



Buzzwords surrounding Data Science

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Rise of Data Science





Outline

- Data Science Community
- Landscape of Data Science Research in Alan Turing Institute
 - What Topics are interesting to research?
- Becoming Data Scientist?
- Fill the Gap between Research and Practice



Data Science: Any new intellectual content?

- What does it mean to Computer Science?
- 1970's: EE + Math \rightarrow Computer Science
- 2010's: CS + Stats + ?? → Data Science
- Is something fundamental emerging here?
- Data Science is a very broad discipline
- Data Science PhD?
 - PhD normally with a narrow field with depth...





Scale of Community Size in ML/AI





NIPS: 8000 Attendees in 2017

- Randomness of Paper acceptance?
- 2016: 2,406 submissions and 568 acceptance (24% acceptance rate)
- 2017: 3,240 submissions and 679 acceptance (21% acceptance rate)
- In 2014, Corinna Cortes and Neil Lawrence ran the NIPS experiment where 1/10th of papers submitted to NIPS went through the NIPS review process twice, and then the accept/reject decision was compared. http://blog.mrtz.org/2014/12/15/the-nips-experiment.html
- In particular, about 57% of the papers accepted by the first committee were rejected by the second one and vice versa. In other words, most papers at NIPS would be rejected if one reran the conference review process (with a 95% confidence interval of 40-75%).





NIPS: Publishing



Google
Carnegie Mellon University
Massachusetts Institute
Microsoft
Stanford University
University of California, Berkeley
DeepMind
University of Oxford
University of Illinois at Urbana-Champaign
Georgia Institute of Technology
Princeton
ETH Zurich
Harvard University
Cornell University
Duke University
Columbia University
University of Cambridge
EPFL
University of Michigan
University of Toronto
University of Southern California
Tsinghua University
Facebook
Riken University of Washington
University of California, Los Angeles
University of Texas at Austin
New York University
University College London
Universite De Montreal
Tecent AI Lab
OpenAl
Adobe



SysML Conference spawn in 2018-2019

- SysML is a conference targeting research at the intersection of systems and machine learning
- Aims to elicit new connections amongst these fields, including identifying best practices and design principles for learning systems, as well as developing novel learning methods and theory tailored to practical machine learning workflows

Steering Committee

Jennifer Chayes Bill Dally Jeff Dean Michael I. Jordan Yann LeCun Fei-Fei Li Alex Smola Dawn Song Eric Xing



SysML 2019: Programming Models Session

Session IV: Programming Models

- (Example: Modular Computation Graphs for Deep Reinforcement Learning Michael Schaarschmidt (University of Cambridge), Sven Mika (rlcore), Kai Fricke (Helmut Schmidt University), Eiko Yoneki (University of Cambridge)
- TensorFlow Eager: A multi-stage, Python-embedded DSL for machine learning Akshay Agrawal (Google Brain), Akshay Naresh Modi (Google Brain), Alexandre Passos (Google Brain), Allen Lavoie (Google Brain), Ashish Agarwal (Google Brain), Asim Shankar (Google Brain), Igor Ganichev

(Google Brain), Josh Levenberg (Google Brain), Mingsheng Hong (Google Brain), Rajat Monga (Google Brain), Shanqing Cai (Google Brain)

• Description AutoGraph: Imperative-style Coding with Graph-based Performance

Dan Moldovan (Google Inc.), James Decker (Purdue University), Fei Wang (Purdue University), Andrew Johnson (Google Inc.), Brian Lee (Google Inc.), Zack Nado (Google Inc.), D Sculley (Google), Tiark Rompf (Purdue University), Alexander B Wiltschko (Google Inc.)

• 🕞 TensorFlow.js: Machine Learning for the Web and Beyond

Daniel Smilkov (Google), Nikhil Thorat (Google), Yannick Assogba (Google), Charles Nicholson (Verily), Nick Kreeger (Google), Ping Yu (Google), Shanqing Cai (Google), Eric Nielsen (Google), David Soegel (Google), Stan Bileschi (Google), Michael Terry (Google), Ann Yuan (Google), Kangyi Zhang (Google), Sandeep Gupta (Google), Sarah Sirajuddin (Google), D Sculley (Google), Rajat Monga (Google), Greg Corrado (Google), Fernanda Viegas (Google), Martin M Wattenberg (Google)



History/Trajectory Data Science





Alan Turing Institute (ATI)

- Established in 2015 in London as a National Institute for Data Science
- >£20M Capital Investment from Government
- Originally 5 Universities formed core body (UCL, Warwick, Edinburg, Oxford and Cambridge) and now expanded to 13 and more universities
- Goal: Data Science and after 2018 changed to Artificial Intelligence

https://www.turing.ac.uk



Driving data futures: Technology and → government – the good, the bad, and the ugly Thursday 02 May 2019 Time: 17:15 - 19:00



 \rightarrow

Turing Lecture: Learning how to learn efficiently Tuesday 30 Apr 2019 Time: 18:00 - 20:30

Nando de Freitas



Lina Dencik | Omar A Guerrero



ATI: Research Programmes

Translating output into practice



Artificial intelligence (AI) → Advancing world-class research into artificial intelligence, its applications and its implications for society, building on our academic network's wealth of expertise.



Data science at scale → Building upon advances in highperformance computer architectures, through algorithm-architecture co-design, with applications including health and life science.



Data science for science → Ensuring that research across science and the humanities can make effective use of state of the art methods in artificial intelligence and data science.



Health and medical sciences → Accelerating the scientific understanding of human disease and improving human health through data-driven innovation in Al and statistical science.



Research Engineering -Connecting research to applications, helping create usable and sustainable tools, practices and systems.



Data-centric engineering → Bringing together world-leading academic institutions and major industrial partners from across the engineering sector, to address new challenges in data-centric engineering.



Defence and security → Collaborating with the defence and security community to deliver an ambitious programme of data science research, to deliver impact in real world scenarios.



Finance and economics — Develop cutting-edge methods to foster financial innovation and deepen our understanding of the economy, to benefit society at large



Urban analytics

Developing data science and AI focused on the process, structure, interactions and evolution of agents, technology and infrastructure within and between cities.



Public policy

Working with policy makers on data-driven public services and innovation to solve policy problems, and developing ethical foundations for data science and AI policymaking.



Landscape of Data Science Research in ATI





Landscape of Data Science Research in ATI





Probabilistic Model

- Probabilistic models incorporate random variables and probability distributions into the model
 - Deterministic model gives a single possible outcome
 - Probabilistic model gives a probability distribution
- Used for various probabilistic logic inference (e.g. MCMCbased inference, Bayesian inference...)

Python based PP:

- Pyro: https://pyro.ai/examples
- Edward: http://edwardlib.org



Probabilistic Programming







TensorFlow Probability

TensorFlow integrated Edward





Save time in model tuning and inference

Avoid re-inventing the wheel

Spend your time hypothesizing, instead of programming

> Use off-the-shelf, performant libraries

Leverage community + scalable cloud compute



Landscape of Data Science Research in ATI





Deep Learning, Machine Learning, and AI...





Machine Learning Timeline

Modern Machine Learning: see Wikipedia-Timeline of machine learning

2009	Achievement	ImageNet	ImageNet is created. ImageNet is a large visual database envisioned by Fei-Fei Li from Stanford University, who realized that the best machine learning algorithms wouldn't work well if the data didn't reflect the real world. ^[40] For many, ImageNet was the catalyst for the AI boom ^[41] of the 21st century.
2010		Kaggle Competition	Kaggle, a website that serves as a platform for machine learning competitions, is launched. ^[42]
2011	Achievement	Beating Humans in Jeopardy	Using a combination of machine learning, natural language processing and information retrieval techniques, IBM's Watson beats two human champions in a Jeopardy! competition. ^[43]
2012	Achievement	Recognizing Cats on YouTube	The Google Brain team, led by Andrew Ng and Jeff Dean, create a neural network that learns to recognize cats by watching unlabeled images taken from frames of YouTube videos. ^{[44][45]}
2014		Leap in Face Recognition	Facebook researchers publish their work on DeepFace, a system that uses neural networks that identifies faces with 97.35% accuracy. The results are an improvement of more than 27% over previous systems and rivals human performance. ^[46]
2014		Sibyl	Researchers from Google detail their work on Sibyl, ^[47] a proprietary platform for massively parallel machine learning used internally by Google to make predictions about user behavior and provide recommendations. ^[48]
2016	Achievement	Beating Humans in Go	Google's AlphaGo program becomes the first Computer Go program to beat an unhandicapped professional human player ^[49] using a combination of machine learning and tree search techniques. ^[50] Later improved as AlphaGo Zero and then in 2017 generalized to Chess and more two-player games with AlphaZero.



Four Great Pictures Illustrating ML Concepts

- Neural Networks: The Backpropagation algorithm
- Cheat Sheet on Probability
- 24 Neural Network Adjustments ->
- Matrix Multiplication in NN

ARCHITECTURE

- Variables type
- Variable scaling
- Cost function
- Neural Network type:
 - RBM,FFN,CNN,RNN...
- Number of layers
- Number of hidden Layers
- Number of nodes
- Type of layers:
 - LSTM, Dense, Highway
 - Convolutional, Pooling...
- Type of weight initialization
- Type of activation function
 - Linear, sigmoid, relu...
- Dropout rate (or not)
- Threshold

HYPERPARAMETER TUNING

- Type of optimizer
- Learning rate (fixed or not)
- Regularization rate (or not)
- Regularization type: L1, L2, ElasticNet
- Type of search for local minima:
 - · Gradient descent, simulated
 - annealing, evolutionary...
- Batch size
- Nesterov momentum (or not)
- Decay rate (or not)
- Momentum (fixed or not)
- Type of fitness measurement:
 - MSE, accuracy, MAE, cross-entropy,
 - precision, recall
- Epochs
- Stop criteria

See https://www.datasciencecentral.com/profiles/blogs/four-great-pictures illustrating-machine-learning-concepts



Landscape of Data Science Research in ATI





Tuning Computer Systems is Complex

- Complex configuration parameter space / increasing # of parameters
- Configurations need tuning to optimise resource utilisation
- Hand-crafted solutions impractical, often left static or configured through extensive offline analysis







Complex and High Dimension Parameter Space









Auto-tuning systems



Properties:

- Many dimensions
- Expensive objective function
- Understanding of the underlying behaviour



Auto-tuning: Large Parameter Space





Bayesian optimisation

Iteratively build a probabilistic model of objective function



Pros:

- ✓ Data efficient: converges in few iterations
- ✓ Able to deal with noisy observations

Cons:

X In many dimensions, model does not converge to the objective function



Bayesian optimisation



Domain



Structured Bayesian Optimisation (SBO)



- ✓ Better convergence
- ✓ Use all measurements
- **BOAT:** a framework to build **B**esp**O**ke **A**uto-**T**uners
- It includes a probabilistic library to express these models

Probabilistic Model written in Probabilistic C++

ruct CassandraModel	: public DAGModel <cassandramodel> {</cassandramodel>
void model(int ygs,	int sr, int mtt){
// Calculate the	size of the heap regions
double es = ygs *	<pre>sr / (sr + 2.0);// Eden space's size</pre>
double ss = ygs /	<pre>(sr + 2.0); // Survivor space's size</pre>
<pre>double rate = double duration =</pre>	<pre>aflow between semi-parametric models output("rate", rate_model, es); output("duration", duration_model, es, ss, mtt); output("latency", latency_model,</pre>
,	rate, duration, es, ss, mtt);
}	
ProbEngine <gcratemo< td=""><td>del> rate_model;</td></gcratemo<>	del> rate_model;
ProbEngine <gcdurati< td=""><td>onModel> duration_model;</td></gcdurati<>	onModel> duration_model;
ProbEngine <latencym< td=""><td><pre>lodel> latency model;</pre></td></latencym<>	<pre>lodel> latency model;</pre>

Developer-specified, model of performance from observed performance + arbitrary runtime characteristics



Semi-parametric Model

3

Time (µs) N

- Easy to use and well suited to SBO
 - Understand general trend of Objective function
 - High precision in region of Optimum for finding highest performance





Example:

Cassandra's garbage collection



Minimise 99th percentile latency of Cassandra



Define DAG Model

Define a directed acyclic graph (DAG) of models



Tune JVM parameters of a database (Cassandra) to minimise latency



Computer Systems Optimisation Models

- Short-term dynamic control: major system components are under dynamic load, such as resource allocation and stream processing, where the future load is not statistically dependent on the current load.
 BaysOpt is sufficient to optimise distinct workloads. For dynamic workload, Reinforcement Learning would perform better.
- Combinatorial optimisation: a set of options to be selected from a larger set under potential rules of combination. There is no straightforward similarity between different combinations. Many problems in device assignment, indexing, compiler optimisation fall in this category. BaysOpt cannot be easily applied. Either learning online if the task is cheap via random sampling, or via RL + pre-training if the task is expensive, or massively parallel online training if the resources are available.

Many systems problems are combinatorial in nature



Problem: Controlling dynamic behaviour

Assume workload dynamic, e.g. seasonality, load spikes, shared resources, failures..

- Algorithm: workload → behavior distribution
- Involves approximations to NP-complete problems,
 e.g. bin packing, subgraph isomorphism, ..





Reinforcement Learning

- Agent interacts with Dynamic environment
- Goal: Maximise expectations over rewards over agent's lifetime
- Notion of Planning/Control, not single static configuration



What makes RL different from other ML paradigms?

- There is no supervisor, only a reward signal
- Feedback is delayed, not instantaneous
- Time really matters (sequential)
- Agent's actions affect the subsequent data it receives

The most similar way to human brain's behaviour...





A brief history of Deep RL software

1. Gen (2014-16): Loose research scripts (e.g. DQN), high expertise required, only specific simulators

2. Gen (2016-17): OpenAI gym gives unified task interface, reference implementations (e.g. OpenAI baselines)

3. Gen (2017-18): Generic declarative APIs, distributed abstractions (Ray RLlib), some standard *flavours* emerge

Problems: Tightly coupled execution/logic, testing, reuse,...




RL Workloads

- Unlike supervised learning, not a single dominant execution pattern
- Distributed workloads: Hierarchies of sync/async data exchange
- Algorithms highly sensitive to hyper-parameters
- From large scale parallel training (e.g. AlphaGo) to single core



RL in Computer Systems: Practical Considerations

- Action spaces do not scale:
 - Systems problems often combinatorial
- Exploration in production system not a good idea
 - Unstable, unpredictable
- Simulations can oversimplify problem
 - Expensive to build, not justified versus gain
- Online steps take too long



Dynamic Control Flow in Current Frameworks

- There are static computation frameworks WITHOUT dynamic control flow (mxnet, cntk) -> dynamic control flow is in the out of graph host program.
- There are dynamic computation graph frameworks WITH dynamic control flow (PyTorch, DyNet) -> graph is only implicitly defined via imperative operations, cannot do static graph optimisations, typically slower but easier to use.
- There is static computation with dynamic differentiable control flow in the graph -> only TensorFlow offers this among modern deep learning frameworks.



RLgraph: Modular Dataflow Composition





RLGraph: Separate Local and Distributed Execution

 High performance RL computation graphs for RL with different distributed backends





OWL Architecture for OCaml



Owl + Actor = Distributed & Parallel Analytics

Owl provides numerical backend; whereas Actor implements the mechanisms of distributed and parallel computing. Two parts are connected with functors.

Various system backends allows us to write code once, then run it from cloud to edge devices, even in browsers.

Same code can run in both sequential and parallel mode with Actor engine.

By Liang Wang in 2018



Pipeline of Data Processing...





Modern Data Scientist: The sexiest job of 21th century





MATH & STATISTICS

- r Machine learning
- ✿ Statistical modeling
 - Experiment design
 - Bayesian inference
 - Supervised learning: decision trees, random forests, logistic regression
- Unsupervised learning: clustering, dimensionality reduction
- Optimization: gradient descent and variants

PROGRAMMING & DATABASE

- 🖈 Computer science fundamentals
- ☆ Scripting language e.g. Python
- ☆ Statistical computing package e.g. R
- 🖨 Databases SQL and NoSQL
- ✿ Relational algebra
- Parallel databases and parallel query processing
- ☆ MapReduce concepts
- ☆ Hadoop and Hive/Pig
- ☆ Custom reducers
- ☆ Experience with xaaS like AWS

COMMUNICATION & VISUALIZATION

- Able to engage with senior management
- ✿ Story telling skills
- Translate data-driven insights into decisions and actions
- ☆ Visual art design
- ✿ R packages like ggplot or lattice
- ☆ Knowledge of any of visualization tools e.g. Flare, D3.js, Tableau







DOMAIN KNOWLEDGE & SOFT SKILLS

- ✿ Passionate about the business
- 🕁 Curious about data
- Influence without authority
- Hacker mindset
- ✿ Problem solver
- Strategic, proactive, creative, innovative and collaborative

senior





Many Courses offered: e.g. Master Certificate

 Data scientist is the pinnacle rank in an analytics organisation. You will be required to understand the business problem, design the analysis, collect and format the required data, apply algorithms or techniques using the correct tools, and finally make recommendations backed by data.







Landscape of Data Science Research in ATI





AutoML: Neural Architecture Search

Current: ML expertise + Data + Computation

AutoML aims turning into: Data + 100X Computation

- Use of Reinforcement Learning, Evolutionary Algorithms
- ..and tune network model?
 - Graph transformation
 - Compression
 - + Hyper parameter tuning



RL Model Building

Current: Simulation based if there is data

World Model:

- Training RL algorithms using variational auto encoders (simulator like)
 - Use randomly collected data as input and train to build a compact model
 - Train the compact model with RNN predict future steps the model, then evolve the controller to maximise the expected cumulative reward of roll out





Modern Theory of Deep Learning

Why does it work so well?

- On the Expressive Power of Deep Neural Networks PMLR 2017: understanding of how and why neural network architectures achieve their empirical successes is still lacking.
- Ali Rahimi's talk at NIPS(NIPS 2017 Test-of-time award presentation)
- Deep Learning works in Practice. But Does it work in Theory? By L. Hoang and R. Guerraoui. (https://arxiv.org/pdf/1801.10437.pdf)
- Understanding deep learning requires rethinking generalisation
- Fundamental theory behind the paradoxical effectiveness of deep learning. Still open research problem...



Gap between Research and Practice



Research opportunities ahead!

http://www.cl.cam.ac.uk/~ey204/

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