



Architecture of ML Systems 10 Model Selection & Management

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Announcements/Org

#1 Video Recording

- Link in TeachCenter & TUbe (lectures will be public)
- Live streaming through TUbe, starting May 08
- Questions: https://tugraz.webex.com/meet/m.boehm



- Status: all project discussions w/ 15 students (~8 PRs)
- Awesome mix of projects (algorithms, compiler, runtime)
- Soft deadline: June 30
- If unable to complete: email to m.boehm@tugraz.at

#3 Course Evaluation

■ Please participate; open period: June 1 – July 15













Recap: The Data Science Lifecycle

Data-centric View:

Application perspective
Workload perspective
System perspective



Data Scientist





Data Integration
Data Cleaning
Data Preparation

Model Selection
Training
Hyper-parameters

Validate & Debug
Deployment
Scoring & Feedback



Exploratory Process

(experimentation, refinements, ML pipelines)







Agenda

- Data Augmentation
- Model Selection Techniques
- Model Management





Data Augmentation





Motivation and Basic Data Augmentation

Motivation Data Augmentation

- Complex ML models / deep NNs need lots of labeled data to avoid overfitting → expensive
- Augment training data by synthetic labeled data

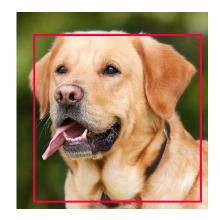
AlexNet

[Alex Krizhevsky, Ilya Sutskever, Geoffrey E. Hinton: ImageNet Classification with Deep Convolutional Neural Networks. NIPS 2012]



Translations & Reflections

- Random 224x224 patches and their reflections (from 256x256 images with known labels)
- Increased data by 2048x
- Test: corner/center patches+ reflections → prediction





Alternating Intensities

- Intuition: object identity is invariant to illumination and color intensity
- PCA on dataset \rightarrow add eigenvalues times a random variable N(0,0.1)





Basic Data Augmentation

Scaling and Normalization

- Standardization: subtract per-channel global pixel means
- Normalization: normalized to range [-1,1] (see min-max)

General Principles

- #1: Movement/selection (translation, rotation, reflection, cropping)
- #2: Distortions (stretching, shearing, lens distortions, color)
- In many different combinations → often trial & error / domain expertise

Excursus: Reducing Training Time

- Transfer learning: Use pre-trained model on ImageNet;
 freeze lower NN layers, fine-tune last layers w/ domain-specific data
- Multi-scale learning: Use cropping and scaling to train 256 x 256 model as starting point for a more compute-intensive 384x384 model

[Karen Simonyan, Andrew Zisserman: Very Deep Convolutional Networks for Large-Scale Image Recognition. ICLR 2015]







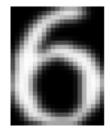
Basic Data Augmentation, cont.

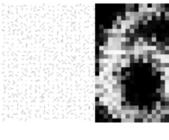
Distortions

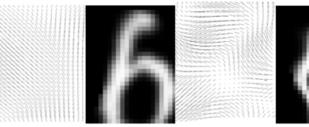
- Translations, rotations, skewing
- Compute for every pixel a new target location via rand displacement fields)



[Patrice Y. Simard, David Steinkraus, John C. Platt: Best Practices for Convolutional Neural Networks Applied to Visual Document Analysis. ICDAR 2003]









- Randomly masking out square regions of input images
- Size more important than shape



[Terrance Devries, Graham W. Taylor: Improved Regularization of Convolutional Neural Networks with Cutout. **Corr 2017**]







Domain Randomization

Training on Simulated Images

- Random rendering of objects with non-realistic textures
- Large variability for generalization to real world objects



[Josh Tobin et al.: Domain randomization for transferring deep neural networks from simulation to the real world. **IROS 2017**]

Pre-Training on Simulated Images

- Random 3D objects and flying distractors w/ random textures
- Random lights and rendered onto random background



[Jonathan Tremblay et al.: Training Deep Networks With Synthetic Data: Bridging the Reality Gap by Domain Randomization. **CVPR Workshops 2018**]

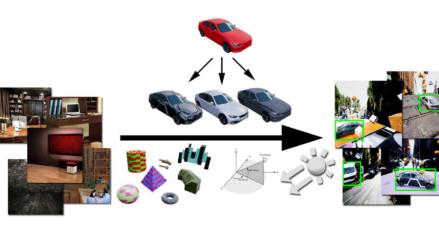














Learning Data Augmentation Policies

AutoAugment

- Search space of augmentation policies
- Goal: Find best augmentation policy (e.g., via reinforcement learning)
- #1: Image processing functions
 (translation, rotation, color normalization)
- #2: Probabilities of applying these functions

Data Augmentation GAN (DAGAN)

- Image-conditional generative model for creating within-class images from inputs
- No need for known invariants



[Antreas Antoniou, Amos J. Storkey, Harrison Edwards: Augmenting Image Classifiers Using Data Augmentation Generative Adversarial Networks. ICANN 2018]

[Ekin Dogus Cubuk, Barret Zoph, Dandelion Mané, Vijay Vasudevan, Quoc V. Le: AutoAugment: Learning Augmentation Policies from Data.

CVPR 2019



→ New state-of-the art top-1 error on ImageNet and CIFAR10

Real input image





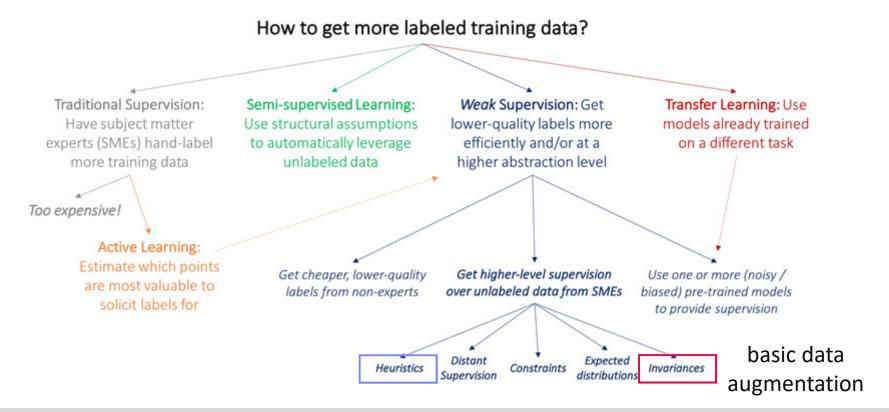


Weak Supervision

Chris Ré, and others: Weak Supervision: A New Programming Paradigm for Machine Learning, ai.stanford.edu/blog/weak-supervision/, 2019]

[Alex Ratner, Paroma Varma, Braden Hancock,

- Heuristically Generated Training Data
 - Hand labeling expensive and time consuming, but abundant unlabeled data
 - Changing labeling guidelines
 labeling heuristics

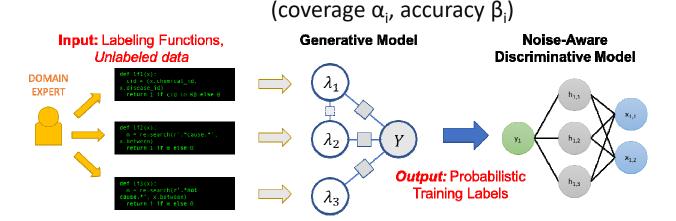






Weak Supervision, cont.

DataProgrammingOverview





[Alexander J. Ratner, Christopher De Sa, Sen Wu, Daniel Selsam, Christopher Ré: Data Programming: Creating Large Training Sets, Quickly. NIPS 2016]



[Alexander Ratner, Stephen H. Bach, Henry R. Ehrenberg, Jason Alan Fries, Sen Wu, Christopher Ré: **Snorkel:** Rapid Training Data Creation with Weak Supervision. **PVLDB 2017**]



[Paroma Varma, Christopher Ré: Snuba: Automating Weak Supervision to Label Training Data. PVLDB 2018]



[Stephen H. Bach, Daniel Rodriguez, Yintao Liu, Chong Luo, Haidong Shao, Cassandra Xia, Souvik Sen, Alexander Ratner, Braden Hancock, Houman Alborzi, Rahul Kuchhal, Christopher Ré, Rob Malkin: **Snorkel DryBell:** A Case Study in Deploying Weak Supervision at Industrial Scale. **SIGMOD 2019**]



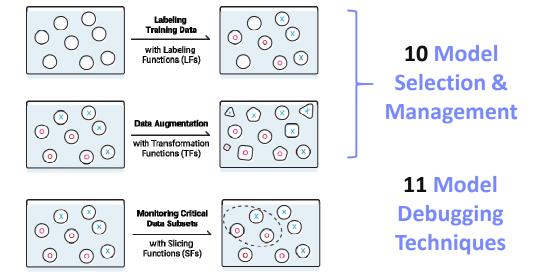
Weak Supervision, cont.

Excursus: Snorkel

[https://www.snorkel.org/]

Programmatically Building and Managing Training Data





Effects of Augmentation

- #1 Regularization for reduced generalization error, not always training error (penalization of model complexity)
- #2 Invariance increase by averaging features of augmented data points

Data Augmentation as a Kernel

- Kernel metric for augmentation selection
- Affine transforms on approx. kernel features

[Tri Dao et al: A Kernel Theory of Modern Data Augmentation. ICML 2019]







Model Selection Techniques





AutoML Overview

[Chris Thornton, Frank Hutter, Holger H. Hoos, Kevin Leyton-Brown: Auto-WEKA: combined selection and hyperparameter optimization of classification algorithms. **KDD 2013**]



Model Selection

 Given a dataset and ML task (e.g., classification or regression)

$$A^* \in \underset{A \in \mathcal{A}}{\operatorname{argmin}} \frac{1}{k} \sum_{i=1}^k \mathcal{L}(A, \mathcal{D}_{\operatorname{train}}^{(i)}, \mathcal{D}_{\operatorname{valid}}^{(i)}),$$

Select the model (type) that performs best
 (e.g.: LogReg, Naïve Bayes, SVM, Decision Tree, Random Forest, DNN)

Hyper Parameter Tuning

Given a model and dataset, $A^{(j)} \in \mathcal{A}, \lambda \in \Lambda^{(j)}$ $k \subseteq A$ find best hyper parameter values (e.g., learning rate, regularization, kernels, kernel parameters, tree params)

$$A^*_{\boldsymbol{\lambda}^*} \in \operatorname*{argmin}_{A^{(j)} \in \mathcal{A}, \boldsymbol{\lambda} \in \boldsymbol{\Lambda}^{(j)}} \frac{1}{k} \sum_{i=1}^k \mathcal{L}(A^{(j)}_{\boldsymbol{\lambda}}, \mathcal{D}^{(i)}_{\text{train}}, \mathcal{D}^{(i)}_{\text{valid}}).$$

Validation: Generalization Error

- Goodness of fit to held-out data (e.g., 80-20 train/test)
- Cross validation (e.g., leave one out \rightarrow k=5 runs w/ 80-20 train/test)

→ AutoML Systems/Services

- Often providing both model selection and hyper parameter search
- Integrated ML system, often in distributed/cloud environments

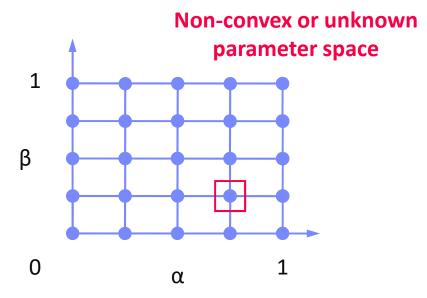


Basic Grid Search



Basic Approach

- Given n hyper parameters $\lambda 1, ..., \lambda n$ with domains $\Lambda 1, ..., \Lambda n$
- Enumerate and evaluate parameter space $\Lambda \subseteq \Lambda_1 \times ... \times \Lambda_n$ (often strict subset due to dependency structure of parameters)
- Continuous hyper parameters → discretization
 - Equi-width
 - Exponential (e.g., regularization 0.1, 0.01, 0.001, etc)
- Problem: Only applicable with small domains
- Heuristic: Monte-Carlo (random search)







Basic Iterative Algorithms

Simulated Annealing

- Decaying temperature schedules: $T_{k+1} = \alpha \cdot T_k$
- #1 Generate neighbor in ε-env of old point

Exploration vs exploitation

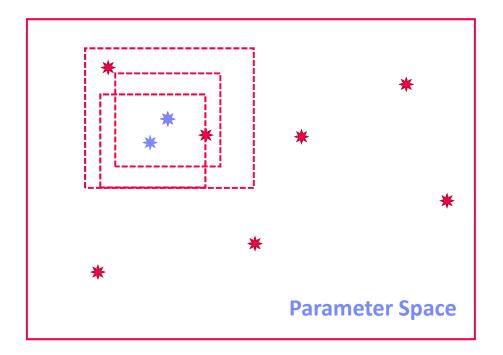
■ #2 Accept better points and worse points w/ $P(T_k) = \frac{1}{1 + \exp((f' - f)/T_{\nu})}$

Recursive Random Search

- Repeated restart
- Sample and evaluate points
- Determine best and shrink area if optimum unchanged
- Realign area if new optimum found



[Tao Ye, Shivkumar Kalyanaraman: A recursive random search algorithm for large-scale network parameter configuration. **SIGMETRICS 2003**]







Bayesian Optimization

Overview BO

- Sequential Model-Based Optimization
- Fit a probabilistic model based on the first n-1 evaluated hyper parameters
- Use model to select next candidate
- Gaussian process (GP) models, or tree-based Bayesian Optimization

[Chris Thornton, Frank Hutter, Holger H. Hoos, Kevin Leyton-Brown: Auto-WEKA: combined selection and hyperparameter optimization of classification algorithms. **KDD 2013**]



Algorithm 1 SMBO

- 1: initialise model \mathcal{M}_L ; $\mathcal{H} \leftarrow \emptyset$
- 2: while time budget for optimization has not been exhausted do
- 3: $\lambda \leftarrow \text{candidate configuration from } \mathcal{M}_L$
- 4: Compute $c = \mathcal{L}(A_{\lambda}, \mathcal{D}_{\text{train}}^{(i)}, \mathcal{D}_{\text{valid}}^{(i)})$
- 5: $\mathcal{H} \leftarrow \mathcal{H} \cup \{(\boldsymbol{\lambda}, c)\}$
- 6: Update \mathcal{M}_L given \mathcal{H}
- 7: end while
- 8: **return** λ from \mathcal{H} with minimal c

Underlying Foundations

- The posterior probability of a model M given evidence E is proportional to the likelihood of E given M multiplied by prior probability of M
- Prior knowledge: e.g., smoothness, noise-free
- P(M|E) = P(E|M)P(M)/P(E) \Rightarrow $P(M|E) \propto P(E|M)P(M)$ after next before
- Maximize acquisition function:
 GP high objective (exploitation) and high prediction uncertainty (exploration)

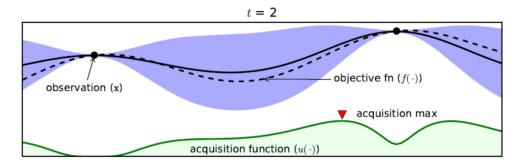


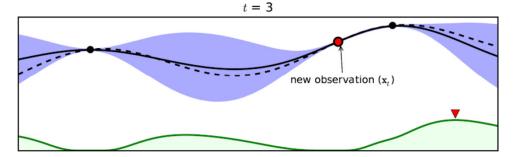


Bayesian Optimization, cont

Example 1D Problem

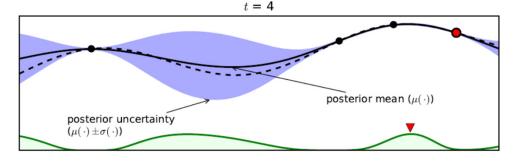
- Gaussian Process
- 4 iterations







[Eric Brochu, Vlad M. Cora, Nando de Freitas: A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning. **Corr 2010**]





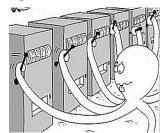


Multi-armed Bandits and Hyperband

Overview Multi-armed Bandits

- Motivation: model types have different quality
- Select among k model types → k-armed bandit problem
- Running score for each arm → scheduling policy

[Credit: blogs.mathworks.com]



[Sébastien Bubeck, Nicolò Cesa-Bianchi: Regret Analysis of Stochastic and Nonstochastic Multi-armed Bandit Problems. Foundations and Trends in Machine Learning 2012]



Hyperband

- Non-stochastic setting, without parametric assumptions
- Pure exploration algorithm for infinite-armed bandits
- Based on Successive Halving
 - Successively discarding the worst-performing half of arms

Talwalkar: Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization. **JMLR 2017**]

[Lisha Li, Kevin G. Jamieson, Giulia DeSalvo, Afshin Rostamizadeh, Ameet



• Extended by doubling budget of arms in each iteration (no need to configure k, random search included)





Selected AutoML Systems

Auto Weka

Bayesian optimization with
 28 learners, 11 ensemble/meta methods

[Chris Thornton et al: Auto-WEKA: combined selection and hyperparameter optimization of classification algorithms. **KDD 2013**]



Ods [Lars Kotthoffet al: Auto-WEKA 2.0: Automatic model selection and hyper-parameter optimization in WEKA. JMLR 2017]



Auto Sklearn

Bayesian optimization with
 15 classifiers, 14 feature prep, 4 data prep

[Matthias Feurer et al: Auto-sklearn: Efficient and Robust Automated Machine Learning. Automated Machine Learning 2019]



TuPaQ

Multi-armed bandit and large-scale

[Evan R. Sparks, Ameet Talwalkar, Daniel Haas, Michael J. Franklin, Michael I. Jordan, Tim Kraska: Automating model search for large scale machine learning. **Socc 2015**]



TPOT

Genetic programming

[Randal S. Olson, Jason H. Moore: TPOT: A Tree-Based Pipeline Optimization Tool for Automating Machine Learning. Automated Machine Learning 2019]



Other Services

- Azure ML, Amazon ML
- Google AutoML, H20 AutoML

[Hantian Zhang, Luyuan Zeng, Wentao Wu, Ce Zhang: How Good Are Machine Learning Clouds for Binary Classification with Good Features? **Corr 2017**]







Selected AutoML Systems, cont.

Alpine Meadow

Curated AutoML

Paper Collections

- Logical and physical ML pipelines
- Multi-armed bandit for pipeline selection
- Bayesian optimization for hyper-parameters

[Zeyuan Shang et al: **Democratizing Data Science** through Interactive Curation of ML Pipelines. SIGMOD 2019]

[Stefan Falkner, Aaron Klein, Frank

Hutter: BOHB: Robust and Efficient

Hyper-parameter Optimization at



- Dabl (Data Analysis Baseline Library)
 - Tools for simple data preparation and ML training
 - Hyperband (successive halving) for optimization

[https://amueller.github.io/ dabl/dev/user guide.html]

Scale. **ICML 2018**]

BOHB

- Bayesian optimization & hyperband
- Queue-based parallelization of successive halving







Neural Architecture Search

Motivation

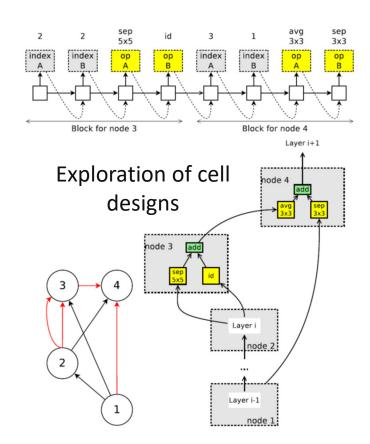
- Design neural networks (type of layers / network) is often trial & error process
- Accuracy vs necessary computation characterizes an architecture
- → Automatic neural architecture search

#1 Search Space of Building Blocks

- Define possible operations (e.g., identity, 3x3/5x5 separable convolution, avg/max pooling)
- Define approach for connecting operations (pick 2 inputs, apply op, and add results)



[Hieu Pham, Melody Y. Guan, Barret Zoph, Quoc V. Le, Jeff Dean: Efficient Neural Architecture Search via Parameter Sharing. ICML 2018]





Neural Architecture Search, cont.

#2 Search Strategy

- Classical evolutionary algorithms
- Recurrent neural networks (e.g., LSTM)
- Bayesian optimization (with special distance metric)

[Barret Zoph, Quoc V. Le: Neural Architecture Search with Reinforcement Learning. ICLR 2017]



[Kirthevasan Kandasamy, Willie Neiswanger, Jeff Schneider, Barnabás Póczos, Eric P. Xing: Neural Architecture Search with Bayesian Optimisation and Optimal Transport. **NeurIPS 2018**]



#3 Optimization Objective

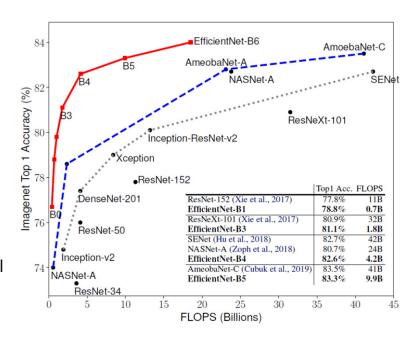
- Max accuracy (min error)
- Multi-objective (accuracy and runtime)

Excursus: Model Scaling

- Automatically scale-up small model for better accuracy
- EfficientNet



[Mingxing Tan, Quoc V. Le: EfficientNet: Rethinking Model Scaling for Convolutional Neural Networks. **ICML 2019**]



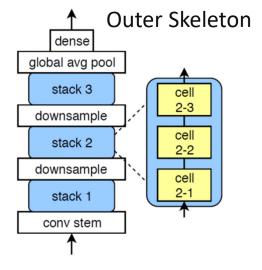


Neural Architecture Search, cont.

- Problem: Computational Resources
 - Huge computational requirements for NAS (even on small datasets)
 - → #1 Difficult to reproduce, and #2 barrier-to-entry
- Excursus: NAS-Bench-101
 - 423K unique convolutional architectures
 - Training and evaluated ALL architectures, multiple times on CIFAR-10
 - Shared dataset: 5M trained models



[Chris Ying, Aaron Klein, Eric Christiansen, Esteban Real, Kevin Murphy, Frank Hutter: NAS-Bench-101: Towards Reproducible Neural Architecture Search. ICML 2019]







Model Management





Overview Model Management

Motivation

- Exploratory data science process → trial and error (preparation, feature engineering, models, model selection)
- Different personas (data engineer, ML expert, devops)

How did you create that model? Did you consider X?





Problems

- No record of experiments, insights lost along the way
- Difficult to reproduce results
- Cannot search for or query models
- Difficult to collaborate



[Manasi Vartak: ModelDB: A system to manage machine learning models, Spark Summit 2017]

Overview

- Experiment tracking and visualization
- Coarse-grained ML pipeline provenance and versioning
- Fine-grained data provenance (data-/ops-oriented)





Background: Data Provenance and Lineage

Overview

- Base query Q(D) = O with database D = $\{R_1, ..., R_n\}$
- Forward lineage query: L_f(R_i", O') from subset of input relation to output
- Backward lineage query: L_b(O', R_i) from subset of outputs to base tables

#1 Lazy Lineage Query Evaluation

- Rewrite (invert) lineage queries as relational queries over input relations
- No runtime overhead but slow lineage query processing

#2 Eager Lineage Query Evaluation

- Materialize annotations (data/transforms) during base query evaluation
- Runtime overhead but fast lineage query processing
- Lineage capture: Logical (relational)
 vs physical (instrumented physical ops)

[Fotis Psallidas, Eugene Wu: Smoke: Fine-grained Lineage at Interactive Speed. **PVLDB 2018**]







Model Management Systems

ModelHub

- Versioning system for DNN models, including provenance tracking
- DSL for model exploration and enumeration queries (model selection + hyper parameters)
- Model versions stored as deltas

[Hui Miao, Ang Li, Larry S. Davis, Amol Deshpande: ModelHub: Deep Learning Lifecycle Management. ICDE 2017]



ModelDB

- Model and provenance logging for ML pipelines via programmatic APIs
- Support for different ML systems (e.g., spark.ml, scikit-learn, others)
- GUIs for capturing meta data and metric visualization

[Manasi Vartak, Samuel Madden: MODELDB: Opportunities and Challenges in Managing Machine Learning Models.

IEEE Data Eng. Bull. 2018]







Model Management Systems, cont.

MLflow



- An open source platform for the machine learning lifecycle
- Use of existing ML systems and various language bindings













- MLflow Tracking: logging and querying experiments
- Mlflow Projects: packaging/reproduction of ML pipeline results
- MLflow Models: deployment of models in various services/tools



[Matei Zaharia, Andrew Chen, Aaron Davidson, Ali Ghodsi, Sue Ann Hong, Andy Konwinski, Siddharth Murching, Tomas Nykodym, Paul Ogilvie, Mani Parkhe, Fen Xie, Corey Zumar: Accelerating the Machine Learning Lifecycle with MLflow. IEEE Data Eng. Bull. 41(4) 2018]





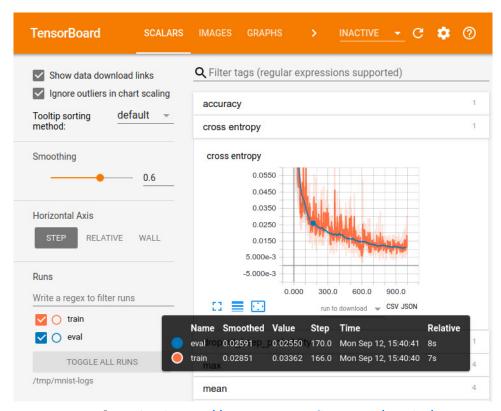
Experiment Tracking

TensorFlow: TensorBoard

- Suite of visualization tools
- Explicitly track and write summary statistics
- Visualize behavior over time and across experiments
- Different folders for model versioning?

Other Tools:

- Integration w/ TensorBoard
- Lots of custom logging and plotting tools



[Credit: https://www.tensorflow.org/guide/ summaries_and_tensorboard]





Provenance for ML Pipelines (fine-grained)

DEX: Dataset Versioning

- Versioning of datasets, stored with delta encoding
- Checkout, intersection, union queries over deltas
- Query optimization for finding efficient plans

[Amit Chavan, Amol Deshpande: DEX: Query Execution in a Deltabased Storage System. SIGMOD 2017]



MISTIQUE: Intermediates of ML Pipelines

- Capturing, storage, querying of intermediates
- Lossy deduplication and compression
- Adaptive querying/materialization for finding efficient plans

Linear Algebra Provenance

- Provenance propagation by decomposition
- Annotate parts w/ provenance polynomials (identifiers of contributing inputs + impact)

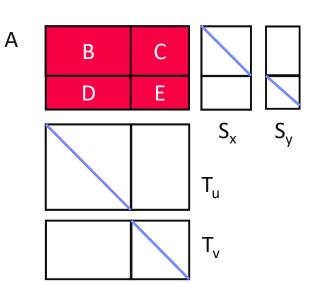
$$A = S_x B T_u + S_x C T_v + S_y D T_u + S_y E T_v$$



[Zhepeng Yan, Val Tannen, Zachary G. Ives: Fine-grained Provenance for Linear Algebra Operators. **TaPP 2016**]

[Manasi Vartak et al: MISTIQUE: A System to Store and Query Model Intermediates for Model Diagnosis. **SIGMOD 2018**]







Provenance for ML Pipelines (coarse-grained)

MLflow

- Programmatic API for tracking parameters, experiments, and results
- autolog() for specific params

```
import mlflow
mlflow.log_param("num_dimensions", 8)
mlflow.log_param("regularization", 0.1)
mlflow.log metric("accuracy", 0.1)
```

mlflow.log artifact("roc.png")

Flor (on Ground)

- DSL embedded in python for managing the workflow development phase of the ML lifecycle
- DAGs of actions, artifacts, and literals
- Data context generated by activities in Ground

[Credit: https://rise.cs.berkeley.edu/ projects/jarvis/]

[Credit: https://databricks.com/

[Joseph M. Hellerstein et al: Ground: A Data Context Service. **CIDR 2017**]



Dataset Relationship Management

- Reuse, reveal, revise, retarget, reward
- Code-to-data relationships (data provenance)
- Data-to-code relationships (potential transforms)

[Zachary G. Ives, Yi Zhang, Soonbo Han, Nan Zheng,: Dataset Relationship Management. CIDR 2019]







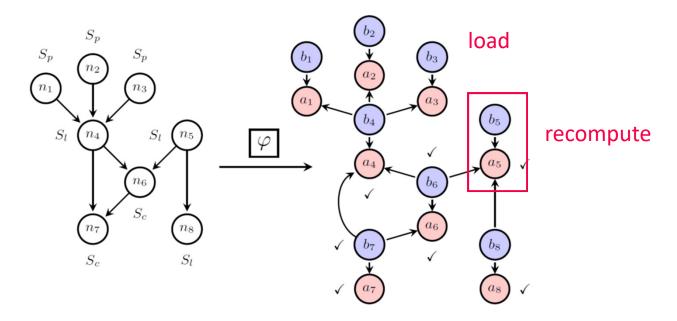
Provenance for ML Pipelines (coarse-grained), cont.

HELIX

- Goal: focus on iterative development
 w/ small modifications (trial & error)
- Caching, reuse, and recomputation
- [Doris Xin, Stephen Macke, Litian Ma, Jialin Liu, Shuchen Song, Aditya G. Parameswaran: Helix: Holistic Optimization for Accelerating Iterative Machine Learning. **PVLDB 2018**]



- Reuse as Max-Flow problem → NP-hard → heuristics
- Materialization to disk for future reuse







Fine-grained Lineage in SystemDS





Problem

- Exploratory data science (data preprocessing, model configurations)
- Reproducibility and explainability of trained models (data, parameters, prep)
- → Lineage/Provenance as Key Enabling Technique:

 Model versioning, reuse of intermediates, incremental maintenance, auto differentiation, and debugging (query processing over lineage)

Efficient Lineage Tracing

- Tracing of inputs, literals, and non-determinism
- Trace lineage of logical operations for all live variables, store along outputs, program/output reconstruction possible:

```
X = eval(deserialize(serialize(lineage(X))))
```

Proactive deduplication of lineage traces for loops

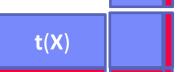




Fine-grained Lineage in SystemDS, cont.

- Full Reuse of Intermediates
 - Before executing instruction, probe output lineage in cache
 Map<Lineage, MatrixBlock>
 - Cost-based/heuristic caching and eviction decisions (compiler-assisted)
- Partial Reuse of Intermediates
 - Problem: Often partial result overlap
 - Reuse partial results via dedicated rewrites (compensation plans)
 - Example: steplm





X

```
O(k(mn^{2}+n^{3})) \rightarrow \\ for(i in 1:numModels) O(mn^{2}+kn^{3}) \\ R[,i] = lm(X, y, lambda[i,], ...)
```

```
m_lmDS = function(...) {
    l = matrix(reg,ncol(X),1)
    A = t(X) %*% X + diag(l)
    b = t(X) %*% y
    beta = solve(A, b) ...}
```

```
m_steplm = function(...) {
  while( continue ) {
    parfor( i in 1:n ) {
       if( !fixed[1,i] ) {
          Xi = cbind(Xg, X[,i])
          B[,i] = lm(Xi, y, ...)
       } }
    # add best to Xg
    # (AIC)
  }
}
```

 $O(n^2(mn^2+n^3)) \rightarrow O(n^2(mn+n^3))$





Summary and Q&A

- Data Augmentation
- Model Selection Techniques
- Model Management
- Next Lectures
 - June 11/12: Corpus Christi (Fronleichnam)
 - 11 Model Debugging Techniques [Jun 19]
 - 12 Model Serving Systems and Techniques [Jun 26]

