Learning Representations for Hyperparameter Transfer Learning

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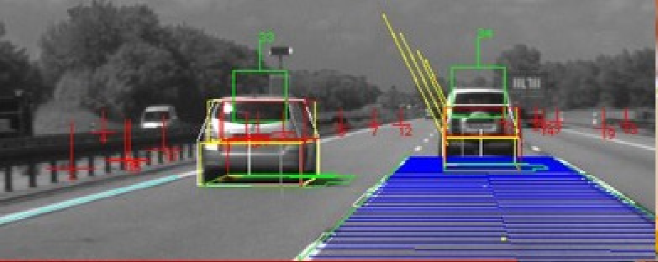

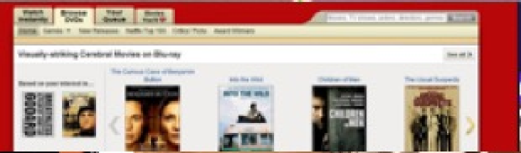
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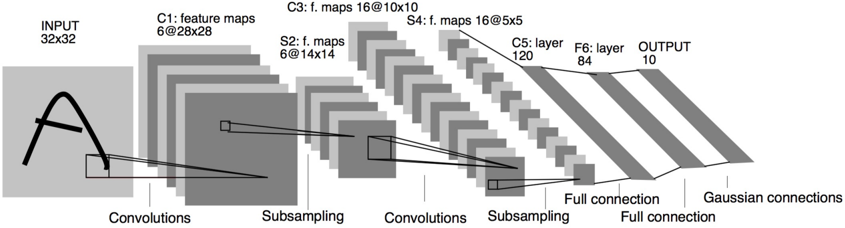
Tuning deep neural nets for optimal performance

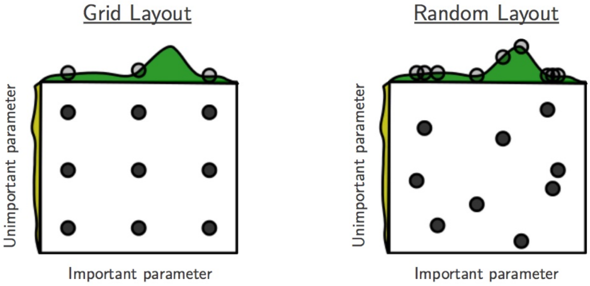


LeNet5 [LBBH98]

The search space $\mathcal{X}$ is large and diverse:

- Architecture: # hidden layers, activation functions, ...
- Model complexity: regularization, dropout, ...
- Optimisation parameters: learning rates, momentum, batch size, ...

Two straightforward approaches



(Figure by Bergstra and Bengio, 2012)

- Exhaustive search on a regular or random grid
- Complexity is exponential in p
- Wasteful of resources, but easy to parallelise
- Memoryless

Can we do better?

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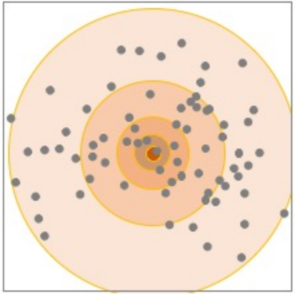
Hyperparameter transfer learning



HPO Job 1

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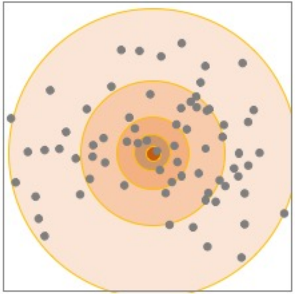
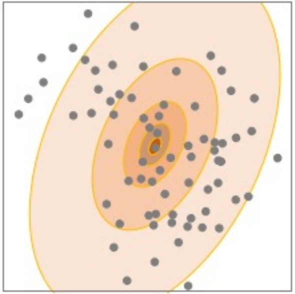
Hyperparameter transfer learning

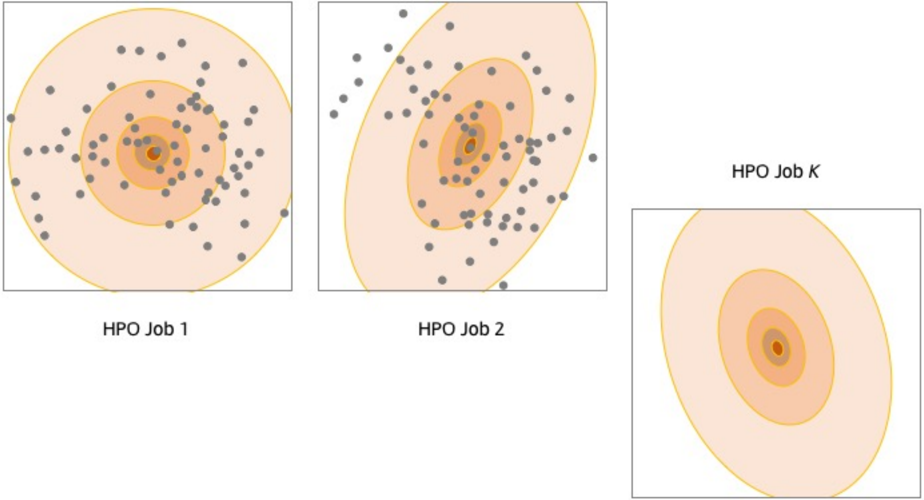


HPO Job 1

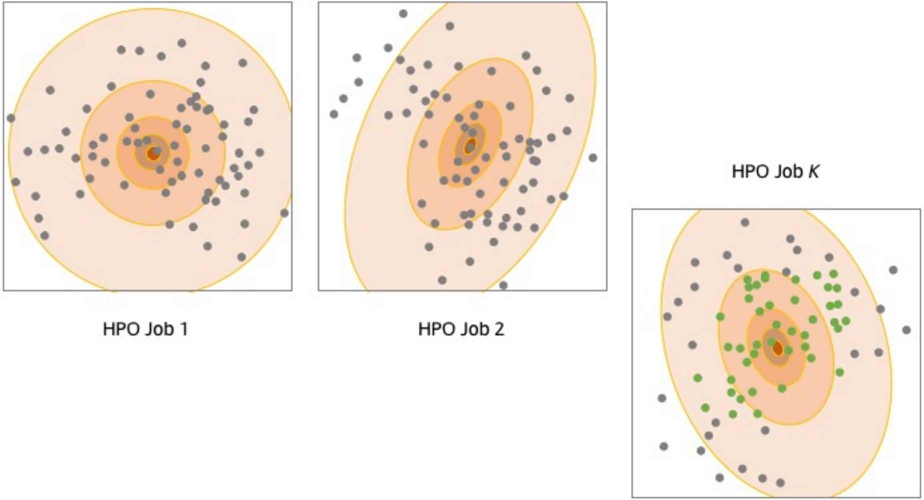


HPO Job 2

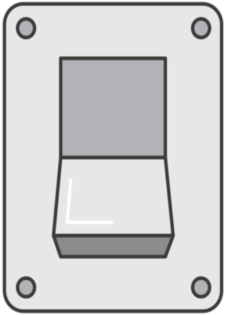
Hyperparameter transfer learning



Hyperparameter transfer learning



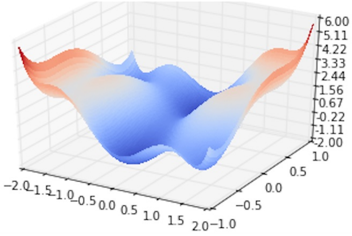
Democratising machine learning



- Abstract away training algorithms
- Abstract away representation (feature engineering)

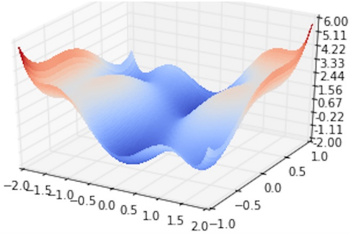
- Abstract away computing infrastructure
- Abstract away memory constraints
- Abstract away network architecture

Black-box global optimisation



- The function f to optimise can be non-convex.
- The number of hyperparameters p is moderate (typically < 20).

Black-box global optimisation



- The function f to optimise can be non-convex.
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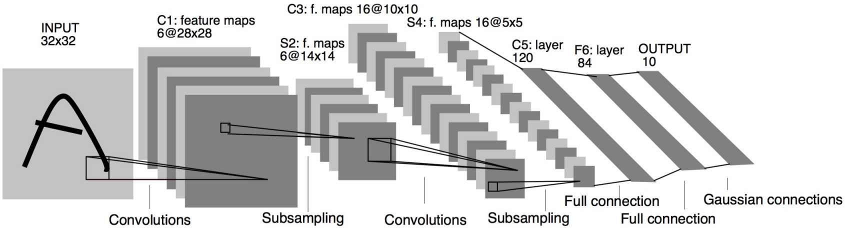
Our goal is to solve the following optimisation problem:

$$\boldsymbol{x}_\star = \operatorname*{argmin}_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x}).$$

- Evaluating $f(\boldsymbol{x})$ is expensive.
- No analytical form or gradient.
- Evaluations may be noisy.

Example: tuning deep neural nets [SLA12, SRS$^+$15, KFB$^+$16]



LeNet5 [LBBH98]

- $f(\mathbf{x})$ is the validation loss of the neural net as a function of its hyperparameters $\mathbf{x}$.
- Evaluating $f(\mathbf{x})$ is very **costly** $\approx$ up to weeks!

Bayesian (black-box) optimisation [MTZ78, SSW+16]

$$\boldsymbol{x}_\star = \operatorname*{argmin}_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x})$$

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Canonical algorithm:

- Surrogate model $\mathcal{M}$ of f `#cheaper to evaluate`
- Set of evaluated candidates $\mathcal{C} = \{\}$

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  - Select candidate $\mathbf{x}_{\text{new}} \in \mathcal{X}$ using $\mathcal{M}$ and $\mathcal{C}$ `#exploration/exploitation`

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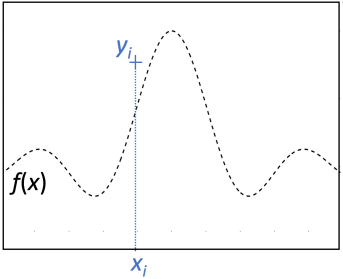
  - Collect evaluation y_{new} of f at $\mathbf{x}_{\text{new}}$ `#time-consuming`
  - Update $\mathcal{C} = \mathcal{C} \cup \{(\mathbf{x}_{\text{new}}, y_{\text{new}})\}$
  - Update $\mathcal{M}$ with $\mathcal{C}$ `#Update surrogate model`
  - Update `BUDGET`

Bayesian (black-box) optimisation with Gaussian processes [JSW98]

1. Learn a probabilistic model of f, which is cheap to evaluate:

$$y_i | f(\boldsymbol{x}_i) \sim \mathrm{Gaussian}\left(f(\boldsymbol{x}_i), \varsigma^2\right), \qquad f(\boldsymbol{x}) \sim \mathcal{GP}(0, \mathcal{K}).$$



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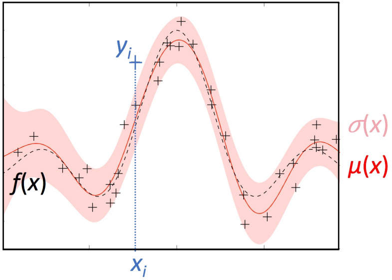
2. Given the observations $\boldsymbol{y} = (y_1, \ldots, y_n)$, compute the predictive mean and the predictive standard deviation:



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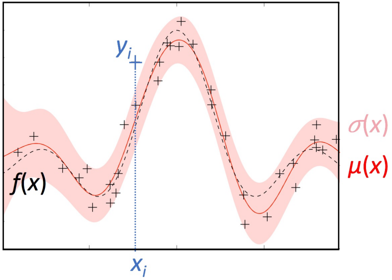
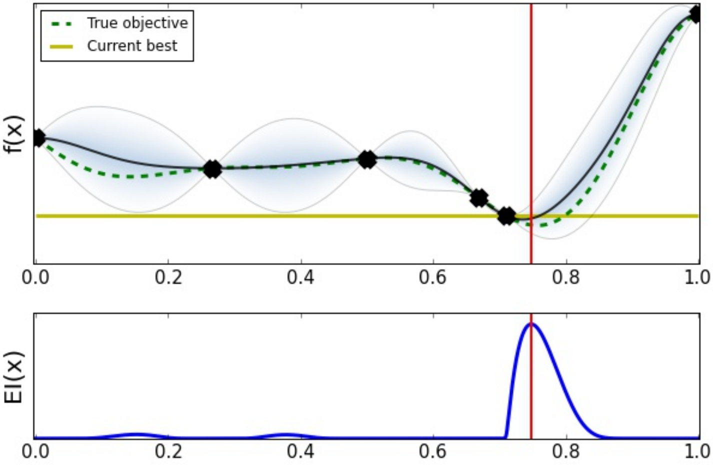


3. Repeatedly query f by balancing **exploitation** against **exploration**!

Bayesian optimisation in practice



(Image credit: Javier González)

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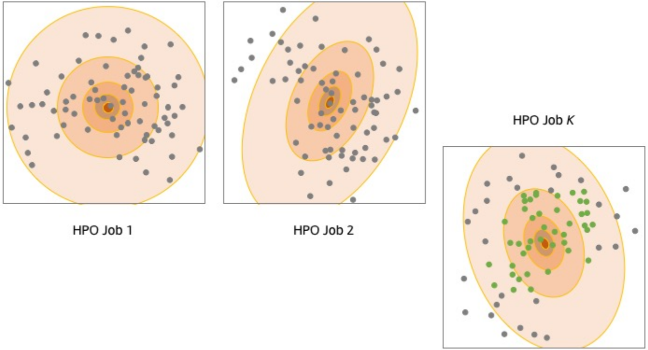
What is wrong with the Gaussian process surrogate?



Scaling is $\mathcal{O}\left(N^3\right)$.

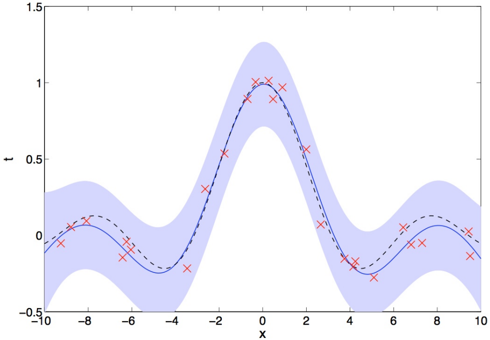
Adaptive Bayesian linear regression (ABLR) [Bis06]

The model:

$$P(\mathbf{y}|\mathbf{w}, \mathbf{z}, \beta) = \prod_n \mathcal{N}(\phi_{\mathbf{z}}(\mathbf{x}_n)\mathbf{w}, \beta^{-1}),$$
$$P(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{0}, \alpha^{-1}\mathbf{I}_D).$$

The predictive distribution:

$$P(y^*|\mathbf{x}^*, \mathcal{D}) = \int P(y^*|\mathbf{x}^*, \mathbf{w})P(\mathbf{w}|\mathcal{D})d\mathbf{w}$$
$$= \mathcal{N}(\mu_t(\mathbf{x}^*), \sigma_t^2(\mathbf{x}^*))$$



Multi-task ABLR for transfer learning

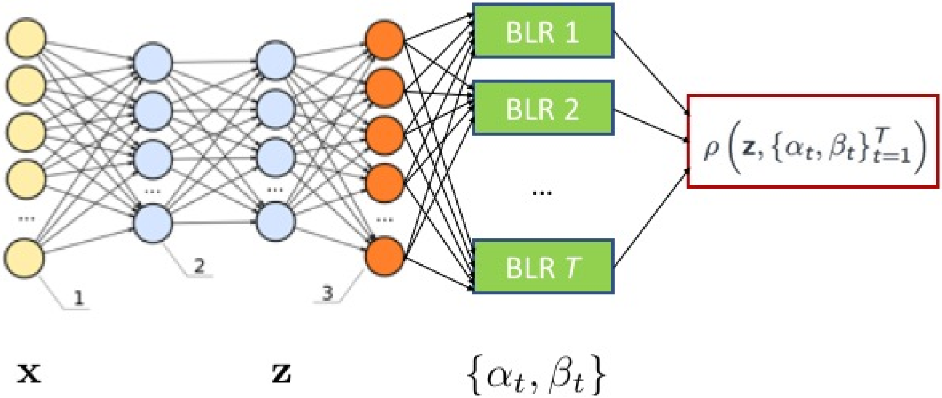
1. Multi-task extension of the model:

$$P(\mathbf{y}_t|\mathbf{w}_t, \mathbf{z}, \beta_t) = \prod_{n_t} \mathcal{N}(\phi_{\mathbf{z}}(\mathbf{x}_{n_t})\mathbf{w}_t, \beta_t^{-1}), \qquad P(\mathbf{w}_t|\alpha_t) = \mathcal{N}(\mathbf{0}, \alpha_t^{-1}\mathbf{I}_D).$$

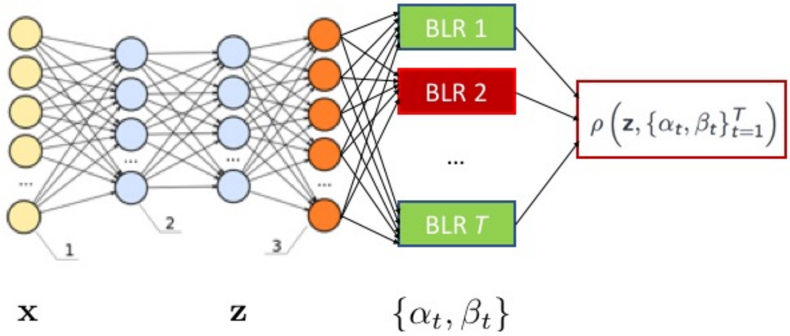
2. Shared features $\phi_{\mathbf{z}}(\mathbf{x})$:
   - Explicit features set (e.g., RBF)
   - Random kitchen sinks [RR+07]
   - Learned by feedforward neural net

3. Multi-task objective:

$$\rho\left(\mathbf{z}, \{\alpha_t, \beta_t\}_{t=1}^{T}\right) = -\sum_{t=1}^{T} \log P(\mathbf{y}_t|\mathbf{z}, \alpha_t, \beta_t)$$

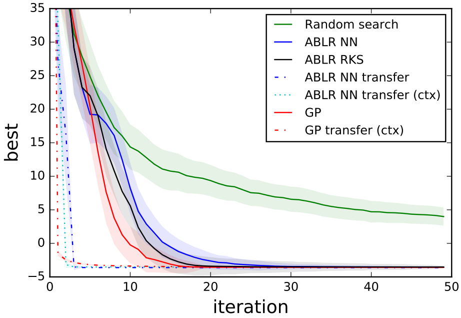

BLR 1
BLR 2
...
BLR T
$\rho\left(\mathbf{z}, \{\alpha_t, \beta_t\}_{t=1}^{T}\right)$
1
2
3
$\mathbf{x}$
$\mathbf{z}$
$\{\alpha_t, \beta_t\}$

Warm-start procedure for hyperparameter optimisation (HPO)

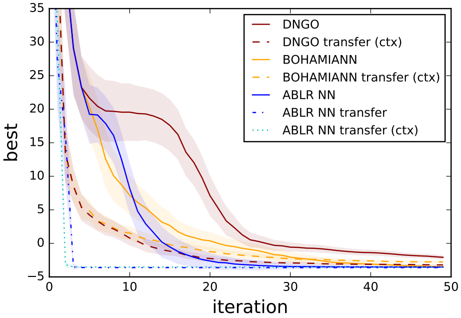


Leave-one-task out.

A representation to optimise parametrised quadratic functions



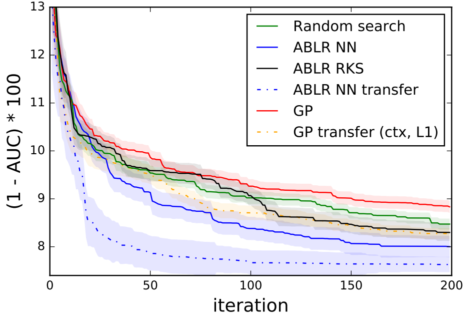
Transfer learning with baselines [KO11].



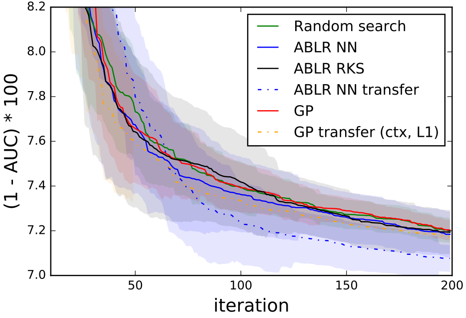
Transfer learning with neural nets [SRS+15, SKFH16].

$$f_t(\boldsymbol{x}) = \frac{a_{2,t}}{2}\|\boldsymbol{x}\|^2 + a_{1,t}\mathbf{1}^\top \boldsymbol{x} + a_{0,t}$$

A representation to warm-start HPO across OpenML data sets

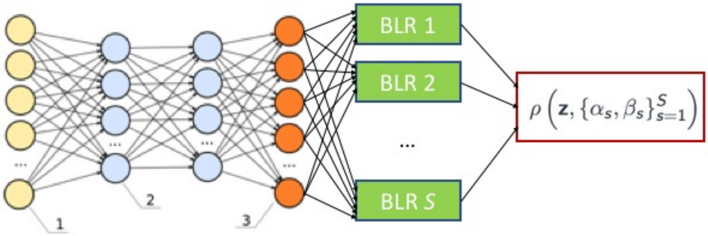


Transfer learning in SVM.



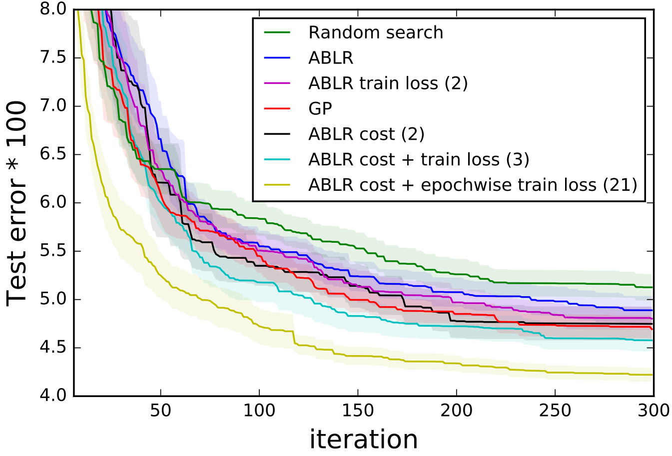
Transfer learning in XGBoost.

Learning better representations by jointly modelling multiple signals



- Tasks are now auxiliary signals (related to the target function to optimise).
- The target is still the validation loss $f(\mathbf{x})$.
- Examples are training cost or training loss.

A representation for transfer learning across OpenML data sets

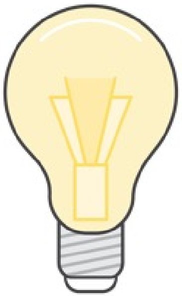


Transfer learning accross LIBSVM data sets.

Conclusion

Bayesian optimisation automates machine learning:

- Algorithm tuning
- Model tuning
- Pipeline tuning



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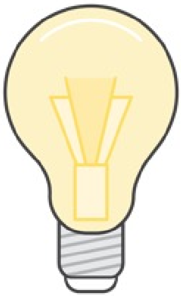

Bayesian optimisation is a model-based approach that can leverage auxiliary information:

- It can exploit dependency structures [JAGS17]
- It can be extended to warm-start HPO jobs [PJSA17]
- It is a key building block of **meta-learning**

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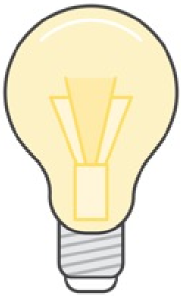
Effective representations for HPO transfer learning can be learned.



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