Scalable Hyperparameter Transfer learning

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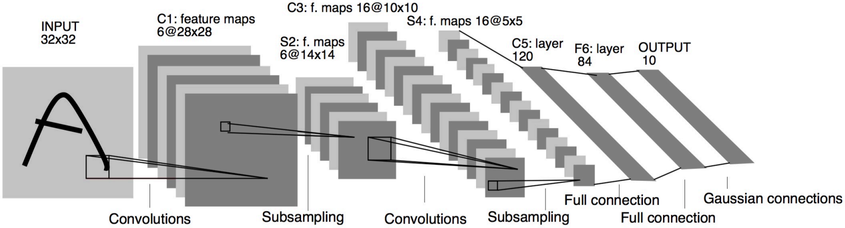
Scalable Hyperparameter Transfer learning. NeurIPS 2018

Tuning deep neural nets for optimal performance

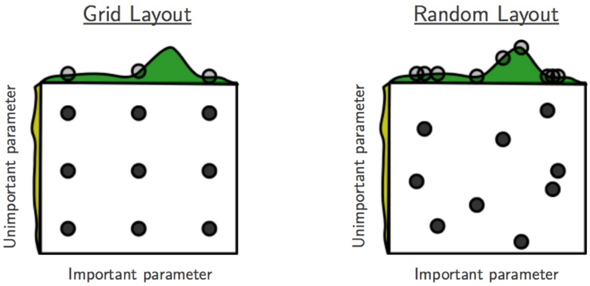


LeNet5 [LBBH98]

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, ...

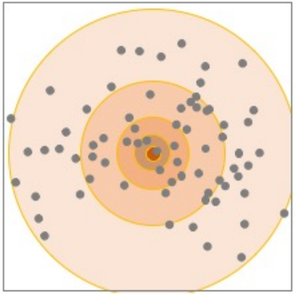
Two straightforward approaches



(Figure by Bergstra and Bengio, 2012)

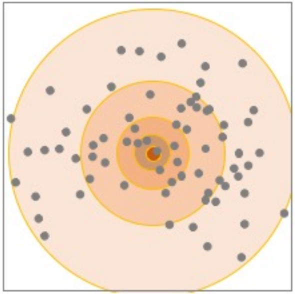
- Exhaustive search on a regular or random grid
- Complexity is exponential in p
- Wasteful of resources, but easy to parallelise
- Memoryless

Hyperparameter transfer learning



HPO Job 1

Hyperparameter transfer learning



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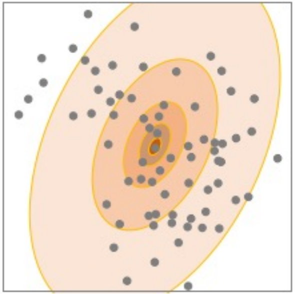
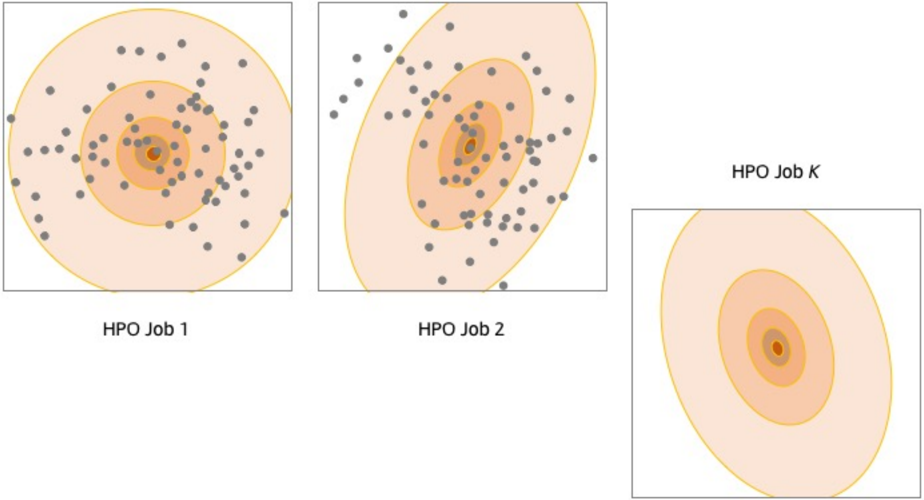
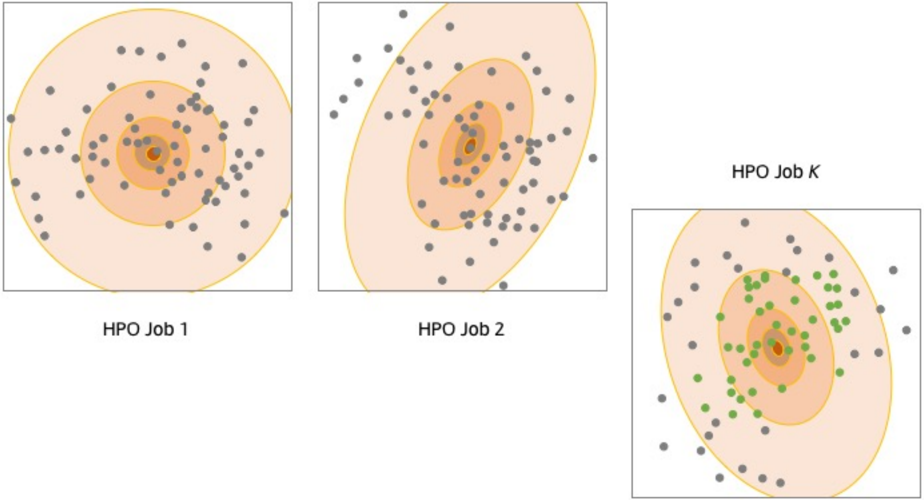


HPO Job 2

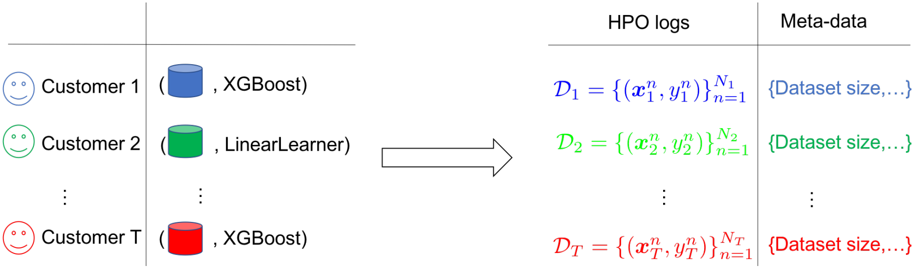
Hyperparameter transfer learning



Hyperparameter transfer learning

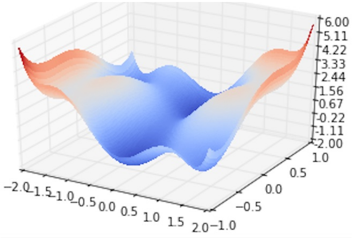


Motivation



- **Transfer learning**: Exploit evaluations of related past tasks
  - A given ML algorithm tuned over different datasets
  - Can we do it in absence of meta-data?
- **Scalability**: Both with respect to
  - #evaluations: $\sum_{t=1}^{T} N_t$
  - #tasks: T

Black-box global optimisation



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

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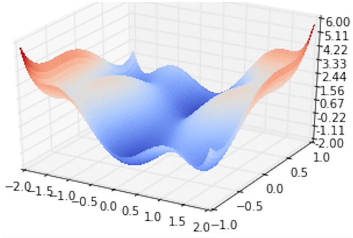

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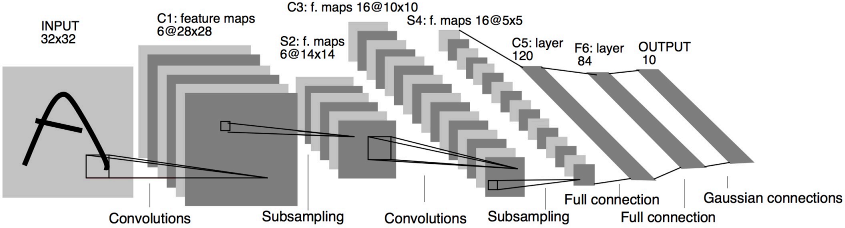
Our goal is to solve the following optimisation problem:

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

- 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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- Set of evaluated candidates $\mathcal{C} = \{\}$

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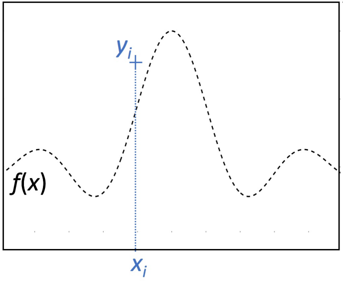
  - Update $\mathcal{C} = \mathcal{C} \cup \{(\mathbf{x}_{\text{new}}, y_{\text{new}})\}$
  - Update $\mathcal{M}$ with $\mathcal{C}$ `#Update surrogate model`
  - Update `BUDGET`

Bayesian (black-box) optimisation with Gaussian processes

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

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



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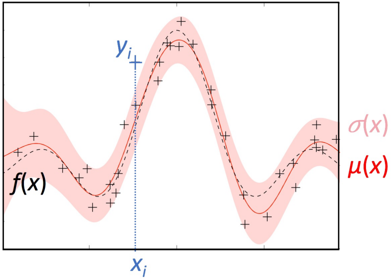

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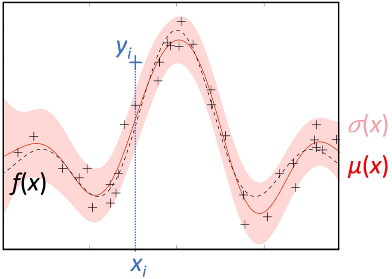
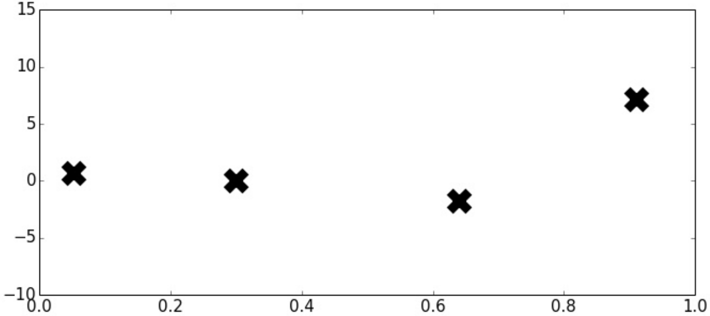
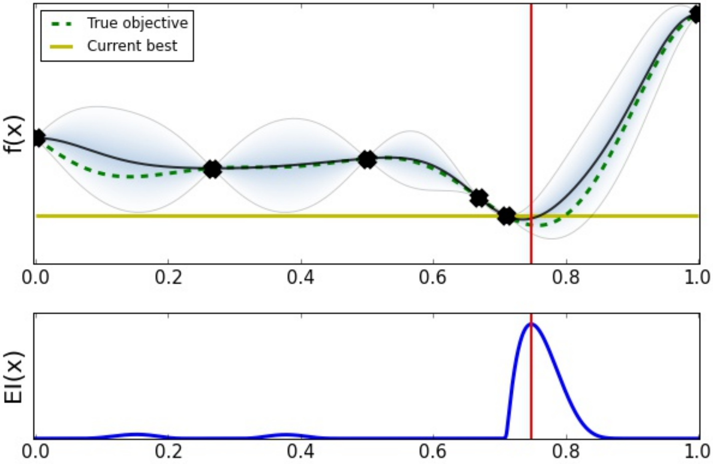


3. Repeatedly query f by balancing **exploitation** against **exploration**

Where is the minimum of $f(x)$?



Bayesian optimisation in practice



(Image credit: Javier González)

Bayesian optimization with transfer learning

Problem statement:

- T functions $\{f_t(\mathbf{x})\}_{t=1}^{T}$ with observations $\mathcal{D}_t = \{(\mathbf{x}_t^n, y_t^n)\}_{n=1}^{N_t}$
- May/may not have meta-data (or contextual features) for $\{f_t(\mathbf{x})\}_{t=1}^{T}$
- **Goal:** Optimize some fixed $f_{t_0}(\mathbf{x})$ while exploiting $\{\mathcal{D}_t\}_{t=1}^{T}$
- (this is not multi-objective!)

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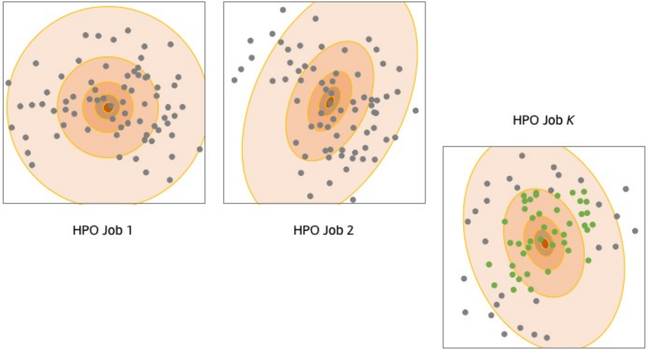
Previous work:

- Multitask GP (Swersky et al. 2013, Poloczek et al. 2016)
- GP + filter evaluations by task similarity (Feurer et al. 2015)
- Various ensemble-based approaches
  - GPs (Feurer et al. 2018)
  - Feedforward NNs (Schilling et al. 2015)

What is wrong with the Gaussian process surrogate?



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

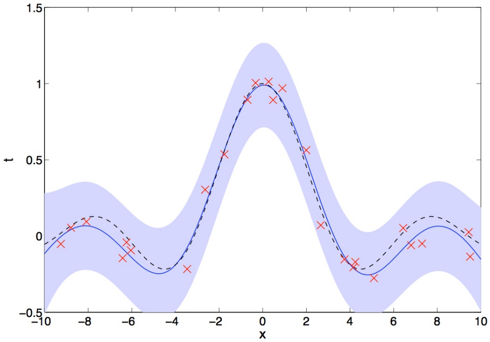
Adaptive Bayesian linear regression (ABLR) [Bis06]

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:

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

Examples of $\phi_{\mathbf{z}}$

Feedforward neural networks:

$$\phi_{\mathbf{z}}(\mathbf{x}) = a_L\left(\mathbf{Z}_L a_{L-1}\left(\ldots \mathbf{Z}_2 a_1\left(\mathbf{Z}_1 \mathbf{x}\right)\ldots\right)\right).$$

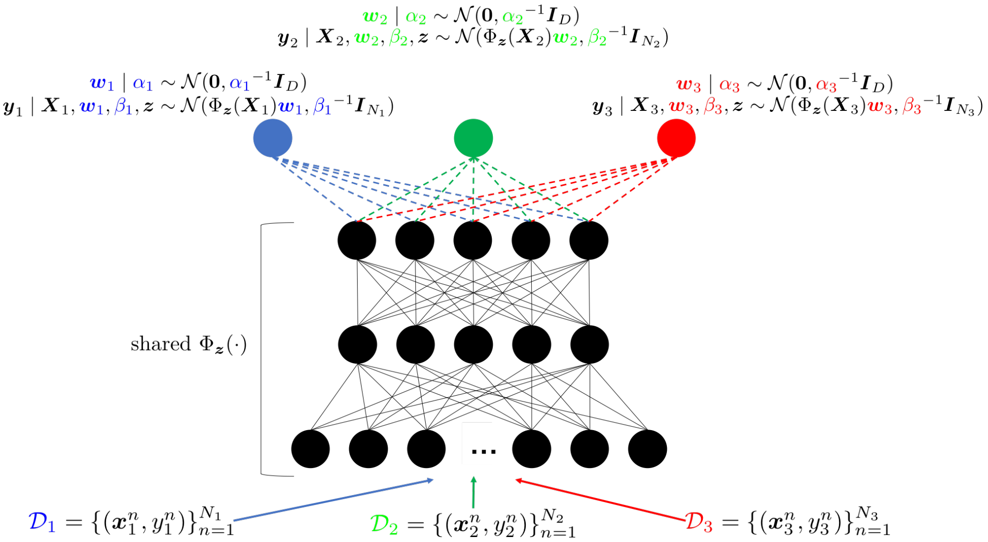
- $\mathbf{z}$ consists of all $\{\mathbf{Z}_l\}_{l=1}^{L}$

Random Fourier features:

$$\phi_{\mathbf{z}}(\mathbf{x}) = \sqrt{2/D}\cos\left\{\frac{1}{\sigma}\mathbf{U}\mathbf{x} + \mathbf{b}\right\}, \quad \text{with} \quad \mathbf{U} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad \text{and} \quad \mathbf{b} \sim \mathcal{U}([0, 2\pi]).$$

- $\mathbf{z}$ only consists of $1/\sigma$

Pictorial summary of ABLR



Posterior inference

Hyperparameters:

- $\{\alpha_t, \beta_t\}_{t=1}^{T}$ for each task t
- $\mathbf{z}$ for the shared basis function

Empirical Bayesian approach:

- Marginalize out the Bayesian linear regression parameters $\{\mathbf{w}_t\}_{t=1}^{T}$
- *Jointly* learn the hyper-parameters of the model $\{\alpha_t, \beta_t\}_{t=1}^{T}$ and $\mathbf{z}$

Minimize

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

Posterior inference (cont'd)

We have closed-forms for posterior mean and variance:

$$\boldsymbol{\mu}_t(\mathbf{x}_t^*; \mathcal{D}_t, \alpha_t, \beta_t, \mathbf{z}) = \frac{\beta_t}{\alpha_t} \phi_{\mathbf{z}}(\mathbf{x}_t^*)^\top \mathbf{K}_t^{-1} \boldsymbol{\Phi}_t^\top \mathbf{y}_t$$
$$\sigma_t^2(\mathbf{x}_t^*; \mathcal{D}_t, \alpha_t, \beta_t, \mathbf{z}) = \frac{1}{\alpha_t} \phi_{\mathbf{z}}(\mathbf{x}_t^*)^\top \mathbf{K}_t^{-1} \phi_{\mathbf{z}}(\mathbf{x}_t^*) + \frac{1}{\beta_t}$$

and marginal likelihood:

$$\rho\left(\mathbf{z}, \{\alpha_t, \beta_t\}_{t=1}^T\right) = -\sum_{t=1}^T \left[\frac{N_t}{2} \log \beta_t - \frac{\beta}{2}\left(||\mathbf{y}_t||^2 - \frac{\beta_t}{\alpha_t}||\mathbf{c}_t||^2\right) - \sum_{i=1}^D \log([\mathbf{L}_t]_{ii})\right]$$

- Cholesky for $\mathbf{K}_t = \frac{\beta_t}{\alpha_t} \boldsymbol{\Phi}_t^\top \boldsymbol{\Phi}_t + \mathbf{I}_D = \mathbf{L}_t {\mathbf{L}_t}^\top$
- $\mathbf{c}_t = {\mathbf{L}_t}^{-1} \boldsymbol{\Phi}_t^\top \mathbf{y}_t$

Leveraging `MXNet`

In Bayesian optimization, derivatives needed for

- Posterior inference: $(\mathbf{z}, \{\alpha_t, \beta_t\}_{t=1}^{T}) \mapsto \rho(\mathbf{z}, \{\alpha_t, \beta_t\}_{t=1}^{T})$
- Acquisition functions $\mathcal{A}$, typically of the form (e.g., EI, PI, UCB,...):

$$\mathbf{x}^* \mapsto \mathcal{A}(\mu_t(\mathbf{x}^*; \mathcal{D}_t, \alpha_t, \beta_t, \mathbf{z}), \sigma_t^2(\mathbf{x}^*; \mathcal{D}_t, \alpha_t, \beta_t, \mathbf{z}))$$

Leverage `MXNet` (Seeger et al. 2017):

- Auto-differentiation
- Backward operator for Cholesky
- Can use any $\phi_{\mathbf{z}}$

Optimization of the marginal likelihood

Optimization properties:

- Number of tasks: $T \approx$ few tens
- Number of points per task: $N_t \gg 1$
- Not standard SGD regime
- We apply `L-BFGS` *jointly* over all parameters $\mathbf{z}$ and $\{\alpha_t, \beta_t\}_{t=1}^{T}$
- Warm-start parameters: Re-convergence in a very few steps

Surrogate models used in Bayesian optimization

Various types of models used:

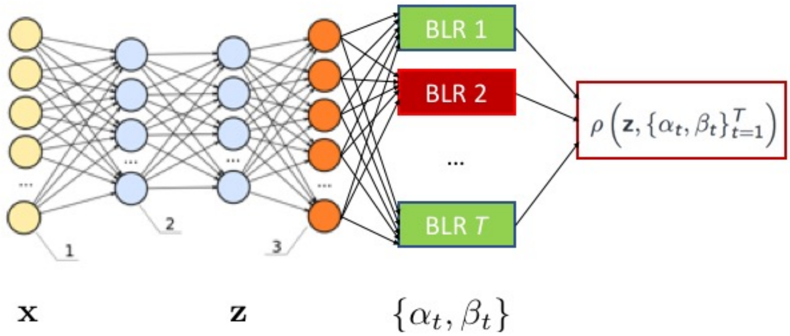
- Gaussian processes (Jones et al. 1998, Snoek et al. 2012,. . .)
- Sparse gaussian processes (McIntire et al. 2016)
- Variants (DKL/KISS-GP) of Gaussian processes (Pleiss et al. 2018)
- Random forests (Hutter et al. 2011)
- (Bayesian) NNs (Snoek et al. 2015, Springenberg et al. 2016)

ABLR

Contributions:

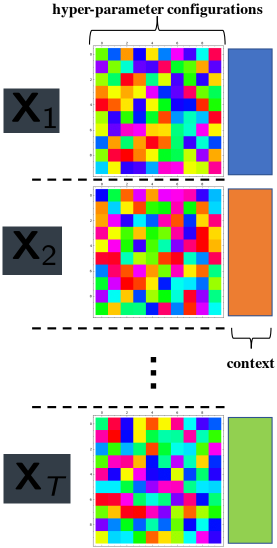
- Simplicity
- Scalability
- Transfer learning in absence of meta-data
- Extend DNGO (Snoek et al. 2015) with:
  - Joint inference
  - Transfer learning and handling of heterogenous tasks

Warm-start procedure for hyperparameter optimisation (HPO)



Leave-one-task out.

Pictorial view of different transfer learning approaches



1. Single marg. likelihood, stack across tasks

$$\begin{bmatrix} \mathbf{X}_1 & \text{context}_1 \\ \vdots & \vdots \\ \mathbf{X}_T & \text{context}_T \end{bmatrix} \in \mathbb{R}^{\sum_{t=1}^{T} N_t \times (P + |\text{context}|)}$$

2. One marg. likelihood per $\mathbf{X}_t$ (no context!)
3. One marg. likelihood per $[\mathbf{X}_t, \text{context}_t]$

Small-scale synthetic example: Transfer learning across quadratic functions

3-dimensional parameterized quadratic functions:

$$f_t(\mathbf{x}) = \frac{1}{2} a_t \|\mathbf{x}\|_2^2 + b_t \mathbf{1}^\top \mathbf{x} + c_t,$$

- One task $=$ one function f_t
- $(a_t, b_t, c_t) \in [0.1, 10]^3$, contextual information
- $T = 30$ tasks
- "Leave-one-task-out"

Experimental protocol

Comparisons with:

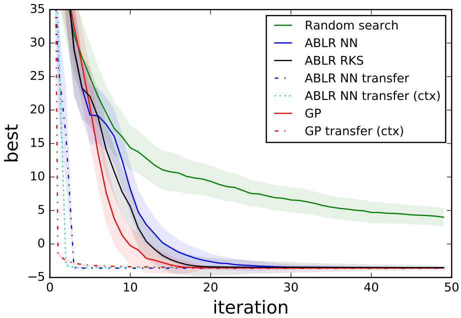
- Random search (Bergstra et al. 2012)
- Gaussian process (based on `GPyOpt` implementation)
- Gaussian process + "L_1 heuristic" (Feurer et al. 2015)
- DNGO[1] (Snoek et al. 2015)
- BOHAMIANN[1] (Springenberg et al. 2016)

Other considerations:

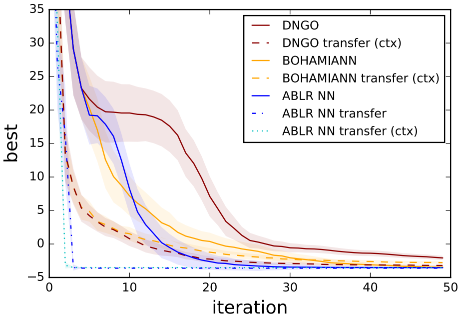
- Results aggregated over 30 replicates.
- Expected improvement used for all model-based approaches.
- Architecture of ABLR is $(50, 50, 50)$ (following Snoek et al. 2015).

[1] Implementation from `https://github.com/automl/RoBO`

Transfer learning across quadratic functions

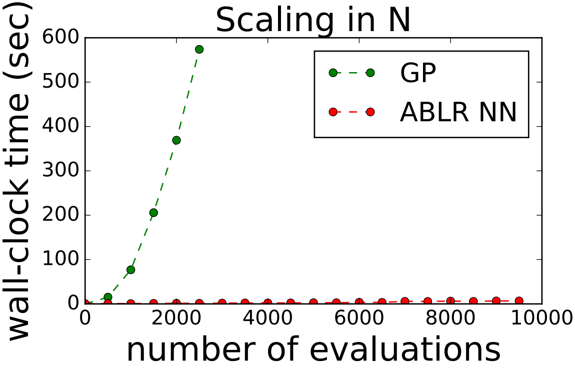


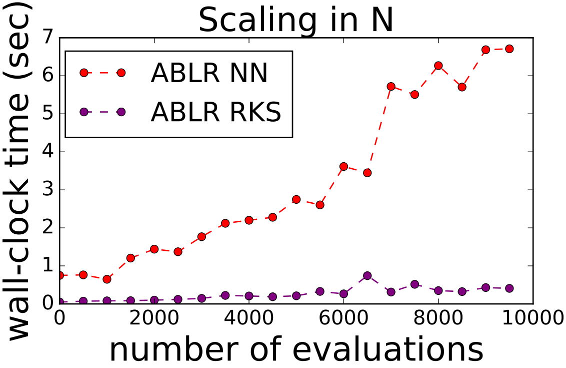
Transfer learning with baselines [KO11].



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

Scalability: GP vs ABLR

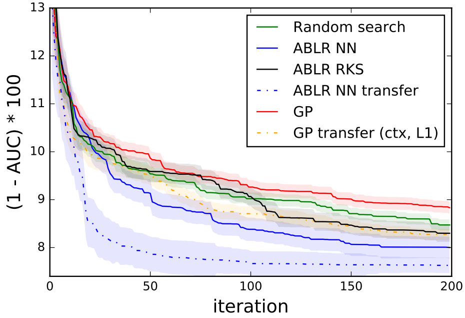




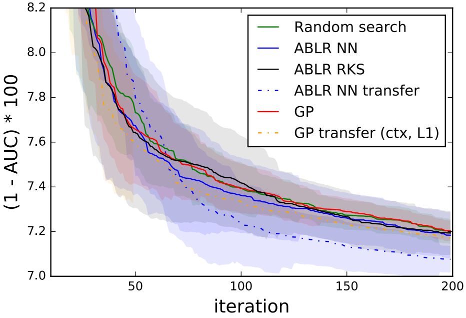
Transfer learning - OpenML data (Vanschoren et al. 2014)

- One task = one dataset
- Collect $\{(\mathbf{X}_t, \mathbf{y}_t)\}_{t=1}^{T}$ from OpenML (Vanschoren et al. 2014)
- `SVM`: 4 HPs, `XGBoost`: 10 HPs
- Take T=30 datasets (`flow_ids`)
  - $\sum_t N_t$ up to 7.5×10^5 evaluations

Transfer learning across OpenML data sets



Transfer learning in SVM.



Transfer learning in XGBoost.

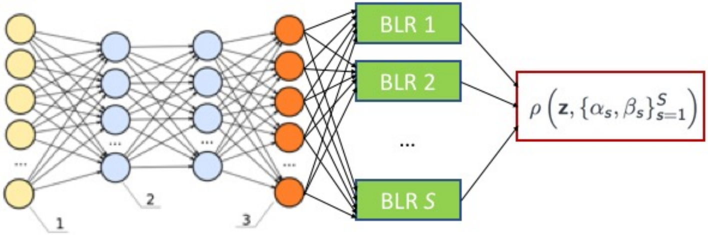
Transfer learning vs. exploiting side signals

	transfer learning	**side signals**
# active task(s)	1	T
# optimized task	1	1
N_t	non-active N_t fixed	growing $N_t = N$
marg. likelihood	a tuning experiment	a signal

Typical use cases

- **Transfer learning**: Reuse data of previous tuning experiments
- **Side signals**: The training of ML models generate multiple signals

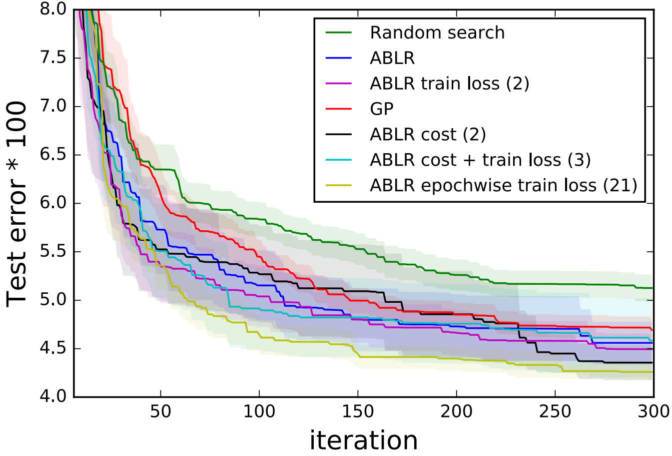
Leveraging multiple signals



Goal: Tune feedforward NNs for binary classification

- Main signal: Validation accuracy
- Side signals: Training accuracy and CPU time ("come for free")
- **Idea**: Side signals can help learn $\phi_{\mathbf{z}}$

Leveraging multiple signals



Transfer learning across LIBSVM data sets.

Conclusion

Bayesian optimisation is a model-based approach that automates machine learning:

- Algorithm tuning
- Model tuning

ABLR [PJSA17]:

- Scalable
- Fully leverages `MXNet`
- Transfers knowledge across tasks and signals

Thank you!

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