Automatic Machine Learning (AutoML): A Tutorial

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Slides available at automl.org/events -> AutoML Tutorial
(all references are clickable links)

Motivation: Successes of Deep Learning

Computer vision in self-driving cars

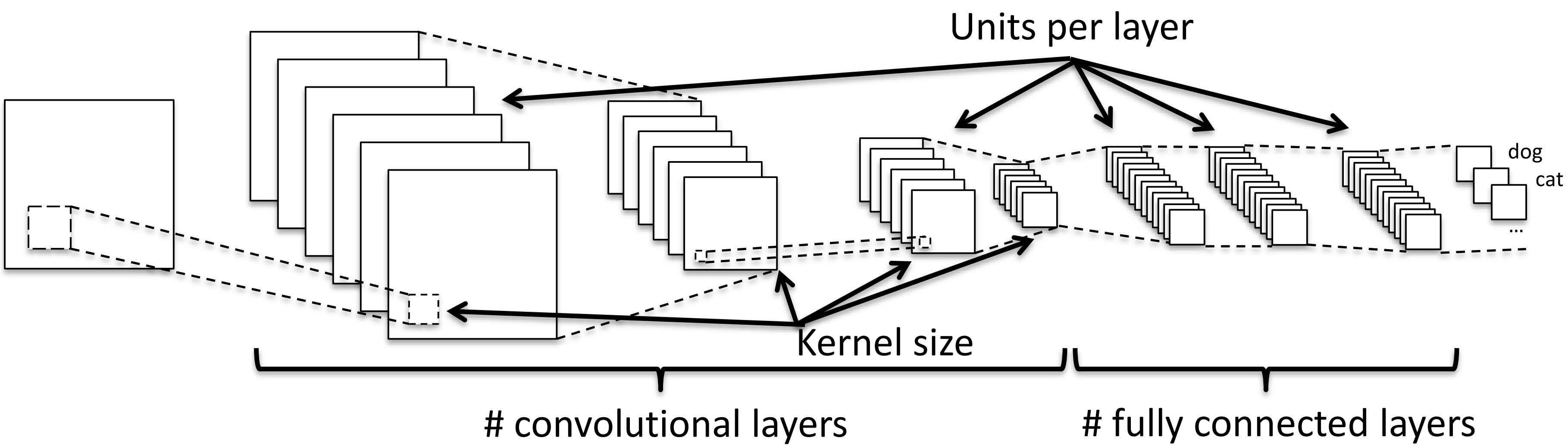
Speech recognition

Reasoning in games

One Problem of Deep Learning

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

- Architectural hyperparameters

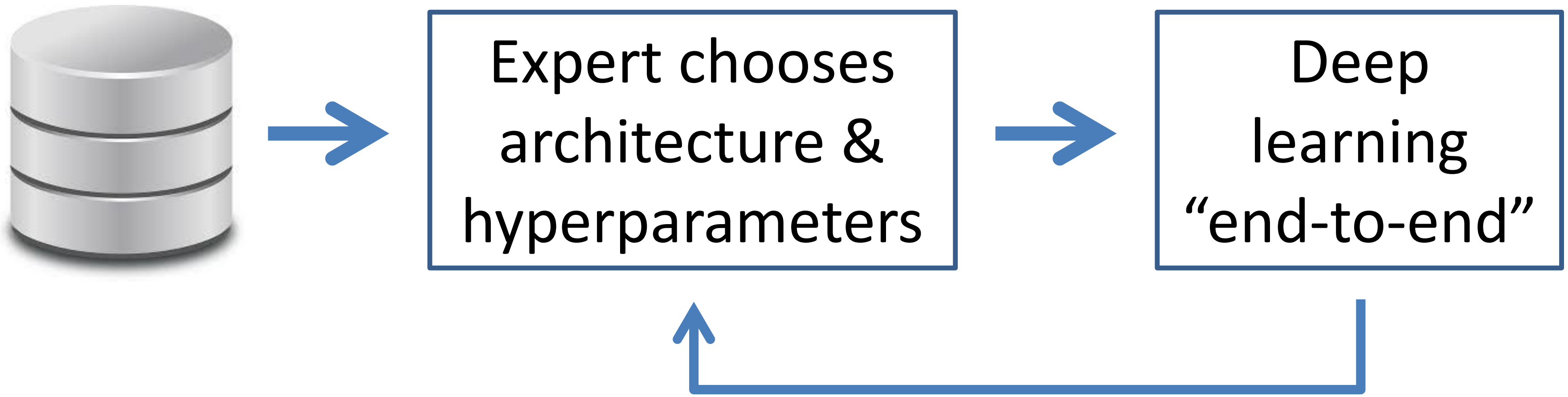


- Optimization algorithm, learning rates, momentum, batch normalization, batch sizes, dropout rates, weight decay, data augmentation, …

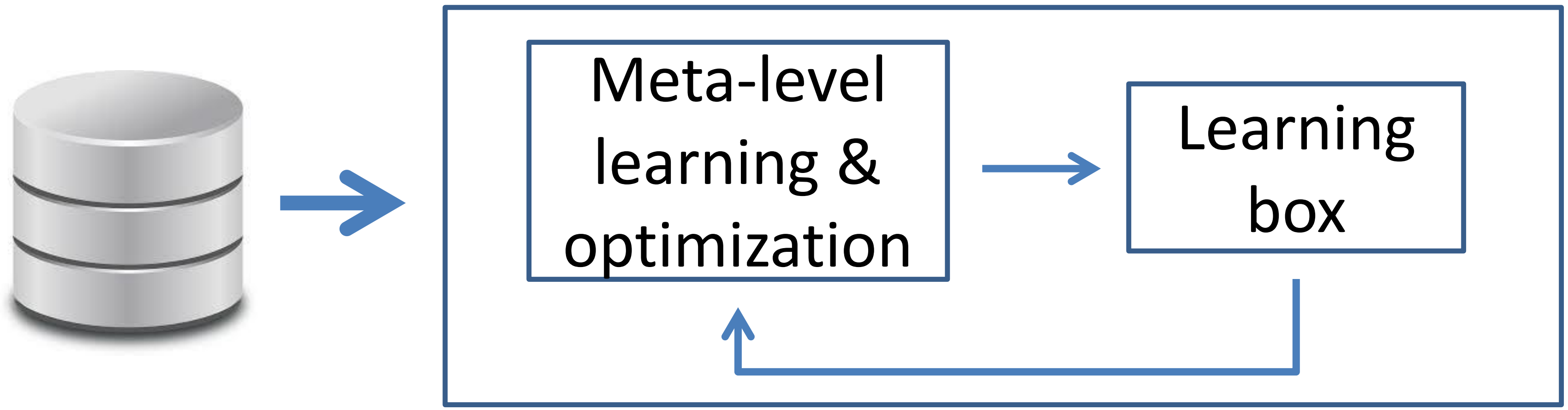
→ **Easily 20-50 design decisions**

Deep Learning and AutoML

Current deep learning practice



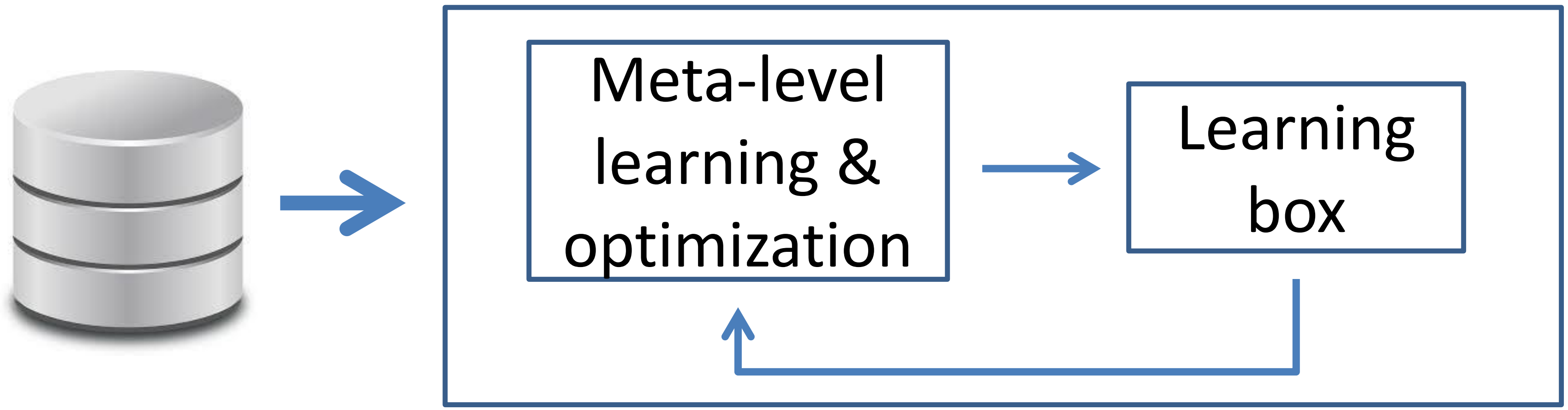
AutoML: true end-to-end learning



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

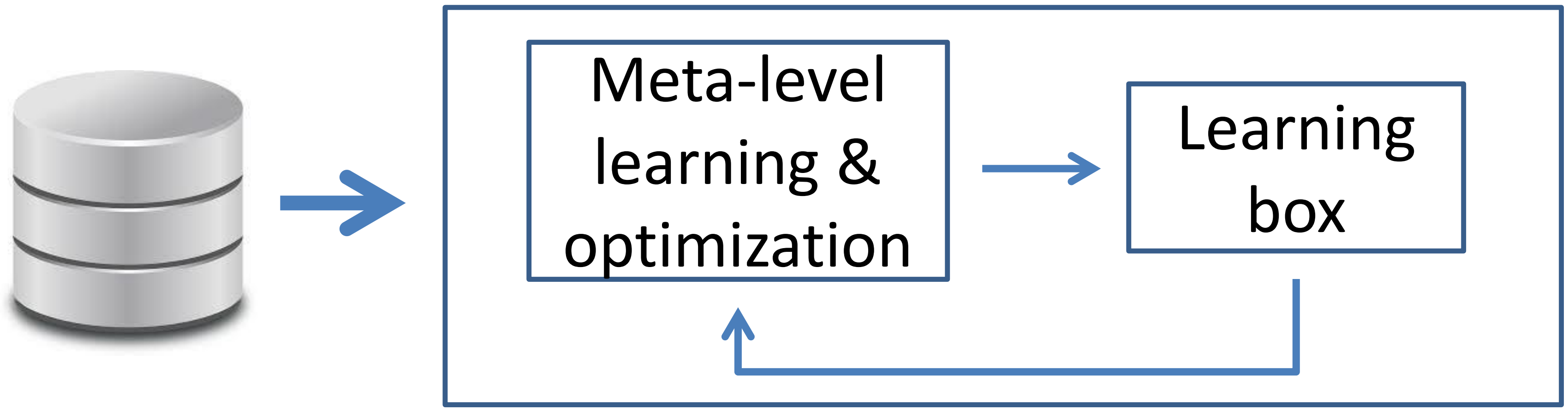


Outline

1. Modern Hyperparameter Optimization
2. Neural Architecture Search
3. Meta Learning

For more details, see: automl.org/book

AutoML: true end-to-end learning



Outline

1. Modern Hyperparameter Optimization

- AutoML as Hyperparameter Optimization
- Blackbox Optimization
- Beyond Blackbox Optimization

Based on: Feurer & Hutter: Chapter 1 of the AutoML book: Hyperparameter Optimization

2. Neural Architecture Search

- Search Space Design
- Blackbox Optimization
- Beyond Blackbox Optimization

Hyperparameter Optimization

Definition: Hyperparameter Optimization (HPO)

Let

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

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

$$\boldsymbol{\lambda}^* \in \operatorname*{arg\,min}_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \mathcal{L}(A_{\boldsymbol{\lambda}}, D_{train}, D_{valid})$$

Types of Hyperparameters

- Continuous
  - Example: learning rate
- Integer
  - Example: #units
- Categorical
  - Finite domain, unordered
    - Example 1: algo ∈ {SVM, RF, NN}
    - Example 2: activation function ∈ {ReLU, Leaky ReLU, tanh}
    - Example 3: operator ∈ {conv3x3, separable conv3x3, max pool, …}
  - Special case: binary

Conditional hyperparameters

- Conditional hyperparameters B are only active if other hyperparameters A are set a certain way
  - Example 1:
    - A = choice of optimizer (Adam or SGD)
    - B = Adam's second momentum hyperparameter (only active if A=Adam)
  - Example 2:
    - A = type of layer k (convolution, max pooling, fully connected, ...)
    - B = conv. kernel size of that layer (only active if A = convolution)
  - Example 3:
    - A = choice of classifier (RF or SVM)
    - B = SVM's kernel parameter (only active if A = SVM)

AutoML as Hyperparameter Optimization

Definition: Combined Algorithm Selection and Hyperparameter Optimization (CASH)

Let

- $\mathcal{A} = \{A^{(1)}, \ldots, A^{(n)}\}$ be a set of algorithms
- $\mathbf{\Lambda}^{(i)}$ denote the hyperparameter space of $A^{(i)}$, for $i = 1, \ldots, n$
- $\mathcal{L}(A^{(i)}_{\boldsymbol{\lambda}}, D_{train}, D_{valid})$ denote the loss of $A^{(i)}$, using $\lambda \in \mathbf{\Lambda}^{(i)}$ 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 $\boldsymbol{\lambda}^* \in \mathbf{\Lambda}^{(i)}$ that minimizes this loss:

$$A^*_{\boldsymbol{\lambda}^*} \in \operatorname*{arg\,min}_{A^{(i)} \in \mathcal{A}, \boldsymbol{\lambda} \in \mathbf{\Lambda}^{(i)}} \mathcal{L}(A^{(i)}_{\boldsymbol{\lambda}}, D_{train}, D_{valid})$$

→ Simply a HPO problem with a top-level hyperparameter (choice of algorithm) that all other hyperparameters are conditional on

- E.g., Auto-WEKA: 768 hyperparameters, 4 levels of conditionality