Automated Machine Learning

DS&AI Conference, 4 October 2022, Bangkok

Matthias König

Universiteit Leiden

This slide deck was prepared together with Mike Huisman

Automated Machine Learning

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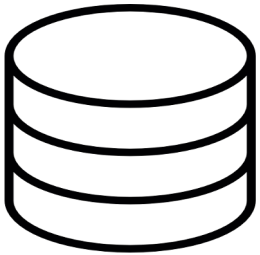
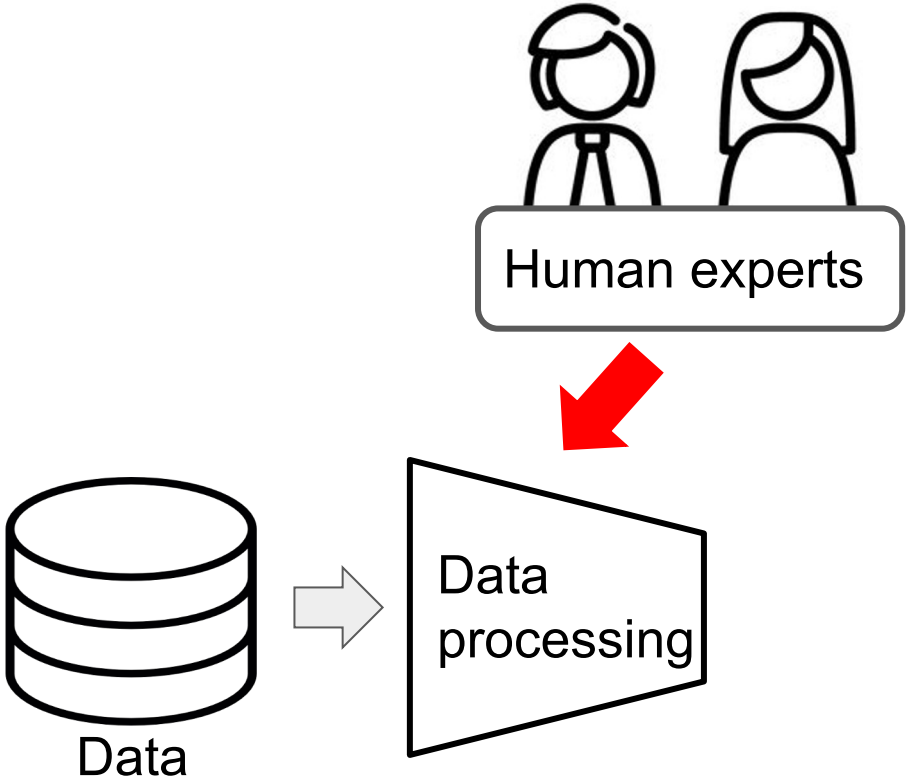
Machine learns to perform task(s) from data

Automated Machine Learning



Data

Automated Machine Learning



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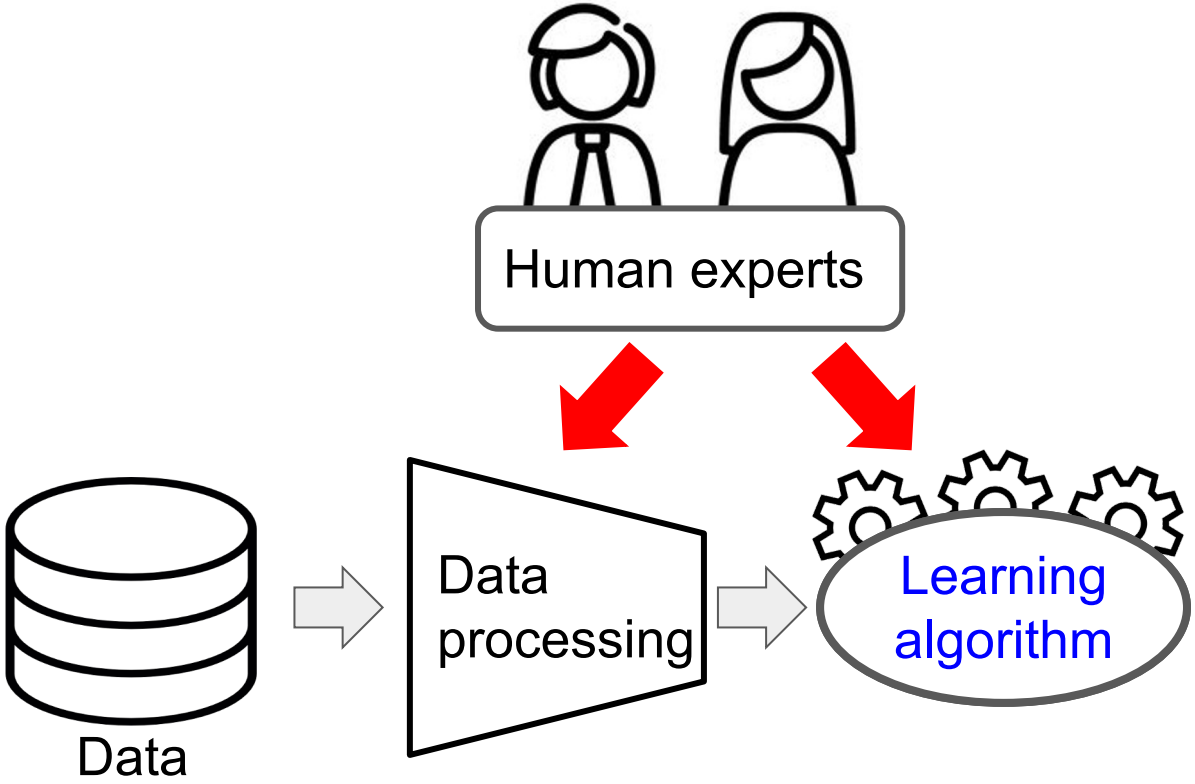

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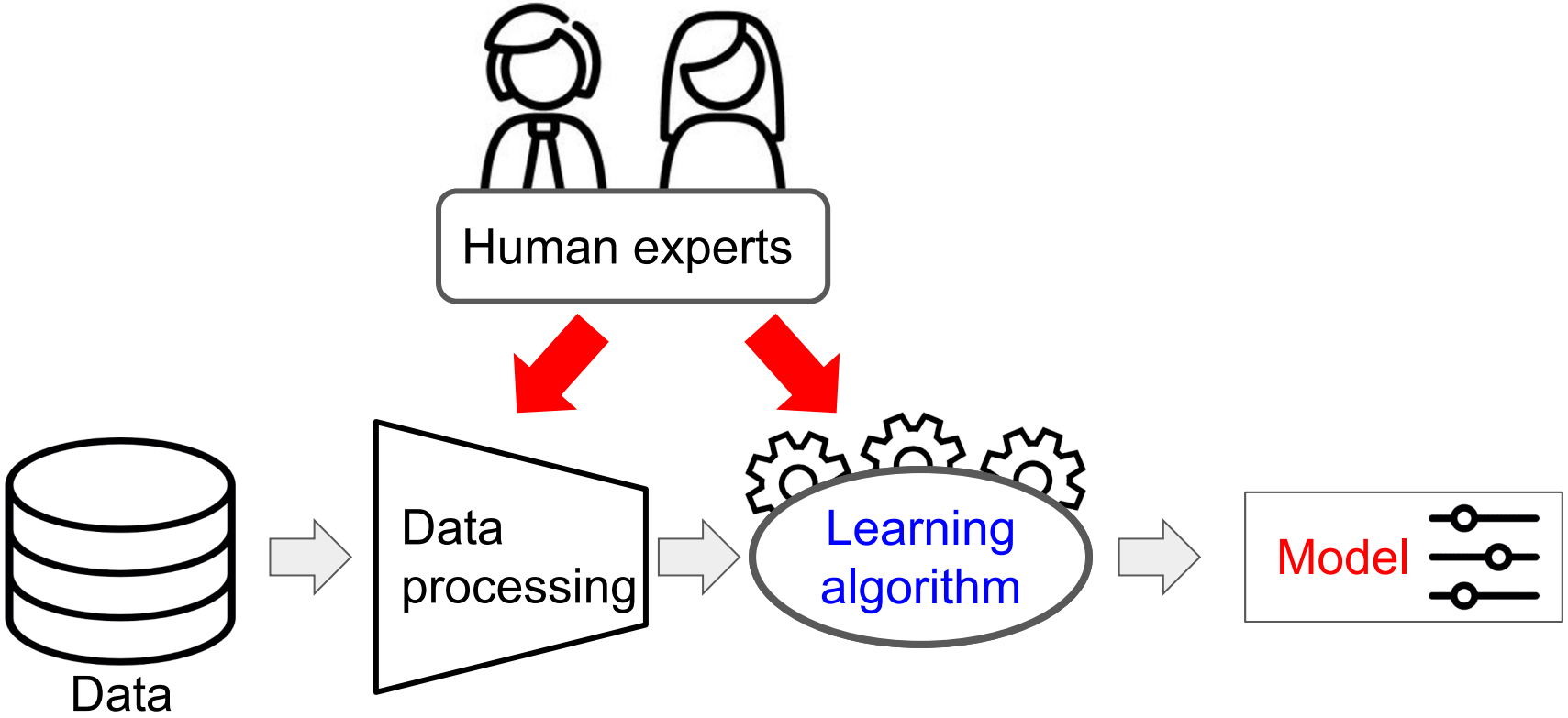

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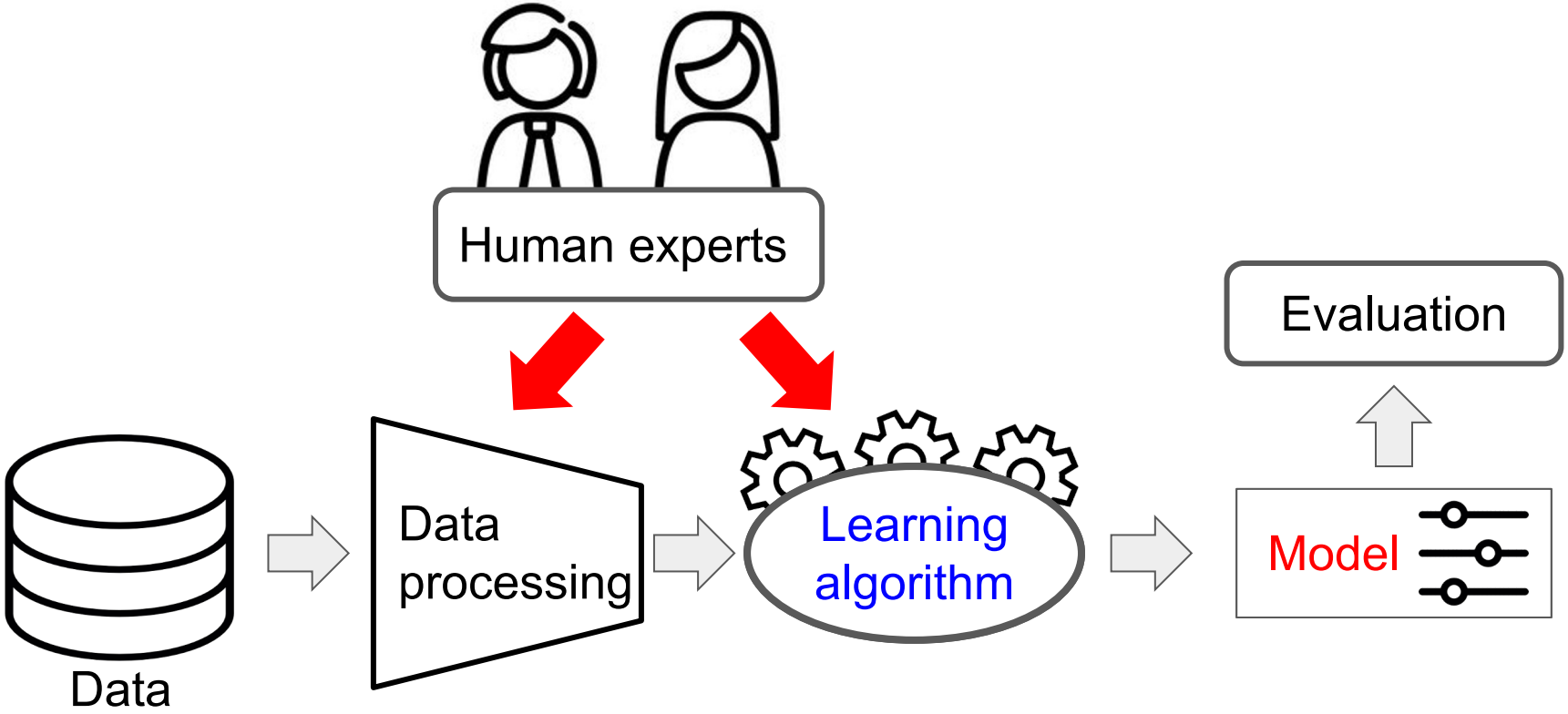

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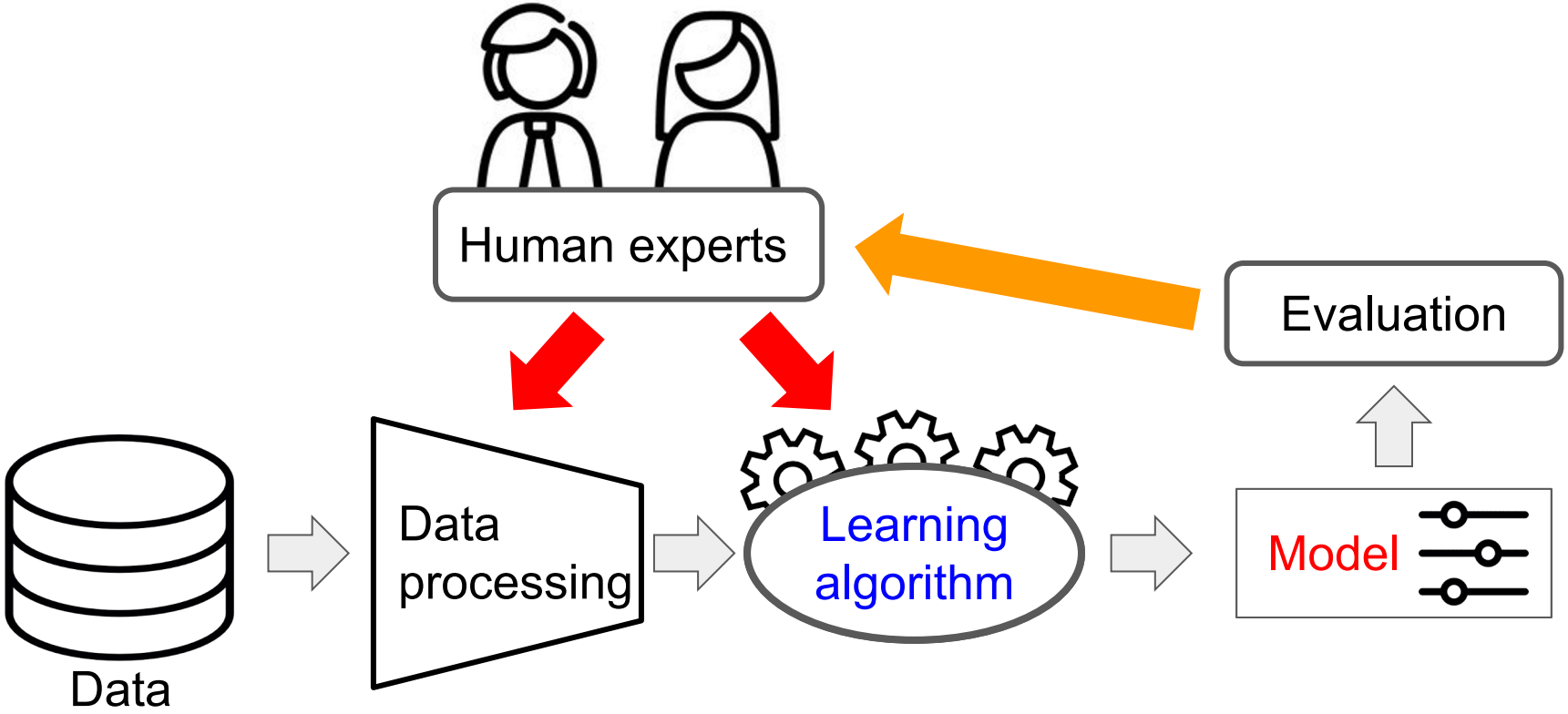
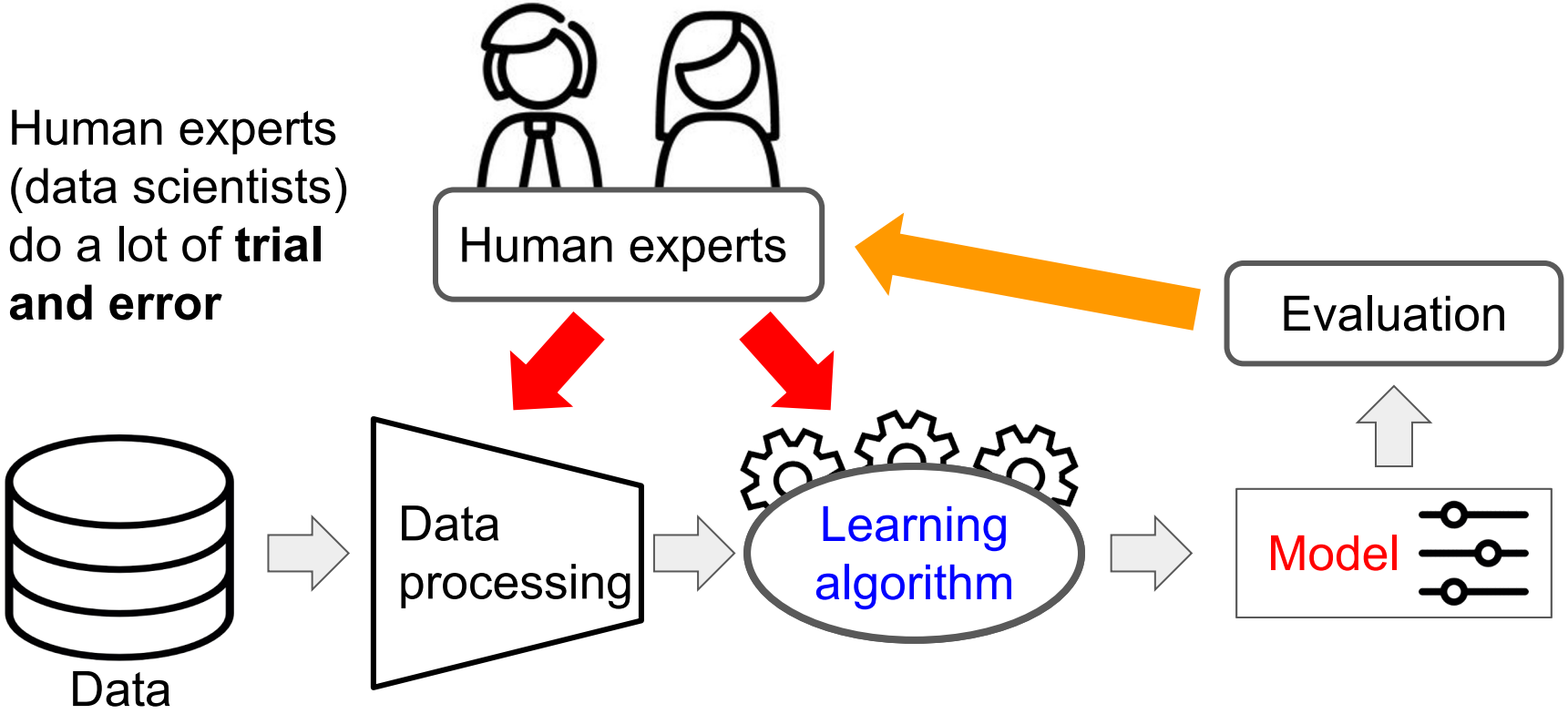


Automated Machine Learning

Human experts (data scientists) do a lot of **trial and error**



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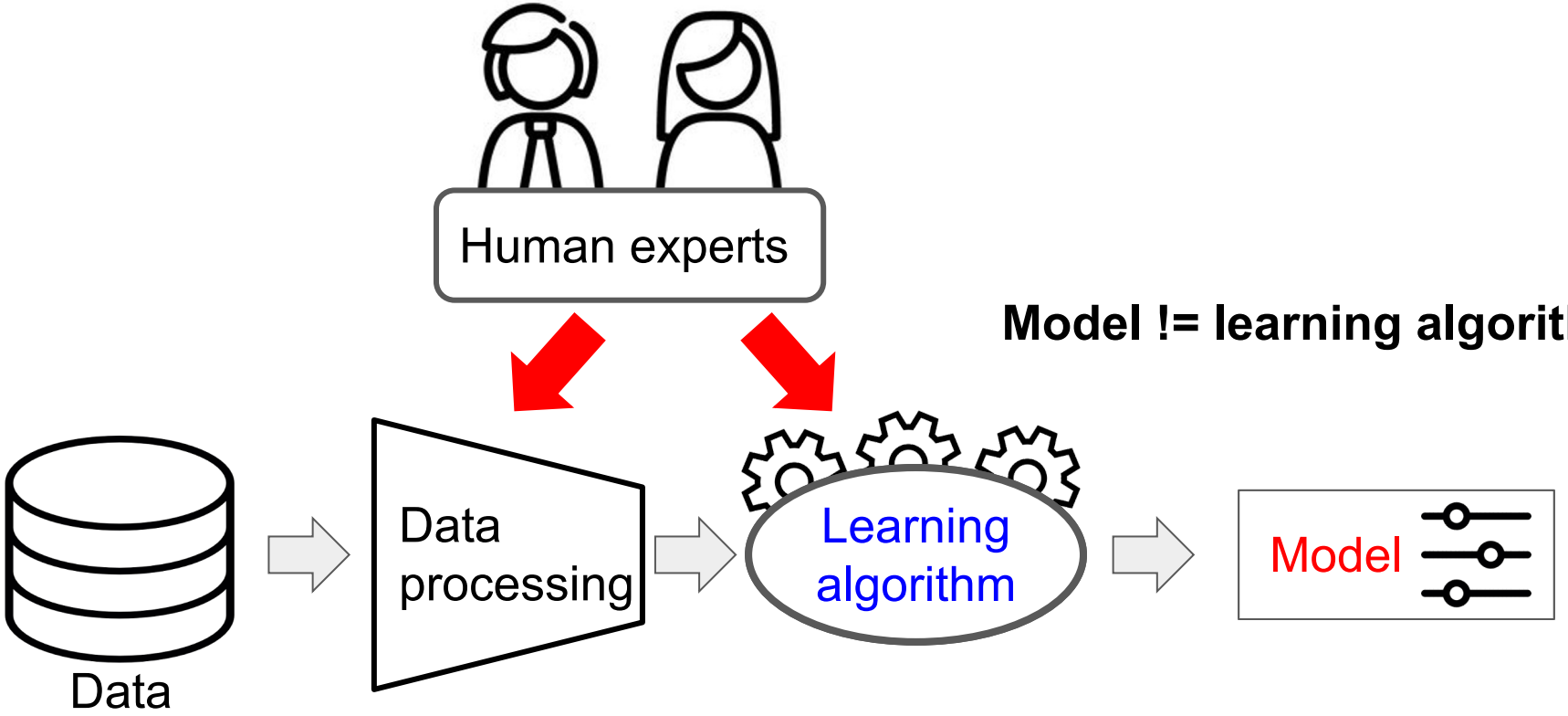

Model != learning algorithm

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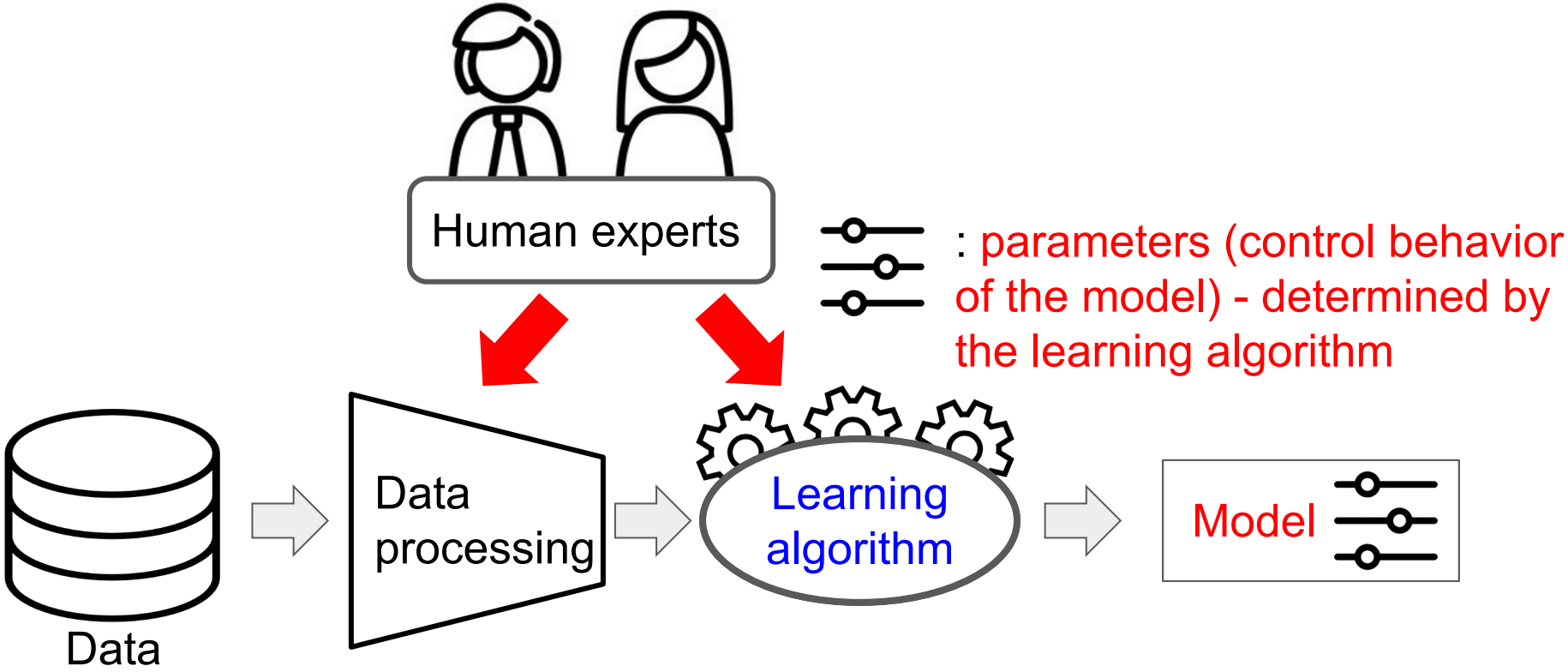

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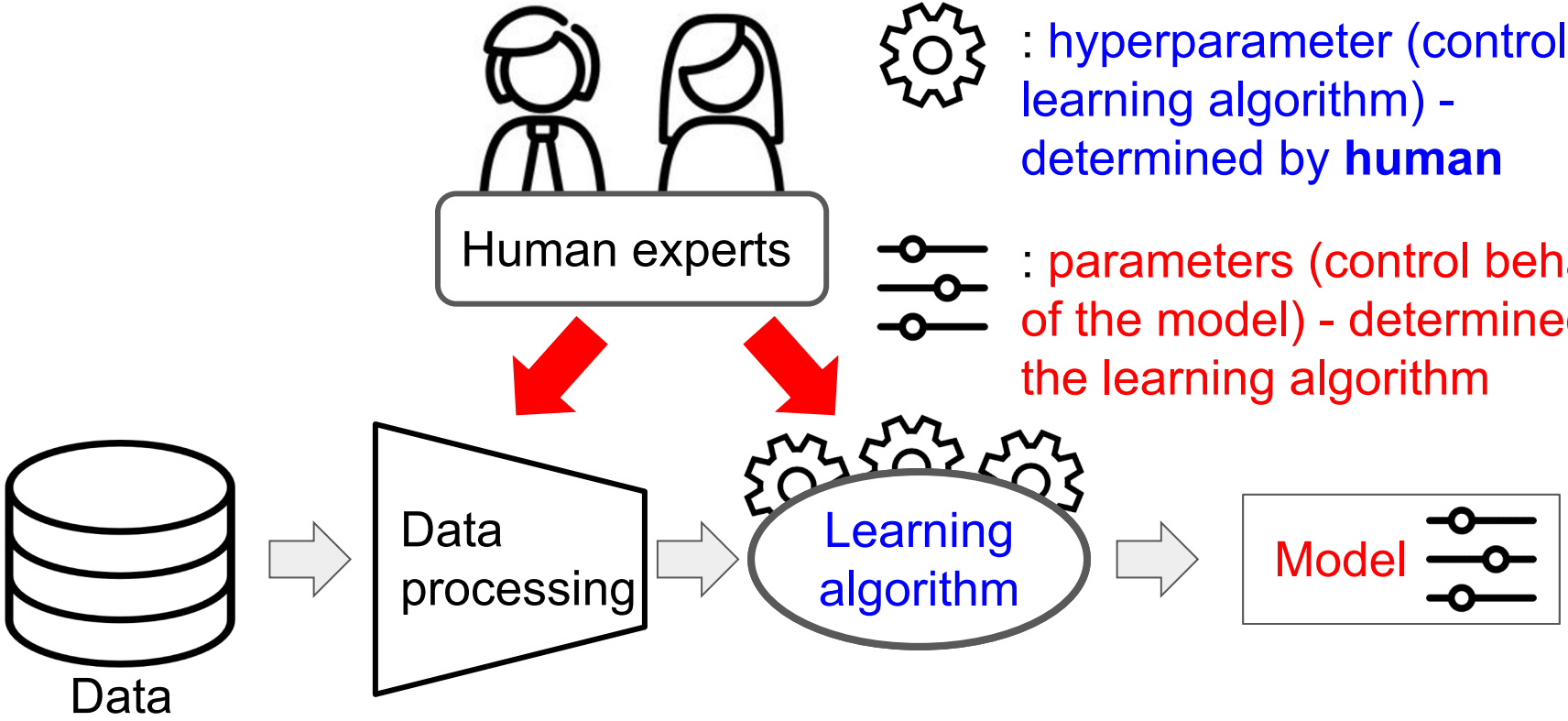

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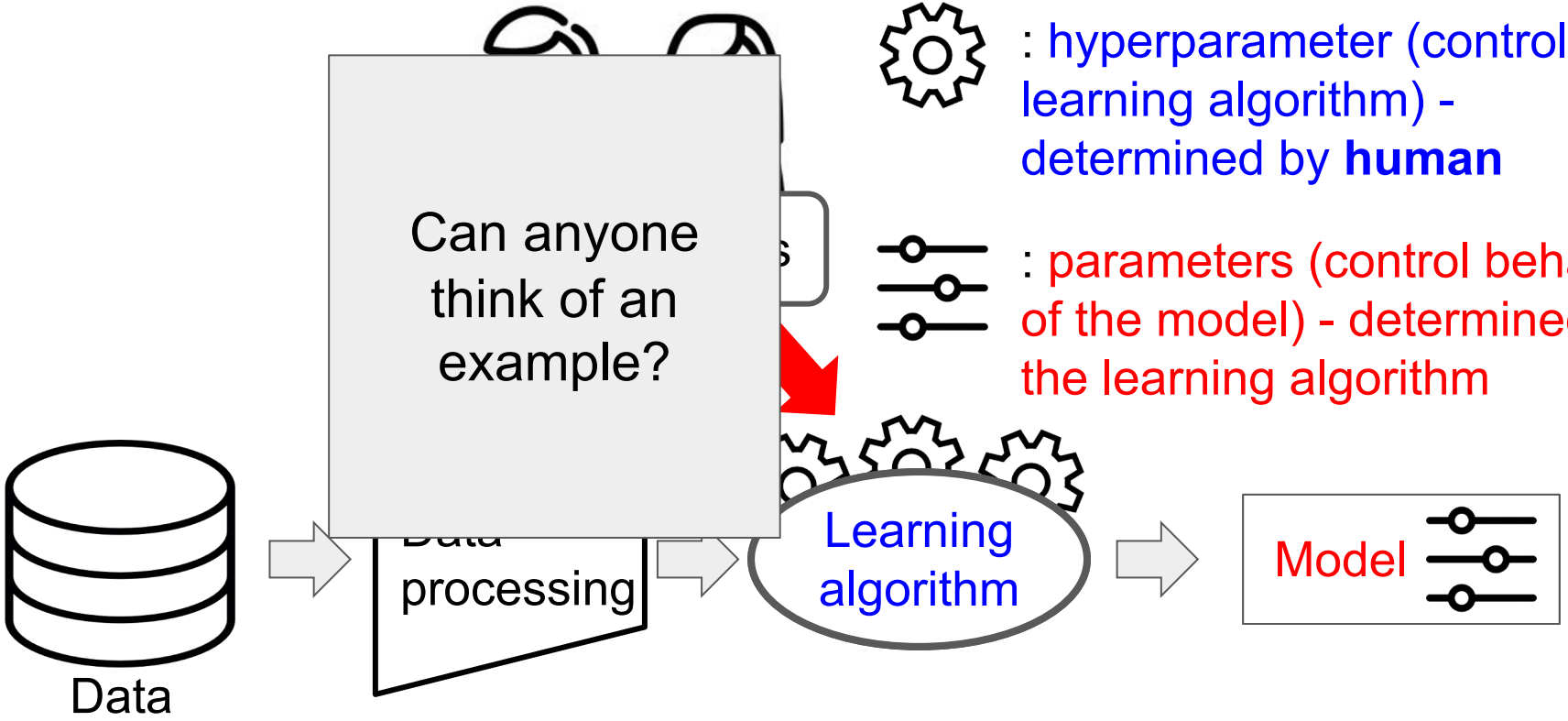

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Automated Machine learning = Automating one or more of these things

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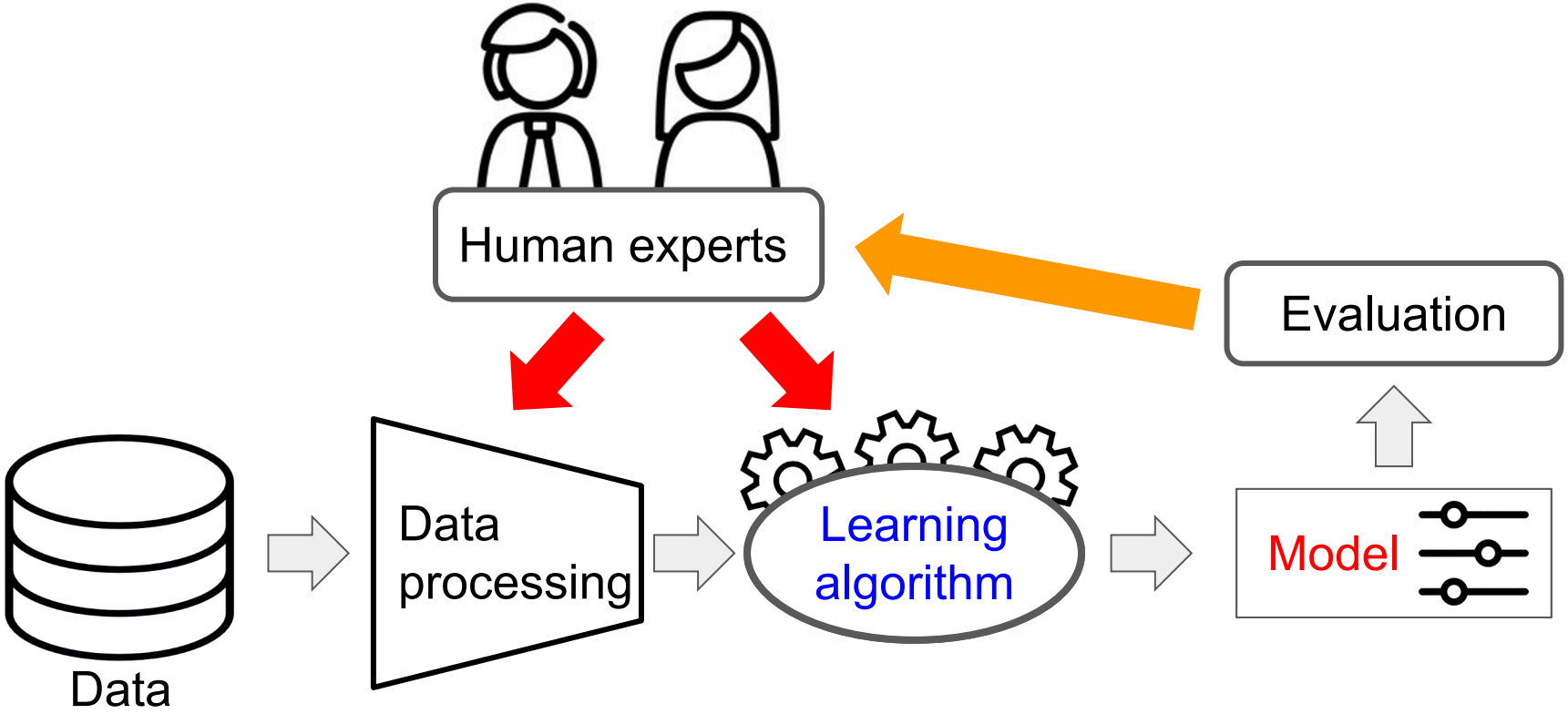

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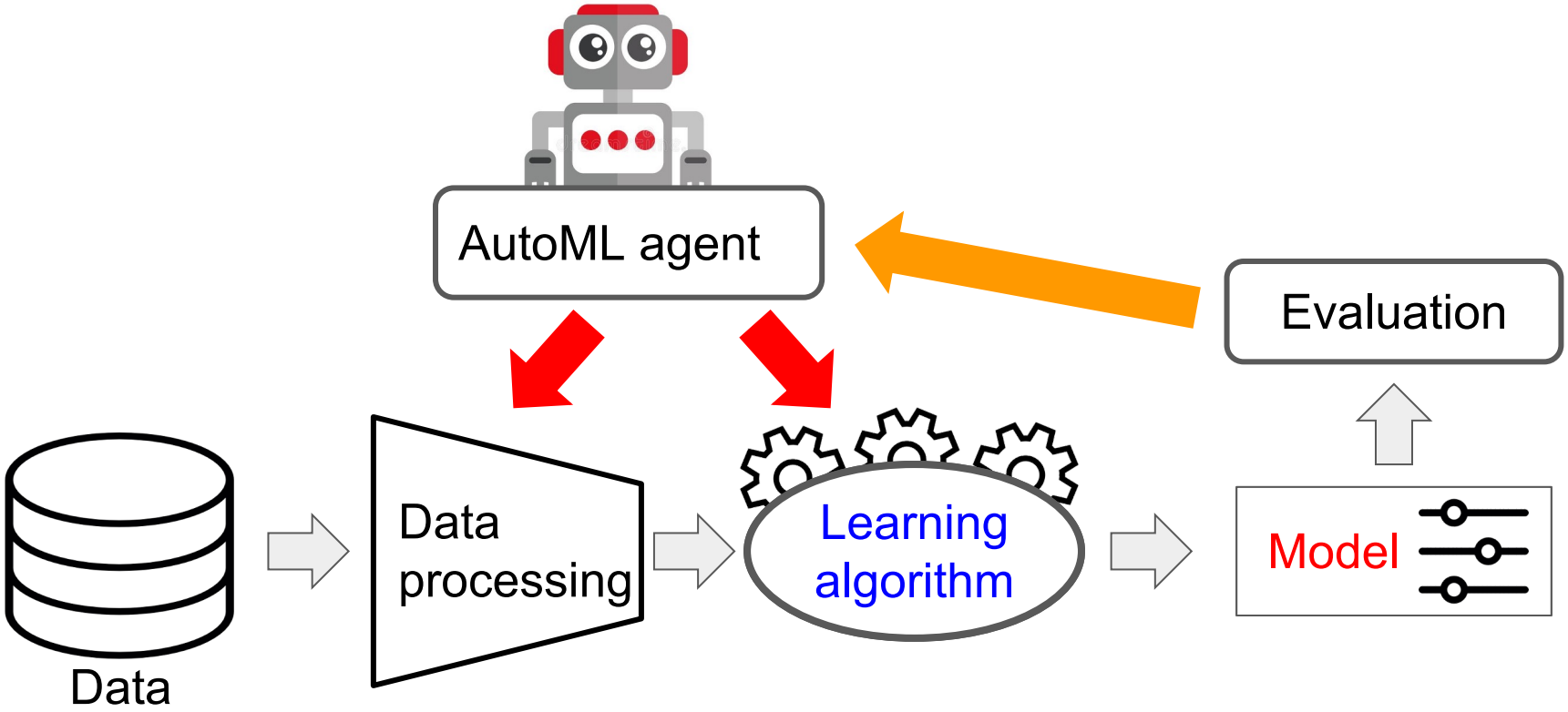

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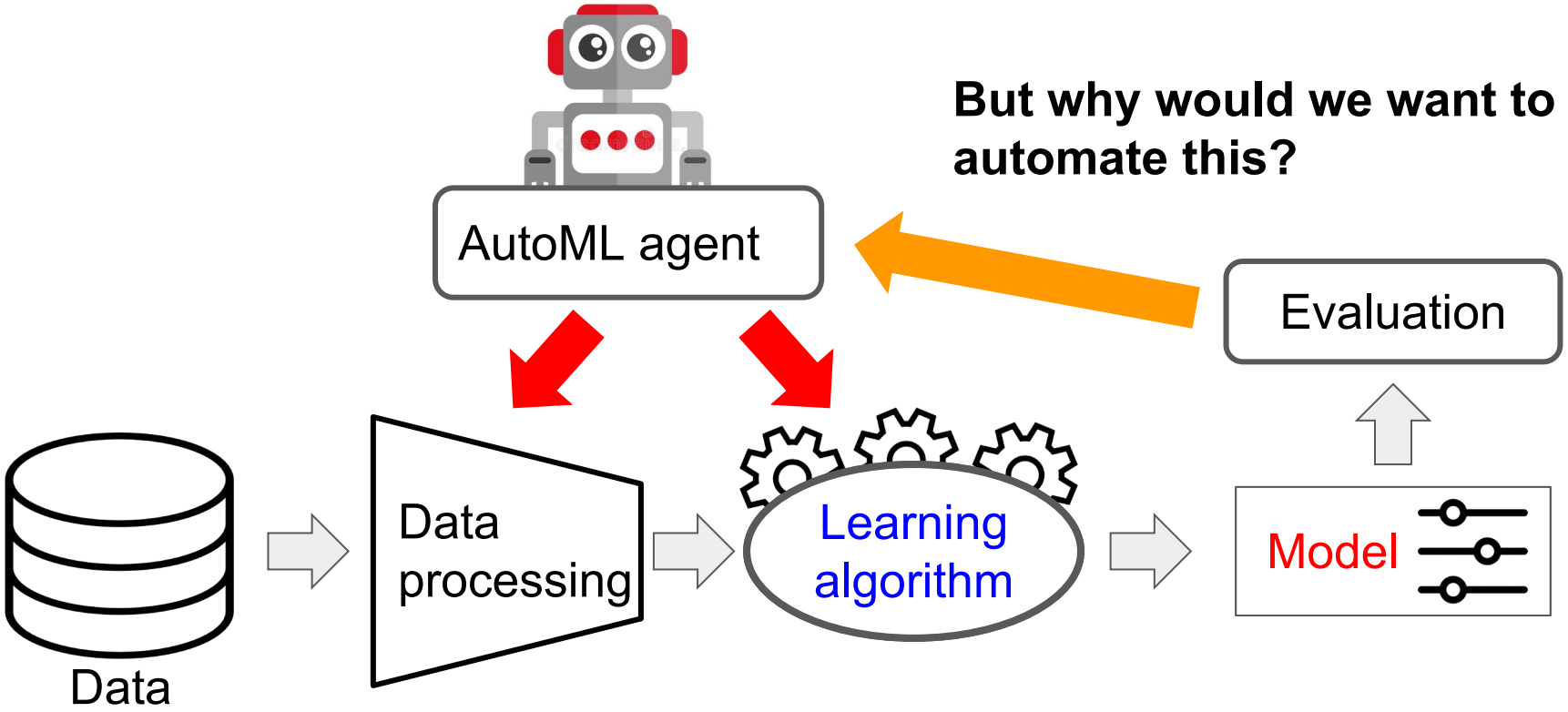

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Choice of preprocessing, learning algorithm, and hyperparameters is **CRUCIAL** for achieving good performance!

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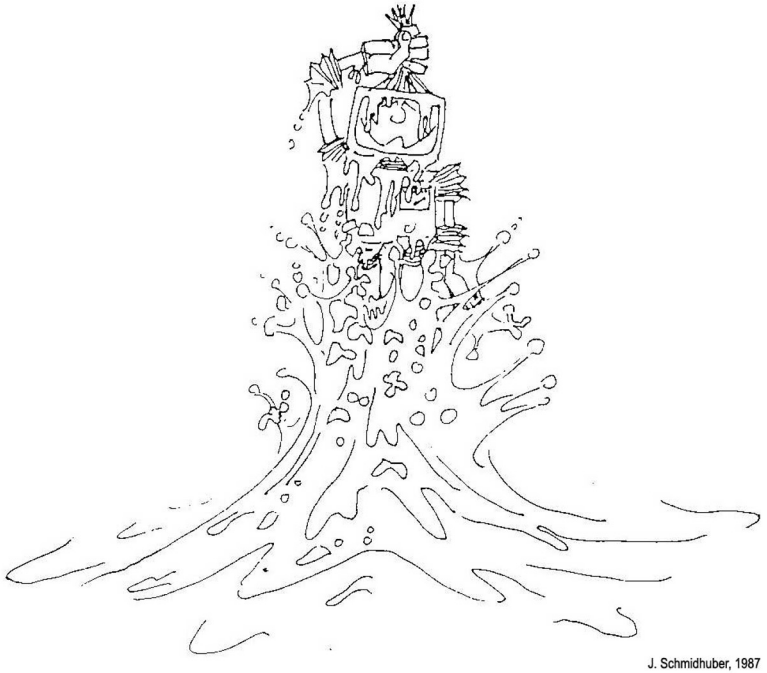
- Takes **a lot of (tedious) effort** and is **expensive** (read this logbook for the creation of a 175B parameter model)
- Suboptimal (machines can do better!)

Automated Machine Learning

- Democratizes the use of machine learning methods (no longer need expert domain knowledge)
- Save human time, effort, money
- Better performance



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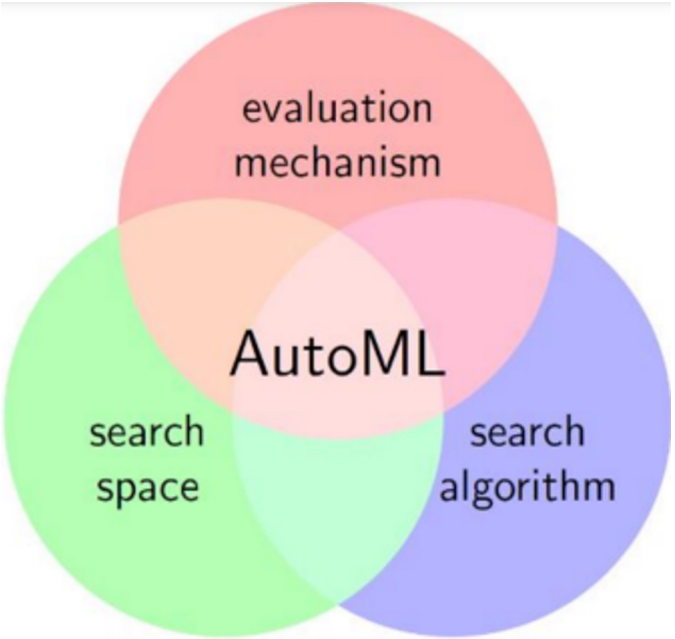

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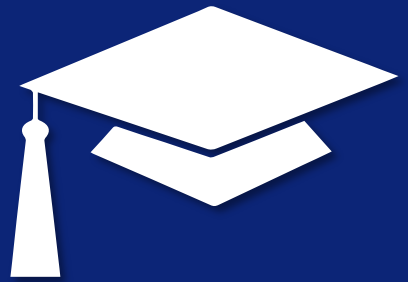
Any questions so far?



Combined Algorithm Selection and Hyperparameter optimization (CASH)

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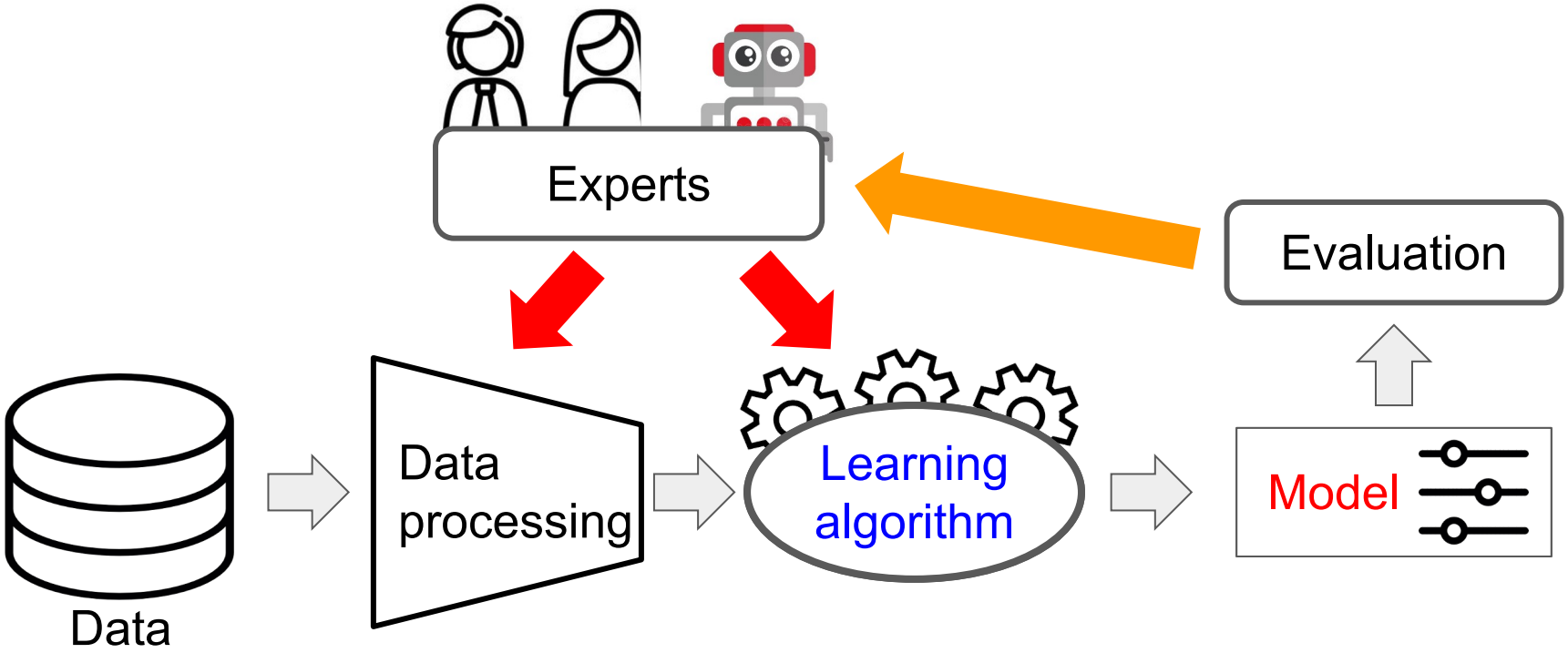

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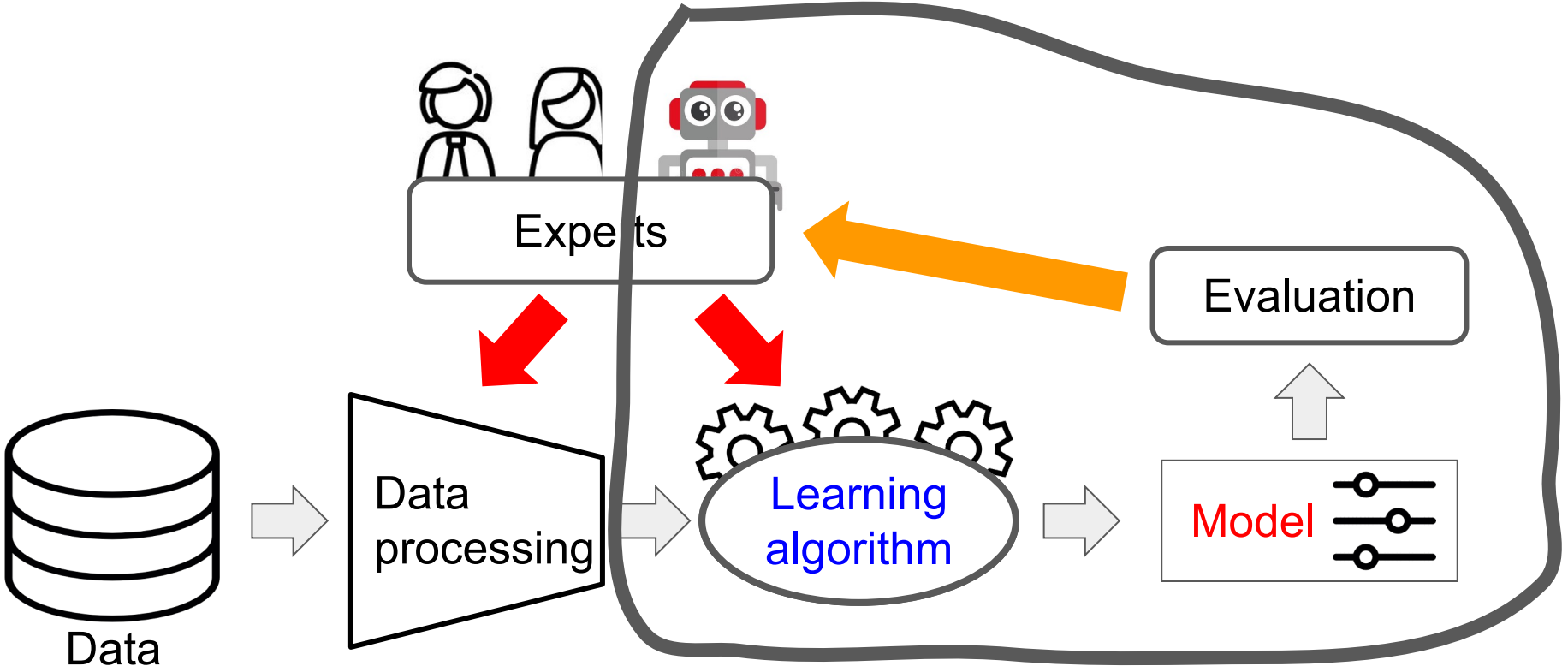

CASH - definition

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Output of learning algorithm = model

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Loss of the model

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Expected/Mean loss of the model

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Hyperparameter vector $\theta = [\theta_1\ \theta_2\ \ldots\ \theta_n]$

E.g., [learning rate, momentum, use_batch_norm]

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= Combined Algorithm and Hyperparameter optimization (CASH)

HPO vs CASH

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HPO vs CASH

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HPO = CASH when including the algorithm as “hyperparameter”

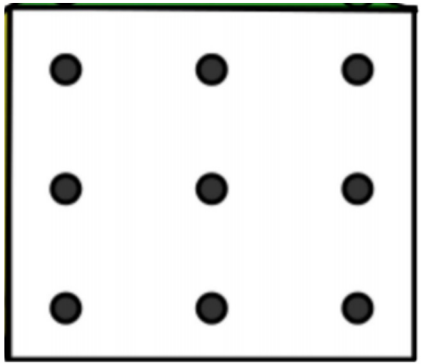
CASH and HPO methods

Methods we look at today:

- Grid search
- Random search
- Successive halving & Hyperband
- Bayesian Optimization (BO)

Grid search

Idea: define sets of values you want to try for some (or all) hyperparameters, evaluate all possible combinations



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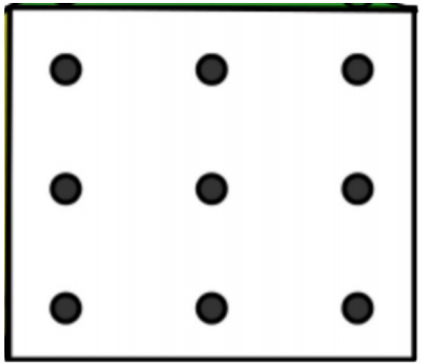
$$v(\theta_1) = \{0.1, 0.01, 0.001\},$$

Value sets:



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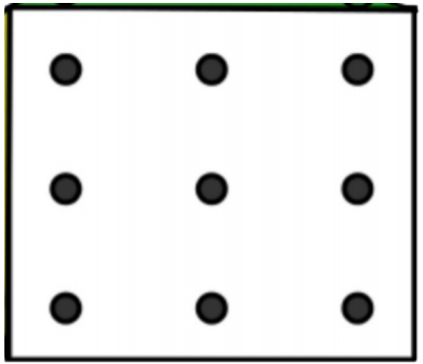

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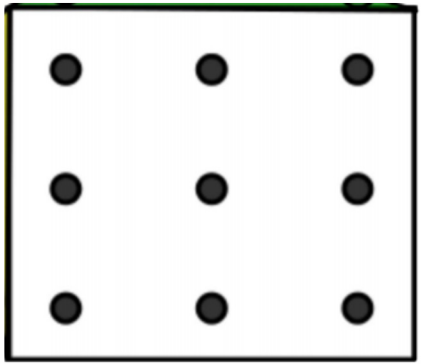
$$v(\theta_n) = \{True, False\}$$



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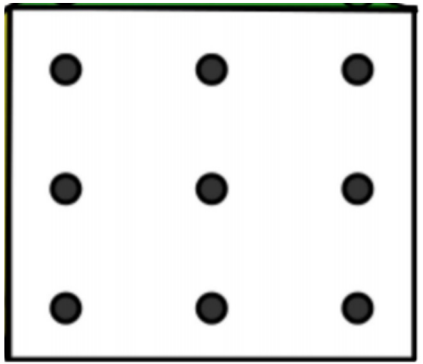
Evaluate: $v(\theta_1) \times v(\theta_2) \times \dots \times v(\theta_n)$



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Pros:

- Simple
- Easy to parallelize

Cons:

- Waste of compute when one or more hyperparameters not important
- Scalability (exponential growth number of combinations)
- How to define the grid?

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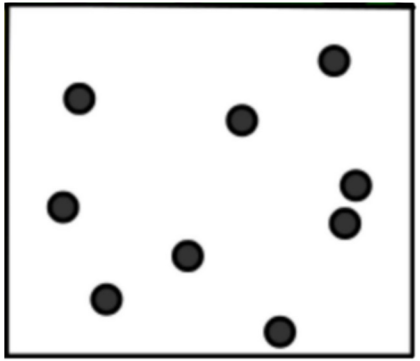

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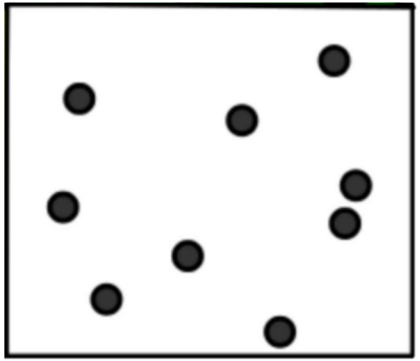
Distributions:



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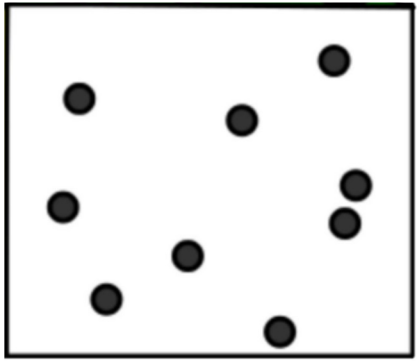
Distributions: $p(\theta_2) = Uniform(0.8, 0.99)$



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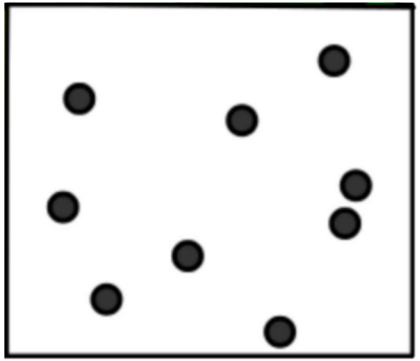

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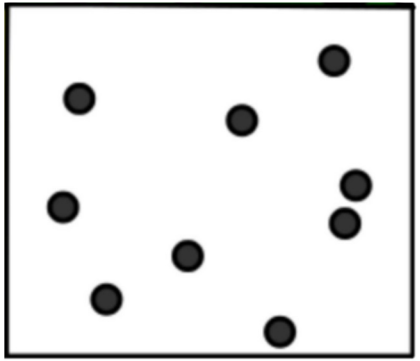


Evaluate M configurations:

$$\theta \backsim p(\theta_1, \theta_2, \dots, \theta_n)$$

Random search

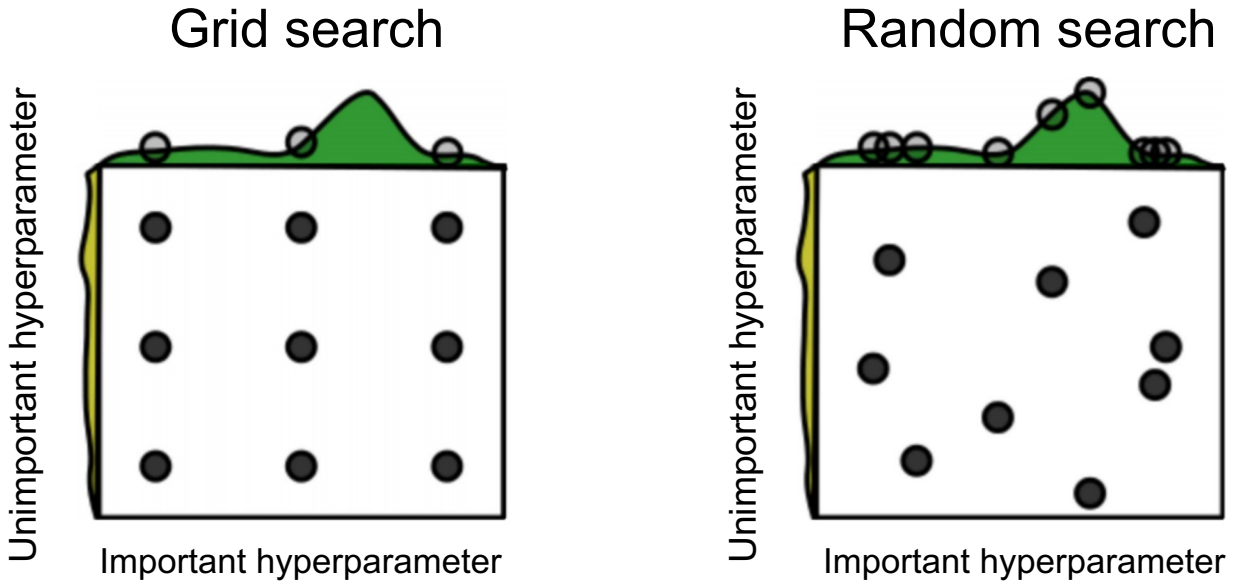
Pros:

- Simple
- Easy to parallelize
- Can set a budget of function evaluations (we evaluate M hyperparameter configurations)
- Theoretical guarantees of convergence with proper ranges

Cons:

- Not data efficient
- Still expensive to perform

Grid search vs Random search



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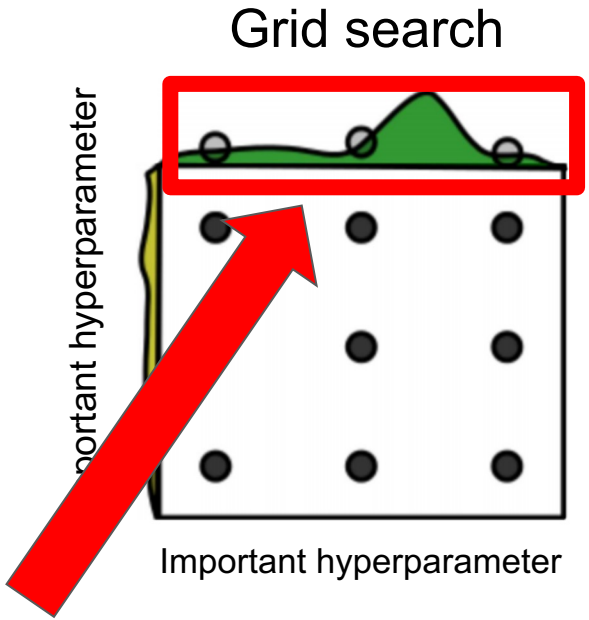
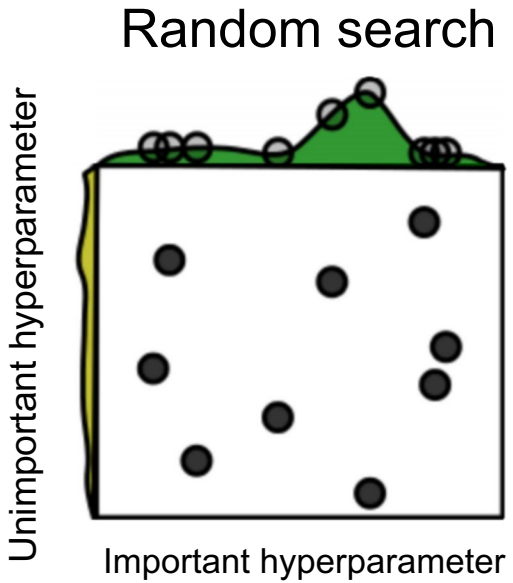
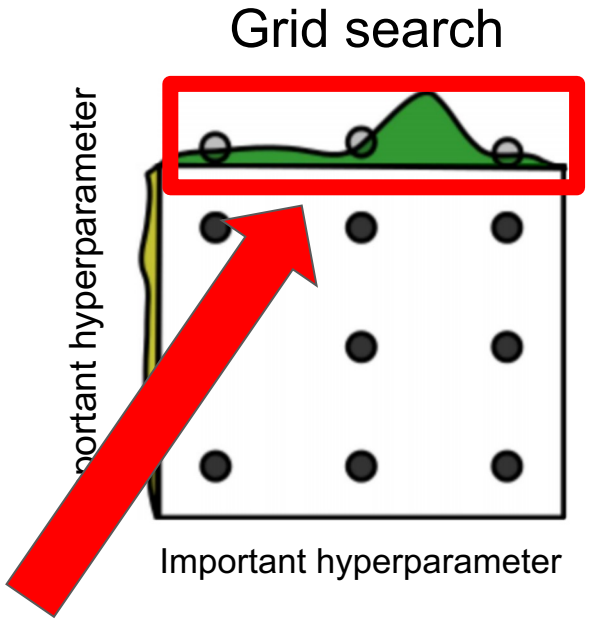




Only 3 useful evaluations

Grid search vs Random search



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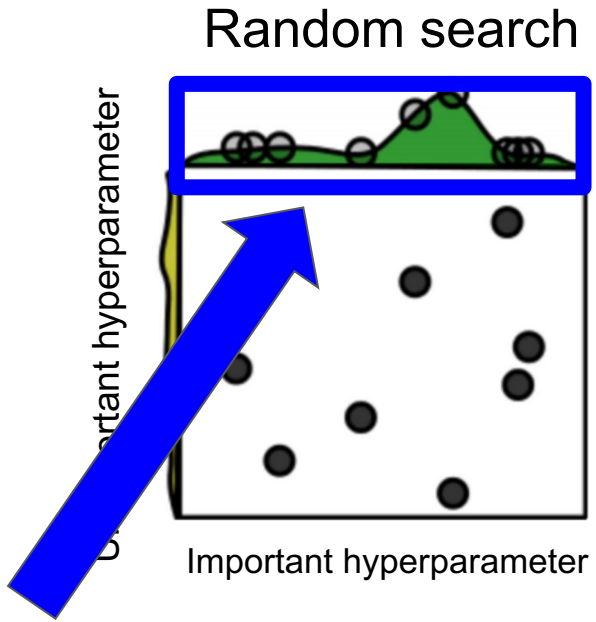

9 useful evaluations

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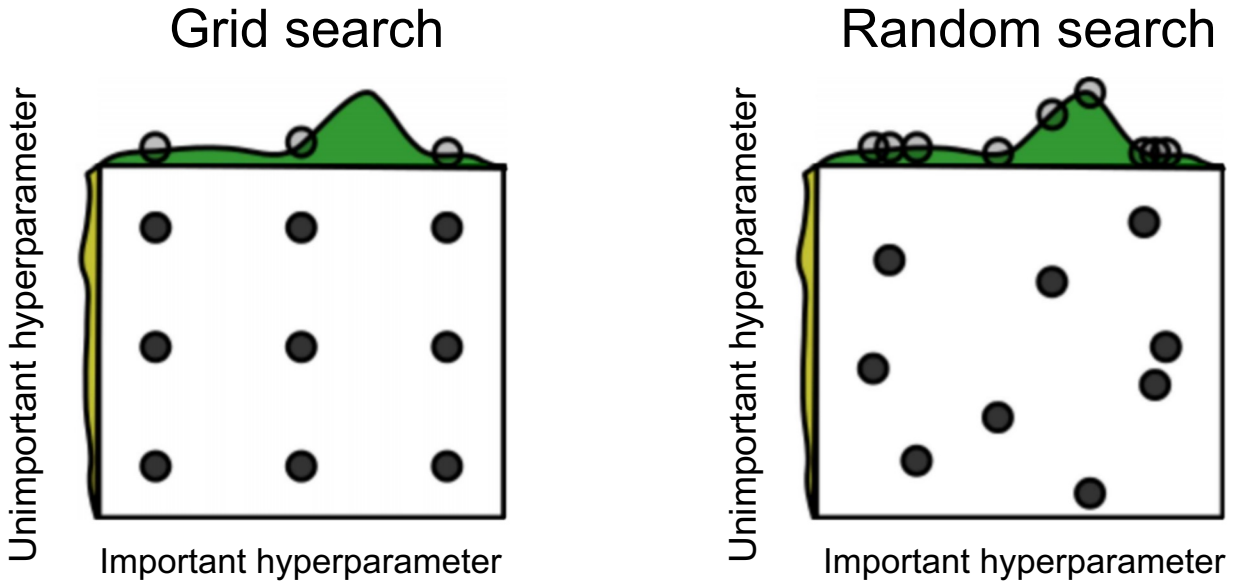
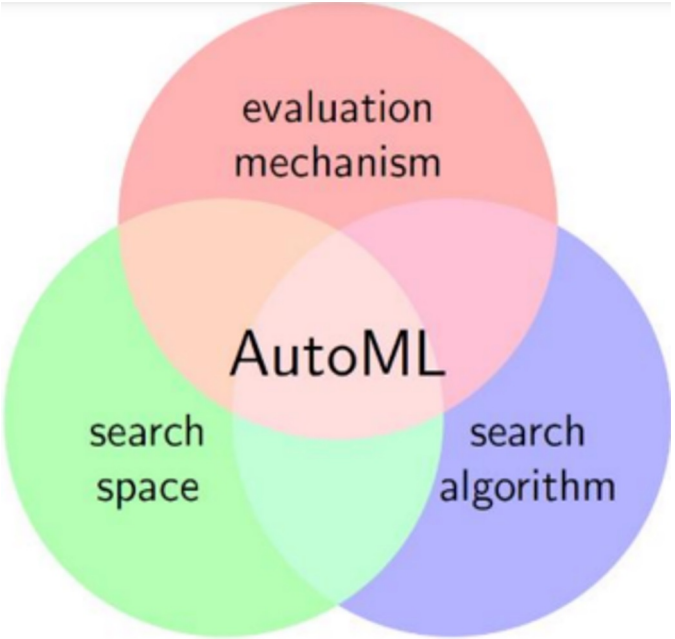


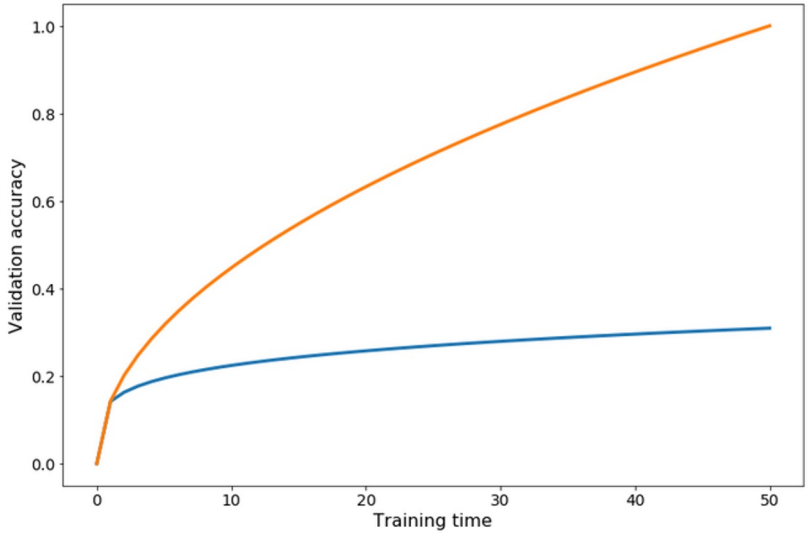
⇒ Random search is more efficient when there are unimportant hyperparameters (better **coverage**)

Automated Machine Learning



Grid search and random search

Downside: Every hyperparameter configuration is fully trained (expensive!)



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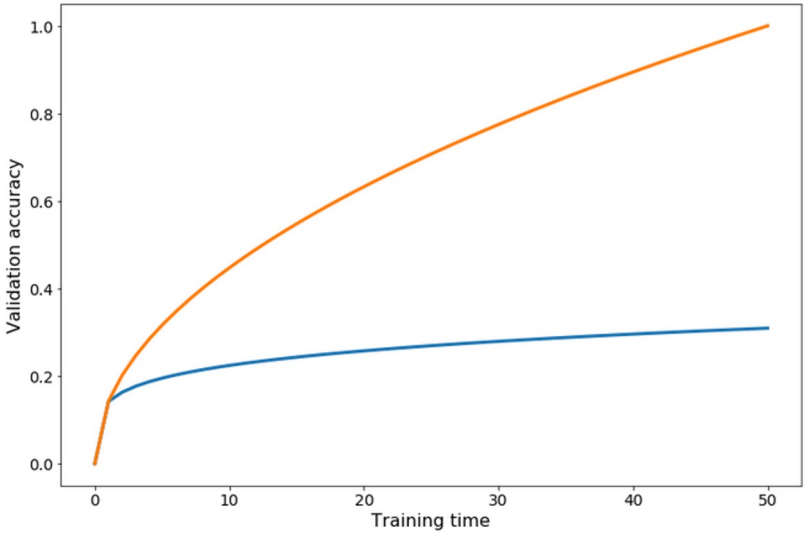

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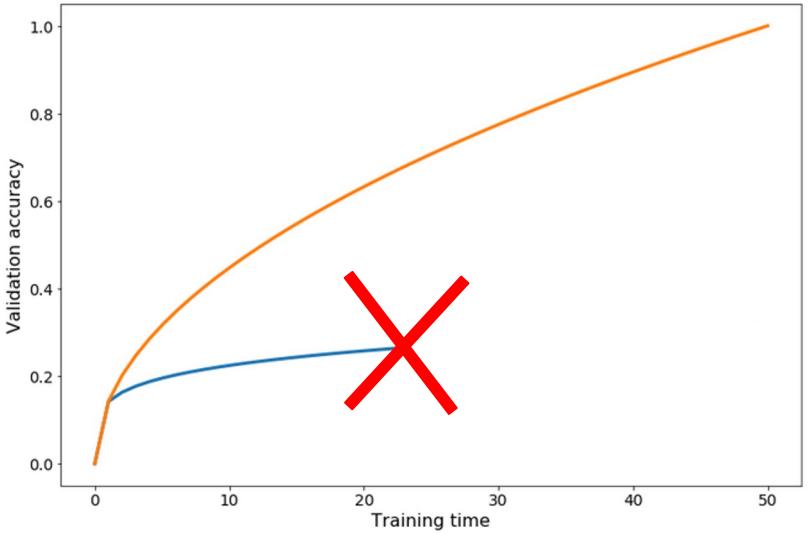
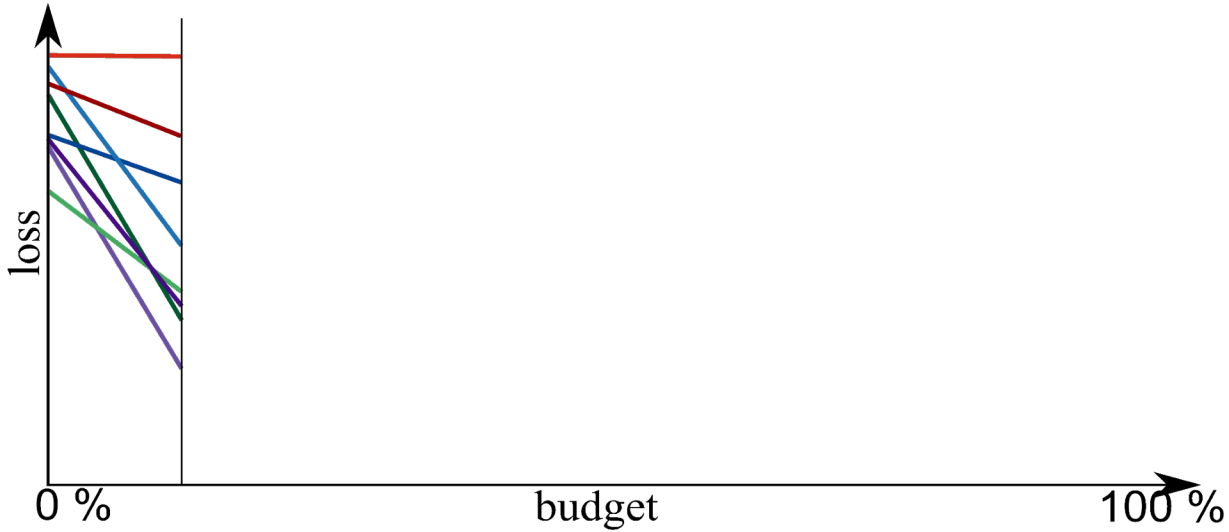


Techniques that do this

- Successive halving (Jamieson and Talwalkar, 2016)
- Hyperband (Li et al., 2018)

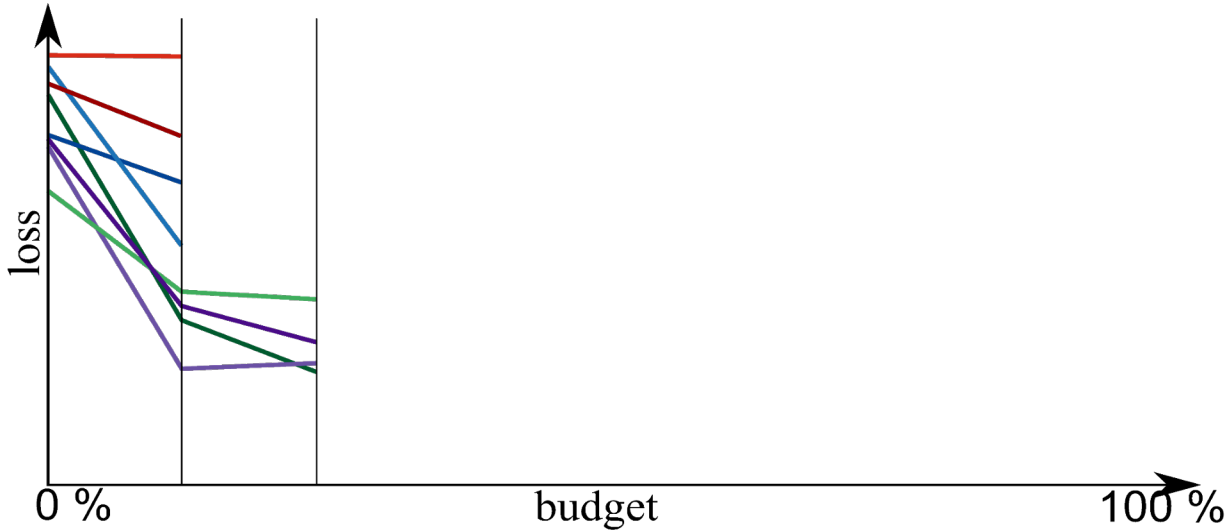
Successive halving

Successive halving



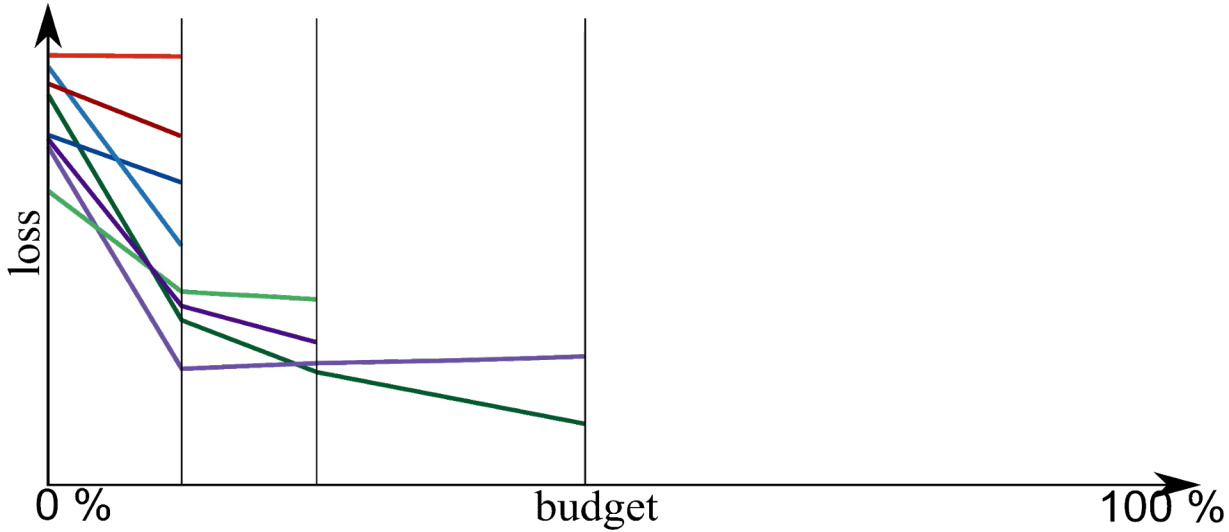
Round 0

Successive halving



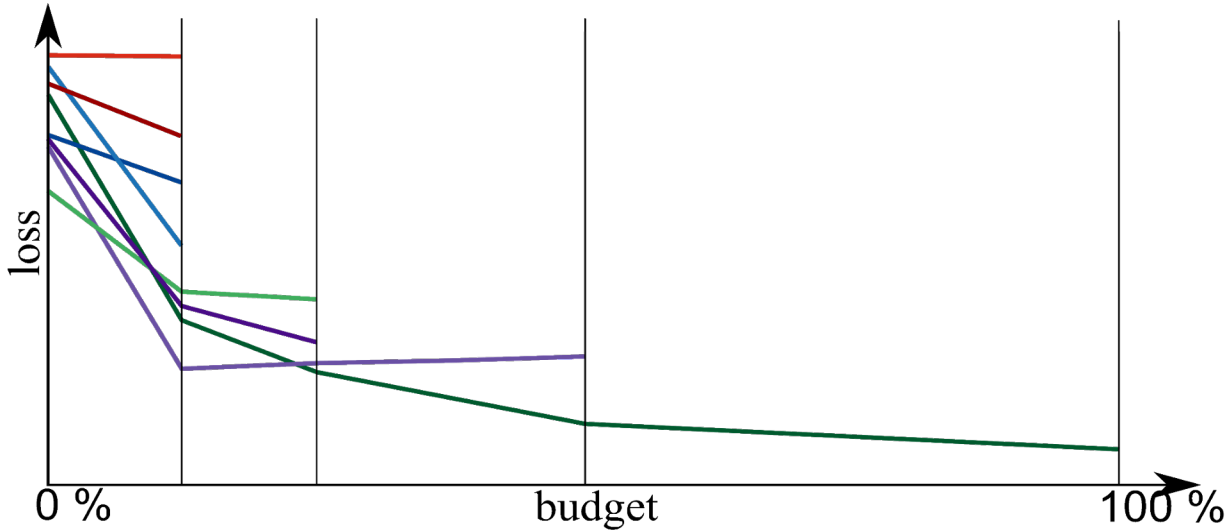
Round 1

Successive halving



Round 2

Successive halving



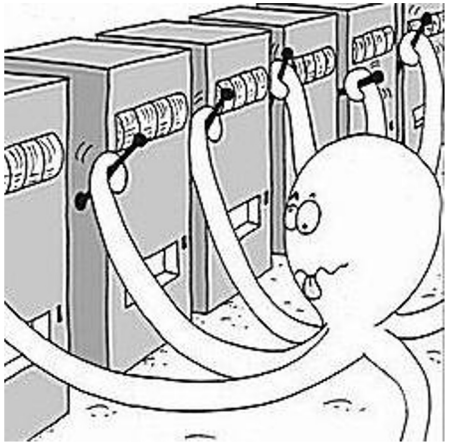
Round 3

Successive halving

This is a bandit-based method

- Different configurations are different one-armed slot machines
- Pull the lever = assign more budget and observe reward

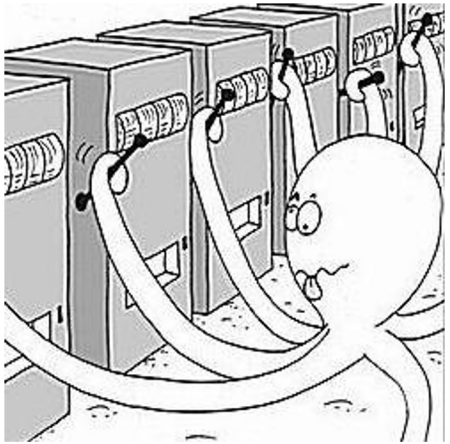
Goal: find the best slot machine (configuration)



Successive halving

Key idea:

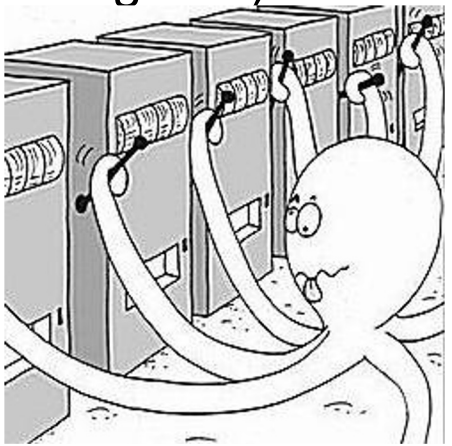
- Start with a set of n random initial configurations $\{A_\theta^{(i)}\}_{i=1}^n$ and a budget B



Successive halving

Key idea:

- Start with a set of n random initial configurations $\{A_\theta^{(i)}\}_{i=1}^{n}$ and a budget B
- Every round the candidate pool size is divided by γ (halving rate)



Successive halving

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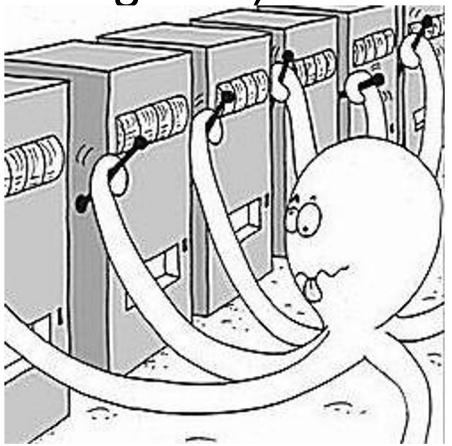
How many rounds are there if we start with n configurations?



Successive halving

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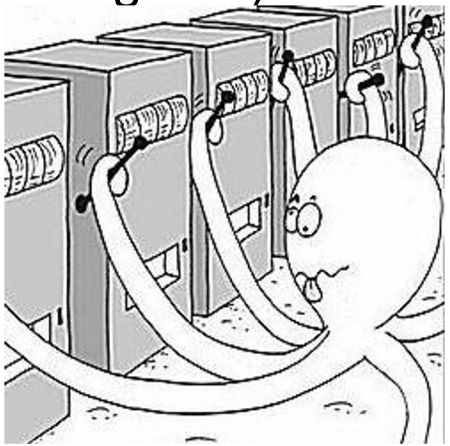

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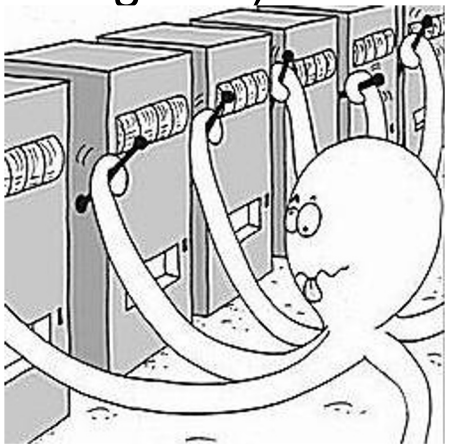

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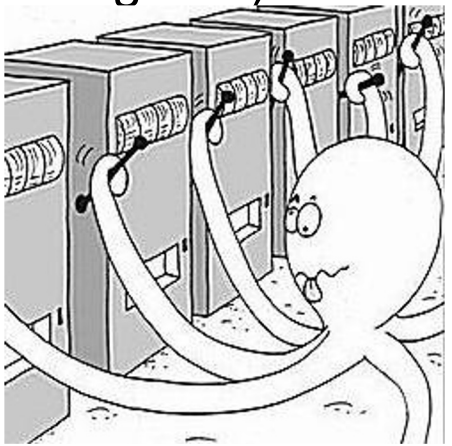
- Budget is divided uniformly over rounds

⇒ We assign exponentially more budget to good configs



Successive halving

Number of initial configs, n=64. Total budget B=384

Halving rate $\gamma = 2$

Successive halving

Number of initial configs, n=64. Total budget B=384

Halving rate γ = 2

k	$\lvert S_k \rvert$	r_k
0		
1		
2		
3		
4		
5		

$\lvert S_k \rvert$: size of candidate pool in round k

r_k : budget in round k per configuration

Successive halving

Number of initial configs, n=64. Total budget B=384

Halving rate $\gamma = 2$

k	$\lvert S_k \rvert$	r_k
0	64	1
1	32	2
2	16	4
3	8	8
4	4	16
5	2	32

Successive halving

Effects of the budget and halving rate

- Higher budget ⇒ Higher budget per config (*more informed decisions*)

Successive halving

Effects of the budget and halving rate

- Higher budget ⇒ Higher budget per config (*more informed decisions*)
- Higher halving rate ⇒ More aggressive pruning (*could be too aggressive and disregard the best candidate early on)*

Successive halving

Pros

- Allows us to work with fixed budget
- Good empirical results
- Strong theoretical foundations
- Parallelizable

Cons

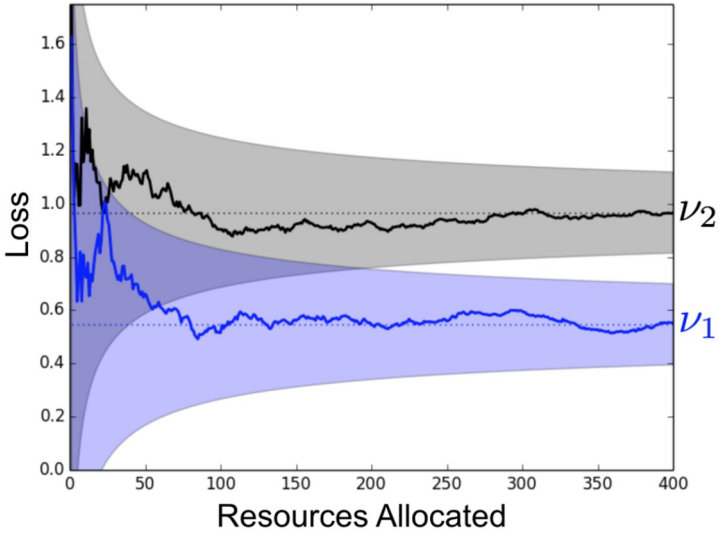
- Learning curves can cross (good candidates to be discarded early)
- n/B trade-off

Successive halving

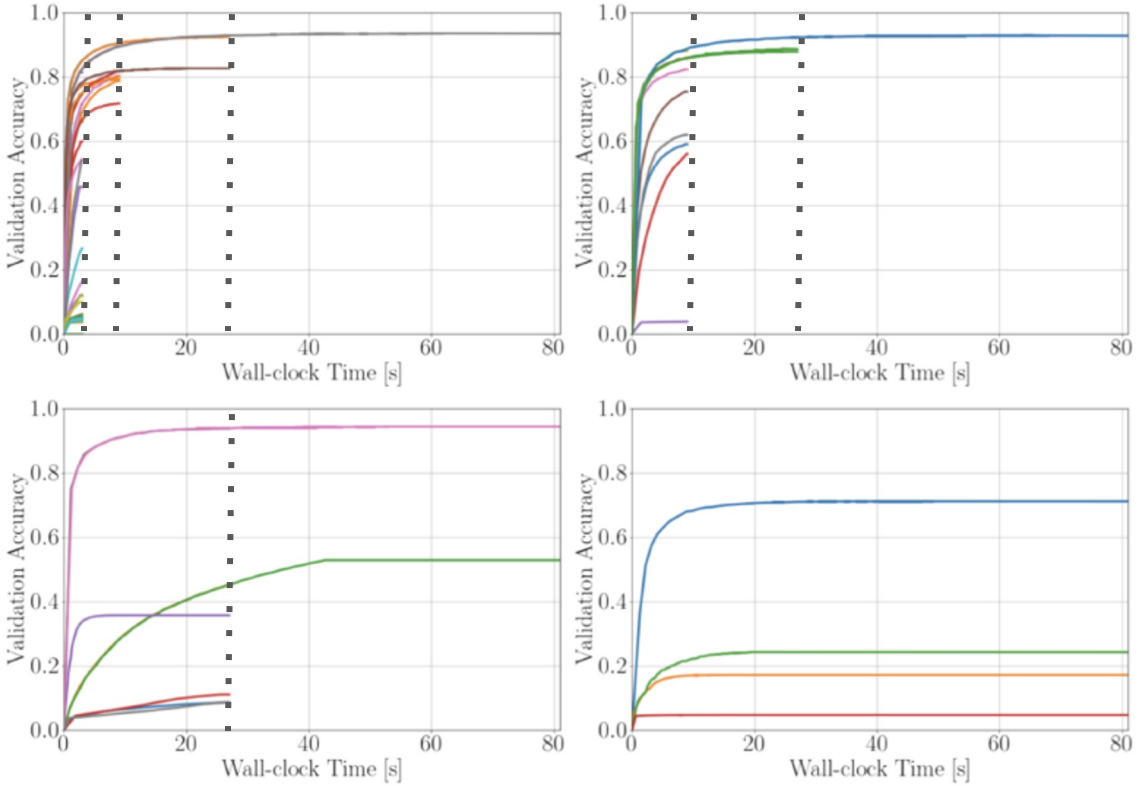
Trade-off: Given a fixed budget B

- Large *n* (num initial configs)? ⇒ small amount of time per configuration
- Small *n?* ⇒ larger amount of time per configuration

⇒ We initially do not know what works best



Hyperband


Validation Accuracy
Wall-clock Time [s]
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80

Hyperband

Idea: Perform different successive halving "*brackets*" $s_{max} + 1$ times with various initial candidate pool sizes *n* for a fixed budget B

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- Every consecutive bracket: reduce *n (more time per configuration)*

Hyperparameters:

- R: maximum resource that can be allocated to a single technique within a round of successive halving
- γ: controls proportion of discarded configs every round

Hyperband

i
0
1
2
3
4

$$\gamma = 3$$

Hyperband

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

First bracket with n=81 (we sample random configurations). Just successive halving.

$$\gamma = 3$$

Hyperband

	$s=4$		$s=3$	
i	n_i	r_i	n_i	r_i
0	81	1	**34**	3
1	27	3	**11**	9
2	9	9	3	27
3	3	27	1	81
4	1	81		

Second bracket with n=34 (new randomly sampled configurations). Just successive halving.

$$\gamma = 3$$

Hyperband

	$s=4$		$s=3$		$s=2$	
i	n_i	r_i	n_i	r_i	n_i	r_i
0	81	1	**34**	3	**15**	9
1	27	3	**11**	9	**5**	27
2	9	9	3	27	1	81
3	3	27	1	81		
4	1	81				

$$\gamma = 3$$

Hyperband

	$s=4$		$s=3$		$s=2$		$s=1$	
i	n_i	r_i	n_i	r_i	n_i	r_i	n_i	r_i
0	81	1	**34**	3	**15**	9	**8**	27
1	27	3	**11**	9	**5**	27	2	81
2	9	9	3	27	1	81		
3	3	27	1	81				
4	1	81						

Various brackets, with $R = 81$ and $\gamma = 3$

Hyperband

	$s=4$		$s=3$		$s=2$		$s=1$		$s=0$	
i	n_i	r_i	n_i	r_i	n_i	r_i	n_i	r_i	n_i	r_i
0	81	1	**34**	3	**15**	9	**8**	27	5	81
1	27	3	**11**	9	**5**	27	2	81		
2	9	9	3	27	1	81				
3	3	27	1	81						
4	1	81								

Hyperband

	$s=4$		$s=3$		$s=2$		$s=1$		$s=0$	
i	n_i	r_i	n_i	r_i	n_i	r_i	n_i	r_i	n_i	r_i
0	81	1	**34**	3	**15**	9	**8**	27	5	81
1	27	3	**11**	9	**5**	27	2	81		
2	9	9	3	27	1	81				
3	3	27	1	81						
4	1	81								

No more intermediate discarding takes place
⇒ **this is random search!!!**

Hyperband

Overview of Hyperband

- Hyperband is a **logfactor** slower than random search to identify the best configuration (effect can be large!!)

Hyperband

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- Random search eventually converges to a solution, and so does Hyperband (the former is embedded in the latter)

Hyperband

Overview of Hyperband

- Hyperband is a **logfactor** slower than random search to identify the best configuration (effect can be large!!)
- Random search eventually converges to a solution, and so does Hyperband (the former is embedded in the latter)
- We explore different values of n for a fixed B ⇒ resolves b/N trade-off in successive halving

Limitation of techniques so far

They **randomly** select (initial) candidates to evaluate

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But if we have already evaluated a set of candidates, can’t we do better than random selection?

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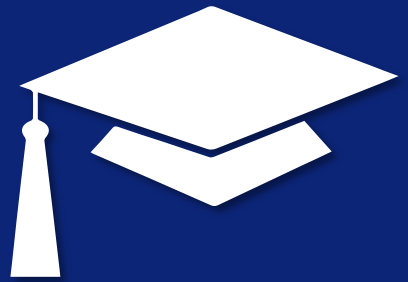
But if we have already evaluated a set of candidates, can't we do better than random selection?

⇒ **Predict promising regions based on history of observations**



Sequential model-based optimization (SMBO)

Sequential model-based optimization

Key idea: Learn a surrogate model that for every configuration $\theta \in \Theta$:

- Predicts the loss (or performance)
- And provides a measure of uncertainty about the prediction

Sequential model-based optimization

Key idea: Learn a surrogate model that for every configuration $\theta \in \Theta$:

- Predicts the loss (or performance)
- And provides a measure of uncertainty about the prediction

$\Rightarrow$ Loosely speaking, the surrogate models $P(y|\theta)$

Sequential model-based optimization

⇒ Update the surrogate model sequentially as new observations (tried configuration, performance) arrive

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Bayesian optimization:

- ❖ Start with a prior distribution

Sequential model-based optimization

⇒ Update the surrogate model sequentially as new observations (tried configuration, performance) arrive

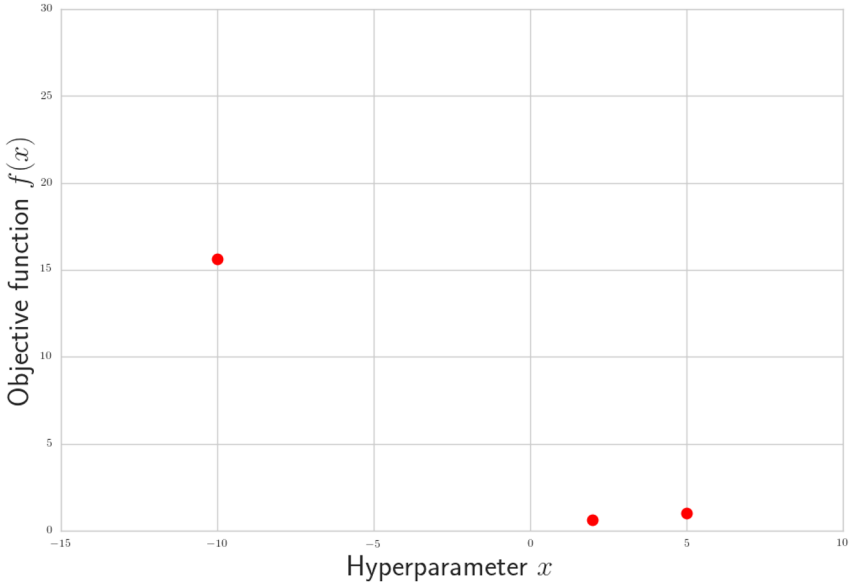
⇒ Use the surrogate model to select new promising configurations to evaluate

Bayesian optimization:

- ❖ Start with a prior distribution
- ❖ Repeat: Update our beliefs about the loss surface

Visualization of Bayesian optimization

1. Fit a surrogate model to observations



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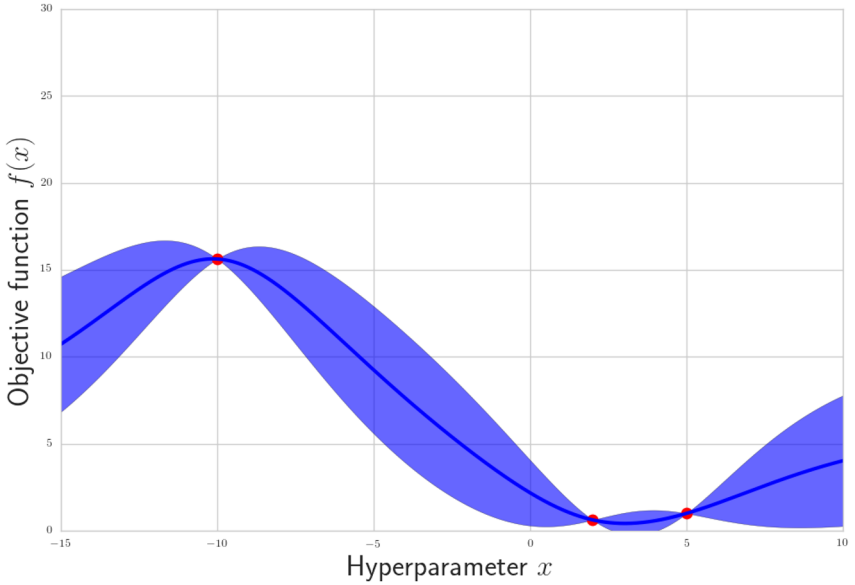
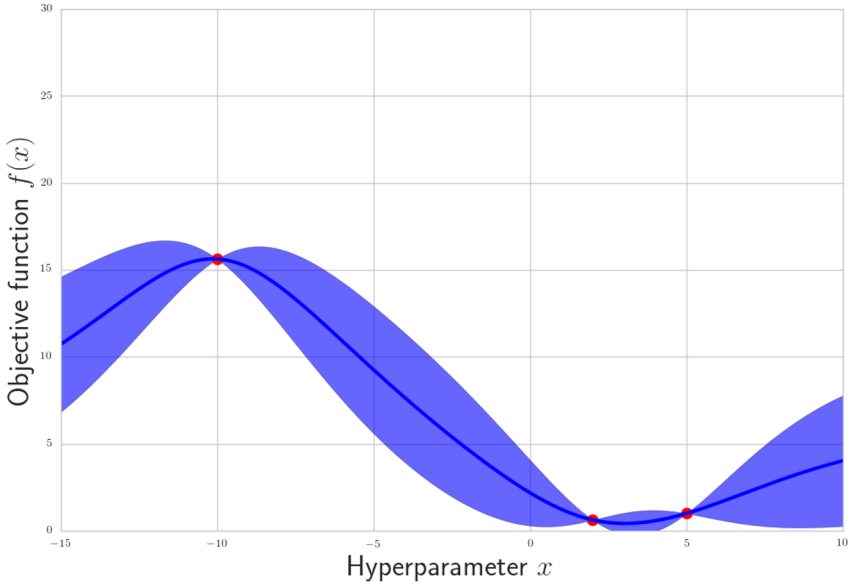


Visualization of Bayesian optimization

1. Fit a surrogate model to observations
2. Compute the **acquisition function** (estimated quality) and select new points accordingly



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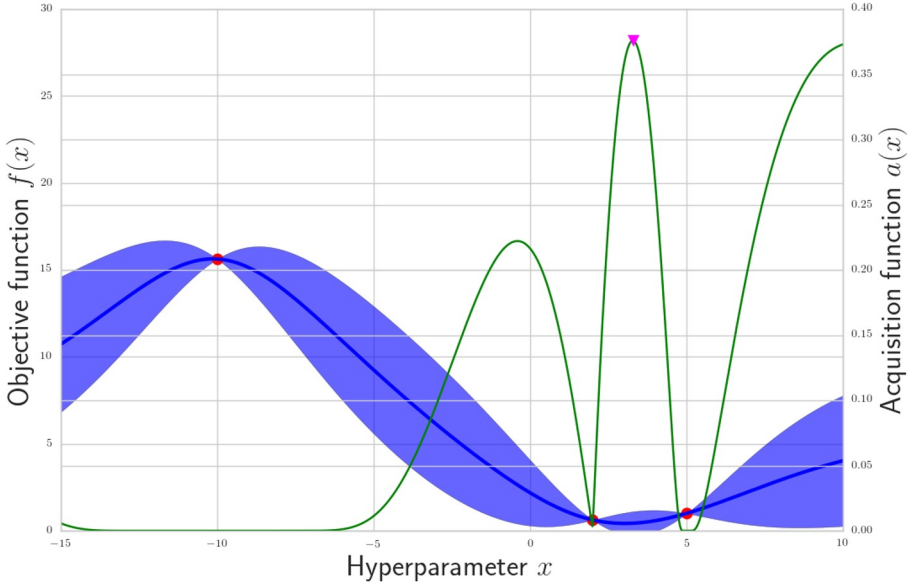
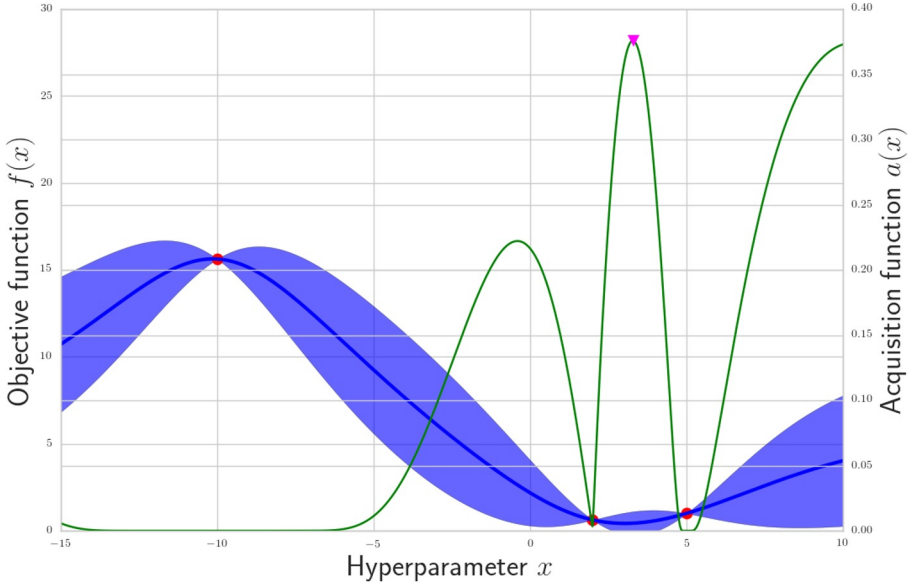


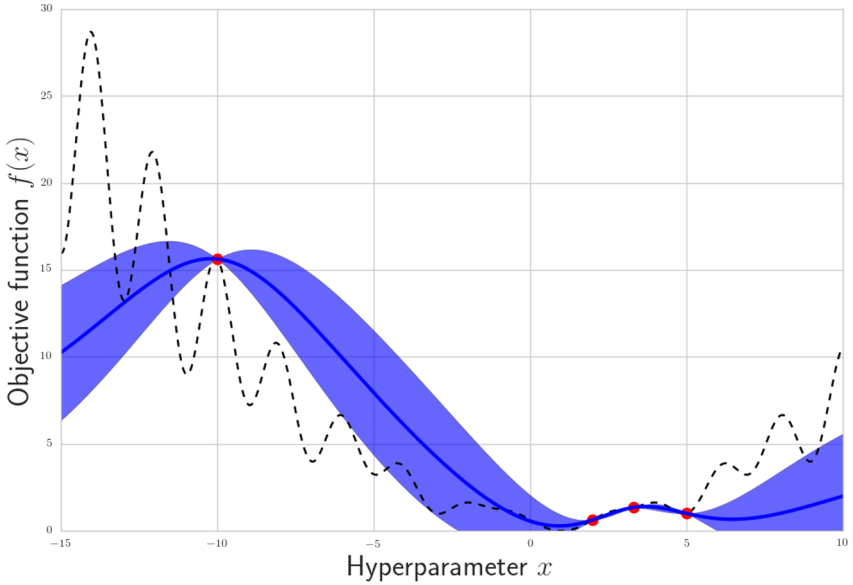
Visualization of Bayesian optimization

1. Fit a surrogate model to observations
2. Compute the **acquisition function** (estimated quality) and select new points accordingly
3. Evaluate new points



Visualization of Bayesian optimization

1. Fit a surrogate model to observations
2. Compute the **acquisition function** (estimated quality) and select new points accordingly
3. Evaluate new points
4. Repeat



Surrogate model - Bayesian optimization

What to use as surrogate model?

- Random forest (categorical and conditional hyperparameters)
- Gaussian process (good confidence bounds - only numerical hyperparameters)

Acquisition function - Bayesian optimization

Many different choices:

- Probability improvement
- Entropy search
- Lower/upper confidence bounds, UCB
- Expected Improvement (EI)

Goal: Compute how promising candidate configurations are

Bayesian optimization

Pros

- Data efficient (surrogate model)
- Convincingly faster than random search

Con: Training of surrogate model (extra time + how to set hyperparameters?)

Extension: Combine with meta-learning (warm-starting the surrogate model)

Overview

Grid Search

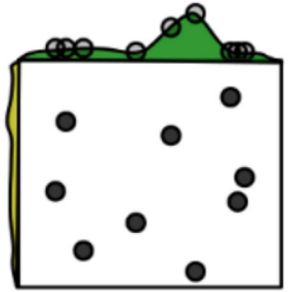
\+

Very simple approach
Can be used to study the problem

\-

Does not scale to high dimensions
Grid needs to be defined

Random Search



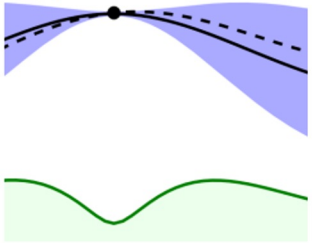
\+

Even more simple
Easily parallelizable
Eventually converges to optimum

\-

Not data efficient
Computationally expensive

Bayesian Optimization



\+

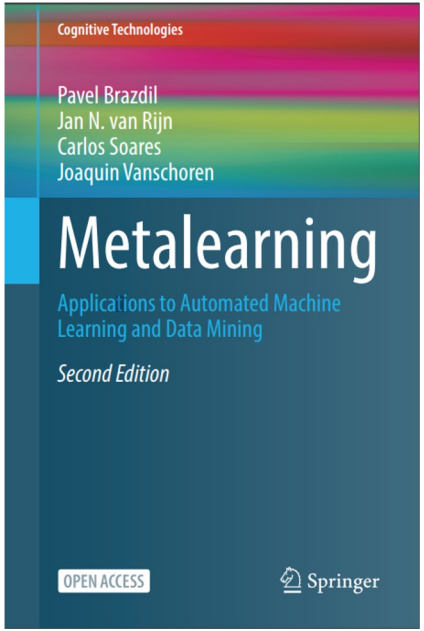
Black-box optimization
Data efficient
State of the art

\-

Not easy to parallelize

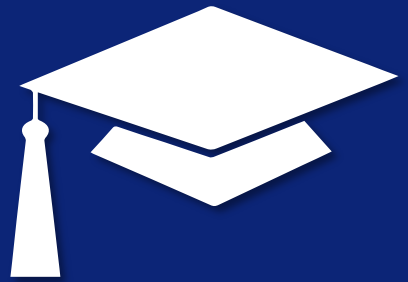
Relevant literature

- Metalearning book (Brazdil et al., 2022)
- Algorithms for Hyper-Parameter Optimization (Bergstra et al., 2011)
- Successive halving paper (Jamieson & Talwalkar, 2016)
- Hyperband paper (Li et al., 2016)
- Blog post on Hyperband



Acknowledgements

- Image by Juergen Schmidhuber
- Animation of TPE made by Alois Bissuel



Appendix

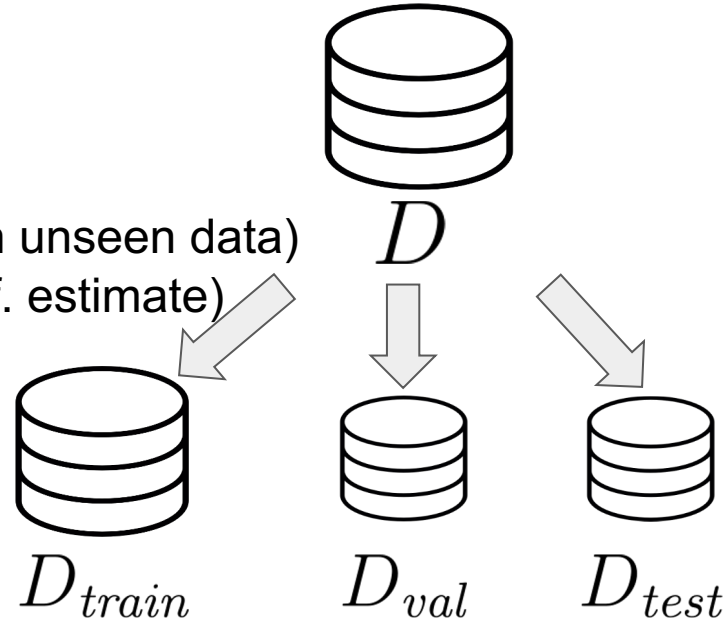
Train/val/test splits

How to compute $\mathbb{E}_{p_{\mathcal{T}}}\left[\mathcal{L}_{\mathcal{T}}(A_\theta(D_{train}))\right]$?

⇒ **Split dataset into 3 parts**

- Training set (fed into learning algorithm)
- Validation set (estimate above quantity on unseen data)
- Test set (never touched, only for final perf. estimate)

⇒ **Goal:** minimize validation loss



Successive halving

Input : Budget B, n arms where $\ell_{i,k}$ denotes the k^{th} loss from the i^{th} *arm*

Successive halving

Input : Budget B, n arms where $\ell_{i,k}$ denotes the k^{th} loss from the i^{th} *arm*

1 Initialize: $S_0 = \{1, 2, \ldots, n\}$ # Initial hyperparameter configurations

Successive halving

Input : Budget B, n arms where $\ell_{i,k}$ denotes the k^{th} loss from the i^{th} *arm*

Initialize: $S_0 = \{1, 2, \ldots, n\}$

for $k = 0, 1, \ldots, \lceil \log_2(n) \rceil - 1$ **do**

  Pull each arm in S_k for $r_k = \lfloor \frac{B}{|S_k| \lceil \log_2(n) \rceil} \rfloor$ additional times and set $R_k = \sum_{j=0}^{k} r_j$

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  Let σ_k be a bijection on S_k such that $\ell_{\sigma_k(1),R_k} \leq \ell_{\sigma_k(2),R_k} \leq \ldots \leq \ell_{\sigma_k(|S_k|),R_k}$

Order configurations by loss

Successive halving

Input : Budget B, n arms where $\ell_{i,k}$ denotes the k^{th} loss from the i^{th} *arm*

Initialize: $S_0 = \{1, 2, \ldots, n\}$

for $k = 0, 1, \ldots, \lceil \log_2(n) \rceil - 1$ **do**

  Pull each arm in S_k for $r_k = \lfloor \frac{B}{|S_k| \lceil \log_2(n) \rceil} \rfloor$ additional times and set $R_k = \sum_{j=0}^{k} r_j$

  Let σ_k be a bijection on S_k such that $\ell_{\sigma_k(1),R_k} \leq \ell_{\sigma_k(2),R_k} \leq \ldots \leq \ell_{\sigma_k(|S_k|),R_k}$

  $S_{k+1} = \{i \in S_k : \ell_{\sigma_k(i),R_k} \leq \ell_{\sigma_k(\lfloor |S_k|/2 \rfloor),R_k}\}$ # Best half continues to next round

end

Successive halving

Input : Budget B, n arms where $\ell_{i,k}$ denotes the k^{th} loss from the i^{th} *arm*

Initialize: $S_0 = \{1, 2, \ldots, n\}$

for $k = 0, 1, \ldots, \lceil \log_2(n) \rceil - 1$ **do**

  Pull each arm in S_k for $r_k = \lfloor \frac{B}{|S_k| \lceil \log_2(n) \rceil} \rfloor$ additional times and set $R_k = \sum_{j=0}^{k} r_j$

  Let σ_k be a bijection on S_k such that $\ell_{\sigma_k(1),R_k} \leq \ell_{\sigma_k(2),R_k} \leq \ldots \leq \ell_{\sigma_k(|S_k|),R_k}$

  $S_{k+1} = \{i \in S_k : \ell_{\sigma_k(i),R_k} \leq \ell_{\sigma_k(\lfloor |S_k|/2 \rfloor),R_k}\}$

end

Output: Singleton element of $S_{\lceil \log_2(n) \rceil}$

Successive halving

Input : Budget B, n arms where $\ell_{i,k}$ denotes the k^{th} loss from the i^{th} *arm*

Initialize: $S_0 = \{1, 2, \ldots, n\}$

for $k = 0, 1, \ldots, \lceil \log_2(n) \rceil - 1$ **do**

  Pull each arm in S_k for $r_k = \lfloor \frac{B}{|S_k| \lceil \log_2(n) \rceil} \rfloor$ additional times and set $R_k = \sum_{j=0}^{k} r_j$

  Let σ_k be a bijection on S_k such that $\ell_{\sigma_k(1),R_k} \leq \ell_{\sigma_k(2),R_k} \leq \ldots \leq \ell_{\sigma_k(|S_k|),R_k}$

  $S_{k+1} = \{i \in S_k : \ell_{\sigma_k(i),R_k} \leq \ell_{\sigma_k(\lfloor |S_k|/2 \rfloor),R_k}\}$

end

Output: Singleton element of $S_{\lceil \log_2(n) \rceil}$

Jamieson and Talwalkar, *Non-stochastic Best Arm Identification and Hyperparameter Optimization*, 2016.

Successive halving

Number of initial configs, n=81. Total budget B=324

Halving rate $\gamma = 3$

k	$\lvert S_k \rvert$	r_k
0	81	1
1	27	3
2	9	9
3	3	27