Deep machines that know when they do not know*



*Thanks for Pedro Domingos for making his slides publically available

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



Third wave of Al



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 Al



Data are now ubiquitous; there is great value from understanding this data, building models and making predictions However, data is not everything



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





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^{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 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 often have no probabilistic semantics. They are not $P(Y|X) \neq P(Y,X)$ calibrated joint distributions.

MNIST て、9563

SVHN

49

SEMEION



Train & Evaluate

Transfer Testing [Bradshaw et al. arXiv:1707.02476 2017]

1622

67



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:

X_{I}	X_2	P (X)
1	1	0.4
1	0	0.2
0	1	0.1
0	0	0.3

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



Alternative Representation:

X_{I}	X_2	P(X)
1	1	0.4
1	0	0.2
0	1	0.1
0	0	0.3

$$P(X) = 0.4 \cdot I[X_1=1] \cdot I[X_2=1]$$

+ 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]



Shorthand using Indicators



<i>X</i> ₁	<i>X</i> ₂	P(X)
1	1	0.4
1	0	0.2
0	1	0.1
0	0	0.3

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



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

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

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

Easy: Set both indicators of X2 to 1



This can be represented as a computational graph







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





Testing independence using a (non-parametric) independency test











Kristian Kersting - Deep Machines that know when they do not know



Random sum-product networks

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

SPNs can have similar predictive performances as (simple) DNNs

RAT-SPN

98.19

89.52

47.8

(8.5M)

(0.65M)

(0.37M)

0.0852

(17M)

0.3525

(0.65M)

1.6954

(1.63M)

MNIST

F-MNIST

20-NG

MNIST

F-MNIST

20-NG

MLP

98.32

90.81

49.05

(2.64M)

(9.28M)

(0.31M)

0.0874

(0.82M)

0.2965

(0.82M)

1.6180

(0.22M)

vMLP

98.09

89.81

48.81

(5.28M)

(1.07M)

(0.16M)

0.0974

(0.22M)

(0.29M)

1.6263

(0.22M)

0.325

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SPNs can distinguish the datasets

input log likelihood

SPNs know when they do not know by design





GRAZ

TECHNISCHE

UNIVERSITÄT



10-3

 10^{-4}

10-5

 10^{-6}

frequency

MNIST

SVHN

SEMEION

-200000 -150000 -100000 -50000



0

[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.

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	2643 ·	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 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 2019]

FASA

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]



chain rule of



[Poon, Domingos UAI'11]



Learn Conditional SPN (CSPNs) by non-parametric conditional independence testing and conditional

clustering [Zhang et al. UAI 2011; Lee, Honovar 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



And SPNs may also provide likelihoods for time series







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

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 X5

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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 | ① ①)? attack



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/

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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

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 implemented in a neural fashion



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



- infinite mixture model
- intractable density
- intractable posterior



"large" but finite mixture model

tractable marginals [Peharz et al., 2015]

tractable posterior [Vergari et al., 2017]

tractable density



(c) Noisy MNIST

(d) Grid MNIST

250

400



There are strong invests into (deep) probabilistic programming

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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.

[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.



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 <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

Indeed, AI has great impact, 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 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, Al is a team sport

= 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

