# Deep Machines that know when they do not know







Getting deep systems that reason and know when they don't know Responsible Al systems that explain their decisions and co-evolve with the humans Open Al systems that are easy to realize and understandable for the domain experts

### Al and ML have a strong 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

Provide the foundations, algorithms, and tools to develop systems that ease or even automate Al model discovery from data as much as possible



#### Potentially much more powerful than shallow architectures, represent computations

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





#### **Differentiable Programming**

Markov Chain (MC)









## Potentially much more powerful than shallow architectures, represent computations

DePhenSe

Bundesanstalt für Landwirtschaft und Ernährung

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

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

[Schramowski, Brugger, Mahlein, Kersting 2019]



# Potentially much more powerful than shallow architectures, represent computations

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





#### They "invent" constrained optimizers

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



1.02k



# Potentially much more powerful than shallow architectures, represent computations

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



SHARE REPORTS PSYCHOLOGY



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

+ See all authors and affiliations

Science 14 Apr 2017: Vol. 356, Issue 6334, pp. 183-186 D0I: 10.1126/science.aal4230

#### They "capture" stereotypes from human language



## Potentially much more powerful than shallow architectures, represent computations

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

#### **The Moral Choice Machine**





#### **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]



## 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 1219562 1125006 7016363

Train & Evaluate





SEMEION



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

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

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

Judea Pearl, UCLA Turing Award 2012 This results in 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



This results in Sum-Product Networks, a deep probabilistic learning framework



... convex sum
 ... product
 ... distribution

completeness sum children: same scope

decomposability product children: non-overlapping scope



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

#### Inference is linear in size of network



### And there is a way to select models

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



[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 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 multiples like commuting matricels, coefficiently and (approximate) most explosed into (MDEs) along with commune.

## **Random sum-product networks**

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

-200000 -150000 -100000 -50000

input log likelihood

UBER AI Labs

Cross-

(1.63M)

(0.22M)

(0.22M)



0



**UNIVERSITY OF** 





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 (µ5)	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	17249		100	696.00	24.44
Audio	20000	4271.78			5.4		B	20317	1		761.00	26.28
Netflix	20000	4892.22			4.8	~		20322	1		654.00	30.58
MSNBC200	388434	15476.05			30.5		1	388900	19		008.00	77.56
MSNBC300	388434	10060.78			41.2		and the	388810	19	8613 ·	933.00	78,74
NLTCS	21574	791.80			31.3	Mr		21904	1		566.00	38.12
Plants	23215	3621.71	6.41	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	29.03
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

# How do we do data science 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 2019]

FASA

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



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]





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]



# Functional weights realized as neural network



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]









## Distribution-agnostic Deep Probabilistic Learning



Use nonparametric independency tests and piece-wise linear approximations



## Distribution-agnostic Deep Probabilistic Learning



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

[Vergari, Molina, Peharz, Ghahramani, Kersting, Valera AAAI 2019]



Max Planck Institute for Intelligent Systems

Federal Ministry
of Education
and Research

TECHNISCHE

UNIVERSITÄT

DARMSTADT

#### The Explorative Automatic Statistician

UNIVERSITY OF

CAMBRIDGE

 X1
 X2
 X3
 X4
 X5

 Xa
 I
 I
 I
 I
 I

 Xa
 I
 I
 I
 I
 I

 Xa
 I
 I
 I
 I
 I
 I
 I

 Xa
 I
 I
 I
 I
 I
 I
 I
 I

 Xa
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I

UBER AI Labs

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









# That is, 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 ....



#### ...and can compile data reports automatically

# P( heart | III )?



# P( heart | attack



)?





# heart attack

Los de Rand

interance Nature



#### **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.



Natarajan, Khot, Kersting, Shavlik. Boosted Statistical Relational Learners. Springer Brief 2015

Relational

#### **Understanding Electronic Health Records**



[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] Natarajan, Khot, Kersting, Shavlik. Boosted Statistical Relational Learners. Springer Brief 2015





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

StARLinGLAB

People

Publications

Projects

Software

Datasets

Blog

Q

#### BOOSTSRIL 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-Senaltive 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

THE UNIVERSITY **OF TEXAS AT DALLAS** 

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: Probabilistic Programming



Problem Statistics					lic IPM	Ground IPM
name	#vars	#constr	nnz(A)	IADDI	time[s]	time[s]
factory	131.072	688.128	4.000.000	1819	6899	516
factory0	524.288	2.752.510	15.510.000	1895	6544	7920
factory1	2.097.150	11.000.000	59.549.700	2406	34749	159730
factory2	4.194.300	22.020.100	119.099.000	2504	36248	$\geq$ 48hrs.
					>4.8x fa	aster

Applies to QPs but here illustrated on MDPs for a factory agent which must paint two objects and connect them. The objects must be smoothed, shaped and polished and possibly drilled before painting, each of which actions require a number of tools which are possibly available. Various painting and connection methods are represented, each having an effect on the quality of the job, and each requiring tools. Rewards (required quality) range from 0 to 10 and a discounting factor of 0. 9 was used used

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):

 

#### (2) Ease the implementation by some highlevel, probabilistic programming language



(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 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]) 

#### (2) Ease the implementation by some highlevel, probabilistic programming language

latent

observed





Sum-Product Network

**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]

## Unsupervised scene understanding

[Stelzner, Peharz, Kersting ICML 2019]

Consider e.g. unsupervised scene understanding using a generative model





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

#### Sum-Product Probabilistic Programming: Making machine learning and data science

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



**Probabilistic Programming:** Easier modelling by programming generative models in a high-level, might be hard, so use a prob. language

**Deep Probabilistic Prog.:** Modelling and inference deep neural network for it



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 son

# Actually, the main idea is to replace the VAEs within AIR by SPNs

VAE

- 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]



#### Sum-Product Attent-Infer Repeat (SuPAIR)



[Stelzner, Peharz, Kersting ICML 2019]



TECHNISCHE UNIVERSITÄT DARMSTADT

#### Sum-Product Attent-Infer Repeat (SuPAIR)

Multi-MNIST

Sprites

Noisy MNIST



[Stelzner, Peharz, Kersting ICML 2019]



### Sum-Product Attent-Infer Repeat (SuPAIR)



[Stelzner, Peharz, Kersting ICML 2019]





# There are strong invests into (deep) probabilistic programming

UBER AI Labs

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





relationalAI Al for the enterprise

## Since we need languages for Systems AI,

the computational and mathematical modeling of complex AI systems.

[Laue et al. NeurIPS 2018; 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.



UBER AI Labs

FI (

Intelligent Systems

Microsoft<sup>®</sup>



#### MORGAN &CLAYTOOL FUBL

Statistical Relational Artificial Intelligence Logic, Probability, and Computation

Luc De Raedt Kristian Kersting Seiraam Natarajar David Poole



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

UNI

GRAZ

**TECHNISCHE** 

UNIVERSITÄT DARMSTADT

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

Open Al 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"



(a) Origina image (b) Explaining a image classification prediction made by Google's Inception network, high lighting positive pixels. The top 3 classes predicted are "Electric Guitar" (p = 0.32), "Acoustic guitar" (p =

Teso, Kersting AIES 2019

AAAI / ACM conference on

**ARTIFICIAL INTELLIGENCE.** 

ETHICS. AND SOCIETY

# Explanation should be understandable by humans

#### 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 <u>Members</u> 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

# Overall, AI/ML/DS indeed refine "formal" science, but ...

- Al is more than deep neural networks. Probabilistic and causal models are whiteboxes that provide insights into applications
- Al is more than a single table. Loops, graphs, different data types, relational DBs, ... are central to data science and highlevel programming languages for DS help to capture this complexity
- Al is more than just Machine Learners and Statisticians

Learning-based programming offers a framework for building systems that help to go beyond, democratize, and even automize traditional AI/ML/DS