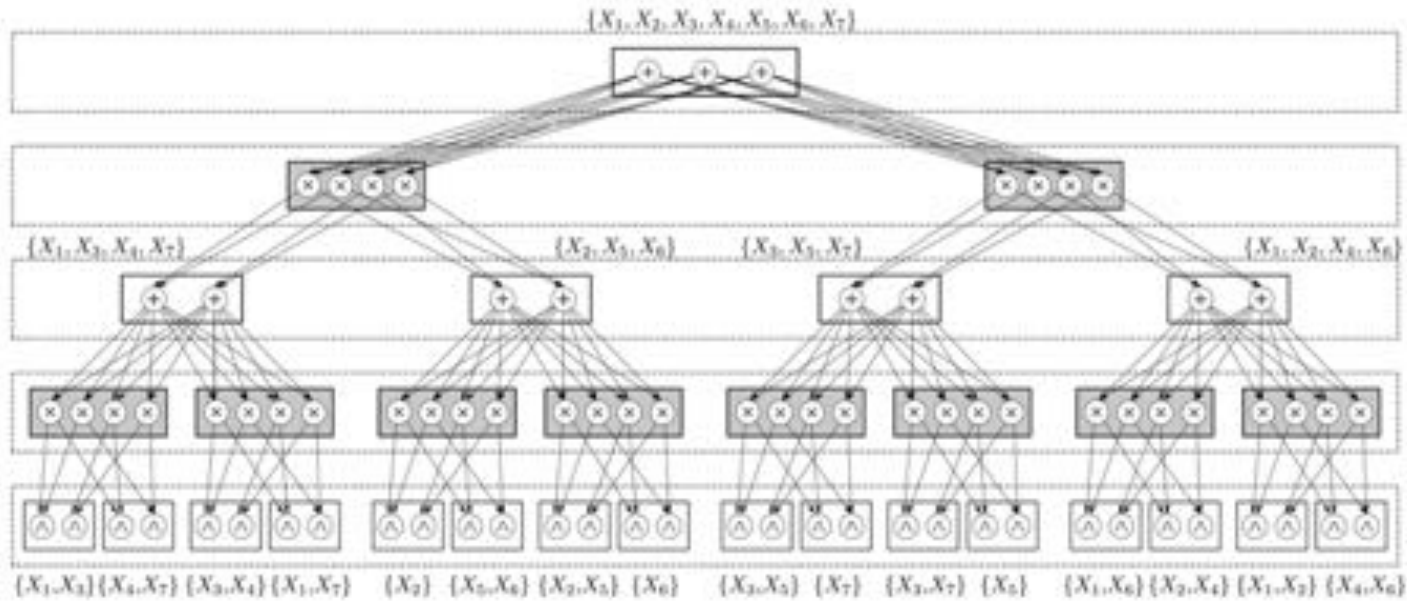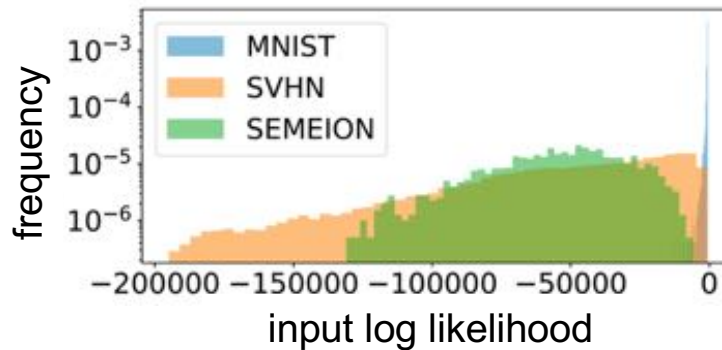
Domain Specific Language, Inference, EM, and Model Selection as well as Compilation of SPNs into TF and PyTorch and also into flat, library-free code even suitable for running on devices: C/C++,GPU, FPGA

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 routines like computing marginals, conditionals and (approximate) most probable explanations (MPEs) along with sampling

Random sum-product networks

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

		RAT-SPN	MLP	vMLP
Accuracy	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)	0.325 (0.29M)
	20-NG	1.6954 (1.63M)	1.6180 (0.22M)	1.6263 (0.22M)

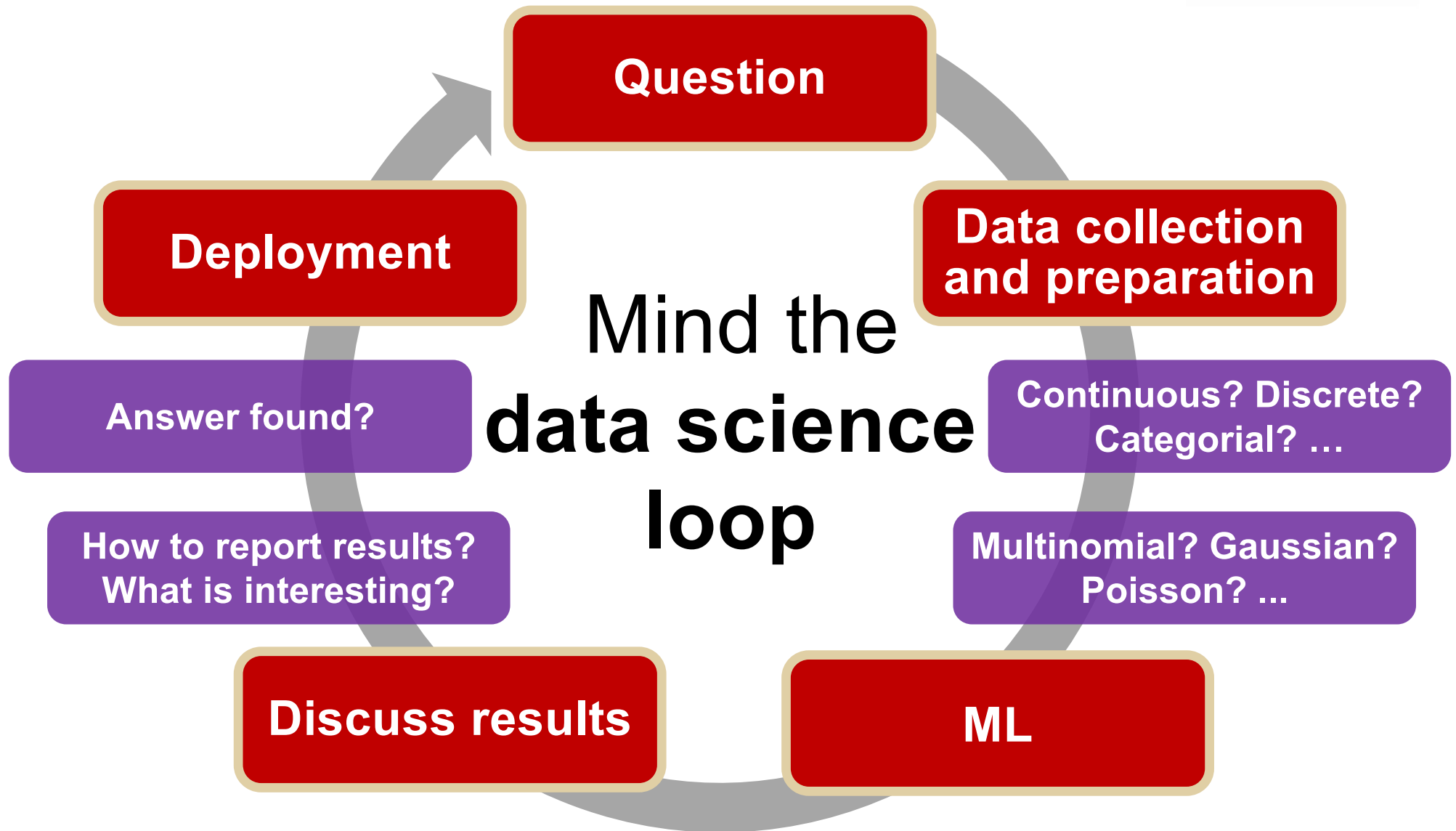outliers
prototypes
outliers
prototypes

Learning the Structure of Autoregressive Deep Models such as PixelCNNs [van den Oord et al. NIPS 2016]
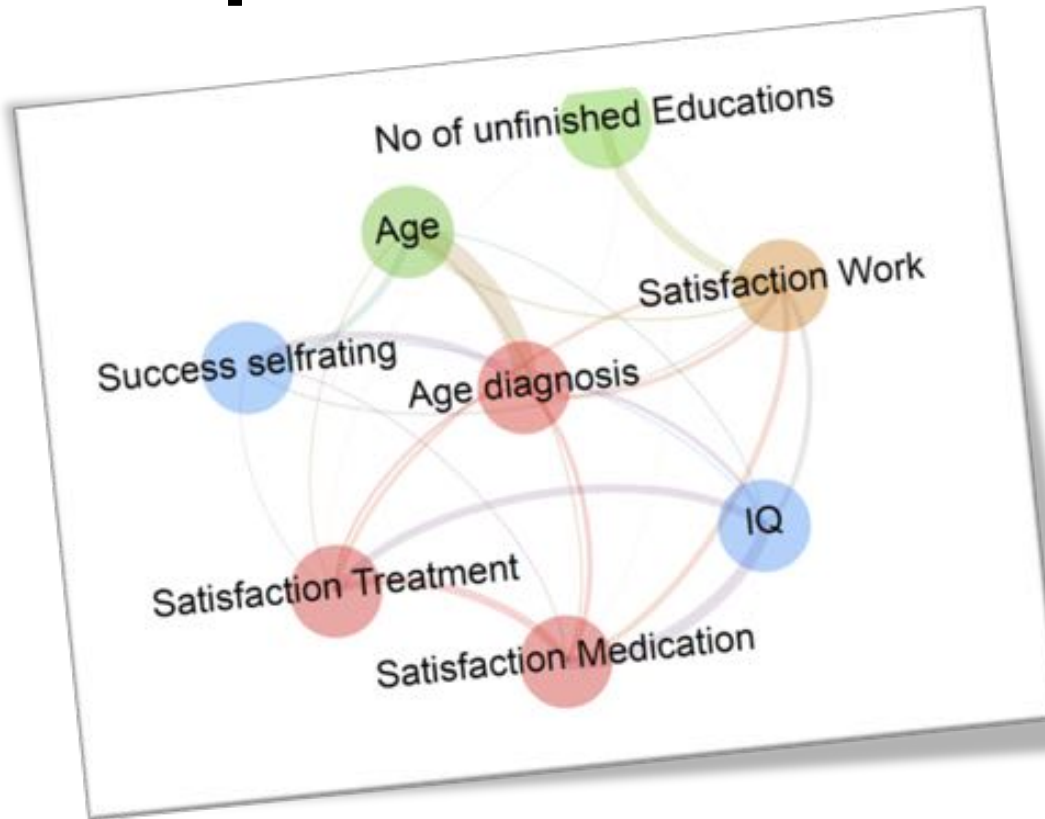
CSPNs
PixelCNNs

Learn Conditional SPN by testing conditional independence and using conditional clustering, using e.g. [Zhang et al. UAI 2011; Lee, Honovar UAI 2017; He et al. ICDM 2017; Zhang et al. AAAI 2018; Runge AISTATS 2018]
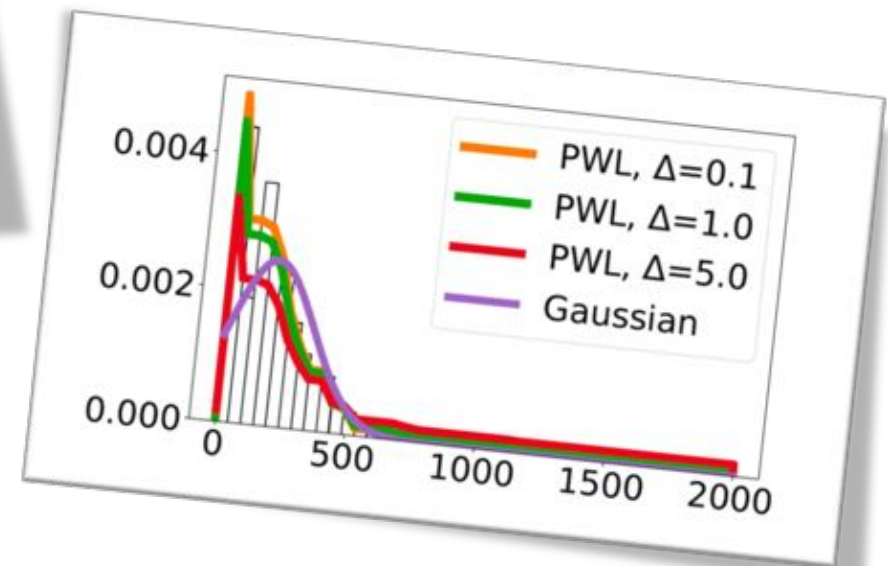
Conditional SPNs
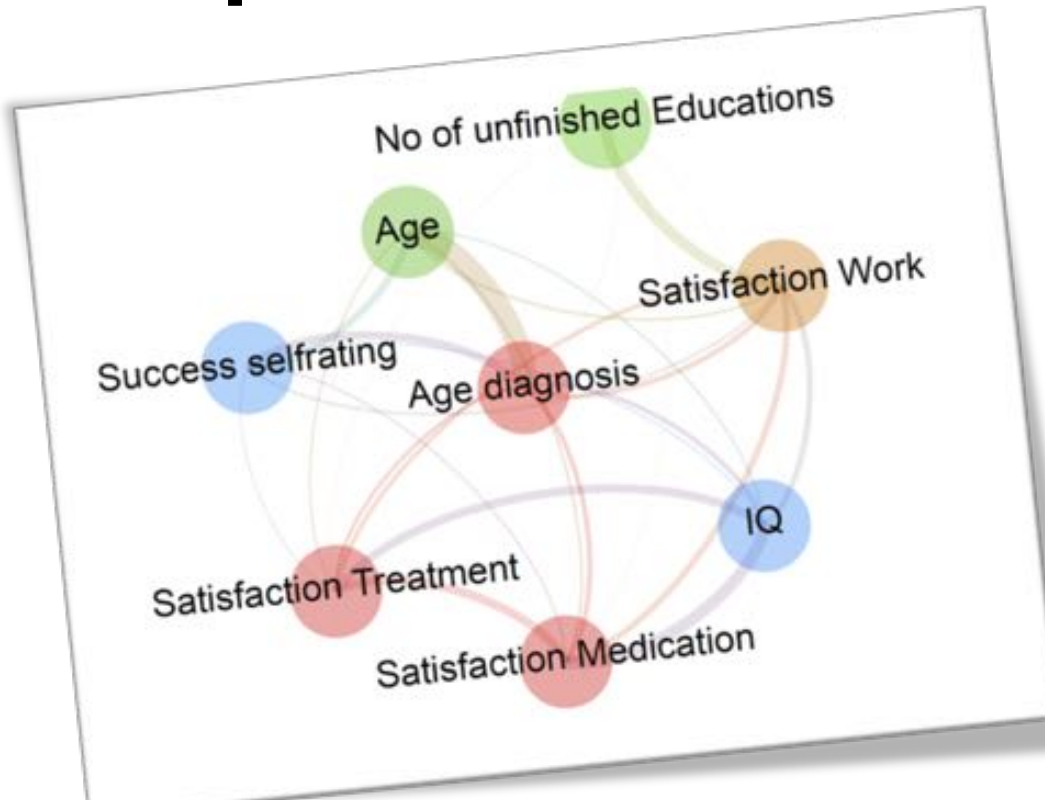[Shao, Molina, Vergari, Peharz, Kersting 2019]

CAML

DFG

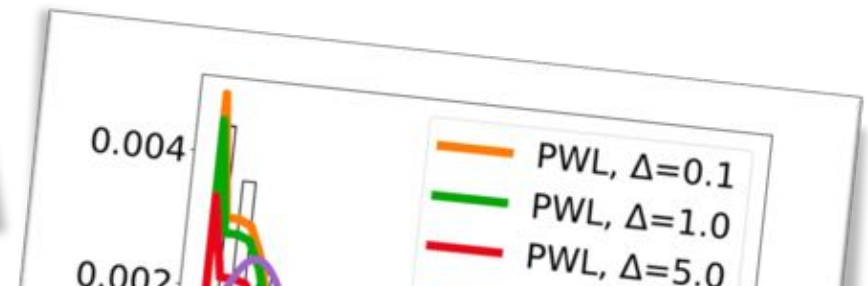# Distribution-agnostic Deep Probabilistic Learning

Use nonparametric independency tests and piece-wise linear approximations

Distribution-agnostic Deep Probabilistic Learning

Use nonparametric independency tests and piece-wise linear approximations
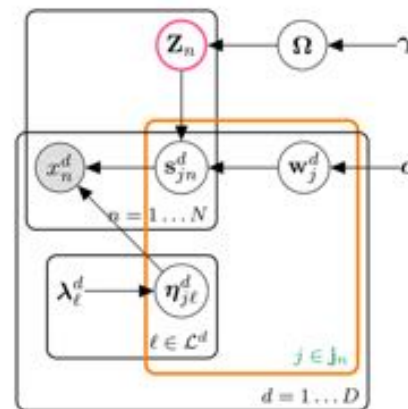

However, we have to provide the statistical types and do not gain insights into the parametric forms of the variables. **Are they Gaussians? Gammas? ...**

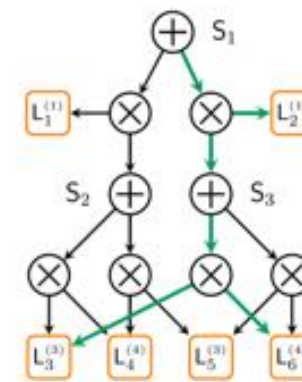# The Explorative Automatic Statistician
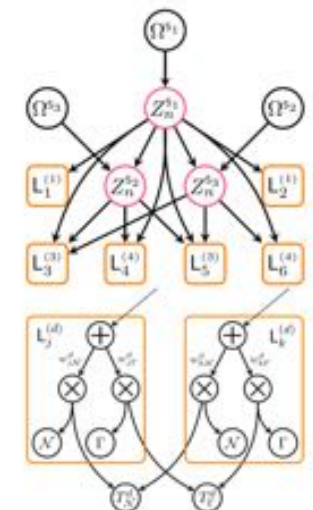

missing value

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 …

Toggle Introduction

Toggle explanations

Toggle Code

Völker: "DeepNotebooks – Interactive data analysis using Sum-Product Networks." MSc Thesis, TU Darmstadt, 2018

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 analyzes. The whole report is generated by fitting a sum product network to the data and extracting all information from this model.

TECHNISCHE UNIVERSITAT DARMSTADT

Report framework created @ TU Darmstadt

…and can compile data reports automatically

P(heart attack |)?

Opinion

A.I. Is Harder Than You Think

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 | ...)?
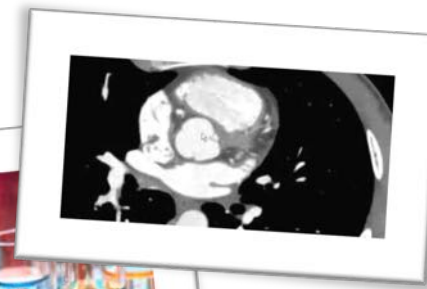
The New York Times

Opinion

A.I. Is Harder Than You Think

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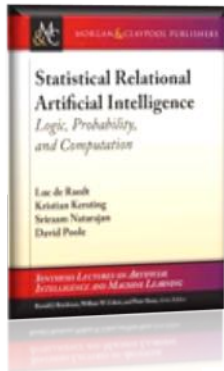Mr. Marcus is a professor of psychology and neural science. Mr. Davis is a professor of computer science.

May 18, 2018

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 and employing domain knowledge

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

KATHOLIEKE UNIVERSITEIT LEUVEN

UTD THE UNIVERSITY OF TEXAS AT DALLAS

TECHNISCHE UNIVERSITÄT DARMSTADT

UBC THE UNIVERSITY OF BRITISH COLUMBIA

Uncertainty

Scaling

Databases/ Logic/ Reasoning

Statistical AI/ML

Heart diseases and strokes – cardiovascular disease – are expensive for the world

According to the World Heart Federation, cardiovascular disease cost the European Union EURO169 billion in 2003 and the USA about EURO310.23 billion in direct and indirect annual costs. By comparison, the estimated cost of all cancers is EURO146.19 billion and HIV infections, EURO22.24 billion

nature REVIEWS

GENETICS

MODERN PHYLOGENETICS

Electronic Health Records A new opportunity for AI to save our Lifes

EHRs are dirty and interconnected

Patient Table

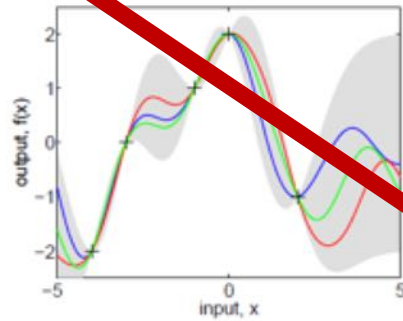| PatientID	Gender	Birthdate
P1	M	3/22/63

Visit Table

PatientID	Date	Physician	Symptoms	Diagnosis
P1	1/1/01	Smith	palpitations	hypoglycemic
P1	2/1/03	Jones	fever, aches	influenza

Lab Tests

Patient ID	Date	Lab Test	Result
P1	1/1/01	blood glucose	42
P1	1/9/01	blood glucose	??

SNP Table

PatientID	SNP1	SNP2	…	SNP500K
P1	AA	AB		BB
P2	AB	BB		AA

Prescriptions

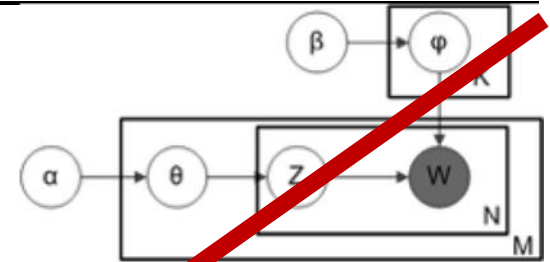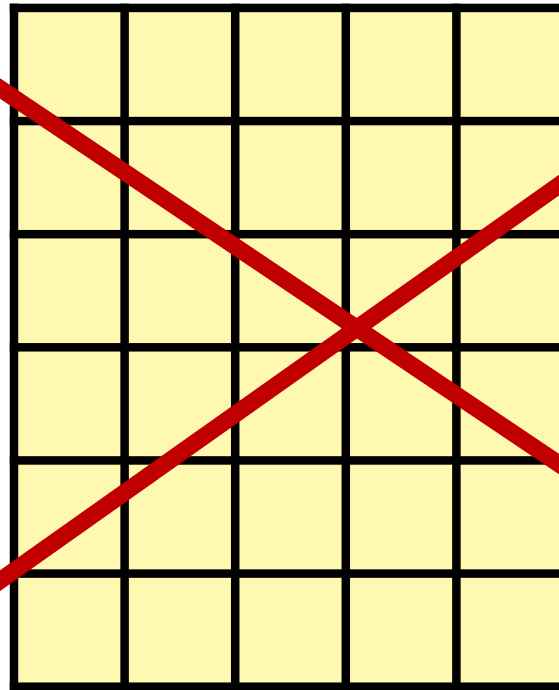| PatientID	Date Prescribed	Date Filled	Physician	Medication	Dose	Duration
P1	5/17/98	5/18/98	Jones	prilosec	10mg	3 months

Standard machine learning

Gaussian Processes
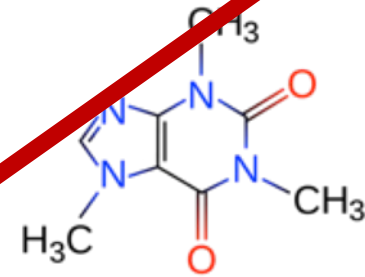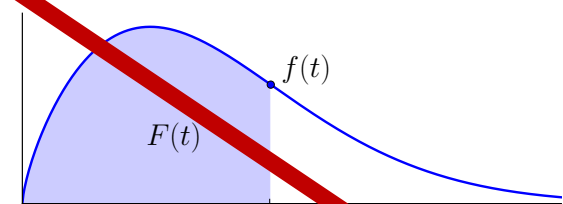
Graphical models

Features

Graph Mining

teaches

Big Model

Small Model

Objects

Boosting

Distillation/LUPI

Encoding DBN

Decoding DBN

Input

Output

Autoencoder, Deep Learning

Big Data Matrix Factorization

$f(t)$

$F(t)$

Diffusion Models

and many more …

Statistical Relational Models

Weighted logical formulas / uncertain databases

Hard constraint

$$\infty \quad Smoker(x) \Rightarrow Person(x)$$

Soft constraint, weight = exp(3.73)

$$3.75 \quad Smoker(x) \wedge Friend(x,y) \Rightarrow Smoker(y)$$

Learning statistical models over databases: Functional Gradient Boosting
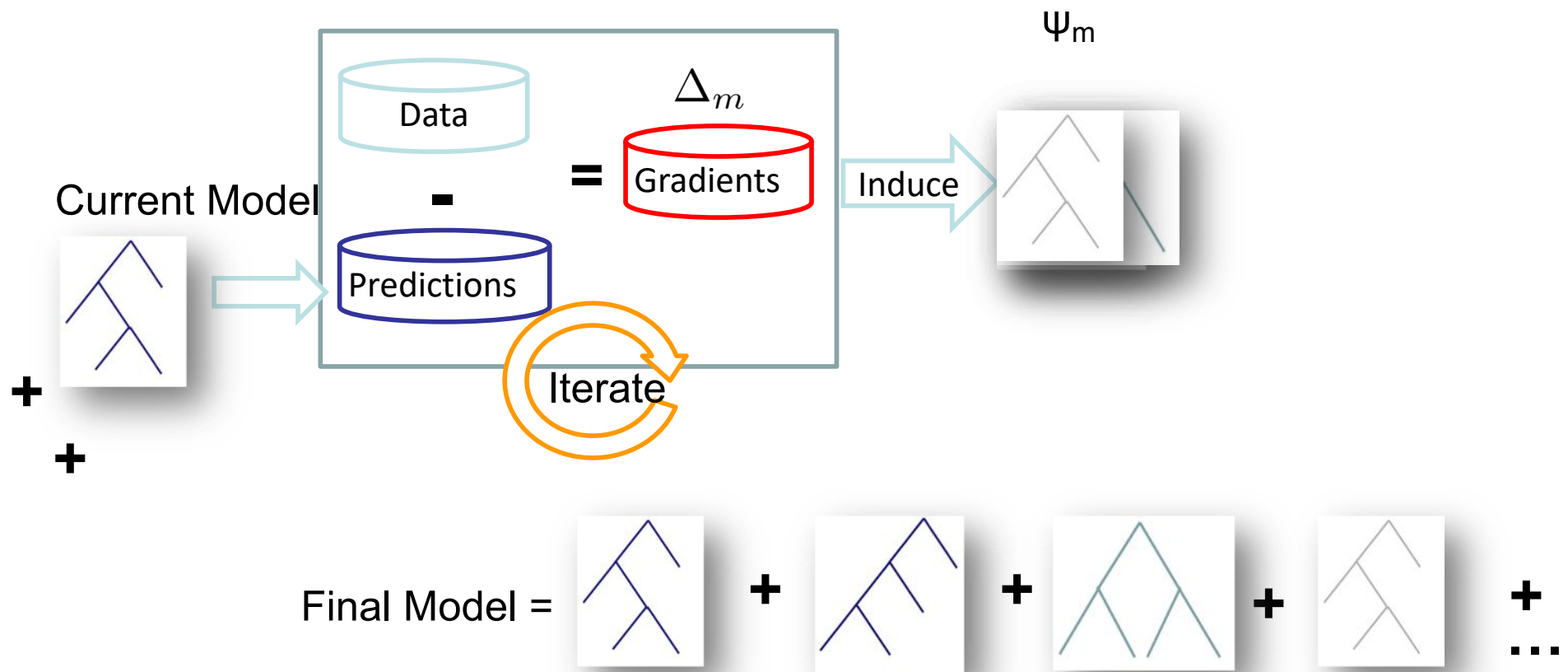
Learn multiple weak is easier than a single complex model

Friedman et al 2001, Dietterich et al. 2004, Natarajan et al. MLJ 2012

Functional Gradients for SRL Models

Pseudo probability of an example

$$P(x_i = true | \mathbf{Pa}(x_i)) = \frac{e^{\psi(x_i; \mathbf{Pa}(x_i))}}{e^{\psi(x_i; \mathbf{Pa}(x_i))} + 1}$$

x	Δ
target(x1)	0.7
target(x2)	-0.2
target(x3)	-0.9

Functional gradient

Maximize e.g. Pseudo Log Likelihood

$$LL(\mathbf{X} = \mathbf{x}) = \sum_{x_i \in \mathbf{x}} \log P(x_i | \mathbf{Pa}(x_i))$$

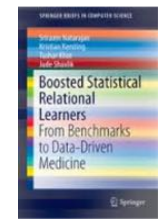Gradient of pseudo log-likelihood w.r.t ψ for learning gradient models

$$\Delta(x_i) = \frac{\partial \log P(\mathbf{X} = \mathbf{x})}{\partial \psi(x_i; \mathbf{Pa}(x_i))} = I(x_i = true; \mathbf{Pa}(x_i)) - P(x_i = true; \mathbf{Pa}(x_i))$$

Sum all gradient models to get final ψ

$$\psi_m = \psi_0 + \Delta_1 + ... + \Delta_m$$

Extended to multiple SRL models & in presence of hidden data

Understanding Electronic Health Records

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

Logical Variables
(Abstraction)
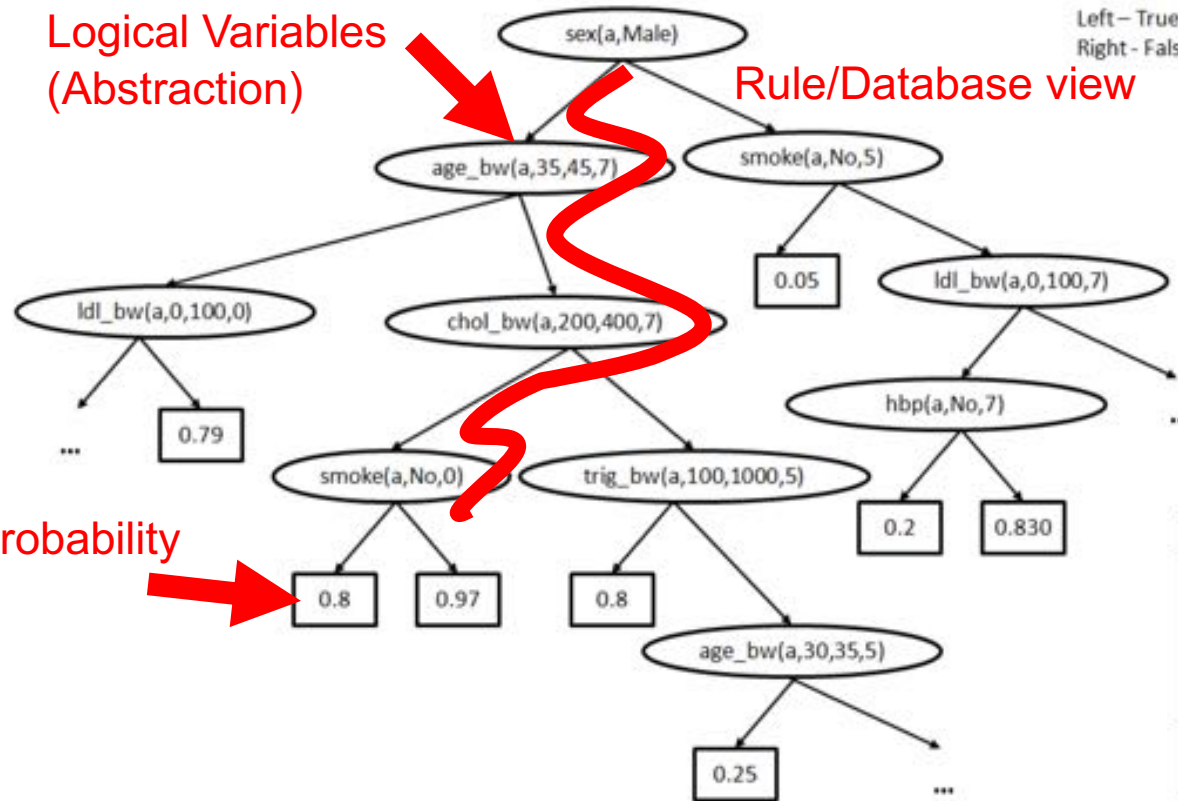
Rule/Database view

Left – True
Right - False

sex(a,Male)

age_bw(a,35,45,7)　　smoke(a,No,5)

ldl_bw(a,0,100,0)　　chol_bw(a,200,400,7)　　0.05　　ldl_bw(a,0,100,7)

0.79

smoke(a,No,0)　　trig_bw(a,100,1000,5)　　hbp(a,No,7)　　...

Probability

0.8　　0.97　　0.8　　0.2　　0.830

age_bw(a,30,35,5)

0.25　　...

Plaque in the left
coronary artery

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

Algorithm	Accuracy	AUC-ROC
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

The higher,
the better

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	state-of-the-art
Boosting	0.81	0.96	0.93	9s	
LSM	0.73	0.54	0.62	93 hrs	

11%　　78%　　50%　　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]

Boosted Statistical Relational Learners
From Benchmarks to Data-Driven Medicine

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UTD
THE UNIVERSITY
OF TEXAS AT DALLAS

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

St✦RLinGLAB   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.

Sriraam 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
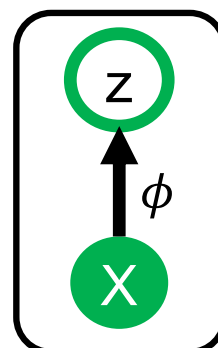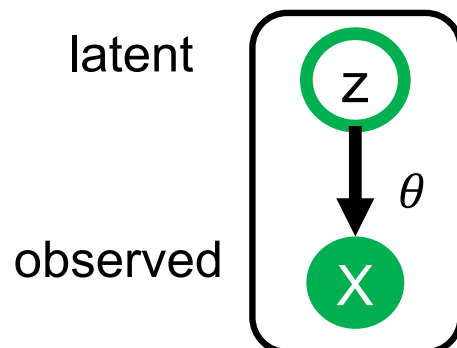
New field: Deep Probabilistic Programming

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.

```python
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])
```

```python
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

latent

observed

Deep Neural Network

(1) Instead of optimizating 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]

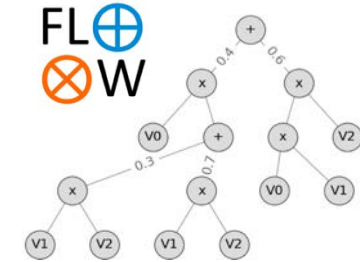# Sum-Product Probabilistic Programming

```
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
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        # observe datapoint i using the bernoulli
        # likelihood Bernoulli(f)
        pyro.sample("obs_{}".format(i), dist.Bernoulli(f), obs=data[i])
```
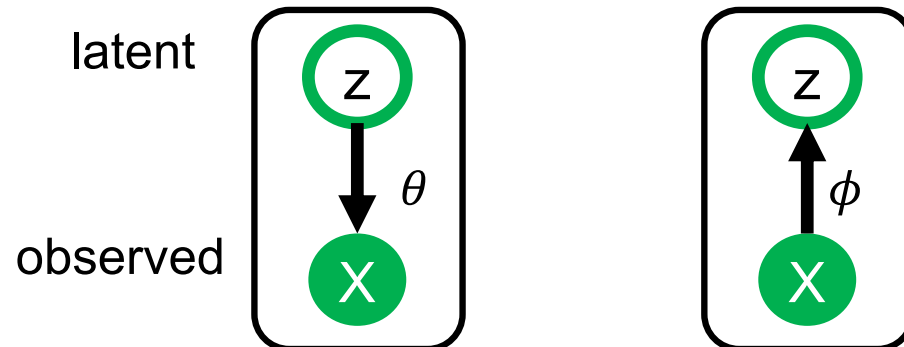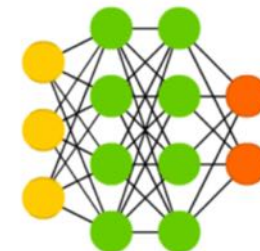
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    pyro.sample("latent_fairness", dist.Beta(alpha_q, beta_q))
```

Sum-Product Network

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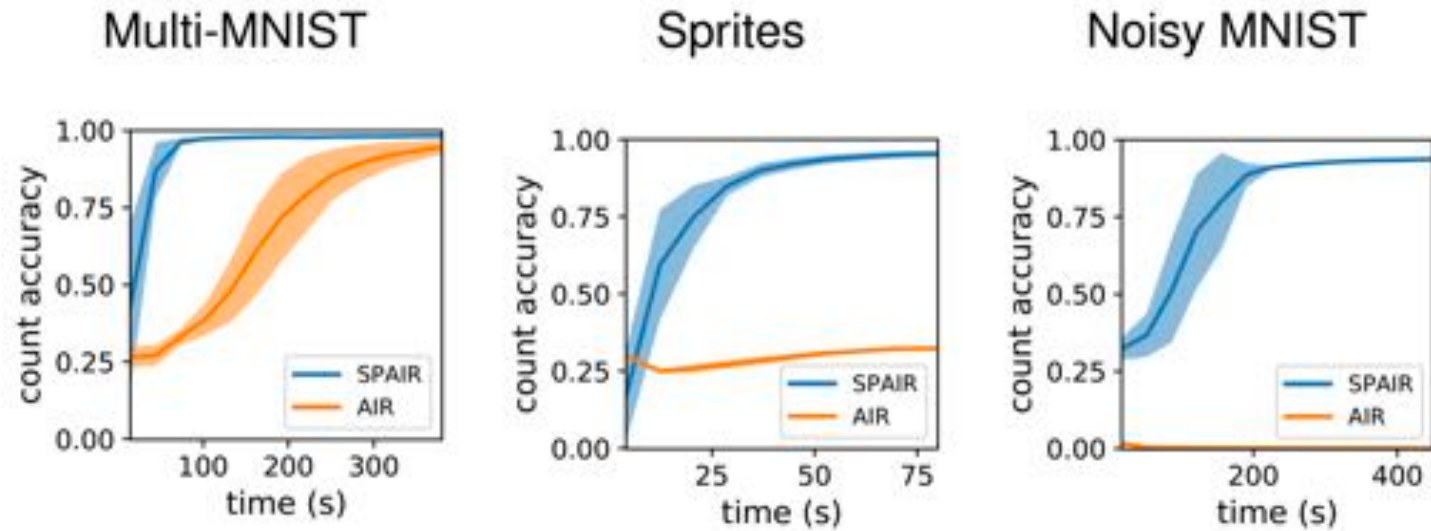
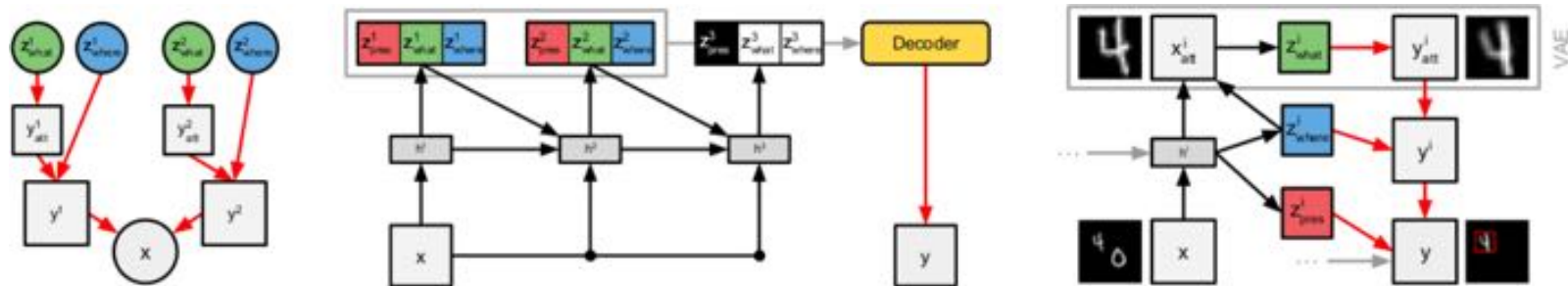latent

θ

observed

Deep Neural Network

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

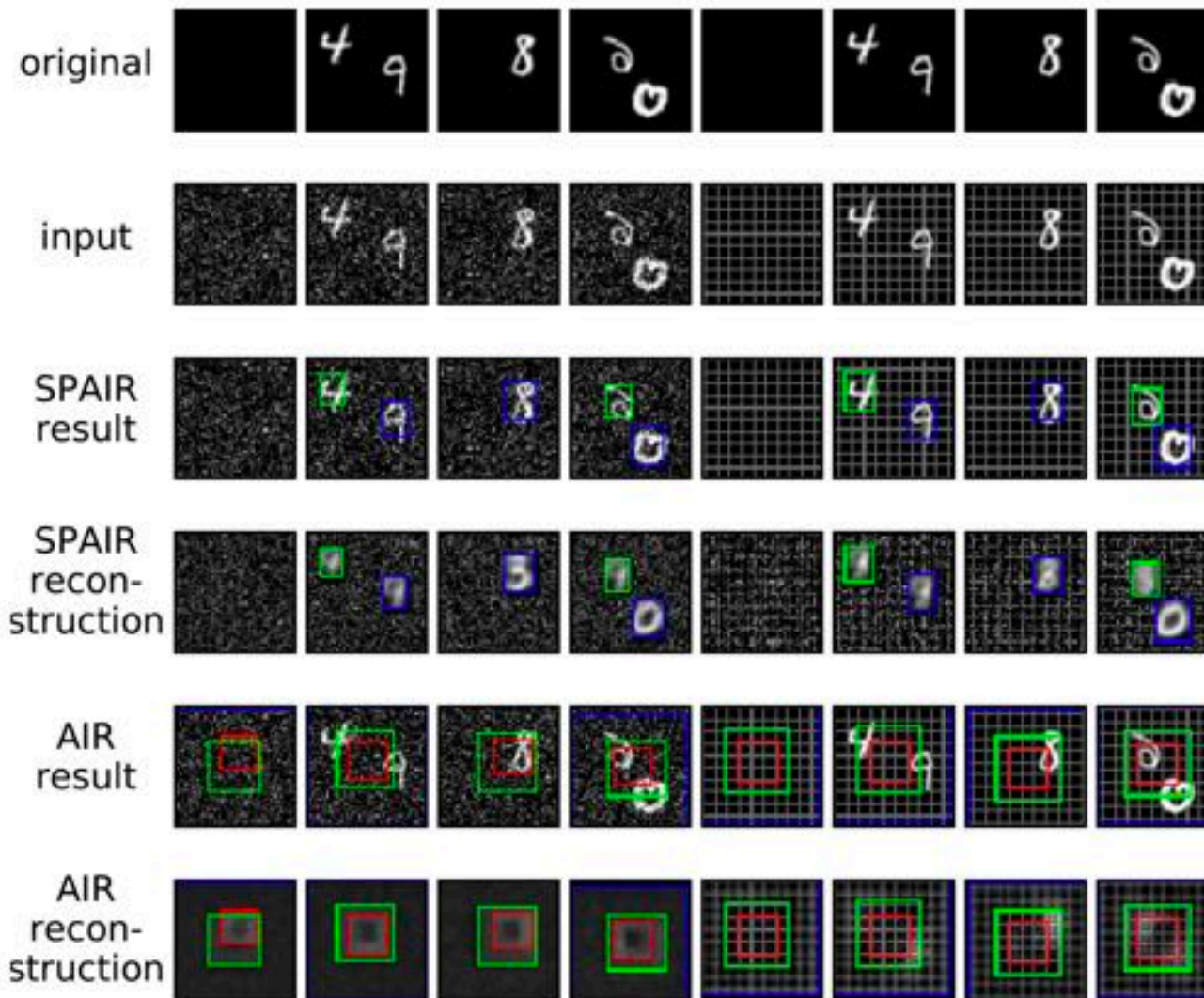# Sum-Product Attent-Infer Repeat

Replace
VAE by
SPN

Multi-MNIST Sprites Noisy MNIST

[Stelzner, Peharz, Kersting ICML 2019]

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A graphical model implemented in neural fashion using an VAE as object represenation [Eslami, Heess, Weber, Tassa, Szepesvari, Kavukcuoglu, Hinton NIPS 2016]

Sum-Product Attent-Infer Repeat

[Stelzner, Peharz, Kersting ICML 2019]
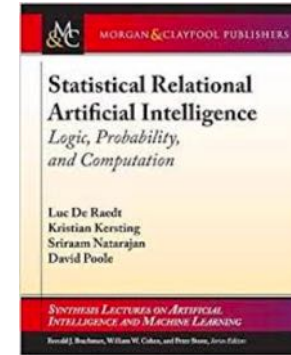
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There are strong invests into (deep) probabilistic programming

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

UBER AI Labs

Get Siri-ous.

No more evasive answers. No more coy innuendos. When you get romantic with Siri Pro, the sparks really fly.

Microsoft® Research

relationalAI
AI for the enterprise

The third wave of AI

- **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 data science, and high-level programming languages for DS help to capture this complexity

- **AI is more than just Machine Learners and Statisticians**

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