Large-scale Data Processing and Optimisation

Overview

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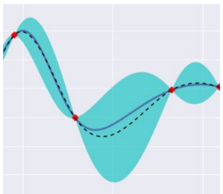

Massive Data: Scale-Up vs Scale-Out

- Popular solution for massive data processing
  → scale and build distribution, combine theoretically unlimited number of machines in single distributed storage
  → Parallelisable data distribution and processing is key
- Scale-up: add resources to single node (many cores) in system (e.g. HPC)
- Scale-out: add more nodes to system (e.g. Amazon EC2)

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Technologies supporting Cluster Computing

- Distributed infrastructure
  - Cloud (e.g. Infrastructure as a service, Amazon EC2, GCP, Azure)
- Storage
  - Distributed storage (e.g. Amazon S3, Hadoop Distributed File System (HDFS), Google File System (GFS))
- Data model/indexing
  - High-performance schema-free database (e.g. NoSQL DB - Redis, BigTable, Hbase, Neo4J)
- Programming model
  - Distributed processing (e.g. MapReduce)

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Data Processing Stack

Data Processing Layer

Streaming Processing
Storm, SEEP, Naiad, Spark Streaming, Flink, Milwheel, Google Dataflow...

Query Language
Pig, Hive, SparkSQL, DryadLINQ..

Machine Learning
Rllib, Caffe, Keras, Torch, MLlib…

Execution Engine
MapReduce, Spark, Tensorflow, Ray, Flumejava…

Graph Processing
Pregel, Giraph, GraphLab, PowerGraph, (Dato), GraphX, X-Stream...

Storage Layer

Distributed File Systems
GFS, HDFS, Amazon S3, Flat FS..

Operational Store/NoSQL DB
Big Table, Hbase, Dynamo, Cassandra, Redis, Mongo, Spanner…

Logging System/Distributed Messaging Systems
Kafka, Flume…

Resource Management Layer

Resource Management Tools
Mesos, YARN, Borg, Kubernetes, EC2, OpenStack…

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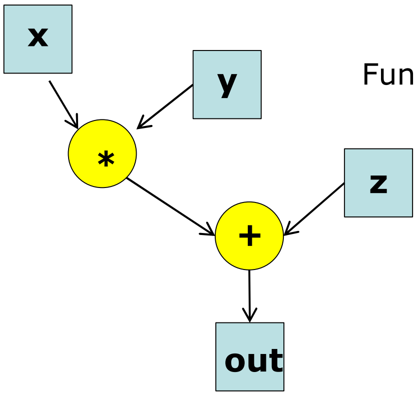
Data Flow Programming

- Non-standard programming models
- Powerful abstraction: mapping computation into dataflow graphs



Function f(x, y, z) = x* y + z

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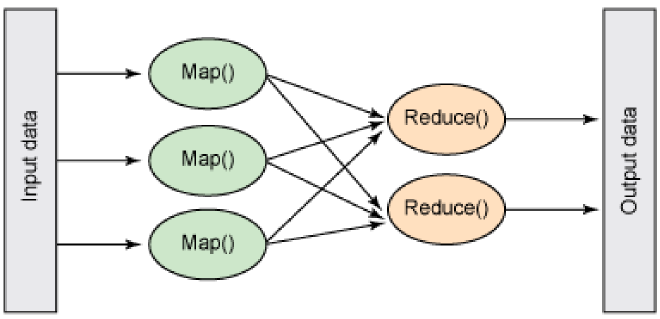
MapReduce Programming

- Target problem needs to be parallelisable
- Split into a set of smaller code (map)
- Next small piece of code executed in parallel
- Results from map operation get synthesised into a result of original problem (reduce)



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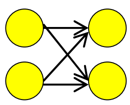
Data Flow Programming Examples

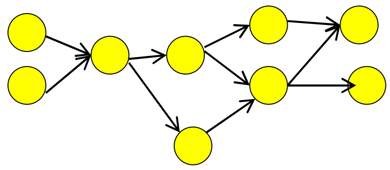
- Data (flow) parallel programming
  - e.g. MapReduce, Dryad/LINQ, NAIAD, Spark, Tensorflow…
  - e.g. ML compiler: computation graphs

MapReduce:
Hadoop

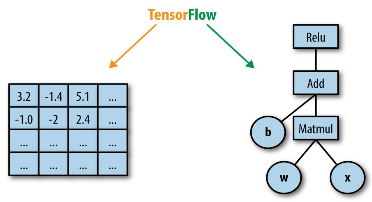


Two-Stage fixed dataflow

DAG (Directed Acyclic Graph)
based: Dryad/Spark…



More flexible dataflow model



Data Flow Programming's Usefulness for ML

- Data flow programming holds the key to natural, modular, streamlined ML specification
- Same language for layer, network, and integration specification
  - For complex NN classes, RL with complex reward, gated networks, attention/transformers, mix of NN and data processing
- Same language for ML algorithmics and compiler design
- Well-established analysis and compilation techniques integrated within existing ML compilers (e.g. MLIR)
  - MLIR (Multi-Level Intermediate Representation) is intended to be a hybrid IR which can support multiple different requirements in a unified infrastructure (https://mlir.llvm.org/)

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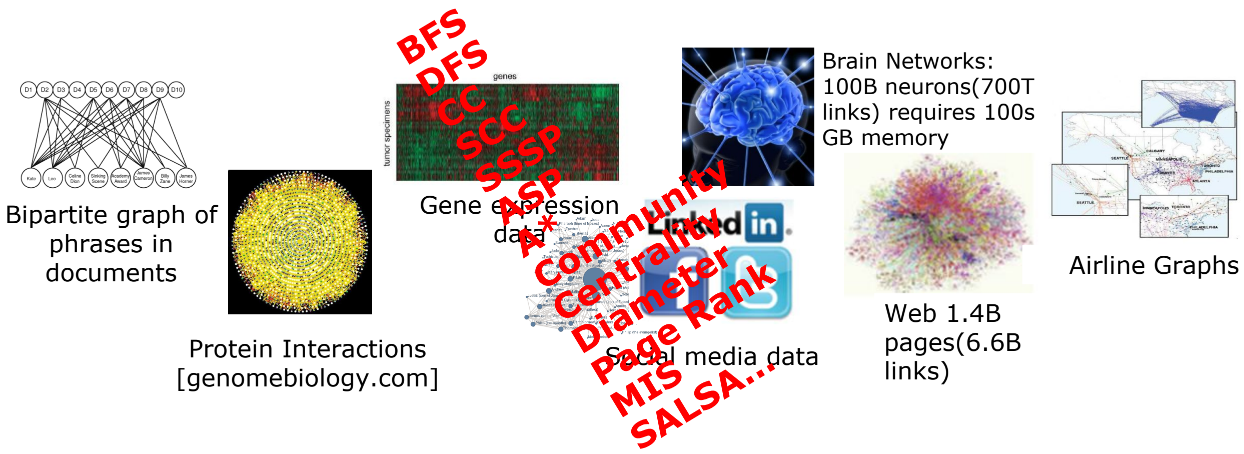
Emerging Massive-Scale Graph Data



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Graph Computation Challenges

1. Graph algorithms (BFS, Shortest path)
2. Query on connectivity (Triangle, Pattern)
3. Structure (Community, Centrality)
4. ML & Optimisation (Regression, SGD)

- Data driven computation: dictated by graph's structure and parallelism based on partitioning is difficult
- Poor locality: graph can represent relationships between irregular entries and access patterns tend to have little locality
- High data access to computation ratio: graph algorithms are often based on exploring graph structure leading to a large access rate to computation ratio

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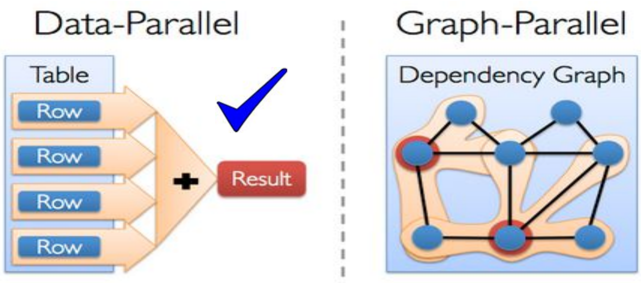
Data-Parallel vs. Graph-Parallel

- *Data-Parallel* for all? *Graph-Parallel* is hard!
  - Data-Parallel (sort/search - randomly split data to feed MapReduce)
  - Not every graph algorithm is parallelisable (interdependent computation)
  - Not much data access locality
  - High data access to computation ratio



Graph-Parallel

- Graph-Parallel (Graph Specific Data Parallel)
  - Vertex-based iterative computation model
  - Use of iterative Bulk Synchronous Parallel Model
    → Pregel (Google), Giraph (Apache), Graphlab, GraphChi (CMU - Dato)
  - Optimisation over data parallel
    → GraphX/Spark (U.C. Berkeley)
  - Data-flow programming – more general framework
    → NAIAD (MSR), TensorFlow…

Bulk synchronous parallel: Example

- Finding the largest value in a connected graph

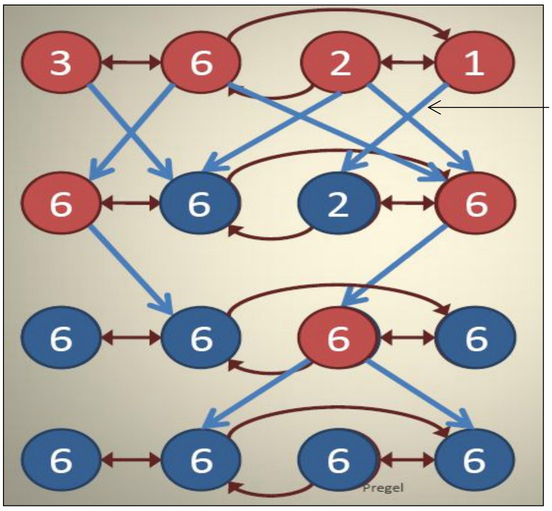
Local Computation

Communication

Local Computation

Communication

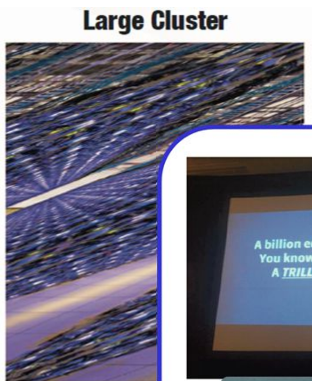
…



Message

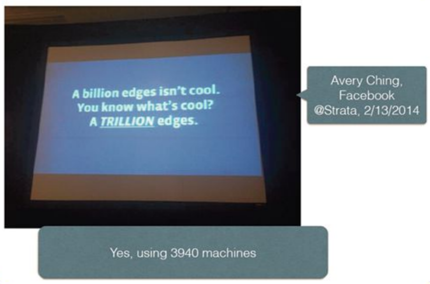
Are Large Clusters and Many cores Efficient?

- Brute force approach really efficiently works?
  - Increase of number of cores (including use of GPU)
  - Increase of nodes in clusters

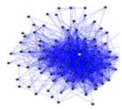


HPC/Graph500 benchmarks (June 2014)

Graph Edges	Hardware
1 trillion	Tsubame
1 trillion	Cray
1 trillion	Blue Gene
1 trillion	NEC



Do we really need large clusters?



- Laptops are sufficient?

Twenty pagerank iterations

System	cores	twitter_rv	uk_2007_05
Spark	128	857s	1759s
Giraph	128	596s	1235s
GraphLab	128	249s	833s
GraphX	128	419s	462s
Single thread	1	300s	651s

Label propagation to fixed-point (graph connectivity)

System	cores	twitter_rv	uk_2007_05
Spark	128	1784s	8000s+
Giraph	128	200s	8000s+
GraphLab	128	242s	714s
GraphX	128	251s	800s
Single thread	1	153s	417s

Fixed-point iteration: All vertices active in each iteration (50% computation, 50% communication)

Traversal: Search proceeds in a frontier (90% computation, 10% communication)

from Frank McSherry HotOS 2015

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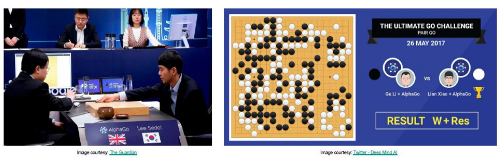
Data Processing Paradigm Change

- Emergence of modern Neural Networks Applications
- Practicalities of training Neural Networks
- Leveraging heterogeneous hardware
- Traditional dataflow programming does not deal with mathematical objects (no deep learning back then), ML application control flow requires to be numerically differentiable (i.e. TensorFlow)
- Now LLM, Agentic systems...

Image Classification

Reinforcement Learning



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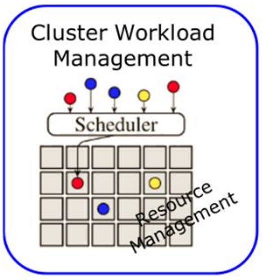
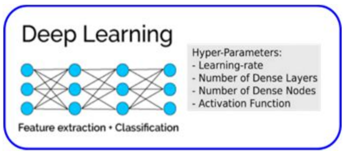
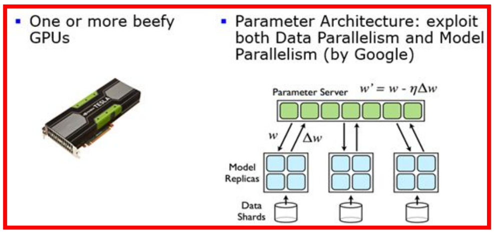
Tuning Computer Systems is Complex

- Complex and High Dimension Parameter Space
- Expensive Objective Functions
- Hand-crafted solutions impractical, often left static or configured through extensive offline analysis
- Not well-tuned system's performance does not scale

→ Necessity of scalable Auto-tuning



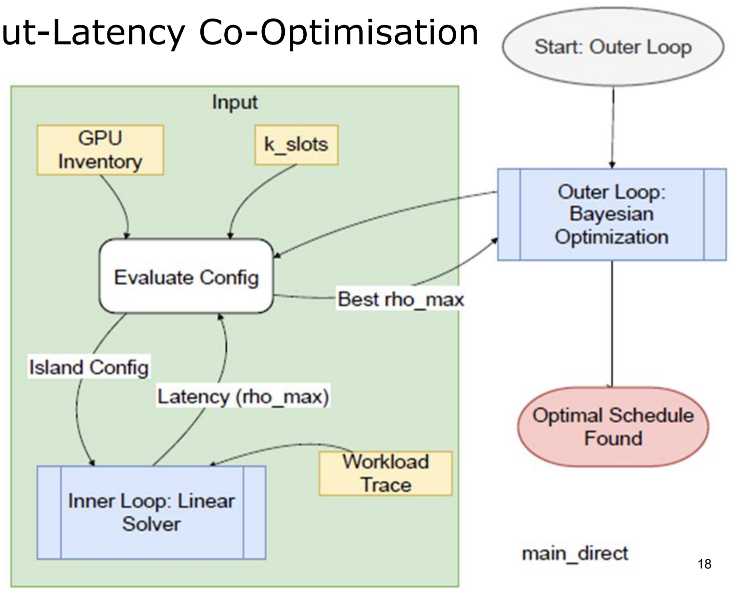




LLM Inference on heterogeneous GPU clusters

- Constrained Throughput-Latency Co-Optimisation

- Find optimal hardware configuration for lowest latency while guaranteeing a specific level of system performance (minimum throughput)
- Outer layer: GPU group
- Inner Layer: Linear Solver



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LLM Optimisation (from algorithms to system resources)

- Smaller LLMs
  - Quantization
  - Distillation
  - Low-Rank Adaptation
  - Weight Sharing
  - Sparse Matrices
  - Layer Dropping
  - Knowledge Transfer
  - Embedding Compression
  - Mixed Sparsity

- Inference Optimisation
  - KV-Caching
  - Speculative Decoding
  - Flash Attention
  - Paged Attention
  - Batch Inference
  - Early Exit Decoding
  - Parallel Decoding
  - Mixed Precision Inference
  - Quantized Kernels
  - Tensor Parallelism
  - Pipeline Parallelism
  - Sequence Parallelism
  - Graph Optimisation

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Challenging: High Performance Computer Systems

- How do we improve performance:
  - Manual tuning
  - Auto-tuning
- What is performance? – objective function of optimisation
  - Resource usage (e.g. time, power)
  - Computational properties (e.g. accuracy, fairness, latency)
  - Large number of parameters
  - Evaluation is slow and expensive
- What is Optimisation Model?
  - Short-term dynamic control (e.g. stream processing: distinct workload or dynamic workload)
  - Combinatorial optimisation (e.g. indexing DB, device assignment)
- Integrate power of Hardware (Accelerator, GPU..)

Many systems problems are combinatorial in nature

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Search Parameter Space

Random search: No risk of 'getting stuck' potentially many samples required

PetaBricks

Evolution strategies: Evaluate permutations against fitness function

Hill Climbing OpenTuner

SPEARMINT

Bayes Opt: Sample efficient, requires continuous function, some configuration

Random Search	Genetic algorithm / Simulated annealing	Bayesian Optimisation
No overhead	Slight overhead	High overhead
High #evaluation	Medium-high #evaluation	Low #evaluation

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Auto-tuning Complex Systems

- Many dimensions
- Expensive objective function
- Hand-crafted solutions impractical (e.g. extensive offline analysis)

Blackbox Optimisation

✓ can surpass human expert-level tuning

- Grid search θ ∈ [1, 2, 3, …]
- Evolutionary approaches (e.g. PetaBricks)
- Hill-climbing (e.g. OpenTuner)
- Bayesian optimisation (e.g. SPEARMINT)

1000s of evaluations of objective function

Computation more expensive

Fewer samples

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Optimisation: Iterative Operation

- Common to use an iterative global search algorithm for optimisation problem
- e.g. Bayesian optimisation algorithm that is capable of simultaneously approximating the target function that is being optimised while optimising it.
- Automated machine learning (AutoML) algorithms being used to choose an algorithm, an algorithm and hyperparameters, or data preparation, algorithm and hyperparameters, with very little user intervention

Machine Learning and Optimisation

- Function Optimisation
  - Find the set of inputs to a target objective function that result in the minimum or maximum of the function
- Function Approximation:
  - Generalise from specific examples to a reusable mapping function for making predictions on new examples
  - **ML can be described as function approximation as approximating the unknown underlying function that maps examples of inputs to outputs in order to make predictions on new data**
  - Function approximation often uses function optimisation
- At the core of many ML algorithms is an optimisation algorithm!

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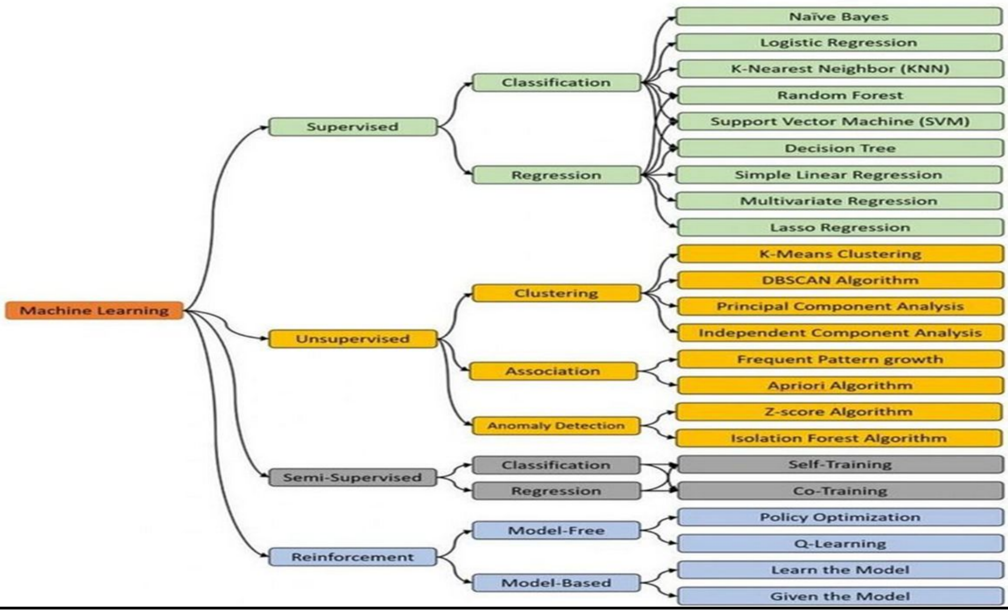
Examples of Machine Learning Algorithms…



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Machine Learning and Optimisation

- Process of working through a predictive modeling involves optimisation at multiple steps:
  - Choosing hyperparameters of a model
  - Choosing transformation to apply to the data prior to modeling
  - Choosing modeling pipeline to use as the final model
- Convert Optimisation Process to Learning
  - A numeric quantity must be predicted in the case of a regression problem, whereas a class label must be predicted in the case of a classification problem…
  - Exploit ML based optimisation practically

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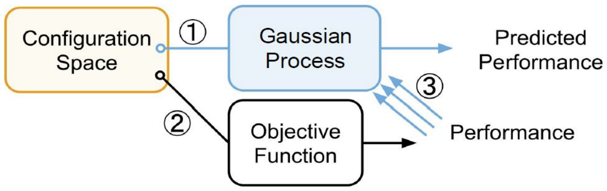
Bayesian Optimisation

- Iteratively builds probabilistic model of objective function
- Typically Gaussian process as probabilistic model
- Data efficient: converges quickly

Input: Objective function $f()$
Input: Surrogate function initial distribution G
Input: Acquisition function $a()$
for $i = 1, 2, \ldots$ **do**
  Sample point: $\boldsymbol{x}_t \leftarrow \arg\max_{\boldsymbol{x}} a(G, \boldsymbol{x})$
  Evaluate new point: $y_t \leftarrow f(\boldsymbol{x}_t)$
  Update surrogate distribution: $G \leftarrow G \mid (\boldsymbol{x}_t, y_t)$
end for



Pros:
✓ Data efficient: converges in few iterations
✓ Able to deal with noisy observations
Cons:
✗ In many dimensions, model does not converge to the objective function

① Find promising point (high performance value in the model)
② Evaluate the objective function at that point
③ Update the model to reflect this new measurement

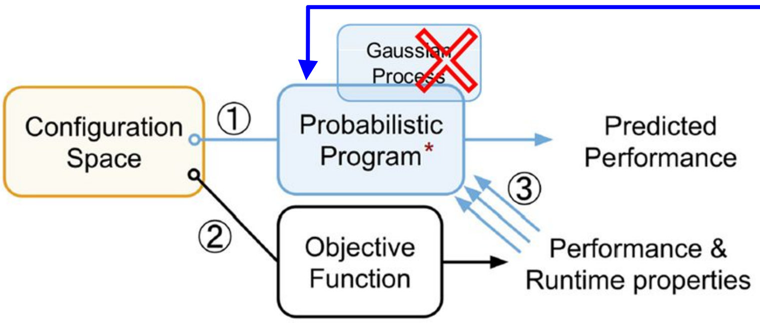
Surrogate Model in Bayesian Optimisation

Table 2.1: Comparison of surrogate models for BO

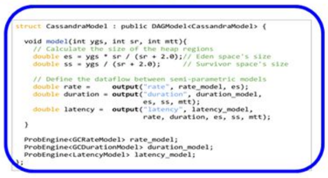
Model	Advantages	Disadvantages
Parametric models	• Quickly fit long-distance trends	• Require known structure of f
Gaussian processes	• Expressive • Flexible	• Fitting is $O(n^3)$ in train-data size • Continuous, non-hierarchical configuration space only
Tree-Parzen estimators	• Fitting is $O(n)$ in train-data size • Categorical and hierarchical configuration space supported	• Less sample efficient than GP
Random forests	• Computationally very cheap • Categorical and hierarchical configuration space supported	• Inaccurately extrapolates uncertainty

- Structural information (e.g. DAG model) improves Optimisation.

Structured Bayesian Optimisation (SBO)



Probabilistic Model written in Probabilistic C++



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

✓ Better convergence
✓ Use all measurements

BOAT: a framework to build **B**esp**O**ke **A**uto-**T**uners

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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. MCMC-based inference, Bayesian inference…)

Tutorial: Session 5 – Guest Lecture by Brooks Paige

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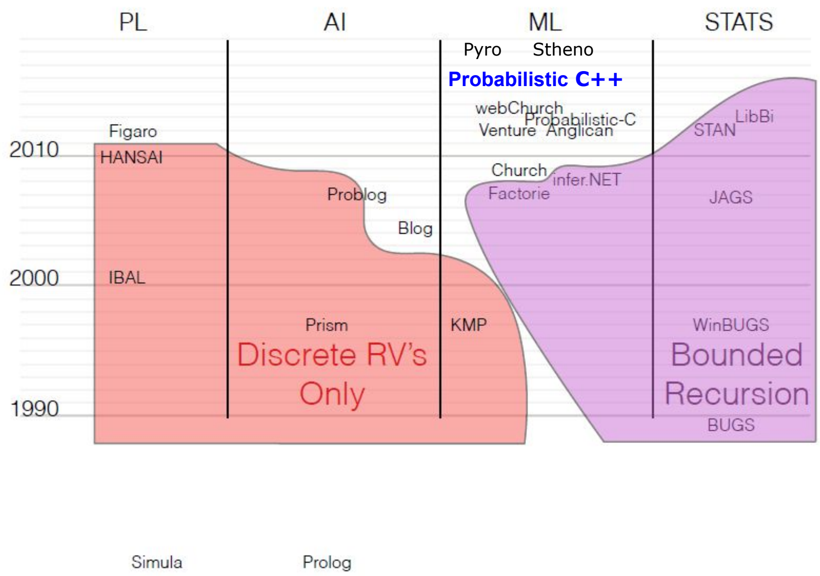
Probabilistic Programming: Probabilistic C++



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Example: JVM Garbage Collection

- Cassandra's garbage collection

Cassandra

JVM

Garbage collection flags:
- Young generation size
- Survivor ratio
- Max tenuring threshold

- Minimise 99th percentile latency of Cassandra

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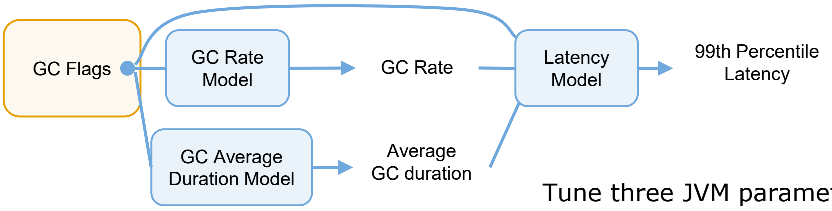
Performance Improvement from Structure

1. User-given probabilistic model structured in semi-parametric model using Directed Acyclic Graph

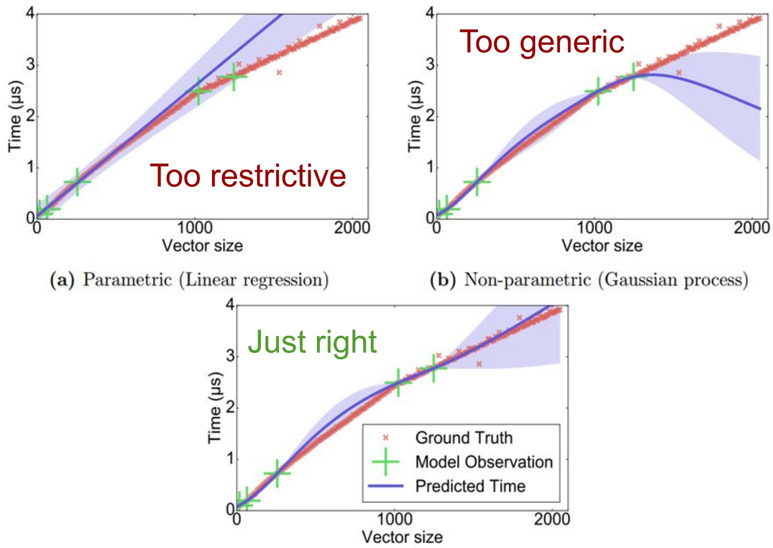


Tune three JVM parameters of database (Cassandra) to minimise latency

2. Sub-Optimisation in numerical optimisation
   - Exploit structure to split optimisation problem into smaller optimisations (e.g. nested optimisation)
   - Provide decomposition mechanisms

Semi-parametric Model

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



(a) Parametric (Linear regression)
(b) Non-parametric (Gaussian process)
(c) Semi-parametric (Combination)

DAG model in BOAT

```
struct CassandraModel : public DAGModel<CassandraModel> {

  void model(int ygs, int sr, int mtt){
    // Calculate the size of the heap regions
    double es = ygs * sr / (sr + 2.0);// Eden space's size
    double ss = ygs / (sr + 2.0);      // Survivor space's size

    // Define the dataflow between semi-parametric models
    double rate =     output("rate", rate_model, es);
    double duration = output("duration", duration_model,
                             es, ss, mtt);
    double latency =  output("latency", latency_model,
                             rate, duration, es, ss, mtt);
  }

  ProbEngine<GCRateModel> rate_model;
  ProbEngine<GCDurationModel> duration_model;
  ProbEngine<LatencyModel> latency_model;
};
```

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GC Rate Semi-parametric model

```
struct GCRateModel : public SemiParametricModel<GCRateModel> {

  GCRateModel() {
    allocated_mbs_per_sec =
     std::uniform_real_distribution<>(0.0, 5000.0)(generator);
    // set the GP parameters here
  }

  double parametric(double eden_size) const {
    // Model the rate as inversely proportional to Eden's size
    return allocated_mbs_per_sec / eden_size;
  }

  double allocated_mbs_per_sec;
};
```

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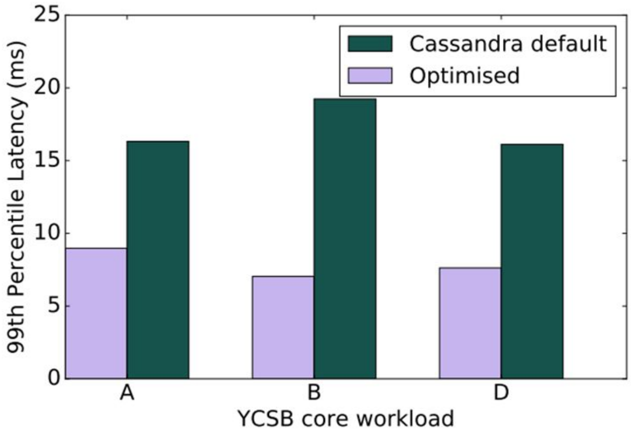
Evaluation: Garbage collection



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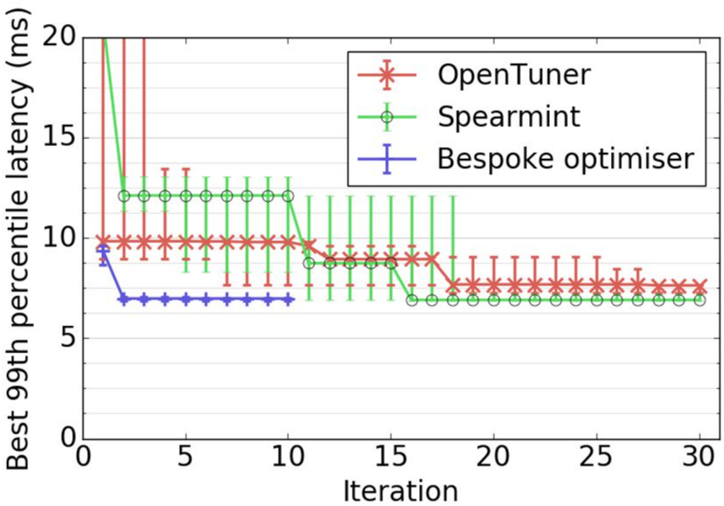
Evaluation: Garbage collection



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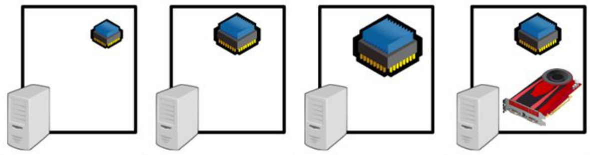
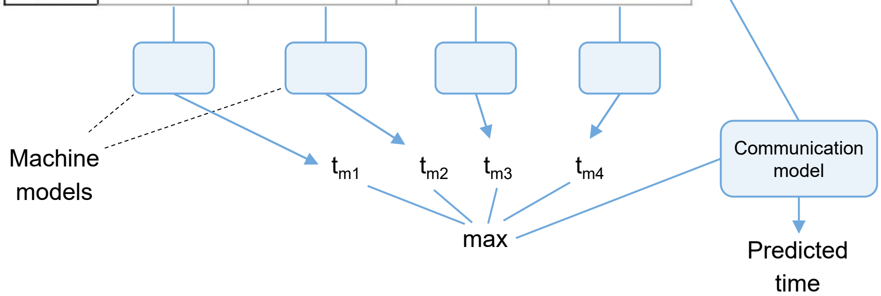
Evaluation: Neural networks (SGD) scheduling



Parameter server	✗	✗	✓	✓
Worker	✗	✓	✓	✓
# Inputs	0	10	16	10 - 28



Load balancing, worker allocation over 10 machines = **~30 parameters**

Use TensorFlow

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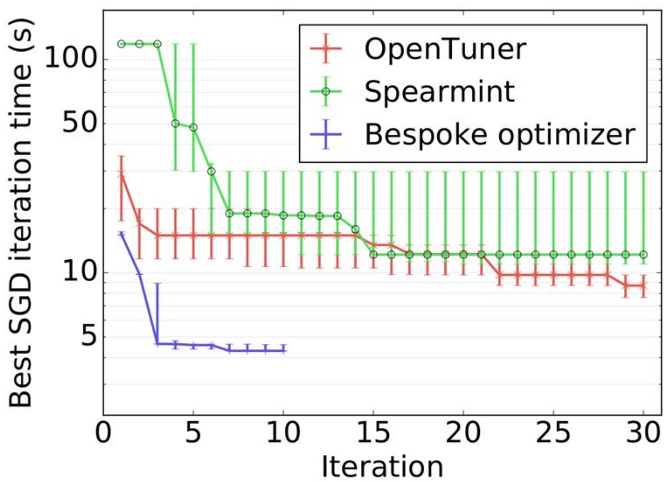
Evaluation: Neural network scheduling



Default configuration: 9.82s
OpenTuner: 8.71s
BOAT: **4.31s**

Existing systems don't converge!

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Further Bayesian Optimisation…

- BO overview/Tutorial
  - https://www.cl.cam.ac.uk/~ey204/teaching/ACS/R244_2024_2025/aid/BO_overview_Archambeau.pdf
  - https://www.cl.cam.ac.uk/~ey204/teaching/ACS/R244_2024_2025/aid/BO_overview_adams.pdf
  - https://www.cl.cam.ac.uk/~ey204/teaching/ACS/R244_2024_2025/aid/BO_overview_gonzalez.pdf
- BO tool with structural information
  - Capable to embed structural information to surrogate model (e.g. BoTorch)
- Papers
  - Review paper by Shahriari, et al. (2016): Taking the Human Out of the Loop: A Review of Bayesian Optimization. Proceedings of the IEEE 104(1):148-175, 2016.
  - Slides by Ryan Adams (2014): A Tutorial on Bayesian Optimization for Machine Learning. CIFAR NCAP Summer School.
  - Slides by Peter Frazier (2010): Tutorial: Bayesian Methods for Global and Simulation Optimization. INFORMS Annual Meeting.

Auto-Tuning

- Manual Tuning
  - User to learn expert knowledge and not transferable
  - e.g. Ottertune (manually selects limited number of parameters then use BO)
- Automated Tuning
  - Divide-and-diverge sampling to explore the configuration space
  - For example, BO uses Gaussian processes, but it struggles to make accurate performance predictions because of high dimensionality

→Generic Auto-Tuning with DAG models

  - Use of DAG models for surrogate model, which mitigates the curse of dimensionality while also retaining all configurable variables
  - Exploit data analysis to identify parameter dependencies
  - Automatic building of DAG models: use of Bayesian Networks

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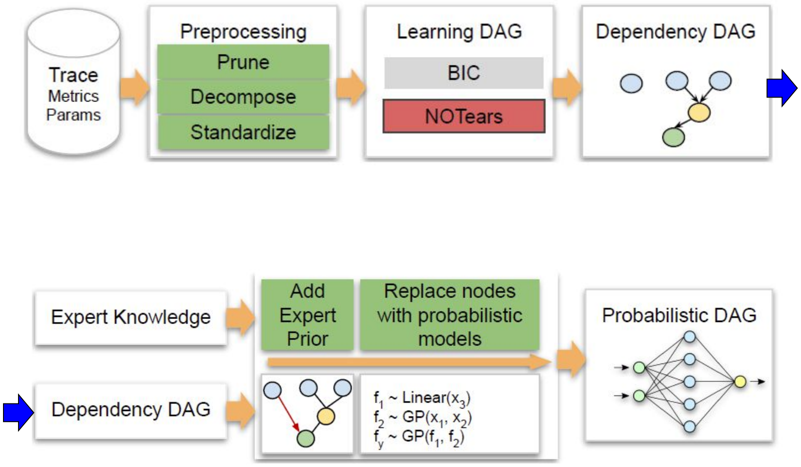
Automation of DAG model building



- System’s inherent structure builds dependency graphs
- Decomposability allows tuning a larger number of parameters, providing interpretable optimisation suggestions
- Natural way to encode expert knowledge in its graph

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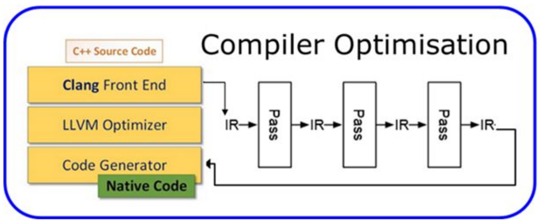
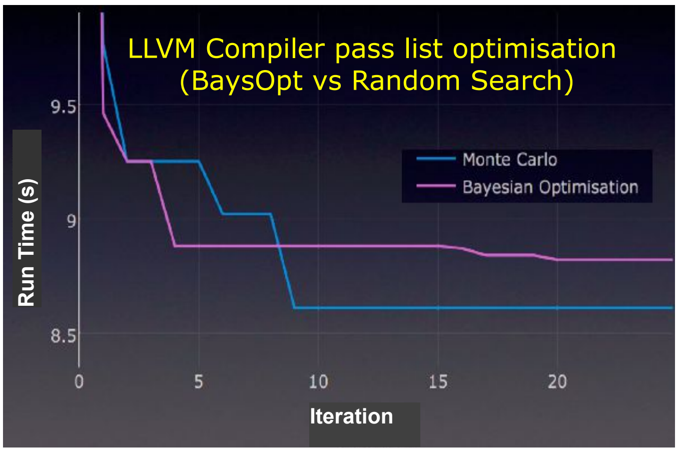
Bayesian Optimisation not for Combinatorial Model





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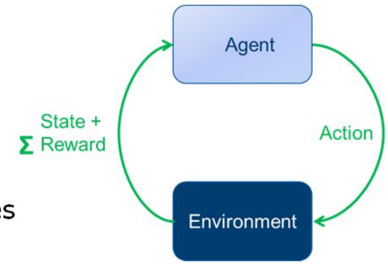
Reinforcement Learning in Computer Systems

- Agent interacts with Dynamic environment
- Goal: Maximise expectations over rewards in 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



Practical Consideration:

- Action spaces do not scale
- Exploration in production system not a good idea
- Simulations can oversimplify problem (Expensive to build)
- Online steps take too long

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Reinforcement Learning for Optimisation

Many problems in systems are sequential Decision Making and/or Combinatorial Problems on graph data

- Compiler Optimisation
  - Input: XLA/HLO graph
  - Objective: Scheduling fusion of ops
- Chip placement
  - Input: Chip netlist graph
  - Objective: placement on 2D of ND grids
- Datacentre resource allocation
  - Input: job - workload graph
  - Objective: Placement on datacentre cells and racks
- Packet Classification
  - Input: network packets
  - Objective: minimise the classification time and memory footprint
- Network congestion control with multiple connections
- Wide range of signals to make decisions (e.g., VM allocation)
- Database: Query optimiser, Dynamic indexing…

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A brief history of Deep RL software

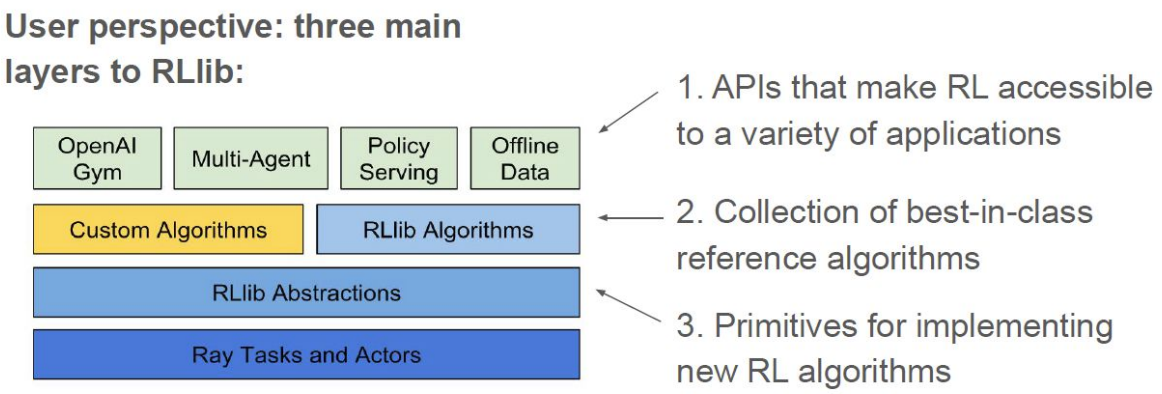
1. Gen (2014-16): Loose research scripts (e.g. DQN), high expertise required, only specific simulators

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

- Good results on some environments (e.g. game), difficult to retool to new domains and execution modes
- Abstractions/Libraries: Not fully reusable, customised towards game simulators, execution coupled with algorithms
- High implementation risk: Lack of systematic testing, performance strongly impacted by noisy heuristics

3. Gen (2017-): Generic declarative APIs, distributed abstractions (Ray Rllib…Coach, Tunic?), some standard *flavours* emerge

RLlib (UC Berkeley) Architecture



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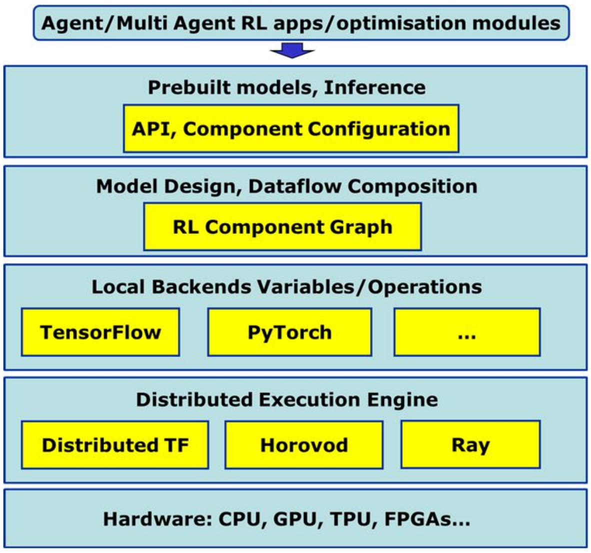
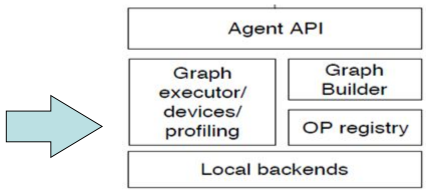
RLgraph: Modular Dataflow Composition





- ... is a programming model to design and execute RL algorithms across execution paradigms
- ... generates incrementally testable, transparently configurable code through a staged build process

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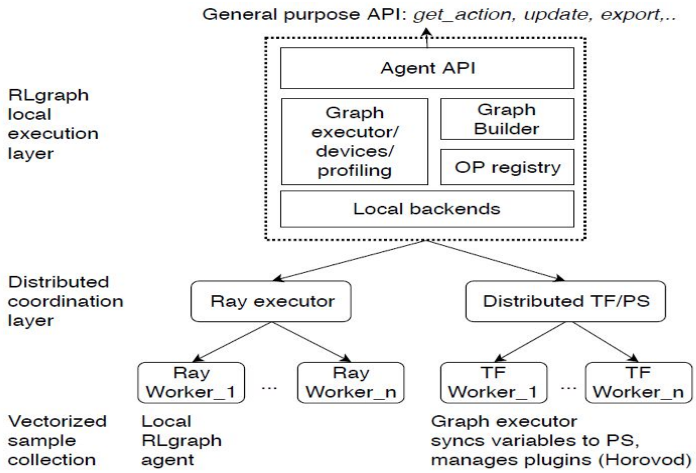
RLGraph: Separate Local and Distributed Execution

- High performance RL computation graphs for RL with different distributed backends



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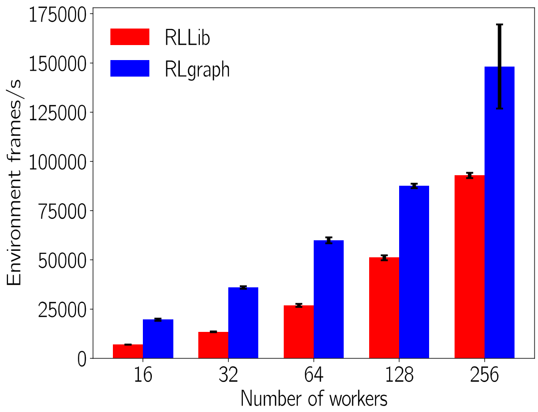
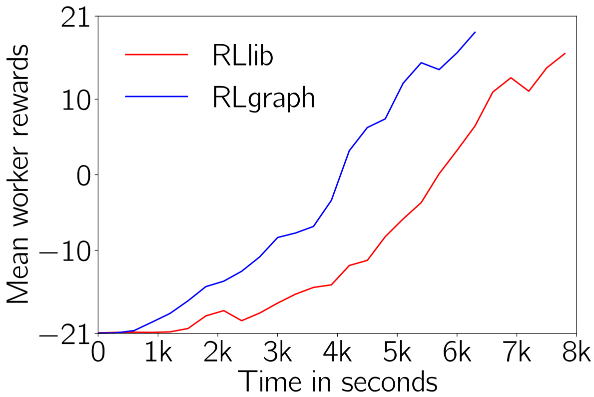
Performance on Apex (Distributed Q-Learning)



Distributed sample performance

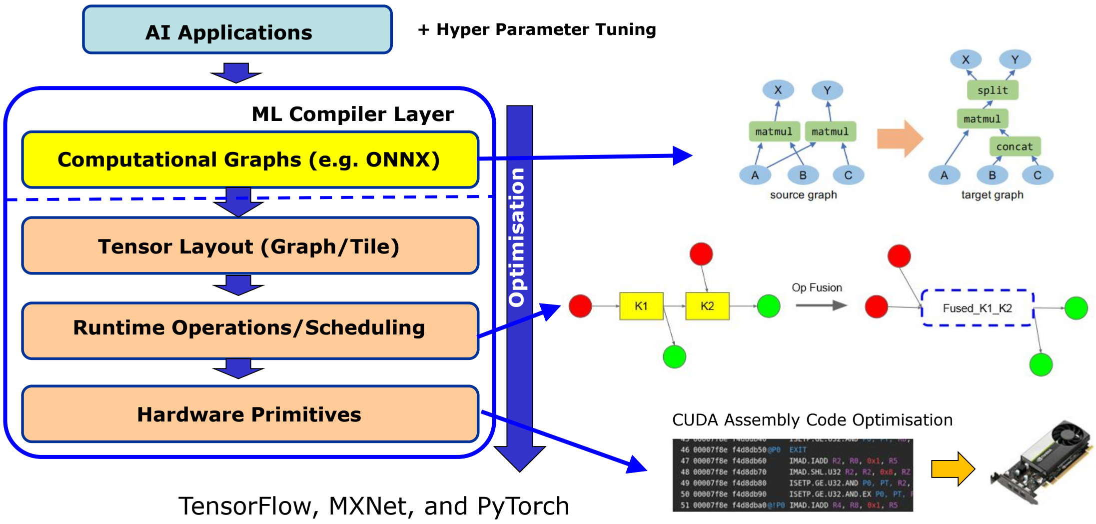


Time to solve Pong (Score ~21)

ML Compiler Challenges

- Fast tensor operation capable compilers: Complex optimisation plays a crucial role for LLM processing
  - Use of ML to optimise ML Compiler
  - Superoptimisation: Deal with massive parameter space
    → use of Equality Saturation (ES), MCTS
    → use of reinforcement Learning
  - Many compiler optimisations are phase ordering problem
- Challenge to bridge the gap between ML models and HW
- Existing ML Compiler
  - Apache TVM
  - NVIDIA TensorRT - CuDNN
  - ONNX runtime
  - LLVM
  - Google MLIR
  - TensorFlow XLA
  - Meta Glow
  - PyTorch nvFuser
  - INTEL pLAIDml
  - Open VINO

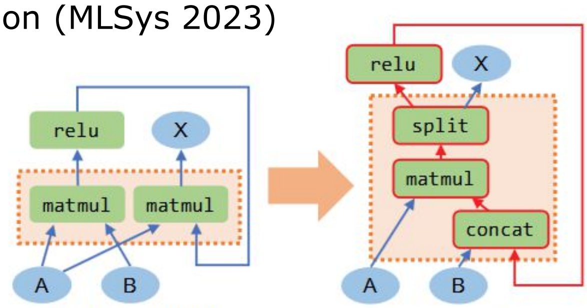
ML Compiler Optimisation



See ML Compiler Tutorial: https://mlc.ai/summer22/schedule
Also Survey: https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=9222299

Optimising DNN Computation with Graph Substitutions

- TASO (SOSP, 2019): Performance improvement by transformation of computation graphs
- PET (OSDI, 2021): Optimizing Tensor Programs with Partially Equivalent Transformations and Automated Corrections
- Equality Saturation for Tensor Graph Superoptimization (MLSys 2021)
- X-RLflow: Graph Reinforcement Learning for Neural Network Subgraph Transformation (MLSys 2023)



(a) before substitution (b) after substitution

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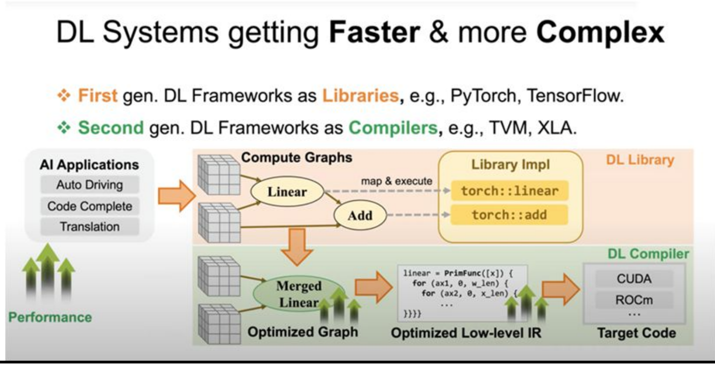
TVM: Deep Learning Compiler

- TVM: end-to-end deep learning compilers
- Operator/expression-level optimisation operates on Tensor Operation Abstraction(TIR)
- Core: Optimising programs through a sequence of transformation
- Automatic optimisation



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CuAsmRL: Optimising CUDA GPU SASS schedules

- Optimising GPU SASS schedules via Deep RL

CUDA kernels compilation pipeline:

C++/CUDA → PTX → SASS → Cubin

SASS: GPU native instructions. GPU architectures-dependent. (SIP optimizes at this level)

- Search space:
  - Original: full permutation of instructions; computationally intractable
  - Pruning: only global read and write memory instructions, e.g. LDG, STG etc.
- Mutation:
  - Randomly select an instruction and reorder an instruction above or below
- Feedback signal:
  - Assemble the mutated SASS and run on GPUs

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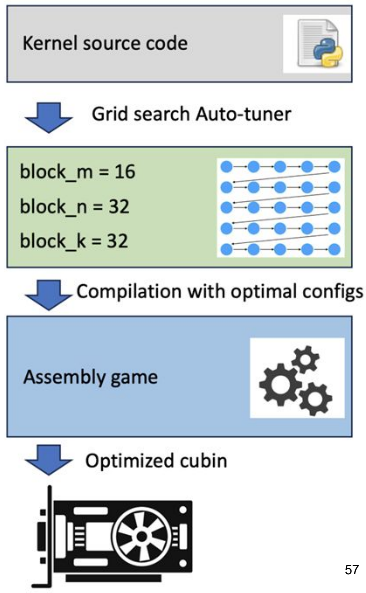
CuAsmRL: Optimising CUDA GPU SASS schedules

- Apply all possible high-level optimisation by reusing compilation pipeline
- Search for optimal schedules by playing the assembly game
  - Each memory instruction can be swapped with the instruction up and down
  - Positive reward is given if the action reduce runtime
  - Iterative optimisation



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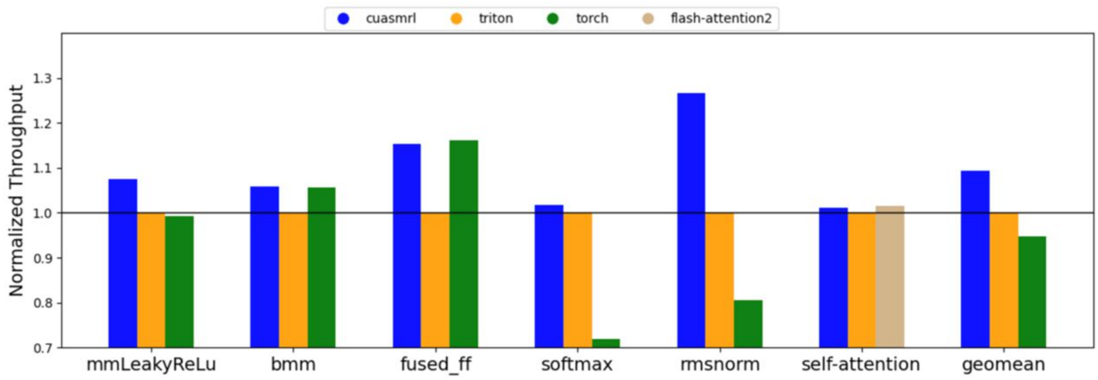
CuAsmRL: Optimising CUDA GPU SASS schedules

- Kernel Throughput



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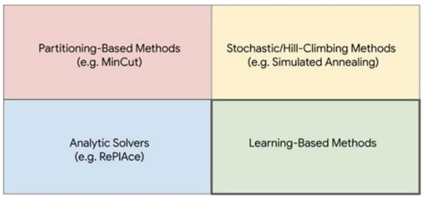
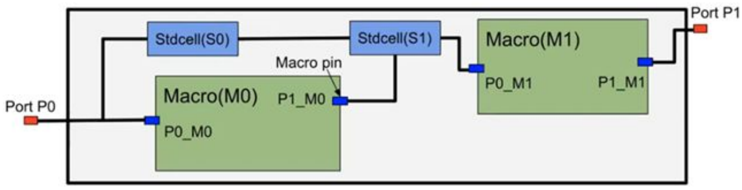
Chip Placement with Reinforcement Learning

- A. Mirhoseini and A. Goldie: A graph placement methodology for fast chip design, Nature, 2021.



- A form of graph resource optimization
- Place the chip components to minimize the latency of computation, power consumption, chip area and cost, while adhering to constraints, such as congestion, cell utilization, heat profile, etc.



Reinforcement Learning for Optimisation

Many problems in systems are sequential decision making and/or combinatorial problems

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- Chip placement
- Datacentre resource allocation
- Network congestion control with multiple connections
- Wide range of signals to make decisions (e.g., VM allocation)
- Database: Query optimiser, Dynamic indexing…
- Emerging Agentic RL…

Summary: Massive Data Processing and Optimisation

→Dataflow is key element used in optimisation

→Parameter space is complex, large and dynamic/combinatorial

- Systems are nonlinear and difficult to model manually → Exploit ML
- Reinforcement Learning to optimise dynamic combinatorial problem
- Key concept behind is Dataflow (~=Computational Graph) structural transformation/Decomposition

→Exploit structural information for model decomposition to accelerate optimisation process and/or transform the structure

→Bayesian Optimisation and Reinforcement Learning are key

→Other ML algorithms would be potentially useful…

Course Schedule

https://www.cl.cam.ac.uk/~ey204/teaching/ACS/R244_2025_2026

Session 1: Introduction

Session 2: Data Flow Programming: Map/Reduce to TensorFlow to ML

Session 3: Hands-on Tutorial: Data Flow Programing

Session 4: Large-scale Graph Data Processing / Search Space

Session 5: Probabilistic Programming + BO : Guest lecture (Brooks Paige)

Session 6: Optimisation of Computer Systems

Session 7: Optimisation in ML Compiler (Superoptimisation…)

Session 8: Project Study Presentation