Automated Machine Learning (AutoML): A Tutorial

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Slides based on material from Frank Hutter and Joaquin Vanschoren
Tutorial based on Chapters 1-3 of the book Automated Machine Learning
Slides available at automl.org/events/tutorials -> AutoML Tutorial
(all references are clickable links)
Motivation: Successes of Deep Learning

Speech recognition

Computer vision in self-driving cars

Reasoning in games

Feurer and Elsken: AutoML
One Problem of Deep Learning

Performance is very **sensitive** to **many hyperparameters**

- Architectural hyperparameters

![Diagram showing architectural parameters](image)

- Units per layer
- Kernel size
- # convolutional layers
- # fully connected layers

Feurer and Elsken: AutoML
One Problem of Deep Learning

Performance is very **sensitive** to **many hyperparameters**

- **Architectural hyperparameters**
  - # convolutional layers
  - # fully connected layers
  - Units per layer
  - Kernel size

- Optimization algorithm, learning rates, momentum, batch normalization, batch sizes, dropout rates, weight decay, data augmentation, ...

❓ **Easily 20-50 design decisions**
Current deep learning practice

1. Expert chooses architecture & hyperparameters
2. Deep learning “end-to-end”
Deep Learning and AutoML

Current deep learning practice

- Expert chooses architecture & hyperparameters
- Deep learning “end-to-end”

Feurer and Elsken: AutoML
Deep Learning and AutoML

Current deep learning practice

Expert chooses architecture & hyperparameters → Deep learning “end-to-end”

AutoML: true end-to-end learning

End-to-end learning

Feurer and Elsken: AutoML
Deep Learning and AutoML

**Current deep learning practice**

- Expert chooses architecture & hyperparameters
- Deep learning “end-to-end”

**AutoML: true end-to-end learning**

- Meta-level learning & optimization
- Learning box

Feurer and Elsken: AutoML
Learning box is not restricted to deep learning

- Traditional machine learning pipeline:
  - Clean & preprocess the data
  - Select / engineer better features
  - Select a model family
  - Set the hyperparameters
  - Construct ensembles of models
  - ...

AutoML: true end-to-end learning
Outline

Part 1: General AutoML (by me, now)
1. AutoML by Hyperparameter Optimization
2. Black-box Hyperparameter Optimization
3. Beyond black-box optimization
4. Meta-learning
5. Examples of AutoML
6. Open issues and future work
7. Wrap-up & Conclusion

Part 2: Neural Architecture Search & Meta-Learning
(by Thomas Elsken, after the break)
Part 1: General AutoML

1. AutoML by Hyperparameter Optimization
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Part 2: Neural Architecture Search & Meta-Learning
**Definition: Hyperparameter Optimization (HPO)**

Let

- \( \lambda \) be the hyperparameters of a ML algorithm \( A \) with domain \( \Lambda \),
- \( \mathcal{L}(A_\lambda, D_{\text{train}}, D_{\text{valid}}) \) denote the loss of \( A \), using hyperparameters \( \lambda \) trained on \( D_{\text{train}} \) and evaluated on \( D_{\text{valid}} \).

The **hyperparameter optimization (HPO)** problem is to find a hyperparameter configuration \( \lambda^* \) that minimizes this loss:

\[
\lambda^* \in \arg \min_{\lambda \in \Lambda} \mathcal{L}(A_\lambda, D_{\text{train}}, D_{\text{valid}})
\]
Types of Hyperparameters

- \{SVM, RF, NN\}
- Example 2: activation function \(\in\) \{ReLU, Leaky ReLU, tanh\}
- Example 3: operator \(\in\) \{conv3x3, separable conv3x3, max pool, \ldots\}

- Special case: binary
Types of Hyperparameters

- **Continuous**
  
  Example: learning rate in NNs or GBMs

- \{SVM, RF, NN\}

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Types of Hyperparameters

- Continuous
  
  Example: learning rate in NNs or GBMs

- Integer
  
  Example: #units, #trees in GBM

- \{SVM, RF, NN\}
  
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- Special case: binary
Types of Hyperparameters

- \{\text{conv3x3}, \text{separable conv3x3}, \text{max pool}, \ldots\}\n- \{\text{ReLU}, \text{Leaky ReLU}, \text{tanh}\}\n- \{\text{SVM, RF, NN}\}\n
- **Continuous**
  
  Example: learning rate in NNs or GBMs

- **Integer**
  
  Example: \#units, \#trees in GBM

- **Categorical**
  
  - Finite domain, unordered
  
  - Special case: binary
    
    - Example 2: activation function \(\in\ \{\text{ReLU, Leaky ReLU, tanh}\}\)
    
    - Example 3: operator \(\in\ \{\text{conv3x3, separable conv3x3, max pool, \ldots}\}\)

  - Special case: binary
**Conditional hyperparameters** B are only active if other hyperparameters A are set a certain way.
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- Example 1:
  - A = choice of optimizer (Adam or SGD)
  - B = Adam’s second momentum hyperparameter (only active if A=Adam)
Conditional hyperparameters B are only active if other hyperparameters A are set a certain way

- **Example 1:**
  - A = choice of optimizer (Adam or SGD)
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- **Example 2:**
  - A = number of layers in a deep neural network
  - B = number of units in layer k (only active if A >= k)
Conditional hyperparameters B are only active if other hyperparameters A are set a certain way

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- **Example 2:**
  - A = number of layers in a deep neural network
  - B = number of units in layer k (only active if A >= k)

- **Example 3:**
  - A = choice of classifier (RF or SVM)
  - B = SVM’s kernel hyperparameter (only active if A = SVM)
Definition: Combined Algorithm Selection and Hyperparameter Optimization (CASH)

Let
- $\mathcal{A} = \{A^{(1)}, \ldots, A^{(n)}\}$ be a set of algorithms
- $\Lambda^{(i)}$ denote the hyperparameter space of $A^{(i)}$, for $i = 1, \ldots, n$
- $\mathcal{L}(A^{(i)}_\lambda, D_{train}, D_{valid})$ denote the loss of $A^{(i)}$, using $\lambda \in \Lambda^{(i)}$ trained on $D_{train}$ and evaluated on $D_{valid}$.

The Combined Algorithm Selection and Hyperparameter Optimization (CASH) problem is to find a combination of algorithm $A^* = A^{(i)}$ and hyperparameter configuration $\lambda^* \in \Lambda^{(i)}$ that minimizes this loss:

$$A^*_\lambda^* \in \arg \min_{A^{(i)} \in \mathcal{A}, \lambda \in \Lambda^{(i)}} \mathcal{L}(A^{(i)}_\lambda, D_{train}, D_{valid})$$
Illustration of the CASH problem in Auto-sklearn:

- 15 base classifiers
- Up to ten hyperparameters each
- Four levels of conditionality
AutoML as Hyperparameter optimization

Not limited to the classification algorithm:

See also Thornton et al. (KDD 2013) which introduced the CASH problem.
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Part 2: Neural Architecture Search & Meta-Learning
Blackbox Hyperparameter Optimization

DNN hyperparameter setting $\lambda$ → Train DNN and validate it → Validation loss $f(\lambda)$
DNN hyperparameter setting $\lambda$ → Validation loss $f(\lambda)$
Blackbox Hyperparameter Optimization

DNN hyperparameter setting $\lambda$ → Blackbox optimizer $\min f(\lambda) \ s.t. \ \lambda \in \Lambda$ → Validation loss $f(\lambda)$
The blackbox function is expensive to evaluate → sample efficiency is important
Grid Search and Random Search

- Both completely uninformed
- Grid search suffers from the curse of dimensionality
- Random search handles low intrinsic dimensionality better
- Example: an additive function \( y = f(x) + g(x) \)

Bergstra and Bengio, JMLR 2012; Image source: Feurer & Hutter, CC-BY 4.0

Feurer and Elsken: AutoML
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Feurer and Elsken: AutoML
Bayesian Optimization

Image source: Feurer & Hutter, CC-BY 4.0
Bayesian Optimization

Iteration 2

objective function

posterior mean

observation

posterior mean +/- stdev

acquisition max

Image source: Feurer & Hutter, CC-BY 4.0
Bayesian Optimization

Objective function

Posterior mean

Posterior mean +/- stdev

Observation

Acquisition max

Iteration 2

Iteration 3

New observation

Acquisition function

Image source: Feurer & Hutter, CC-BY 4.0
Bayesian Optimization

Iteration 2

- Objective function
- Posterior mean
- Acquisition max
- Observation
- Posterior mean +/- stddev

Iteration 3

- Objective function
- New observation
- Acquisition function

Iteration 4

- Posterior uncertainty
- Posterior mean

Image source: Feurer & Hutter, CC-BY 4.0
Acquisition Function: Expected Improvement

\[ f(x^+) \]

\[ \mu(x_1) - \sigma(x_1) \]

\[ \mu(x_2) \]

\[ \mu(x_2) - \sigma(x_2) \]

\[ \mu(x_3) \]

\[ \mu(x_3) + \sigma(x_3) \]

Image source: Brochu et al., arXiv:1012.2599
Bayesian Optimization

Approach

- Conduct an initial design
- Iteratively:
  - Fit a probabilistic model to the function evaluations $\langle \lambda, f(\lambda) \rangle$, most often a Gaussian process
  - Use that model to trade off Exploration vs. Exploitation in an acquisition function

Popular since Mockus [1974]

- Sample-efficient
- Works when objective is nonconvex, noisy, has unknown derivatives, etc
- Recent convergence results [Srinivas et al, 2010; Bull 2011; de Freitas et al, 2012; Kawaguchi et al, 2016; Nguyen et al., 2017; Berkenkamp et al., 2019]
- Excellent reviews by Shahriari et al. (IEEE, 2016) and Frazier (arXiv:1807.02811)
During the development of AlphaGo, its many hyperparameters were tuned with Bayesian optimization multiple times.

This automatic tuning process resulted in substantial improvements in playing strength. For example, prior to the match with Lee Sedol, we tuned the latest AlphaGo agent and this improved its win-rate from 50% to 66.5% in self-play games. This tuned version was deployed in the final match.

Of course, since we tuned AlphaGo many times during its development cycle, the compounded contribution was even higher than this percentage.

[Chen et al., arXiv:1812.06855]
Problems for standard Gaussian Process (GP) approach:

– **Complex hyperparameter space**
  * High-dimensional (low effective dimensionality) [e.g., Wang et al., 2013]
  * Mixed continuous/discrete hyperparameters [e.g., Hutter et al., 2011]
  * Conditional hyperparameters [e.g., Jenatton et al., 2017]

– **Noise**: sometimes heteroscedastic, large, non-Gaussian

– Model **overhead** (budget is runtime, not function evaluations)
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Simple solution used in SMAC: **random forests** [Breiman, 2001]

- Frequentist uncertainty estimate: variance across individual trees’ predictions [Hutter et al, 2011]
Simple solution used in SMAC: random forests [Breiman, 2001]

- Frequentist uncertainty estimate: variance across individual trees’ predictions [Hutter et al, 2011]
Other methods

- \( p(y | \lambda) \) is good) and \( p(\lambda \text{ is bad}) \), rather than \( p(y | \lambda) \).
Two recent promising models for Bayesian optimization

- Neural networks with Bayesian linear regression using the features in the output layer [Snoek et al, ICML 2015]
- Fully Bayesian neural networks, trained with stochastic gradient Hamiltonian Monte Carlo [Springenberg et al, NIPS 2016]

- $p(\lambda \text{ is good})$ and $p(\lambda \text{ is bad})$, rather than $p(y|\lambda)$
Other methods

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- Tree Parzen Estimator [Bergstra et al., 2011]
  - Ratio is proportional to Expected Improvement
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- Population-based methods
  - Genetic algorithms, evolutionary algorithms, evolutionary strategies, particle swarm optimization
  - Embarassingly parallel, conceptually simple
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- See **Chapter 1 of the AutoML book** for more information.
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Beyond Blackbox Hyperparameter Optimization

DNN hyperparameter setting $\lambda$ → Blackbox optimizer $\max f(\lambda) \quad \lambda \in \Lambda$ → Validation performance $f(\lambda)$
Beyond Blackbox Hyperparameter Optimization

DNN hyperparameter setting $\lambda$ → Blackbox optimizer $\underset{\lambda \in \Lambda}{\text{max}} f(\lambda)$ → Validation performance $f(\lambda)$

Too slow for DL / big data

Feurer and Elsken: AutoML
Main Approaches Going Beyond Blackbox HPO

- Extrapolation of learning curves
- Multi-fidelity optimization
- Meta-learning [next part]
- Hyperparameter gradient descent [see AutoML book]
- Parametric learning curve models [Domhan et al, IJCAI 2015]
- Bayesian neural networks [Klein et al, ICLR 2017]
- Linear combination of previous curves [Chandrashekaran and Lane, ECML2017]
Probabilistic Extrapolation of Learning Curves

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Use cheap approximations of the blackbox, performance on which correlates with the blackbox, e.g.

- Subsets of the data
- Fewer epochs of iterative training algorithms (e.g., SGD)
- Fewer trials in deep reinforcement learning
- Downsampled images in object recognition
Multi-Fidelity Optimization

- Use cheap approximations of the blackbox, performance on which correlates with the blackbox, e.g.
  - Subsets of the data
  - Fewer epochs of iterative training algorithms (e.g., SGD)
  - Fewer trials in deep reinforcement learning
  - Downsampling images in object recognition

- Also applicable in different domains, e.g., fluid simulations:
  - Less particles
  - Shorter simulations
Multi-fidelity Optimization

- Make use of cheap low-fidelity evaluations
  - E.g.: subsets of the data (here: SVM on MNIST)
Multi-fidelity Optimization

• Make use of cheap low-fidelity evaluations
  – E.g.: subsets of the data (here: SVM on MNIST)

                      0.0078% data       6.25% data       25% data       100% data

\[ \log(C) \quad \log(C) \quad \log(C) \quad \log(C) \]

\[ \log(\gamma) \quad \log(\gamma) \quad \log(\gamma) \quad \log(\gamma) \]

Size of subset (of MNIST)
Multi-fidelity Optimization

- **Make use of cheap low-fidelity evaluations**
  - E.g.: subsets of the data (here: SVM on MNIST)
    - 0.0078% data
    - 6.25% data
    - 25% data
    - 100% data

- Many cheap evaluations on small subsets
- Few expensive evaluations on the full data
- Up to 1000x speedups [Klein et al, AISTATS 2017]
Multi-fidelity Optimization

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Size of subset (of MNIST)

Feurer and Elsken: AutoML
Multi-fidelity Optimization

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  Fit a Gaussian process model $f(\lambda, b)$ to predict performance as a function of hyperparameters $\lambda$ and budget $b$
Multi-fidelity Optimization

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- Fit a Gaussian process model \( f(\lambda, b) \) to predict performance as a function of hyperparameters \( \lambda \) and budget \( b \)
- Choose both \( \lambda \) and budget \( b \) to maximize “bang for the buck”

A Simpler Approach: Successive Halving (SH)

Size of subset (of MNIST)

Feurer and Elsken: AutoML
**A Simpler Approach: Successive Halving (SH)**

- **Idea:** Use a bandit to allocate more budget to promising configurations

Size of subset (of MNIST)

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A Simpler Approach: Successive Halving (SH)

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- **Successive Halving** [Jamieson & Talwalkar, AISTATS 2016]
  - Randomly sample N configurations & evaluate on cheapest fidelity
  - Keep the top half, double its budget (or top third, triple budget)

![Graphs showing log validation error at different points](image_url)
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![Log Validation error at $s_{max}$](image1.png)
![Log Validation error at $s_{max}$](image2.png)
![Log Validation error at $s_{max}$](image3.png)
![Log Validation error at $s_{max}$](image4.png)

Size of subset (of MNIST)

Feurer and Elsken: AutoML
A Simpler Approach: Successive Halving (SH)

[Jamieson & Talwalkar, AISTATS 2016]

![Graph showing validation accuracy over wall-clock time](image-url)
Hyperband (its first 4 calls to SH)

[Li et al, JMLR 2018]
Hyperband (its first 4 calls to SH)

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Hyperband (its first 4 calls to SH)
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Each call to Successive Halving takes roughly the same amount of wallclock time!

[Li et al, JMLR 2018]
Advantages of Hyperband

- Strong anytime performance
- General-purpose
  - Low-dimensional continuous spaces
  - High-dimensional spaces with conditionality, categorical dimensions, etc
- Easy to implement
- Scalable
- Easily parallelizable

[Bohb: Bayesian Optimization & Hyperband][Falkner, Klein & Hutter, ICML 2018]

Feurer and Elsken: AutoML
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Advantage of Bayesian optimization: strong final performance
Advantages of Hyperband

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Advantage of Bayesian optimization: strong final performance

Combining the best of both worlds in BOHB

- Bayesian optimization
  - for choosing the configurations to evaluate (using a TPE variant)
- Hyperband
  - for deciding how to allocate budgets
Hyperband vs. Random Search

Biggest advantage: much improved **anytime performance**

Auto-Net on dataset adult

Feurer and Elsken: AutoML
Hyperband vs. Random Search

Biggest advantage: much improved anytime performance

Auto-Net on dataset adult

Feurer and Elsken: AutoML
Hyperband vs. Random Search

Biggest advantage: much improved *anytime performance*

Auto-Net on dataset adult

Feurer and Elsken: AutoML
Bayesian Optimization vs Random Search

Biggest advantage: much improved **final performance**

Auto-Net on dataset adult

Feurer and Elsken: AutoML
Bayesian Optimization vs Random Search

Biggest advantage: much improved final performance

Auto-Net on dataset adult

Feurer and Elsken: AutoML
Combining Bayesian Optimization & Hyperband

Best of both worlds: strong anytime and final performance

Auto-Net on dataset adult

Feurer and Elsken: AutoML
Combining Bayesian Optimization & Hyperband

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Feurer and Elsken: AutoML
Combining Bayesian Optimization & Hyperband

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Auto-Net on dataset adult
Combining Bayesian Optimization & Hyperband

Best of both worlds: strong *anytime and final performance*

Auto-Net on dataset adult

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Task $T_T$
Blackbox Hyperparameter Optimization

DNN hyperparameter setting $\lambda$ → Blackbox optimizer \[ \min_{\lambda \in \Lambda} f(\lambda) \] → Validation loss $f(\lambda)$

Task $T_T$

Meta-knowledge

Previous Task $T_0$  Previous Task $T_1$  ...  Previous Task $T_{T-1}$
Analogy to manual hyperparameter optimization:
• Accumulate knowledge over time
• Use Knowledge when optimizing on a new dataset
Task-independent recommendations

- Idea: learn a sorted list of defaults

- Advantages:
  - Easy to share and use
  - Strong anytime performance
  - Embarrassingly parallel

- Disadvantages:
  - Not adaptive

[Wistuba et al., 2015a, b, Feurer et al., 2018, Pfisterer et al., 2018]
Task-independent recommendations

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Task-independent recommendations

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  - Disadvantages:
    - Not adaptive

  - Method:
    - Mostly greedy

  - Results
    - Improves over Random Search and Bayesian Optimization

[Wistuba et al., 2015a,&b, Feurer et al., 2018, Pfisterer et al., 2018]
Joint model for Bayesian optimization

• Jointly train a “deep” neural network on all tasks
• Have a separate output layer (head) for each task
• Each head is a Bayesian linear regression
• Feature extraction on hyperparameter configurations
Joint model for Bayesian optimization

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[Perone et al., NeurIPS 2018]
Joint model for Bayesian optimization

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[Perrone et al., NeurIPS 2018]
Analyzing the effect of hyperparameters

- Search Space Pruning [Wistuba et al., ECMLPKDD 2015]
  - Rate all candidate configurations by their potential on past datasets
  - Drop the ones with low potential (plus some space around)
Analyzing the effect of hyperparameters

- **Search Space Pruning** [Wistuba et al., ECMLPKDD 2015]
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- **Hyperparameter importance** [van Rijn and Hutter, KDD 2018]
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What can be automated?

Image credit: Rich Caruana, AutoML 2015
Example I – Data cleaning and ingestion

- Automatically detect the dialect of CSV files [van den Burg et al., arXiv:1811.11242]
- Automatically classify data types [Valera and Ghahramani, ICML 2017]
- Automatically detect mistakes in the data gathering process [Sutton et al., KDD 2018]
- Check out the talk of Charles Sutton@AutoML Workshop 2019
Example II – Feature Engineering

- From relational data bases:
  - Automatically aggregates information, can for example generate the *average sum of orders*
  - Requires post-hoc pruning of the features
    - [Kanter and Veeramachaneni, DSAA 2015]
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- From featurized data:
  - Generate candidate features by applying
    - unary (normalization, discretization, sqrt, square, log etc.)
    - binary (+,-,*,/)
    - higher order (GroupByThen)
  - Use search mechanism to perform guided exploration
  - Use feature selection to remove unnecessary features again
    - [Smith and Bull, GP&EM 2005, Katz et al., ICDM 2016]
Example III: Off-the-shelf Algorithms

- Reduce the amount of tuning:
  - Random Forests are excellent default classifiers
  - Learning rate adaption
    - rProp
    - RMSProp
    - ...
    - Adam
    - ...
    - Ranger (look ahead + rectified Adam)
  - Pre-trained Neural Networks
  - Better defaults
  - ...

Feurer and Elsken: AutoML
Part 1: General AutoML

1. AutoML by Hyperparameter Optimization
2. Black-box Hyperparameter Optimization
3. Beyond black-box optimization
4. Meta-learning
5. Examples of AutoML
6. Open issues and future work
7. Wrap-up & Conclusion

Part 2: Neural Architecture Search & Meta-Learning
While a commonly cited reason for the pressing need for effective and efficient data mining algorithms is the growing number of huge databases, the data mining research community almost never gets to see those databases. **Most databases available for empirical studies are ridiculously small.** Unless a number of realistic and big databases become publically available, the only way to fill the gap seems to be the use of artificially generated databases.

Johann Petrak, 2000
Access to real-world large-scale datasets

• The current state:
Access to real-world large-scale datasets

• The current state:
  • Many image datasets available -> good for NAS
Access to real-world large-scale datasets

- The current state:
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• What do we need:
  • Large real-world datasets
  • Many of them
  • Machine readable description
Access to real-world large-scale datasets

• The current state:
  • Many image datasets available -> good for NAS
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• What do we need:
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  • Many of them
  • Machine readable description

• Call for contribution:
  • If you have a paper which introduces a new dataset
  • or if you have a paper which uses large datasets
  • or if you have large datasets at hand
  ⇒ upload them to OpenML.org
• Collaborative machine learning
• Share:
  • Datasets
  • Tasks
  • Runs
• APIs in Python, R and Java
• Learn more on OpenML.org & get involved today!

[Van den Bosch et al., SIGKDD 2014]
Search space representation

Bounded representation

1. Creation of bounds still requires expert knowledge
2. Dynamic extension possible, but not widely used
   [Bergstra et al., NeurIPS 2011, Shahriari et al., AISTATS 2015]
3. AutoML tools ship with search spaces
4. If you release an algorithm, also release the search space and make magic constants tunable, too [Hoos, 2012]

Pipeline construction?
• See https://www.slideshare.net/JoaquinVanschoren/automl-lectures-acdl-2019

Feurer and Elsken: AutoML
Overfitting on HPO level possible

Alleviate by:

- More data [Levesque, 2018]
- Reshuffle the train-valid split each iteration [Levesque, 2018]
- Separate selection split [Zeng and Luo, Hiss 2017; Mohr et al., ML 2018; Levesque, 2018]
- Stable optima [Nguyen et al., PAKDD 2017]
- Ensembling [Momma and Bennett, 2002; Escalante et al., 2009; Bürger and Pauli, 2015; Feurer et al., 2015]
What can be automated?

Image credit: Rich Caruana, AutoML 2015
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Image credit: Rich Caruana, AutoML 2015
What can be automated?

$\{X_{train}, Y_{train}, X_{test}, L\}$

meta-learning

Bayesian optimizer

data preprocessor

feature preprocessor

classifier

ML framework

AutoML system

build ensemble

$\hat{Y}_{test}$

Problem Definition

Data Collection

Data Cleaning

Data Coding

Metric Selection

Algorithm Selection

Parameter Optimization

Post-Processing

Deployment

Online Evaluation

Debug

Image credit: Rich Caruana, AutoML 2015
Outline

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Part 2: Neural Architecture Search & Meta-Learning
If you have access to multiple fidelities

- We recommend **BOHB** [Falkner et al, ICML 2018]
- [https://github.com/automl/HpBandSter](https://github.com/automl/HpBandSter)
- Combines the advantages of Bayesian optimization and Hyperband

If you do not have access to multiple fidelities

- Low-dim. continuous: GP-based BO (e.g., BoTorch, MLRMBO, Sigopt, GP version of SMACv3)
- High-dim, categorical, conditional: SMAC or Hyperopt
- Purely continuous, budget >10x dimensionality: CMA-ES
Open-source AutoML Tools based on HPO

- **Auto-WEKA** [Thornton et al, KDD 2013]
  - 768 hyperparameters, 4 levels of conditionality
  - Based on WEKA and SMAC

- **Hyperopt-sklearn** [Komer et al, SciPy 2014]
  - Based on scikit-learn & TPE

- **Auto-sklearn** [Feurer al, NeurIPS 2015]
  - Based on scikit-learn & SMAC
  - Uses meta-learning and posthoc ensembling
  - Won AutoML competitions 2015-2016 & 2017-2018

- **H2O AutoML** [no reference]
  - Uses implementations from H2O.ai
  - Based on random search and stacking

- **TPOT** [Olson et al, EvoApplications 2016]
  - Based on scikit-learn and evolutionary algorithms

- **ML-PLAN** [Mohr et al., Machine Learning 2018]
  - Based on WEKA and Hierarchical Task Networks
Auto-sklearn also won the last two phases of the AutoML challenge human track (!)

- It performed better than up to 130 teams of human experts
- It is open-source (BSD) and trivial to use:
Auto-sklearn also won the last two phases of the AutoML challenge human track (!)

- It performed better than up to 130 teams of human experts
- It is open-source (BSD) and trivial to use:

```python
import autosklearn.classification as cls
automl = cls.AutoSklearnClassifier()
automl.fit(X_train, y_train)
y_hat = automl.predict(X_test)
```

[automl.github.io/auto-sklearn](https://automl.github.io/auto-sklearn)
What have we learned?

1. **AutoML by Hyperparameter Optimization**
   AutoML can be phrased as an HPO problem

2. **Black-box Hyperparameter Optimization**
   We reviewed Bayesian optimization

3. **Beyond black-box optimization**
   Practically applicable by using domain knowledge

4. **Meta-learning**
   Increase practicality by using previous data

5. **Examples**
   AutoML can be used in almost every step of the ML pipeline

6. **Open issues and future work**
   Datasets, search space representation & overfitting
Further reading

- Automated Machine Learning: Methods, Systems, Challenges
  - Edited by Frank Hutter, Lars Kotthoff and Joaquin Vanschoren
  - Contains introductions to HPO, Meta-Learning and NAS

- Various literature reviews on arXiv:
  - 1908.05557: Focus on open source software
  - 1810.13306: General and comprehensive
  - 1908.00709: Focuses mostly on NAS
  - 1905.01392: NAS survey

- AutoML workshop video recordings
  - icml2019.automl.org
Thank you for your attention!

Special thanks to Frank Hutter and Joaquin Vanschoren for providing me with the slides this presentation is based on.

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