Architecture of ML Systems
01 Introduction and Overview

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Agenda

- Motivation and Goals
- Data Management Group
- Course Organization
- Course Outline and Projects
- Overview Apache SystemML
Motivation and Goals
Example ML Applications (Past)

- **Transportation / Space**
  - Lemon car detection and reacquisition (classification, seq. mining)
  - Airport passenger flows from WiFi data (time series forecasting)
  - Satellite sensor analytics (regression and correlation)

- **Finance**
  - Water cost index based on various influencing factors (regression)
  - Insurance claim cost per customer (model selection, regression)
  - Financial analysts survey correlation (bivariate stats w/ new tests)

- **Health Care**
  - Breast cancer cell grow from histopathology images (classification)
  - Glucose trends and warnings (clustering, classification)
  - Emergency room diagnosis / patient similarity (classification, clustering)
  - Patient survival analysis and prediction (Cox regression, Kaplan-Meier)
A Car Reacquisition Scenario

Motivation and Goals

- Warranty Claims
- Repair History
- Diagnostic Readouts

Features | Labels
--- | ---

- Machine Learning Algorithm
- Algorithm
- Algorithm
- Algorithm

- Class skew
- Low precision

+ custom loss functions
+ hyper-parameter tuning

→ 25x improved accuracy
Example ML Applications (Past), cont.

- **Other Domains**
  - **Machine data: errors and correlation** (bivariate stats, seq. mining)
  - Smart grid: energy demand/RES supply, weather models (forecasting)
  - Visualization: dimensionality reduction into 2D (auto encoder)

- **Information Extraction**
  - **NLP contracts → rights/obligations** (classification, error analysis)
  - **PDF table recognition and extraction** (NMF clustering, custom)
  - OCR: optical character recognition (preprocessing, classification)

- **Algorithm Research** (+ various state-of-the-art algorithms)
  - **User/product recommendations** via various forms of NMF
  - Localized, supervised metric learning (dim reduction and classification)
  - Learning word embeddings via orthogonalized skip-gram
  - Learning first-order rules for explainable classification
What is an ML System?

**ML Applications**
(Entire KDD/DS lifecycle)

- Statistics
- Data Mining
- Machine Learning (ML)

**Runtime Techniques**
(Execution, Data Access)

- Distributed Systems
- Data Management
- Operating Systems

**Rapidly Evolving**

- Classification
- Regression
- Recommenders
- Clustering
- Assoc. Rules
- Dim Reduction

- Hardware Architecture
- Accelerators

**Compilation Techniques**

- HPC
- Prog. Language Compilers
What is an ML System?

- **ML System**
  - **Narrow focus**: SW system that executes ML applications
  - **Broad focus**: Entire system (HW, compiler/runtime, ML application)
  - Trade-off **runtime/resources** vs **accuracy**
  - Early days: no standardizations, lots of different languages and system architectures, but many shared concepts

- **Course Objectives:**
  - Architecture and internals of modern (large-scale) ML systems
  - #1 Understanding of characteristics → better evaluation / usage
  - #2 Understanding of effective techniques → build/extend ML systems
Data Management Group
About Me

- **09/2018 TU Graz, Austria**
  - BMVIT endowed chair for data management
  - *Data management for data science*  
    (ML systems internals, end-to-end data science lifecycle)

- **2012-2018 IBM Research – Almaden, USA**
  - Declarative large-scale machine learning
  - Optimizer and runtime of *Apache SystemML*

- **2011 PhD TU Dresden, Germany**
  - Cost-based optimization of integration flows
  - Systems support for time series forecasting
  - In-memory indexing and query processing

https://github.com/tugraz-isds/systemds
Data Management Courses

- **SS: Databases / Databases 1 (DM)**
  - Data management from user/application perspective
  - VU 1.5/1.5 (4 ECTS), and VU 1/1 (3 ECTS)

- **SS: Architecture of ML Systems (AMLS)**
  - Internals of machine learning systems
  - VU 2/1 (5 ECTS), master, [github.com/tugraz-isds/systemds](https://github.com/tugraz-isds/systemds)

- **WS: Data Integration and Large-Scale Analysis (DIA)**
  - Distributed data and information systems
  - VU 2/1 (5 ECTS), bachelor/master

- **WS: Architecture of Database Systems (ADBS)**
  - Internals of database management systems
  - VU 2/1 (5 ECTS), master
Course Organization
Basic Course Organization

- **Staff**
  - Lecturer: Univ.-Prof. Dr.-Ing. Matthias Boehm, ISDS
  - Assistant: M. Tech. Arnab Phani, ISDS

- **Language**
  - Lectures and slides: **English**
  - Communication and examination: **English/German**

- **Course Format**
  - VU 2/1, **5 ECTS** (2x 1.5 ECTS + 1x 2 ECTS), master only
  - Weekly lectures (**start 12.15pm**, including **Q&A**), attendance optional
  - Mandatory programming project (2 ECTS)
  - **Recommended papers** for additional reading on your own
Course Logistics

- **Exam**
  - **Completed project** (merged PRs and project presentation)
  - **Final oral exam** (by appointment)
  - **Grading** (40% project, 60% exam)

- **Communication**
  - **Informal language** (first name is fine)
  - Please, **immediate feedback** (unclear content, missing background)
  - Newsgroup: [news://news.tugraz.at/tu-graz.lv.aml](news://news.tugraz.at/tu-graz.lv.aml) (email for private issues)
  - Office hours: by appointment or after lecture

- **Website**
  - [https://mboehm7.github.io/teaching/ss19_aml/index.htm](https://mboehm7.github.io/teaching/ss19_aml/index.htm)
  - All course material (lecture slides, list of projects) and dates
Course Organization

Course Logistics, cont.

- **Open Source Projects**
  - Programming project in context of open source projects
    - SystemDS: [https://github.com/tugraz-isds/systemds](https://github.com/tugraz-isds/systemds)
    - SystemML: [https://github.com/apache/systemml](https://github.com/apache/systemml)
  - Other open source projects possible, **but harder to merge PRs**
  - Commitment to **open source and open communication** (discussion on PRs, mailing list, etc)
  - **Remark**: Don’t be afraid to ask questions / develop code in public
Course Outline
Part A-C: Architecture, Compiler, Runtime

A: Introduction

- 01 Introduction and Overview [Mar 15]
- 02 Languages, Architectures, and System Landscape [Mar 22]

B: Rewrites and Optimization

- 03 Size Inference, Rewrites, and Operator Selection [Mar 29]
- 04 Operator Fusion and Runtime Adaptation [Apr 05]

C: Execution Strategies

- 05 Data- and Task-Parallel Execution [Apr 12]
- 06 Parameter Servers [May 03]
- 07 Hybrid Execution and HW Accelerators [May 10]
Part D-F: Data Access and ML Lifecycle

D: Data Storage and Access
- 08 Formats, Caching, Partitioning, and Indexing [May 17]
- 09 Lossy and Lossless Compression [May 24]

E: ML Lifecycle Systems
- 10 Data Acquisition, Cleaning, and Preparation [Jun 07]
- 11 Model Selection and Management [Jun 14]
- 12 Model Deployment and Serving [Jun 21]

F: Wrap-Up
- 14 Project Presentations, Conclusions, Q&A [Jun 28]
Project Overview

- Team
  - Individuals or two-person teams (w/ clearly separated responsibilities)

- Objectives
  - Non-trivial feature in an open source ML system (2 ECTS → 50 hours)
  - OSS processes: Break down into 3-7 tasks, code/tests/docs, PR per task, code review, incorporate review comments, etc

- Target Systems
  - Preferred: SystemDS, or Apache SystemML
  - Other options: Julia, TensorFlow, PyTorch, <your_favorite_project>

- Timeline
  - Mar 22: List of projects and discussions
  - Apr 05: Project selection
  - Last lecture: 5-10min project presentation, including demo!
Example Projects

- **#1: Auto Differentiation**
  - Implement auto differentiation for deep neural networks
  - Integrate auto differentiation framework in compiler or runtime

- **#2: Sparsity-Aware Optimization of Matrix Product Chains**
  - Integrate sparsity estimators into DP algorithm
  - Extend DP algorithm for DAGs and other operations

- **#3 Parameter Server Update Schemes**
  - New PS update schemes: e.g., stale-synchronous, Hogwild!
  - Language and local/distributed runtime extensions

- **#4 Extended I/O Framework for Other Formats**
  - Implement local readers/writers for NetCDF, HDF5, libsvm, and/or Arrow

- **#5: LLVM Code Generator**
  - Extend codegen framework by LLVM code generator
  - Native vector library, native operator skeletons, JNI bridge
Overview Apache SystemML

Declarative Large-Scale Machine Learning
Common Large-Scale ML Challenges

- **#1 Custom ML Algorithms**
  - Huge diversity of existing ML algorithms
  - Cutting- / bleeding-edge algorithms
  - Domain-specific extensions init/loss

Overview Apache SystemML

Data Scientist → Systems Programmer → Dist. Prog. → Spark

- Hinders quick iteration
- NeurIPS, ICLR, ICML, KDD, JMLR
Common Large-Scale ML Challenges

- **#1 Custom ML Algorithms**
  - Huge diversity of existing ML algorithms
  - Cutting- / bleeding-edge algorithms
  - Domain-specific extensions init/loss

- **#2 Changing Environment**
  - Sample vs large-scale datasets (data size)
  - Dense/sparse, #features (data characteristics)
  - Single-node vs cluster (cluster characteristics)

- **#3 Integration and Deployment**
  - Data preparation and feature engineering
  - Batch and mini-batch training/scoring
  - Low-latency scoring (streaming)
  - Scale-up, scale-out, GPUs (hardware)

“Hellerstein’s Inequality”

\[
\frac{\Delta_{\text{env}}}{\Delta t} \gg \frac{\Delta_{\text{app}}}{\Delta t}
\]
Apache SystemML

- **05/2017** Apache Top-Level Project
- **11/2015** Apache Incubator Project
- **08/2015** Open Source Release
- **01/2012** Integration in IBM BigInsights
- **01/2010** Project Kickoff

Data Scientist → R / Python → SystemML → Spark
Example: Linear Regression Conjugate Gradient

Note:
#1 Data Independence
#2 Implementation-Agnostic Operations

1: X = read($1); # n x m matrix
2: y = read($2); # n x 1 vector
3: maxi = 50; lambda = 0.001;
4: intercept = $3;
5: ...
6: r = -(t(X) %*% y);
7: norm_r2 = sum(r * r); p = -r;
8: w = matrix(0, ncol(X), 1); i = 0;
9: while(i<maxi & norm_r2>norm_r2_trgt)
10: {
11:   q = (t(X) %*% (X %*% p)) + lambda*p;
12:   alpha = norm_r2 / sum(p * q);
13:   w = w + alpha * p;
14:   old_norm_r2 = norm_r2;
15:   r = r + alpha * q;
16:   norm_r2 = sum(r * r);
17:   beta = norm_r2 / old_norm_r2;
18:   p = -r + beta * p; i = i + 1;
19: }
20: write(w, $4, format="text");
**High-Level SystemML Architecture**

- **APIS:** Command line, JMLC, Spark MLContext, Spark ML, (20+ scalable algorithms)
- **DML Scripts**
- **Language**
- **Compiler**
- **Runtime**
- **In-Memory Single Node** (scale-up)
- **Hadoop or Spark Cluster** (scale-out)

**APIs and Literature:***
- [SIGMOD’15,’17,’19]
- [PVLDB’14,’16a,’16b,’18]
- [ICDE’11,’12,’15]
- [CIDR’17]
- [VLDBJ’18]
- [DEBull’14]
- [PPoPP’15]

**In-Progress:**
- GPU

**Timeline:**
- 05/2017 Apache Top-Level Project
- 11/2015 Apache Incubator Project
- 08/2015 Open Source Release
Overview Apache SystemML

Basic HOP and LOP DAG Compilation

LinregDS (Direct Solve)

X = read($1);
y = read($2);
intercept = $3;
lambda = 0.001;
...

if( intercept == 1 ) {
    ones = matrix(1, nrow(X), 1);
    X = append(X, ones);
}

I = matrix(1, ncol(X), 1);
A = t(X) %*% X + diag(I)*lambda;
b = t(X) %*% y;
beta = solve(A, b);
...
write(bbeta, $4);

HOP DAG (after rewrites)

Scenario:
X: $10^8 \times 10^3, 10^{11}$
y: $10^8 \times 1, 10^8$

Cluster Config:
- driver mem: 20 GB
- exec mem: 60 GB

Distributed Matrices
- Fixed-size (squared) matrix blocks
- Data-parallel operations

Hybrid Runtime Plans:
- Size propagation / memory estimates
- Integrated CP / Spark runtime
- Dynamic recompilation during runtime

LOP DAG (after rewrites)
Static and Dynamic Rewrites

- **Example Static Rewrites** (size-indep.)
  - Common Subexpression Elimination
  - Constant Folding / Branch Removal / Block Sequence Merge
  - **Static Simplification Rewrites**
    - Right/Left Indexing Vectorization
    - For Loop Vectorization
    - Spark checkpoint/repartition injection

- **Example Dynamic Rewrites** (size-dep.)
  - **Dynamic Simplification Rewrites**
  - **Matrix Mult Chain Optimization**

\[
\text{trace}(X\%\%Y) \rightarrow \sum(X\ast t(Y))
\]

\[
\begin{align*}
O(n^3) & \quad Y \\
X & \quad \rightarrow \\
O(n^2) & \\
\end{align*}
\]

\[
\begin{align*}
\sum(\lambda \ast X) & \rightarrow \lambda \ast \sum(X) \\
\sum(X+Y) & \rightarrow \sum(X)+\sum(Y)
\end{align*}
\]

- \(2,002\) MFLOPs
- \(4\) MFLOPs

Size propagation and sparsity estimation
Selected Research Results

- **#1 SystemML’s Optimizer**
  - rewrites, operator selection, size propagation, memory estimates, dynamic recompilation (DEBull’14)

- **#2 Task-Parallel Parfor Loops**
  - hybrid parallelization strategies (PVLDB’14)

- **#3 Resource Optimization**
  - for automatic resource provisioning (SIGMOD’15)

- **#4 Compressed Linear Algebra**
  - (PVLDB’16, SIGMOD Record’17, VLDB Journal’18, CACM’19)

- **#5 Optimizing Operator Fusion Plans**
  - (PPoPP’15, CIDR’17, PVLDB’18)

- **#6 Advanced Optimization**
  - sum-product (CIDR’17), sparsity estimation (SIGMOD’19)
  - GPU, meta learning, numerical stability, parameter servers, etc
Lessons on Declarative Specification

- **L1: Importance of Data Independence and Logical Operations**
  - Protection of investments (adaptation to changing technology stack)
  - Simplification of development (especially libs) and deployment
  - Adaptation to data/cluster characteristics, **but** harder to optimize
  - Allows optimizations such as resource op, compression and fusion

- **L2: User Categories** (|Alg. Users| >> |Alg. Developers|)
  - Algorithm developers/researchers → Linear algebra
  - Algorithm users → ML libraries
  - Domain experts → ML tasks / AutoML

- **L3: Importance of Real Applications and Users**
  - Language for ML is wild west, **no standards** (PMML, PFA, ONNX)
  - Unseen data and algorithm characteristics
  - Source of new APIs, features and optimizations
  - Variety of apps / use cases → **balance generality / specialization**
Lessons on Data Model

- **L4: Diversity** of ML Algorithms / Applications
  - Broad range of algorithms (stats, ML, 2\textsuperscript{nd}-order optim)
  - Model choice often a **cost-benefit tradeoff**
  - Complex ML applications (rules, models, etc)
  - Opportunities of **data programming and augmentation**

- **L5: Users want Consolidated Lifecycle / Structured Data**
  - **Boundary crossing** for data integration, cleaning, feature engineering, training, and scoring is obstacle
  - Heterogeneous input/output data, with **structure**
  - Poor support for **provenance and model versioning**
  - APIs for embedded, low-latency scoring

- **L6: Data Model very Difficult to Change**
  - Internal format extensions (e.g., dense/sparse, type) are major efforts
  - All combinations of data representations virtually impossible to test
  - **Deep integration of tensors** equivalent to new system
SystemDS™ Overview

- **Overview**
  - Open source System for end-to-end Data Science lifecycle
  - Data integration/cleaning, ML training, serving

- **Stack of Declarative Languages**
  - Language hierarchy for tasks and users
  - Unified DSL and layering for interop., reuse, opt
  - **Data model**: Heterogeneous tensors (w/ schema)

- **Key Features**
  - #1: Data integration and cleaning, outliers, feature engineering
  - #2: ML model training, tuning, validation, and serving
  - #3: Data provenance and model versioning → explainability
  - #4: ML+Rules: incorporate domain-expert and compliance rules
  - Hybrid runtime plans: local/distributed, data/task/PS/federated
  - Horizontal and vertical optimization; sparsity exploitation

https://github.com/tugraz-isds/systemds