Architecture of ML Systems (AMLS)
10 Model Selection and Management

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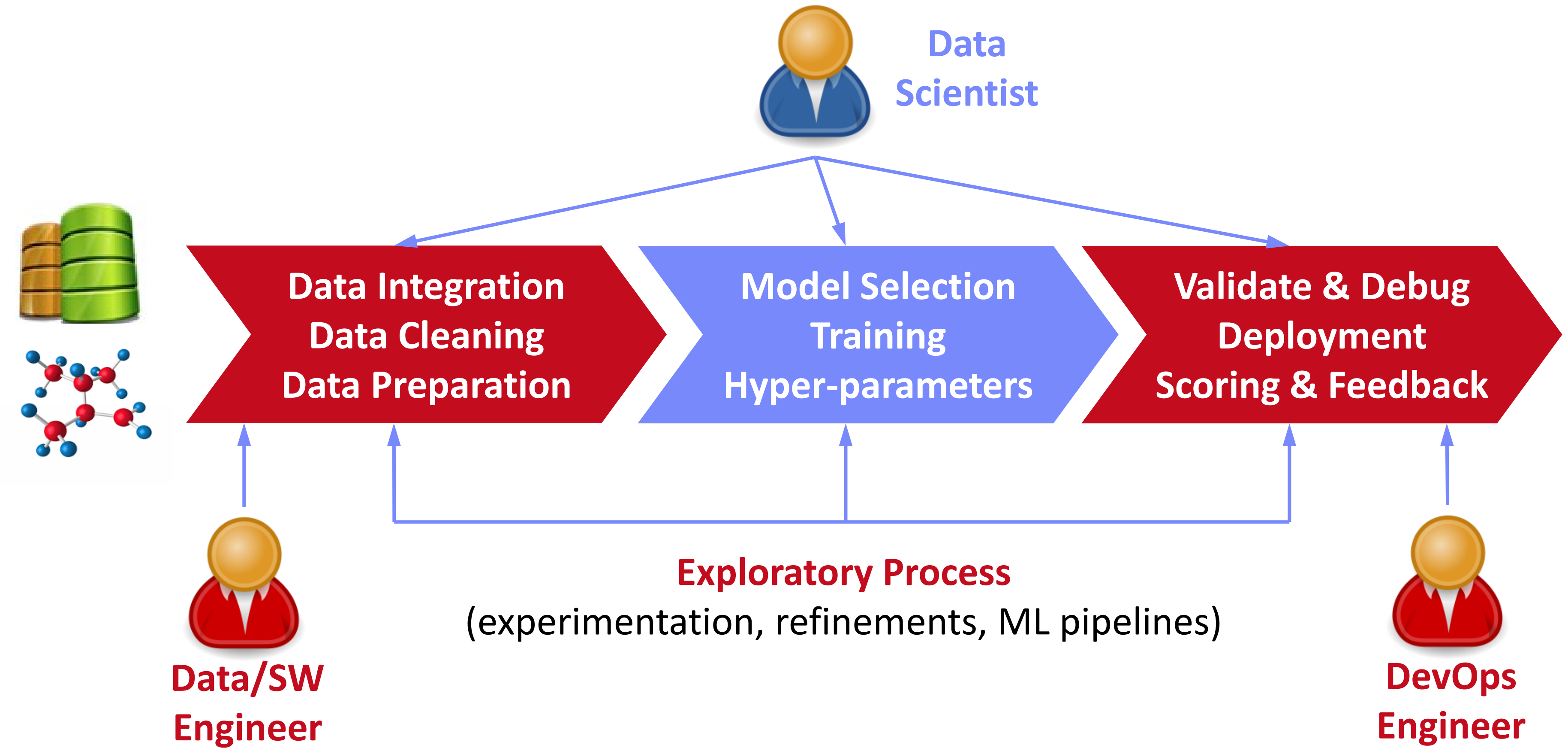
Announcements / Org

- **#1 Hybrid & Video Recording**
  - Hybrid lectures (in-person, zoom) with optional attendance https://tu-berlin.zoom.us/j/9529634787?pwd=R1ZsN1M3SC9BOU1OcFdmem9zT202UT09
  - Zoom **video recordings**, links from website https://mboehm7.github.io/**teaching**/ss23_amls/index.htm

- **#2 Virtual Lectures June 22**
  - **Thu, June 29, 6.30pm-8.30pm** due to BMBF visit at BIFOLD
  - **Virtual lecture and video recording**

- **#3 Project/Exercise Submission**
  - Original Deadline: **July 4** → **24h before individual exam slot**
  - Pull requests (SystemDS/DAPHNE); ISIS submission or email (for TU Graz students)
  - Please, deregister your exam slot if you can't make it

Recap: The Data Science Lifecycle (aka KDD Process, aka CRISP-DM)



Agenda

- Data Augmentation
- Model Selection Techniques
- Model Management & Provenance

Data Augmentation

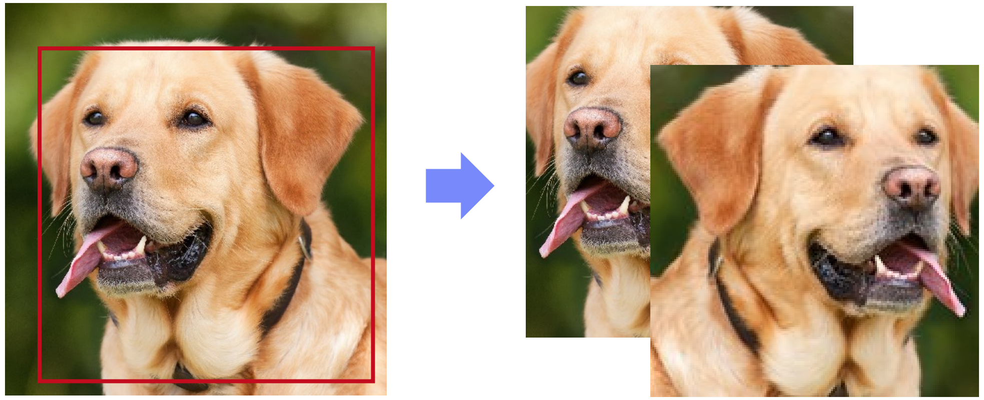
Motivation and Basic Data Augmentation

- **Motivation Data Augmentation**
  - Complex ML models / deep NNs need lots of labeled data to avoid overfitting ➔ **expensive**
  - Augment training data by **synthetically generated labeled data**

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

AlexNet (see Section 4.1)

- **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 → add eigenvalues times a random variable N(0,0.1)

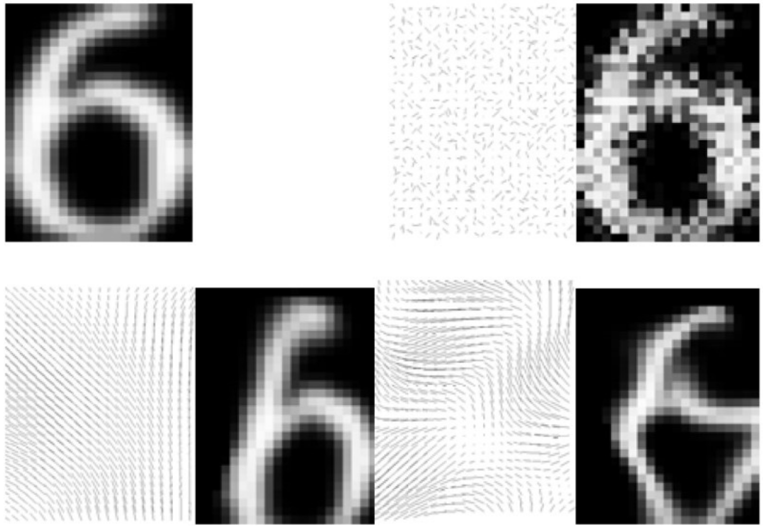
Basic Data Augmentation

- **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, mixup of images)
  - 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 Convolu-tional Networks for Large-Scale Image Recognition. **ICLR 2015**]

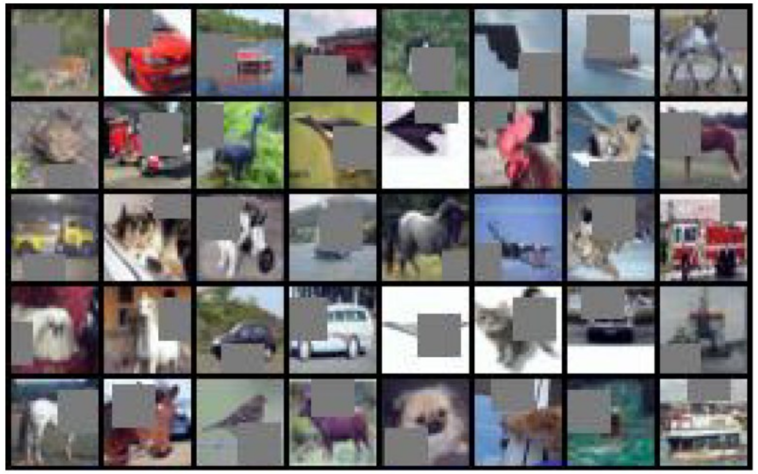
Basic Data Augmentation, cont.

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



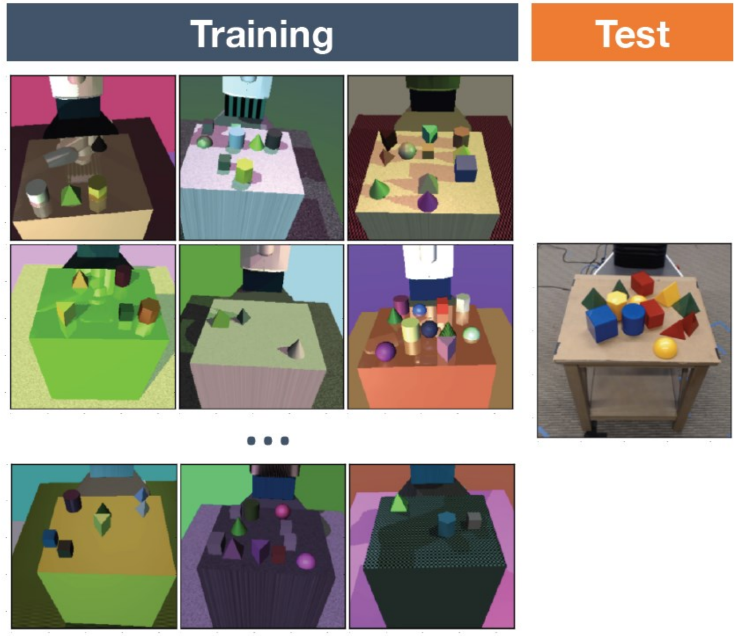
[Patrice Y. Simard, David Steinkraus, John C. Platt: Best Practices for Convolutional Neural Networks Applied to Visual Document Analysis. **ICDAR 2003**]

- **Cutout**
  - 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**]

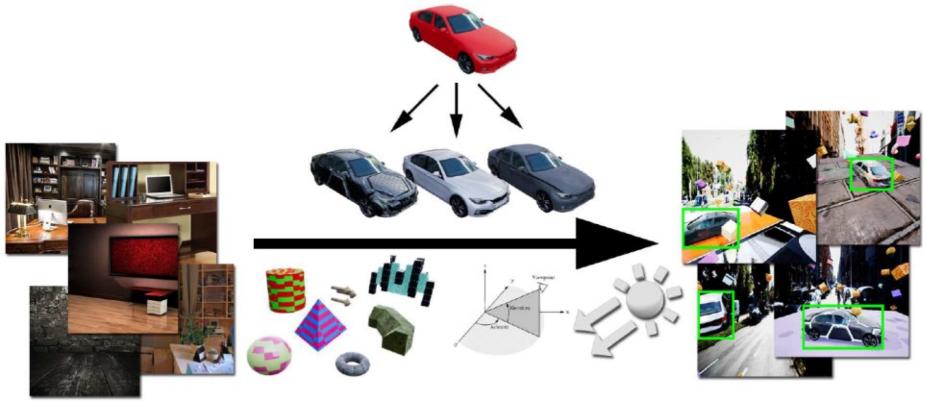
Domain Randomization



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

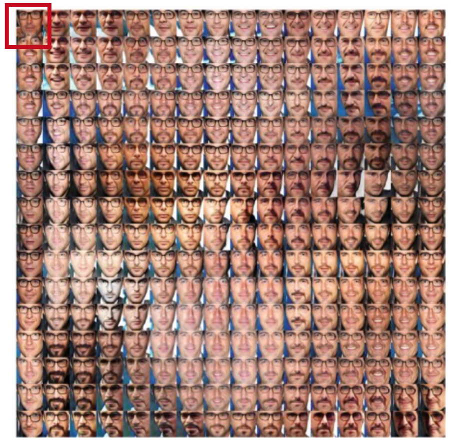
[Ekin Dogus Cubuk, Barret Zoph, Dandelion Mané, Vijay Vasudevan, Quoc V. Le: AutoAugment: Learning Augmentation Policies from Data. **CVPR 2019**]

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

- **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**]

Real input image

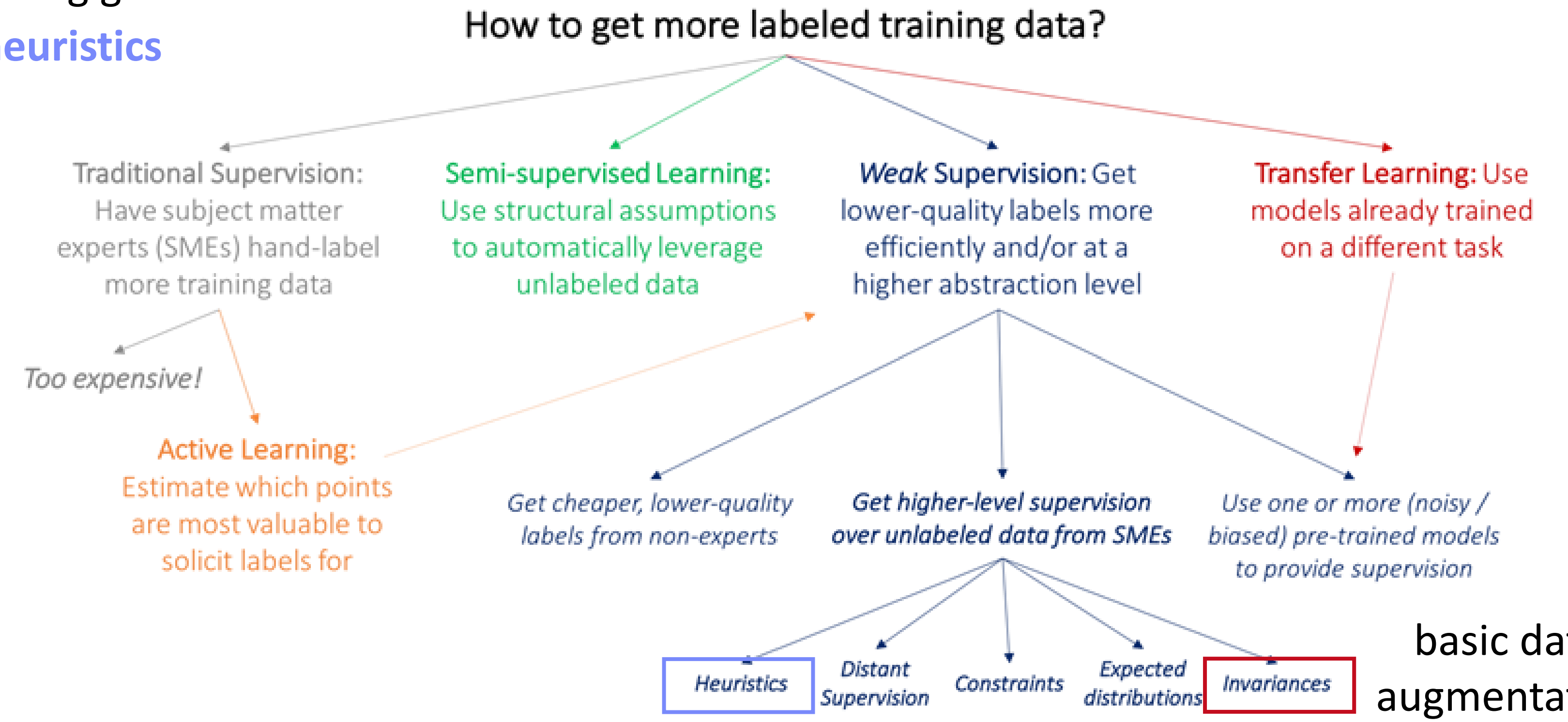


Weak Supervision

[Alex Ratner, Paroma Varma, Braden Hancock, Chris Ré, and others: Weak Supervision: A New Programming Paradigm for Machine Learning, ai.stanford.edu/blog/weak-supervision/, 2019]

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

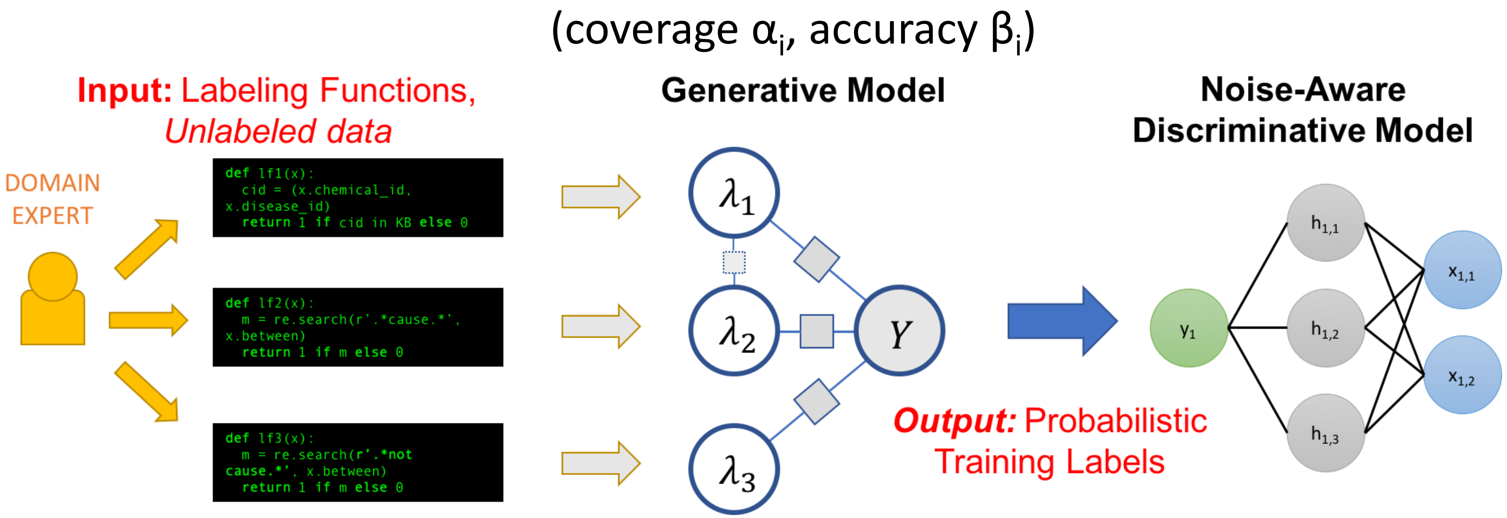
    ➔ labeling heuristics



basic data augmentation

Weak Supervision, cont.

- **Data Programming Overview**



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

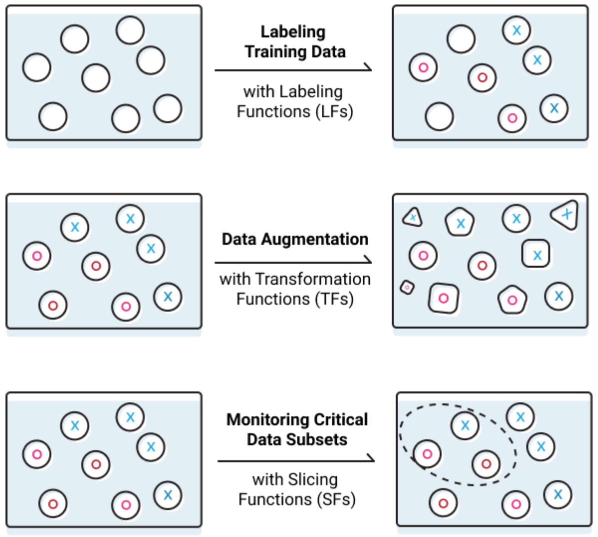
[Alexander Ratner, Stephen H. Bach, Henry R. Ehrenberg, Jason Alan Fries, Sen Wu, Christopher Ré: **Snorkel:** Rapid Training Data Creation with Weak Supervision. **PVLDB 2017**]

[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



10 Model Selection & Management

11 Model Debugging Techniques

- **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**]

- **#1 Model Selection**
  - Given a dataset and ML task (e.g., classification or regression)
  - Select the model (type) that performs best (e.g.: LogReg, Naïve Bayes, SVM, Decision Tree, Random Forest, DNN)

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

- **#2 Hyper Parameter Tuning**
  - Given a model and dataset, 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 → 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

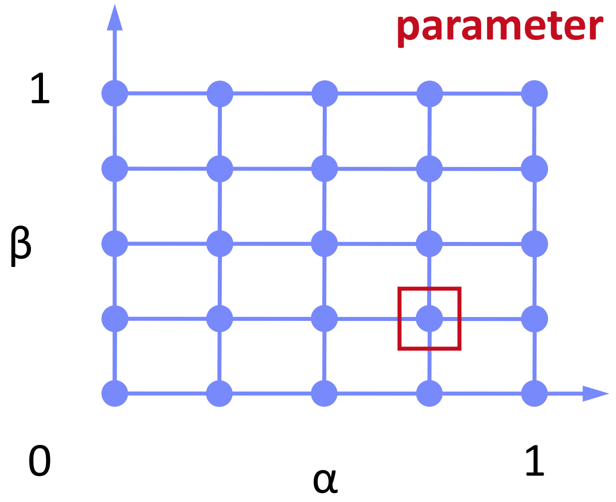
Basic Grid Search

`gridSearch()` `GridSearchCV()`

- **Basic Approach**
  - Given n hyper parameters $\lambda_1, \ldots, \lambda_n$ with domains $\Lambda_1, \ldots, \Lambda_n$
  - Enumerate and evaluate parameter space $\Lambda \subseteq \Lambda_1 \times \ldots \times \Lambda_n$ (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, anytime)**

Non-convex or unknown parameter space



Basic Grid Search, cont.

- **Example Adult Dataset** (train 32,561 x 14)
  - Binary classification (>50K), https://archive.ics.uci.edu/ml/datasets/adult
  - **#1** MLogReg defaults w/ one-hot categoricals — Accuracy (%): 82.35
  - **#2** MLogReg defaults w/ one-hot + binning — Accuracy (%): 84.73
  - **#3** GridSearch MLogReg: — Accuracy (%): 90.07

```
params = list("icpt", "reg", "numBins");
paramRanges = list(seq(0,2), 10^seq(3,-6), 10^seq(1,4));
```

- **Example SystemDS** `gridSearch`

```
HP = matrix(0, numConfigs, numParams);
parfor( i in 1:nrow(HP) ) {
  for( j in 1:numParams )
    HP[i,j] = paramVals[j,as.scalar(((i-1)/cumLens[j,1])%%paramLens[j,1]+1)];
}
```

 # Materialize Configs

```
parfor( i in 1:nrow(HP) ) {
  # a) replace training arguments
  largs = trainArgs;
  for( j in 1:numParams )
    largs[as.scalar(params[j])] = as.scalar(HP[i,j]);
  # b) core training/scoring and write-back
  lbeta = t(eval(train, largs))
  Rbeta[i,1:ncol(lbeta)] = lbeta;
  Rloss[i,] = eval(predict, list(X, y, t(lbeta)));
}
```

05 Data- and Task-Parallel Execution

Basic Iterative Algorithms

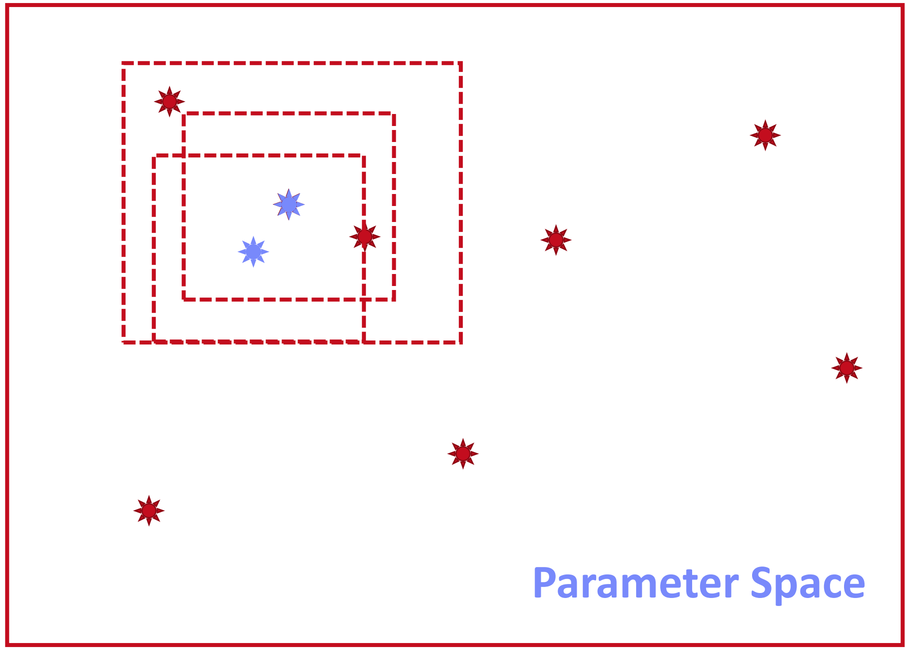
- **Simulated Annealing**
  - Decaying temperature schedules: $T_{k+1} = \alpha \cdot T_k$
  - **#1** Generate neighbor in **ε-env** of old point
  - **#2** Accept better points and worse points w/

Exploration vs exploitation

$$P(T_k) = \frac{1}{1 + \exp((f' - f)/T_k)}$$

- **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

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

- **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

Algorithm 1 SMBO

initialise model $\mathcal{M}_L$; $\mathcal{H} \leftarrow \emptyset$
while time budget for optimization has not been exhausted **do**
  $\boldsymbol{\lambda} \leftarrow$ candidate configuration from $\mathcal{M}_L$
  Compute $c = \mathcal{L}(A_{\boldsymbol{\lambda}}, \mathcal{D}^{(i)}_{\text{train}}, \mathcal{D}^{(i)}_{\text{valid}})$
  $\mathcal{H} \leftarrow \mathcal{H} \cup \{(\boldsymbol{\lambda}, c)\}$
  Update $\mathcal{M}_L$ given $\mathcal{H}$
end while
return $\boldsymbol{\lambda}$ 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
  - **Maximize acquisition function:**
    GP high objective (exploitation) and high prediction uncertainty (exploration)

$$P(M|E) = P(E|M)P(M)/P(E)$$

$$\rightarrow$$

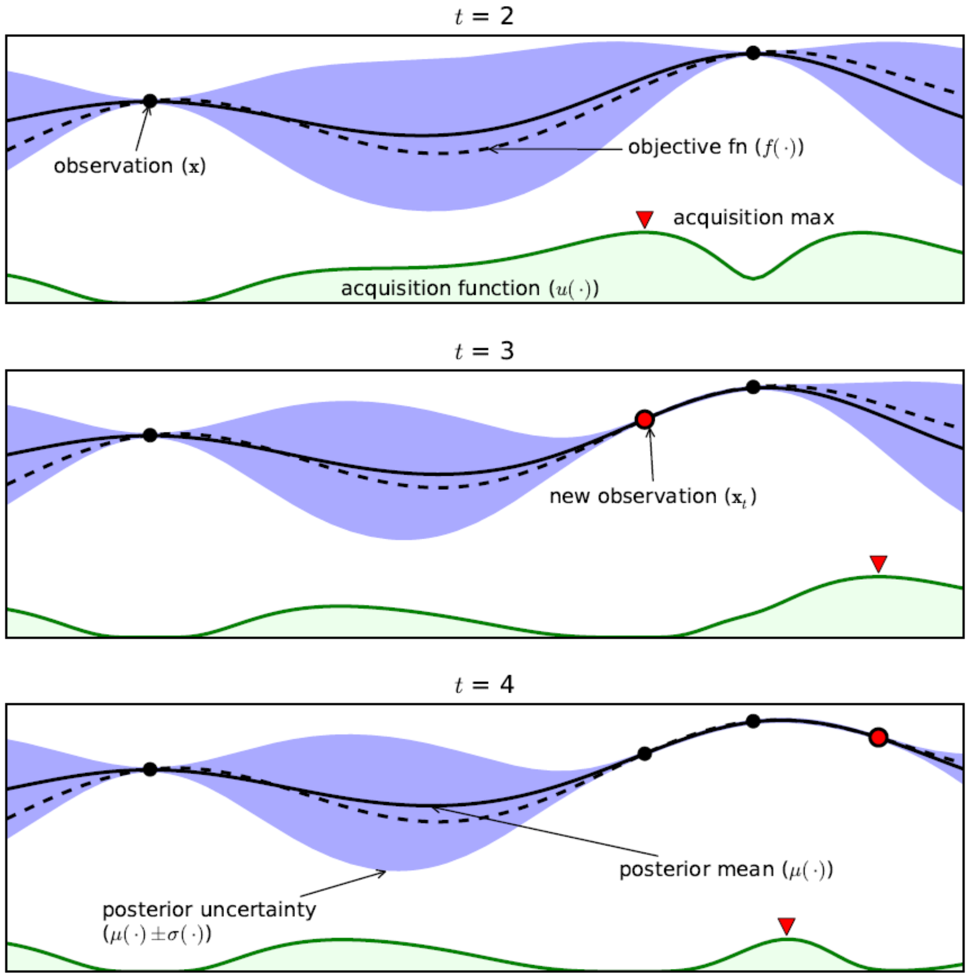
$$P(M|E) \propto P(E|M)P(M)$$

after next before

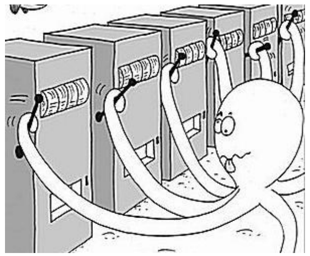
Bayesian Optimization, cont.

- **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



[Credit: blogs.mathworks.com]

- **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**

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

[Lisha Li, Kevin G. Jamieson, Giulia DeSalvo, Afshin Rostamizadeh, Ameet Talwalkar: Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization. **JMLR 2017**]

5 buckets with R=81 resources and η = 3 (**exploitation** vs **exploration**)

	$s=4$		$s=3$		$s=2$		$s=1$		$s=0$	
i	n_i	r_i	n_i	r_i	n_i	r_i	n_i	r_i	n_i	r_i
0	81	1	27	3	9	9	6	27	5	81
1	27	3	9	9	3	27	2	81		
2	9	9	3	27	1	81				
3	3	27	1	81						
4	1	81								

Selected AutoML Systems

- **Auto Weka**
  - **Bayesian optimization** with 28 learners, 11 ensemble/meta methods
- **Auto Sklearn**
  - **Bayesian optimization** with 15 classifiers, 14 feature prep, 4 data prep
- **TuPaQ**
  - **Multi-armed bandit** and large-scale
- **TPOT**
  - Genetic programming
- **Other Services**
  - Azure ML, Amazon ML
  - Google AutoML, H20 AutoML

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

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

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

[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**]

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

[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**
  - 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**]

- **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]

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

[Stefan Falkner, Aaron Klein, Frank Hutter: BOHB: Robust and Efficient Hyper-parameter Optimization at Scale. **ICML 2018**]

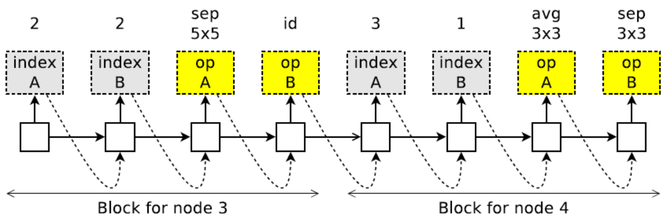
- **AutoML** (https://www.automl.org/) **Paper Collections/Benchmarks**
  - HPOBench/NASBench

AutoML.org Freiburg-Hannover

AutoML Freiburg-Hannover

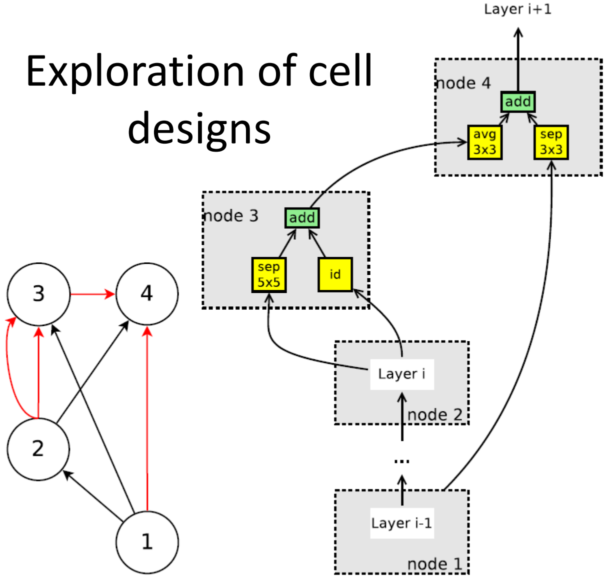
Neural Architecture Search

- **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)

Exploration of cell designs



[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.

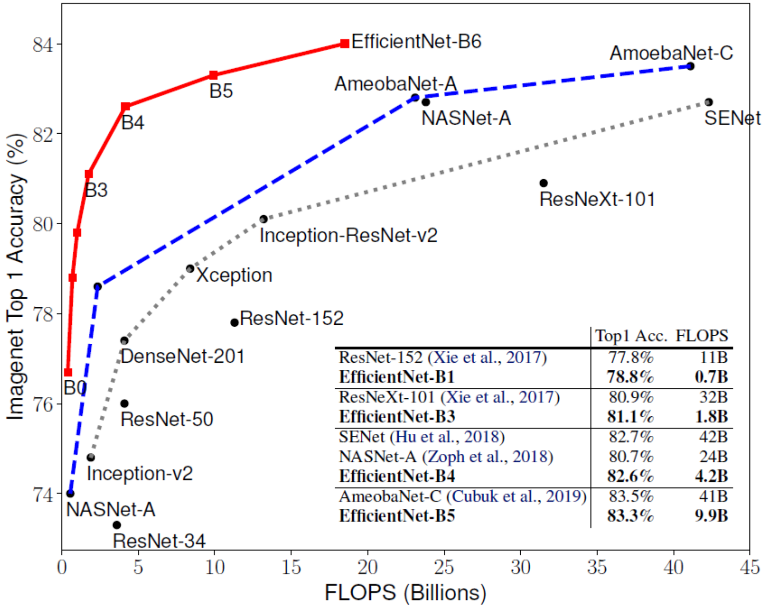
- **#2 Search Strategy**
  - Classical evolutionary algorithms
  - Recurrent neural networks (e.g., LSTM)
  - Bayesian optimization (with special distance metric)

[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



	Top1 Acc.	FLOPS
ResNet-152 (Xie et al., 2017)	77.8%	11B
EfficientNet-B1	**78.8%**	**0.7B**
ResNeXt-101 (Xie et al., 2017)	80.9%	32B
EfficientNet-B3	**81.1%**	**1.8B**
SENet (Hu et al., 2018)	82.7%	42B
NASNet-A (Zoph et al., 2018)	80.7%	24B
EfficientNet-B4	**82.6%**	**4.2B**
AmeobaNet-C (Cubuk et al., 2019)	83.5%	41B
EfficientNet-B5	**83.3%**	**9.9B**

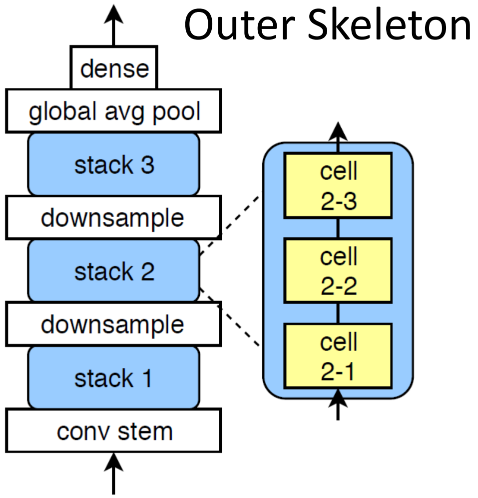
[Mingxing Tan, Quoc V. Le: EfficientNet: Rethinking Model Scaling for Convolutional Neural Networks. **ICML 2019**]

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**]

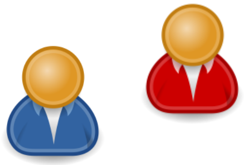


Model Management & Provenance

Overview Model Management

- **Motivation**
  - **Exploratory data science process** → trial and error (preparation, feature engineering, model selection)
  - **Different personas** (data engineer, ML expert, devops)
- **Problems**
  - No record of experiments, insights lost along the way
  - Difficult to reproduce results
  - Cannot search for or query models
  - Difficult to collaborate
- **Overview**
  - Experiment tracking and visualization
  - Coarse-grained ML pipeline provenance and versioning
  - Fine-grained data provenance (data-/ops-oriented)

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



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

Model Management Systems (MLOps)

- **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 → Verta.ai**
  - **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**]

[Verta Enterprise MLOps Platform https://www.verta.ai/platform/]

Model Management Systems (MLOps), cont.

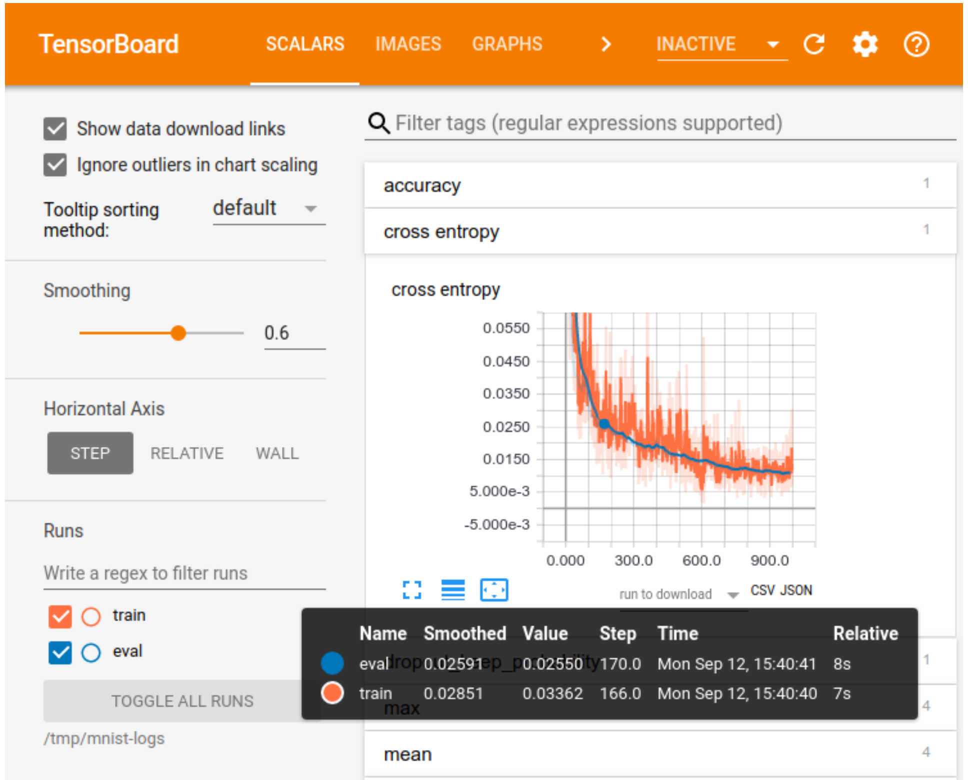
- **MLflow**
  - An open source platform for the machine learning lifecycle
  - Use of existing ML systems and various language bindings
  - **MLflow Tracking:** logging and querying experiments
  - **MLflow Projects:** packaging/reproduction of ML pipeline results
  - **MLflow Models:** deployment of models in various services/tools
  - **MLflow Model Registry:** cataloging models and managing deployment

[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**]

[Andrew Chen, Andy Chow, Aaron Davidson, Arjun DCunha, Ali Ghodsi, Sue Ann Hong, Andy Konwinski, Clemens Mewald, Siddharth Murching, Tomas Nykodym, Paul Ogilvie, Mani Parkhe, Avesh Singh, Fen Xie, Matei Zaharia, Richard Zang, Juntai Zheng, Corey Zumar: Developments in MLflow: A System to Accelerate the Machine Learning Lifecycle. **DEEM@SIGMOD 2020**]

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



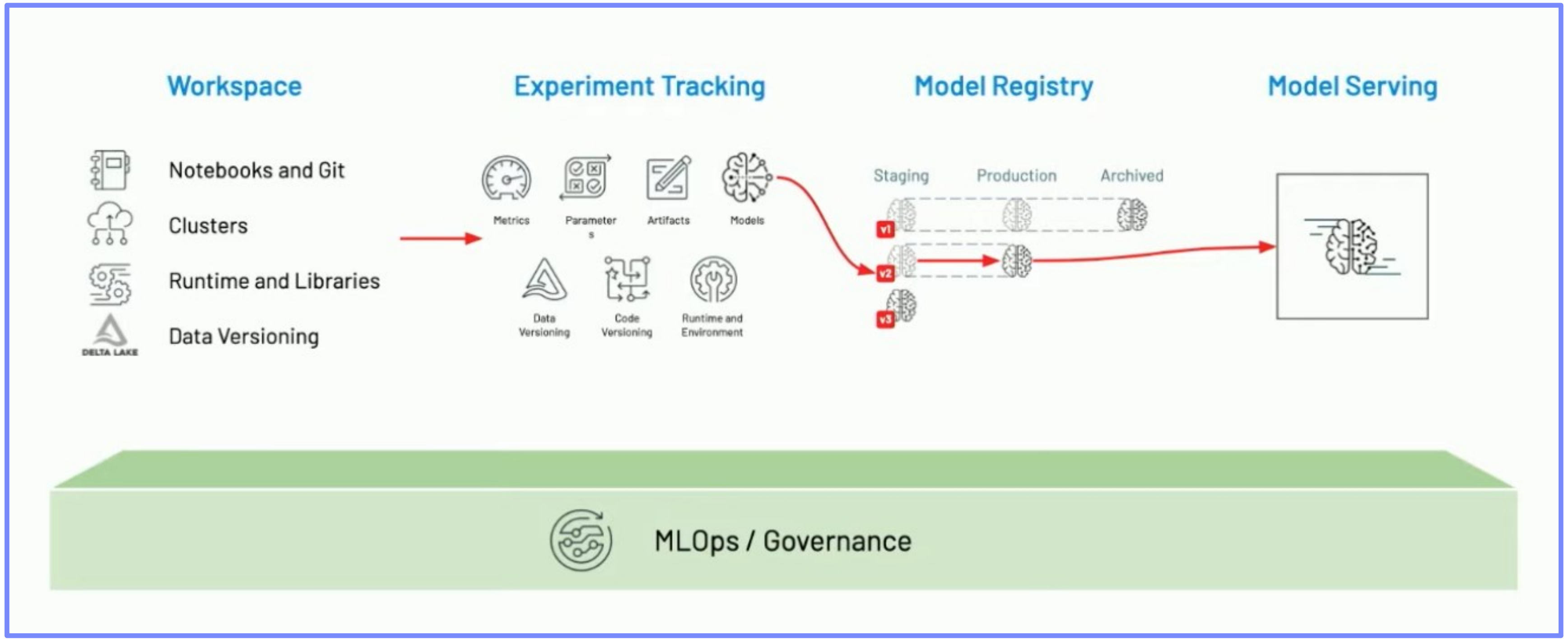
[**Credit:** https://www.tensorflow.org/guide/summaries_and_tensorboard]

ML Lifecycle Management

[Clemens Mewald: Announcing Databricks Machine Learning, Feature Store, AutoML, **Keynote Data+ AI Summit 2021**]

- **Databricks Machine Learning**
  - MLOps, Feature Store, AutoML

```
MLOps = DataOps + DevOps + ModelOps
```

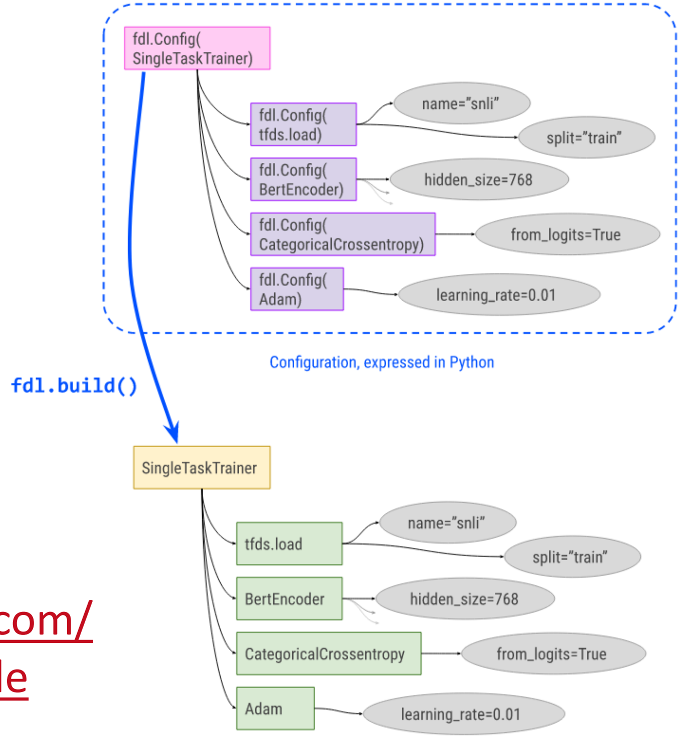


Configuration Management

- **#1 ML Collections**
  - Dictionary-like data structures for configurations of experiments and models (hyper-parameters, loss, optimizer)
  - `ConfigDict` and `FrozenConfigDict`

https://github.com/google/ml_collections

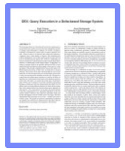
- **#2 Fiddle**
  - **Configurations for model training** with `build()` for creating training instances
  - **Auto-config** for creating a config object from a (control-flow-free) function
  - Explain and visualization



https://github.com/google/fiddle

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 Delta-based Storage System. **SIGMOD 2017**]

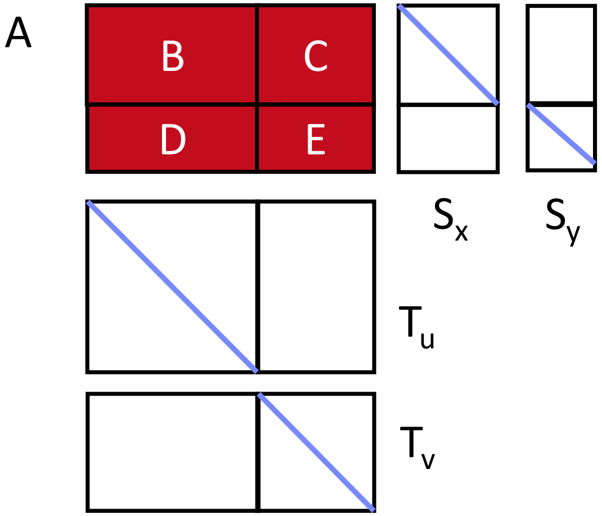
- **MISTIQUE: Intermediates of ML Pipelines**
  - Capturing, storage, querying of intermediates
  - **Lossy deduplication and compression**
  - Adaptive querying/materialization for finding efficient plans

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

- **Linear Algebra Provenance**
  - Provenance propagation by decomposition
  - Annotate parts w/ provenance polynomials (contributing inputs + impact)

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

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



Provenance for ML Pipelines (coarse-grained)

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

[**Credit:** https://databricks.com/blog/2018/06/05]

```
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

https://rise.cs.berkeley.edu/projects/jarvis/

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

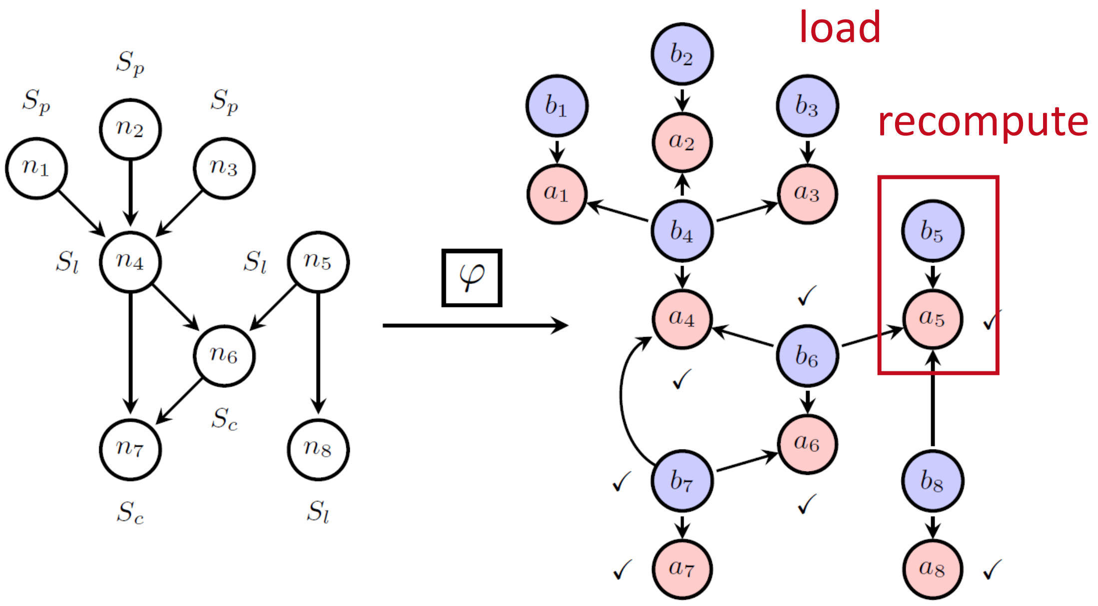
- **Dataset Relationship Management**
  - **Reuse**, **reveal**, **revise**, **retarget**, **reward**
  - Code-to-data relationships (data provenance)
  - Data-to-code relationships (potential transforms)

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

[Doris Xin, Stephen Macke, Litian Ma, Jialin Liu, Shuchen Song, Aditya G. Parameswaran: Helix: Holistic Optimization for Accelerating Iterative Machine Learning. **PVLDB 2018**]



- **Collaborative Optimizer**

[Behrouz Derakhshan, Alireza Rezaei Mahdiraji, Ziawasch Abedjan, Tilmann Rabl, Volker Markl: Optimizing Machine Learning Workloads in Collaborative Environments. **SIGMOD 2020**]

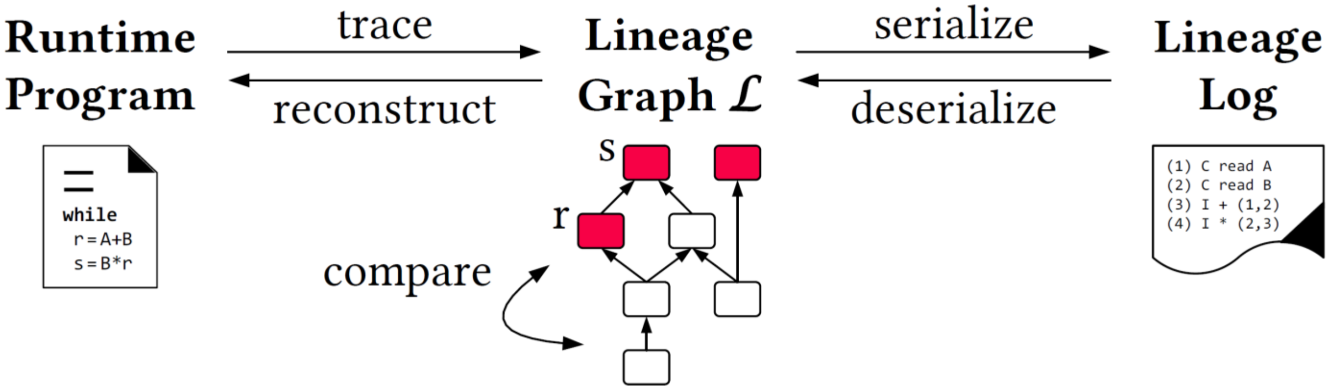
Lineage Tracing & Reuse in SystemDS

- **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)

[Arnab Phani, Benjamin Rath, Matthias Boehm: LIMA: Fine-grained Lineage Tracing and Reuse in Machine Learning Systems, **SIGMOD 2021**]

- **Efficient Lineage Tracing**
  - Tracing of inputs, literals, and **non-determinism**
  - **Trace lineage of logical operations**
  - **Deduplication** for loops/functions
  - Program/output reconstruction

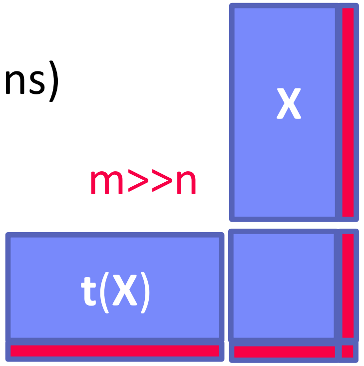


Lineage Tracing & Reuse in SystemDS, cont.

- **Multi-level, Lineage-based Reuse**
  - Lineage trace uniquely identifies intermediates
  - Reuse intermediates at function / block / operation level
- **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
- **Next Steps:** multi-backend, unified mem mgmt

```
for( i in 1:numModels )
  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)
} }
```

Summary & QA

- **Data Augmentation**
- **Model Selection Techniques**
- **Model Management & Provenance**

- **Next Lectures** (Part B)
  - **11 Model Debugging, Fairness, Explainability** [Jul 06]
  - **12 Model Serving Systems and Techniques** [Jul 13]