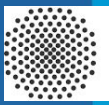


Universität Stuttgart

Latent Space Bayesian Optimization with Transfer Learning

Jagan Shanmugam

Outline

- Motivation
- Problem statement
- Background
  - Bayesian Optimization
- Existing methods
  - Random Embeddings for Bayesian Optimization
  - Multi-Task Adaptive Bayesian Linear Regression (ABLR)
- Latent space models and Joint learning
  - Projection Multi-Task ABLR
  - Auto Encoder Multi-Task ABLR
- Latent space Bayesian Optimization with Transfer Learning
- Experiments
  - Synthetic functions
  - Results

Motivation

- Hyperparameters of industrial processes **(black-box functions)** are manually tuned in different context/settings
- Oftentimes, only a subset or linear/nonlinear combination of parameters are relevant
- Should adapt to unseen tasks by learning from previous evaluations (metadata)

Goal: Find the optimal parameters of a black-box function by optimizing in low dimensional space and leveraging collected information from previous runs

Optimization run	***Settings/Context in Welding process***	***Dataset***
Run/Task 1	*Material type 1, Electrode type 1, Size, ..*	*Dataset 1*
Run/Task 2	*Material type 2, Electrode type 2, Size, ..*	*Dataset 2*
…..	…..	…..
Run/Task T	***Material type T, Electrode type 1, Size, ..***	***Warm start from previous runs/tasks, to increase sample efficiency in Task T***

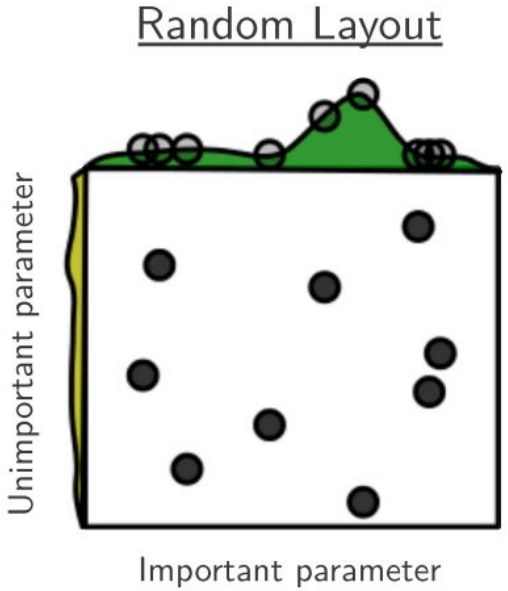
Problem statement

- Following black-box optimization problem:

$$x^* = \arg\min_{x \in \mathcal{X}} f(x)$$

  - Evaluation is expensive and noisy
  - No analytical form or gradient, possibly non-convex
  - Parameter space $\mathcal{X}$ - high but *Intrinsically low dimensional*

- Leverage data from evaluations of related black-box functions: $\{(\mathrm{f}_t)\}_{t=1}^{T}$



Random layout of parameters in a function with one important and one unimportant parameter*

*Image source: Bergstra, J. & Bengio, Y. (2012). Random Search for Hyper-Parameter Optimization. *J. Mach. Learn. Res.*, 13, 281-305.

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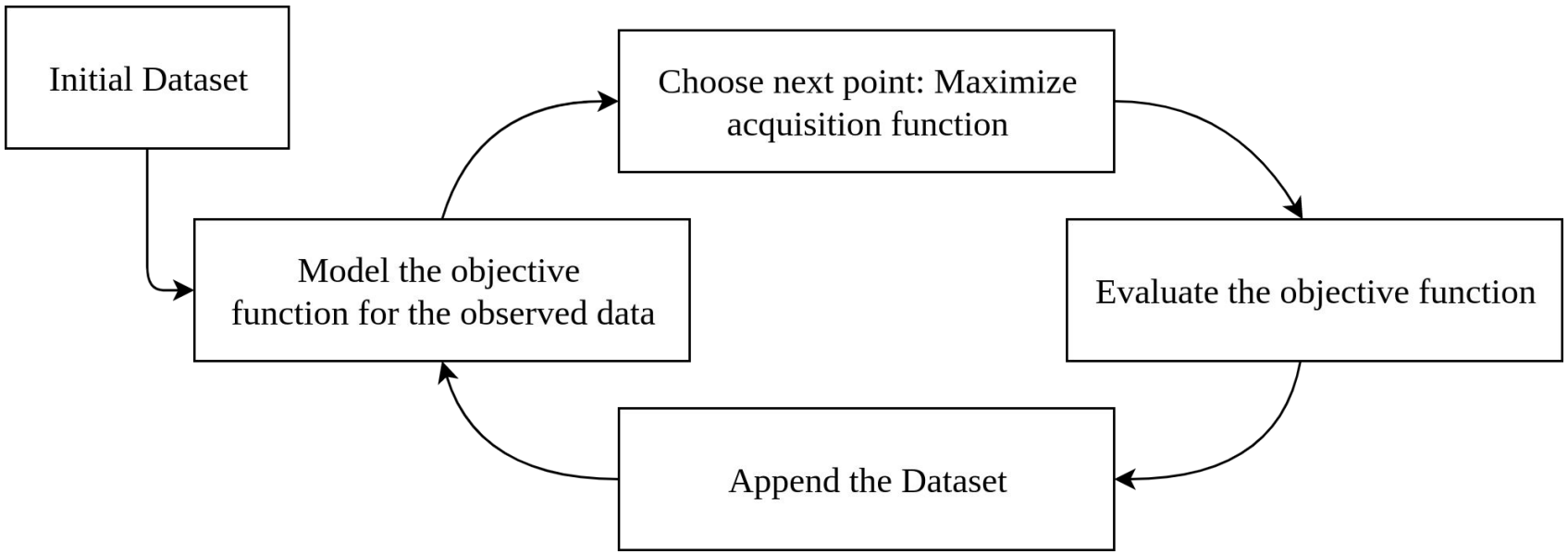
Bayesian Optimization (BO)

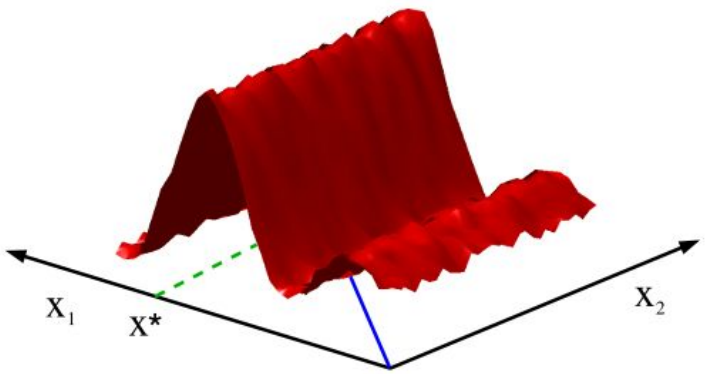


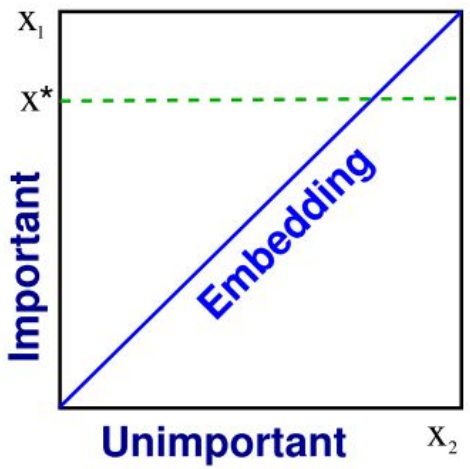
Limitations:

- Cold start problem: When started from scratch, initial iterations explore the input space randomly
- High Dimensional BO: Maximizing nonconvex acquisition function in high dimensional input spaces does not lead to reliable estimate of next input point to evaluate

Existing methods -

Random Embeddings for BO (REMBO)





- Random projection matrix, $A \in \mathbb{R}^{D \times d}, d < D$
- Sample a point $z \in \mathbb{R}^d$ in low dimensional embedding within $[-\sqrt{d}, \sqrt{d}]^d$ to optimize the acquisition function in low dimensional space
- Evaluate on the function: $f(Az)$

*2D function with 1 effective dimension, d=1, D=2

*Image source: Ziyu Wang, Frank Hutter, Masrour Zoghi, David Matheson, and Nando De Freitas. 2016. Bayesian optimization in a billion dimensions via random embeddings.

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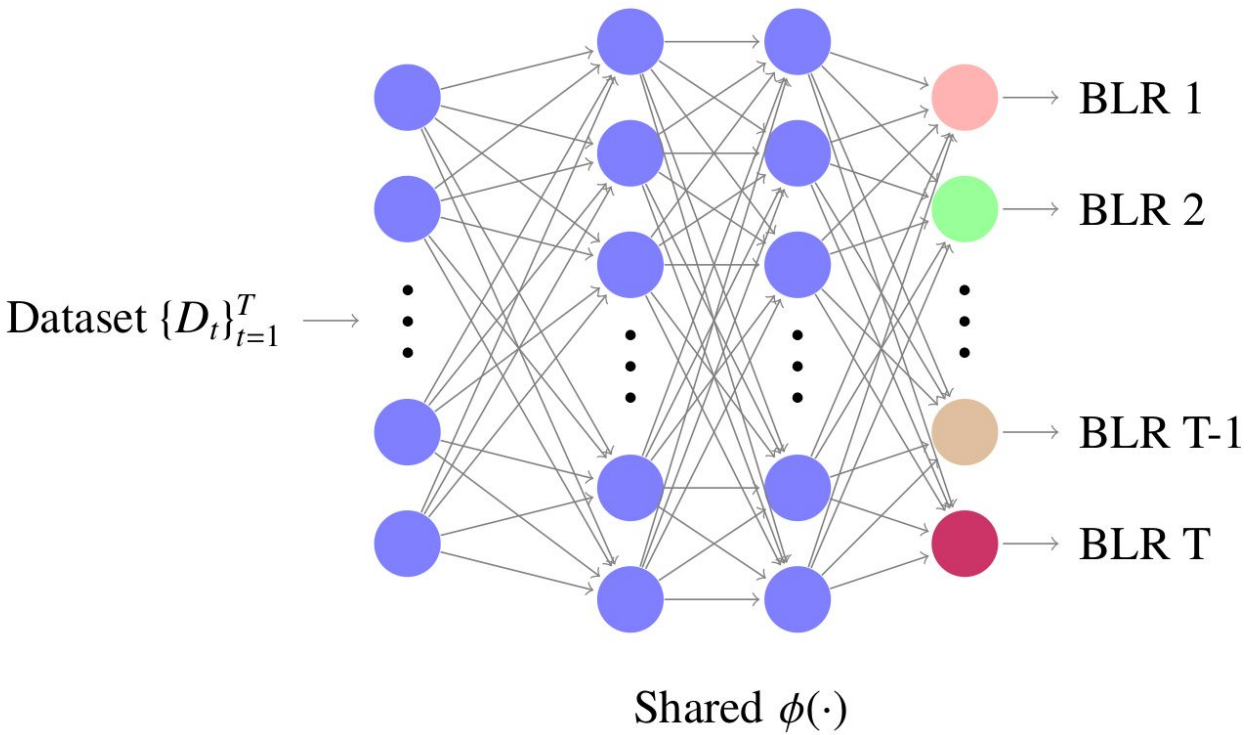
Existing methods -

Multi-Task Adaptive Bayesian Linear Regression (ABLR)



- Extension of Adaptive Bayesian Linear Regression to multi-task cases
- Shared feature learning network for all tasks
- One Bayesian Linear Regressor as a last layer for each task
- **Training:** By minimizing the sum of Negative Log Likelihood of all tasks with points from one task forming a batch

Existing methods -

Multi-Task Adaptive Bayesian Linear Regression (ABLR)

T Black-box functions: $\{(\mathrm{f}_t)\}_{t=1}^{T}$

Data evaluated on each function: $\mathrm{D}_t = \{(x_t^n, y_t^n)\}_{n=1}^{N_t}$

Dataset: $\{\mathrm{D}_t\}_{t=1}^{T}$

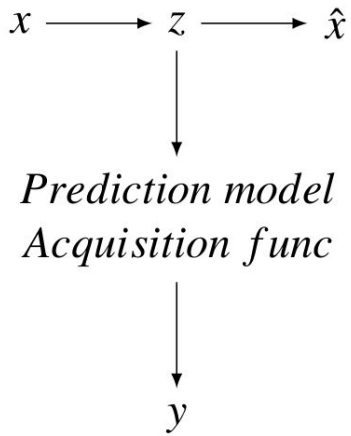
$$P(w_t \mid \alpha_t) = \mathcal{N}(0,\, \alpha_t^{-1}\mathbb{I}_P)$$
$$P(y_t \mid w_t, z, \beta_t) = \mathcal{N}(\Phi_t w_t,\, \beta_t^{-1}\mathbb{I}_{N_t})$$

$$\Phi_t = [\phi_z(x_t^n)]_n \in \mathbb{R}^{N_t \times D}$$

$$\beta_t > 0,\ \alpha_t > 0$$

Latent space models

Idea: Joint learning of low dimensional latent space and prediction model on the latent space by learning shared features from the latent space



➔ Enables BO in the low dimensional space

➔ Speeds up BO by learning from other tasks in multi-task cases

Joint training: Minimizing the sum of Negative Log Likelihood and MSE for all tasks

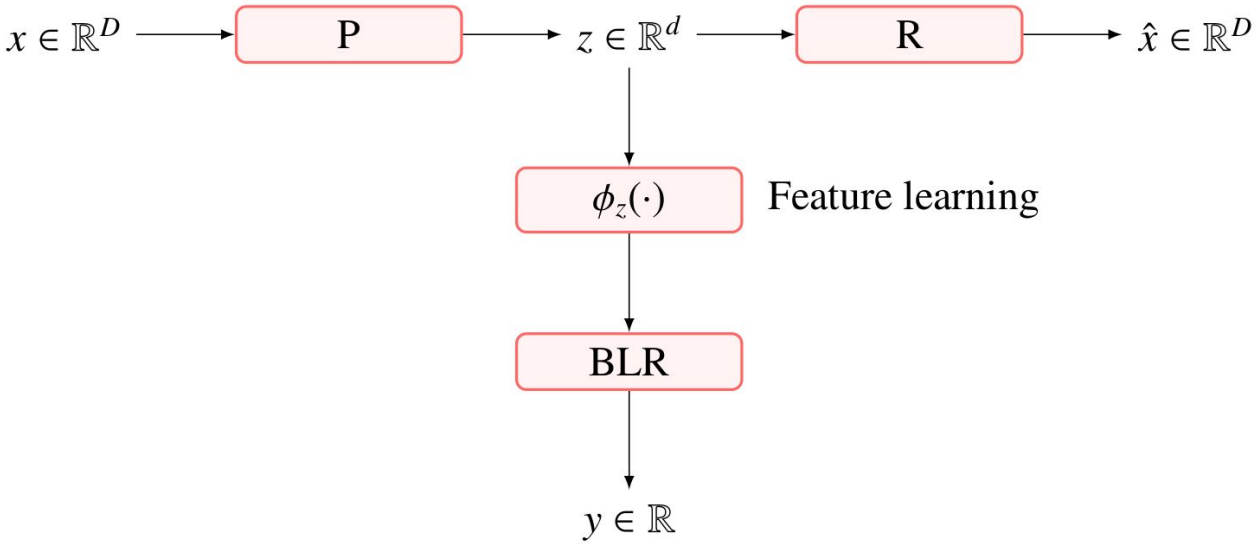
$$Total\ loss = \sum_{t=1}^{T}[-log\ P(y_t/z, \alpha_t, \beta_t) + \|x_t - \hat{x}_t\|_2^2]$$

Two variants:

- Projection ABLR model
- Auto Encoder ABLR model

Latent space models -

Projection ABLR model



- Single Task case - Typical BO
- Linear transformation of input space to latent space and vice-versa
- Projection (*P*) and Reconstruction (*R*) matrices are learned during BO

Latent space models -

Projection Multi-Task ABLR model

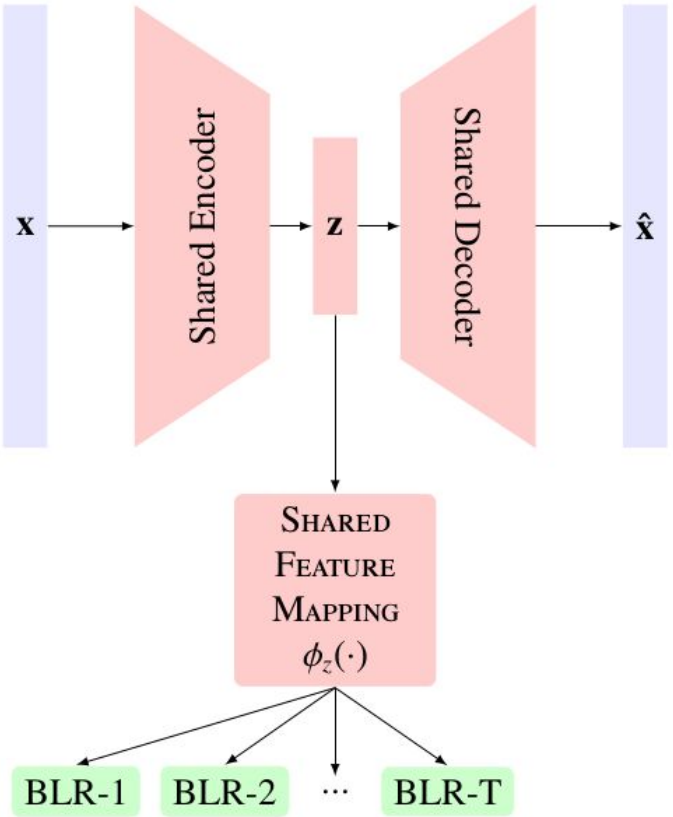
- Learn shared Projection and Reconstruction matrices for all tasks along with ABLR parameters from metadata

$$z = Px \qquad \mathrm{P} \in \mathbb{R}^{d \times D}$$
$$\hat{x} = Rz \qquad \mathrm{x} \in \mathbb{R}^{D}$$
$$\mathrm{z} \in \mathbb{R}^{d}$$
$$\mathrm{R} \in \mathbb{R}^{D \times d}$$

- With one BLR layer for each task and learning a linear shared Projection/Reconstruction mapping from metadata, a Multi-Task model is constructed

Latent space models -

Auto Encoder Multi-Task ABLR model



- Shared Encoder, Decoder, Feature mapping for all tasks
- Nonlinear transformation of input space to latent space
- Constrain the latent space to be gaussian using Variational Auto Encoder approach, a variant implemented and tested, which is conceptually similar to VAE-BO

Latent space Bayesian Optimization

while *current step <= max iterations* **do**
- *Train the Latent model: Target-train*
  - Dimensionality reduction: $z = Mapping(x)$
  - Learn the low dimensional surface: $p(f_z/z, y)$
- *Select next input for evaluation:*
  - Maximize Acquisition function over: z_{next}
  - Map z_{next} to input space: x_{next}
  - Clip x_{next} if projected outside bounds
- Evaluate x_{next} on Target Task T
- Append the dataset $D_T = \{x_{next}, f_T(x_{next})\}$
- Increment current step by 1

- Model resides in low dimensional space -> Acquisition function is optimized in low dimensional latent space
- During BO, point to evaluate on the target task's objective function in input space is reconstructed from the point in latent space
- **Latent Space BO with Transfer Learning**: Multi-Task model is trained on metadata offline
  - Mapping (Projection or AE model) is learned during meta-training and adapted during BO
  - Shared features are learned from latent space by using Multi-Task ABLR model

Experiments -

Synthetic functions

- Parameterized Quadratic function:
  - Multiple tasks are generated by sampling the parameters (a, b, c)

$$f(z) = \frac{1}{2}a||z||^2 + b\mathbf{1}^T z + 3c$$

- Parameterized Rosenbrock function (log-scaled):
  - Number of settings: n_s (Values of settings differentiate tasks)

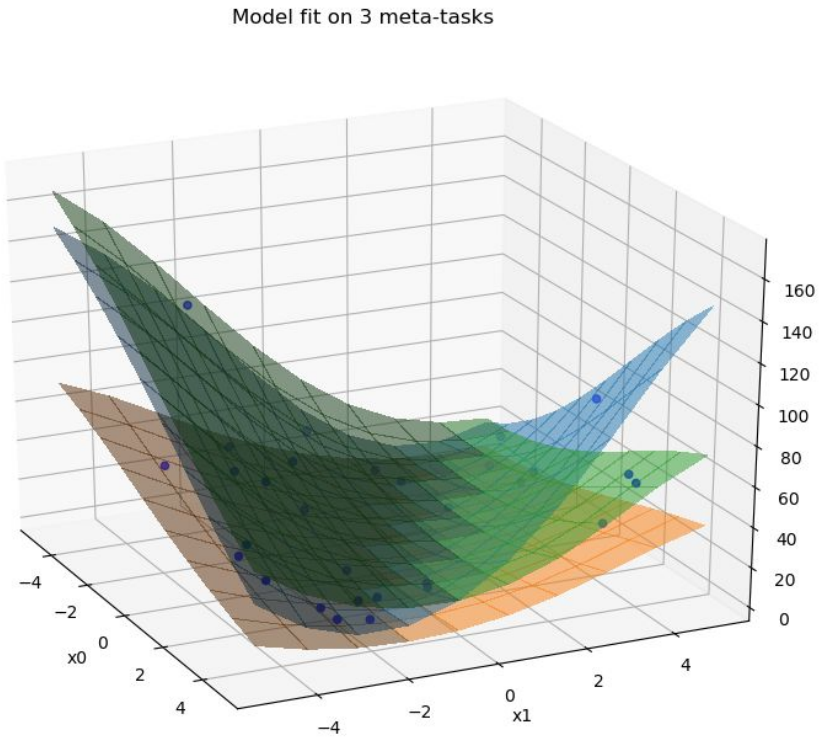
$$f(z) = \sum_{i=1}^{(n_s+d)-1} [100(z_{i+1} - z_i^2)^2 + (z_i - 1)^2]$$

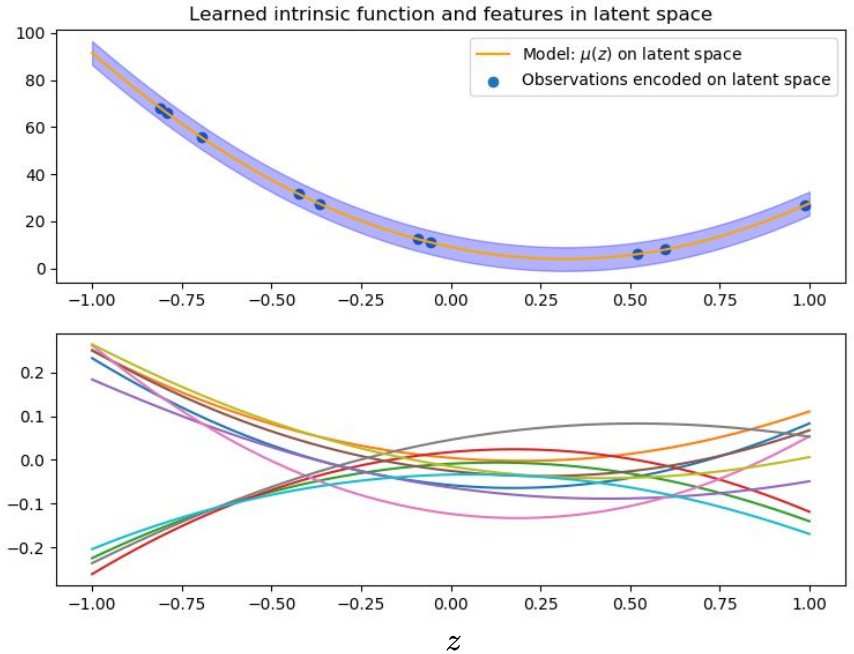
- **High dimensional function with low intrinsic dimensionality**, with matrix $A \in \mathbb{R}^{d \times D}$ with orthogonal rows

$$f_X(x) = f(z) = f(Ax)$$

Experiments -

Meta-learning the intrinsic function





Projection-MT-ABLR model trained on metadata (30 tasks and 10 points each) of 2D Quadratic function with 1D intrinsic space

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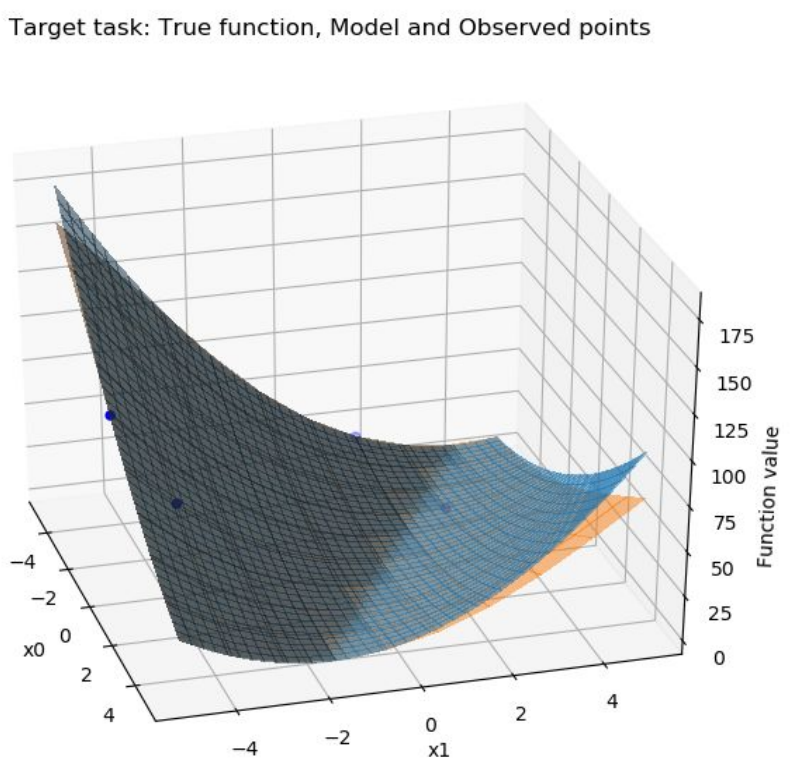
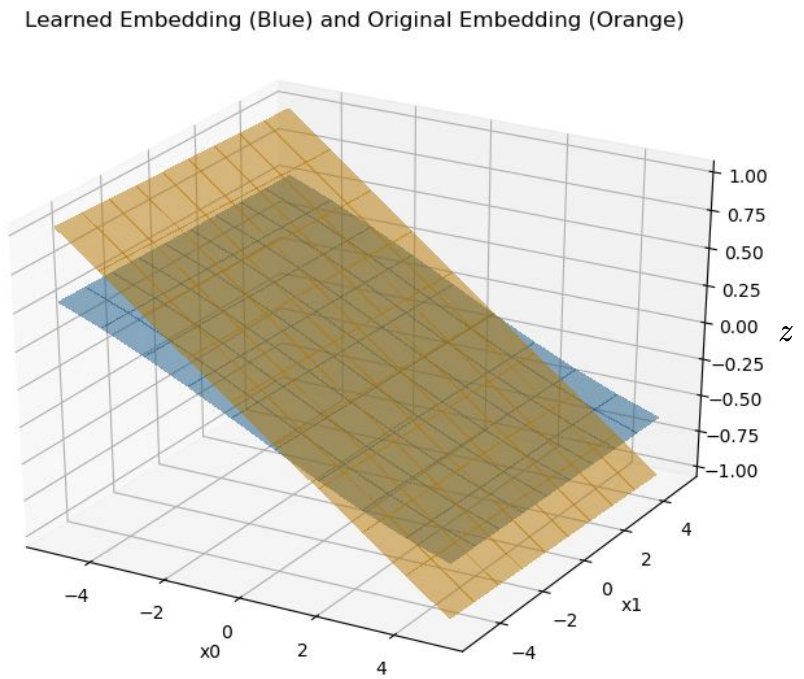
Experiments -

Meta-learning the intrinsic function



Projection-MT-ABLR model on Target task with only 4 randomly sampled points:Original function (Orange), Model fit (Blue)



Learned and Original linear embedding in the input space: Every point in 2D input space is mapped via learned projection matrix to latent space

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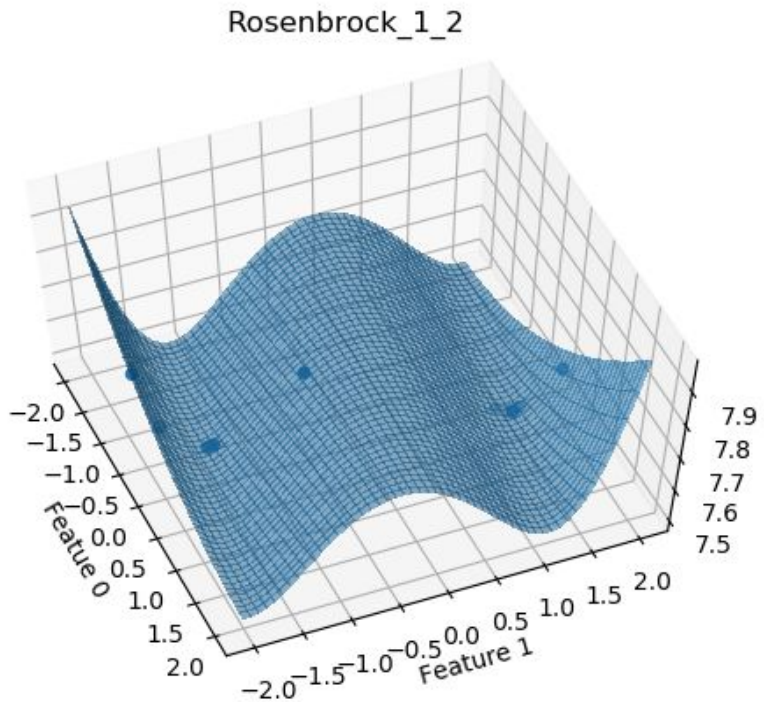
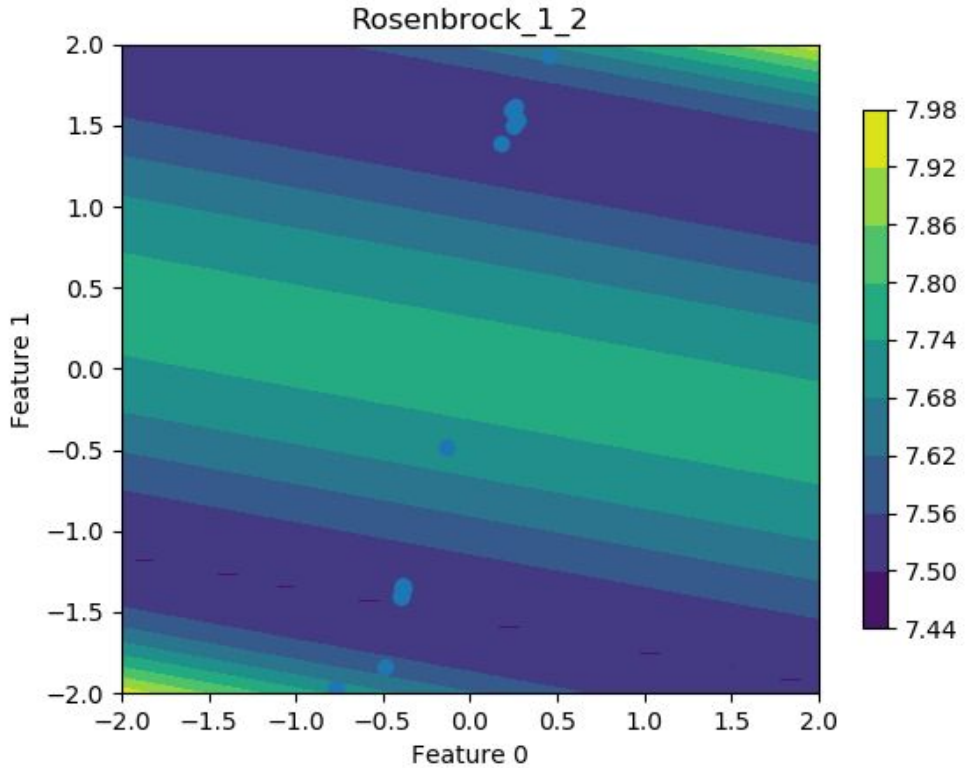
Experiments -

Low dimensional BO with Transfer Learning





2D Rosenbrock function with intrinsic dimensionality of one and points sampled during BO in the corresponding contour plot

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Results

High Dimensional BO for parameterized Quadratic and Rosenbrock functions for two cases:

1. without Transfer Learning
2. with Transfer Learning

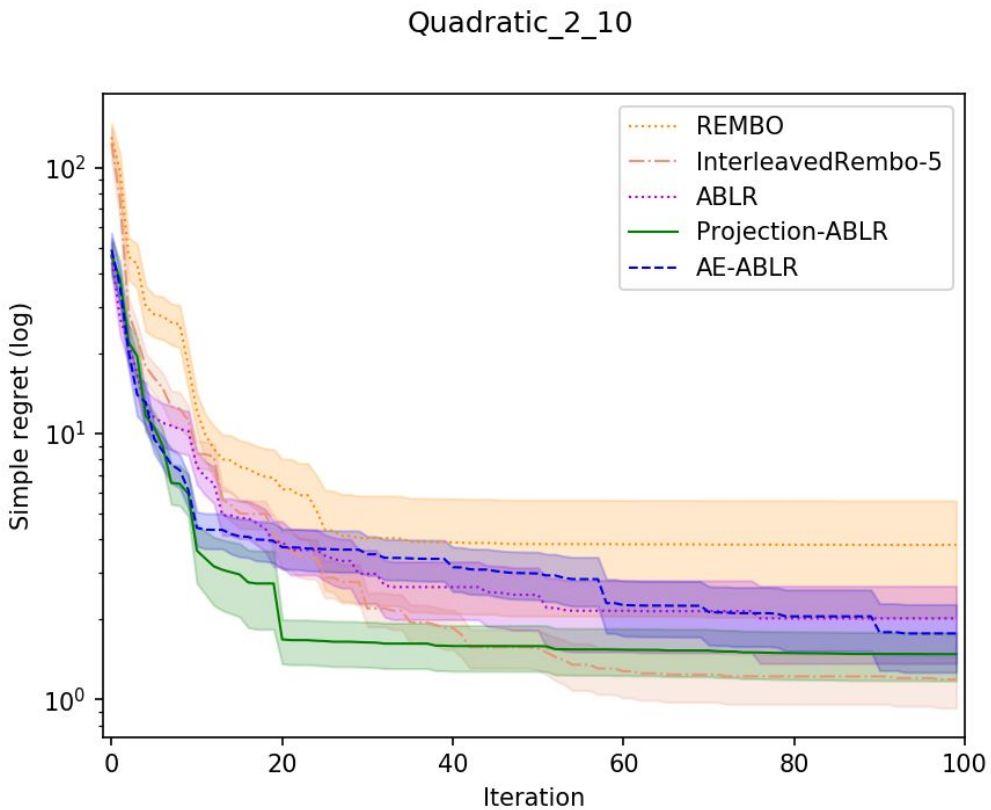
Metric for comparison - Simple regret or Optimality gap

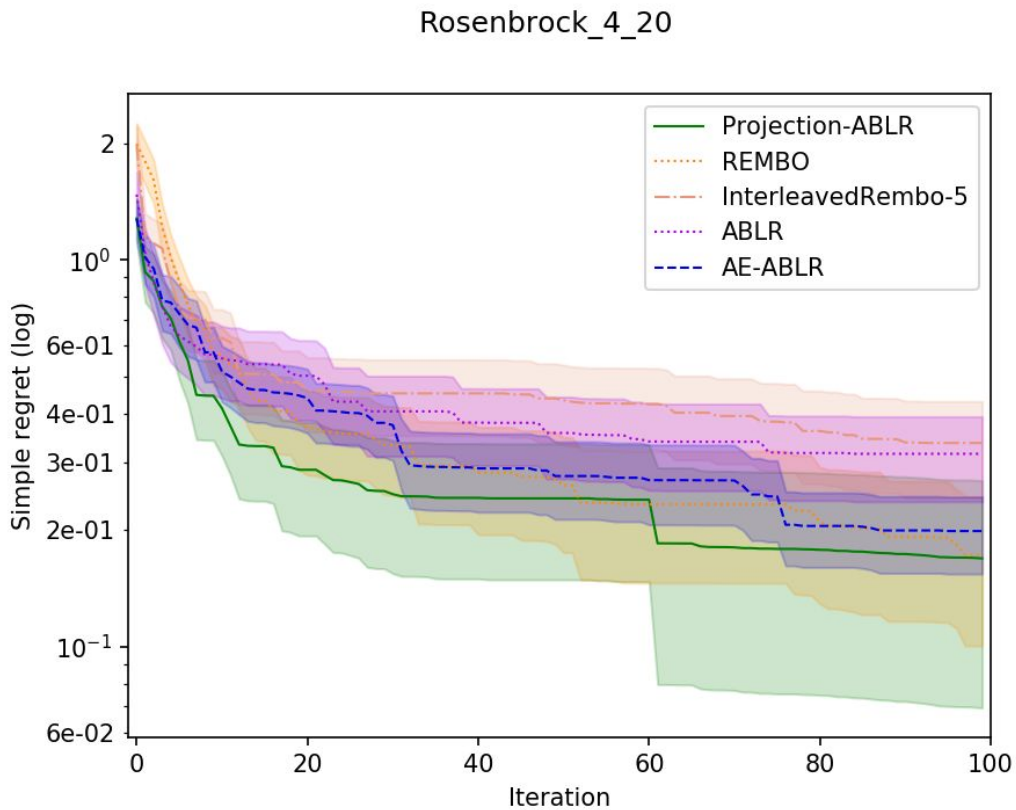
$$\text{Simple regret} = y_{current\_best} - y_{optimum}$$

Display format of benchmarks: *<function>_<d>_<D>*, where *d* is the intrinsic dimensionality and *D* is the actual number of input dimensions.

Results -

High Dimensional BO - without Transfer Learning





Typical HD-BO without meta-training the model

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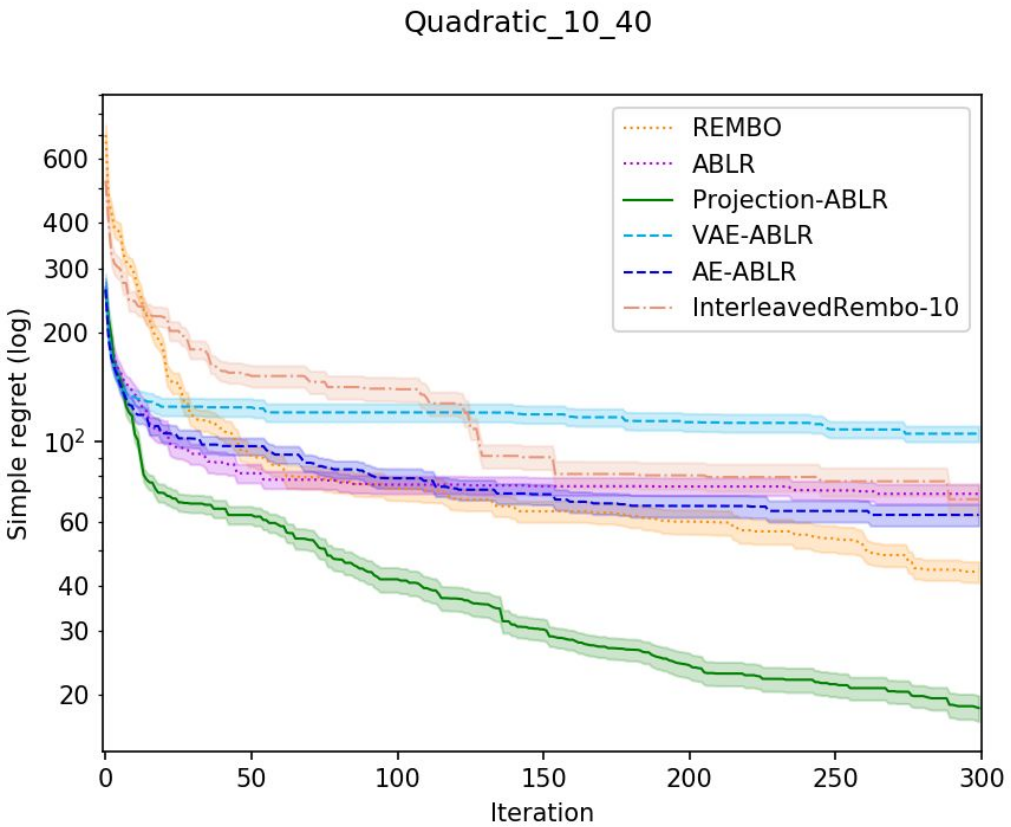
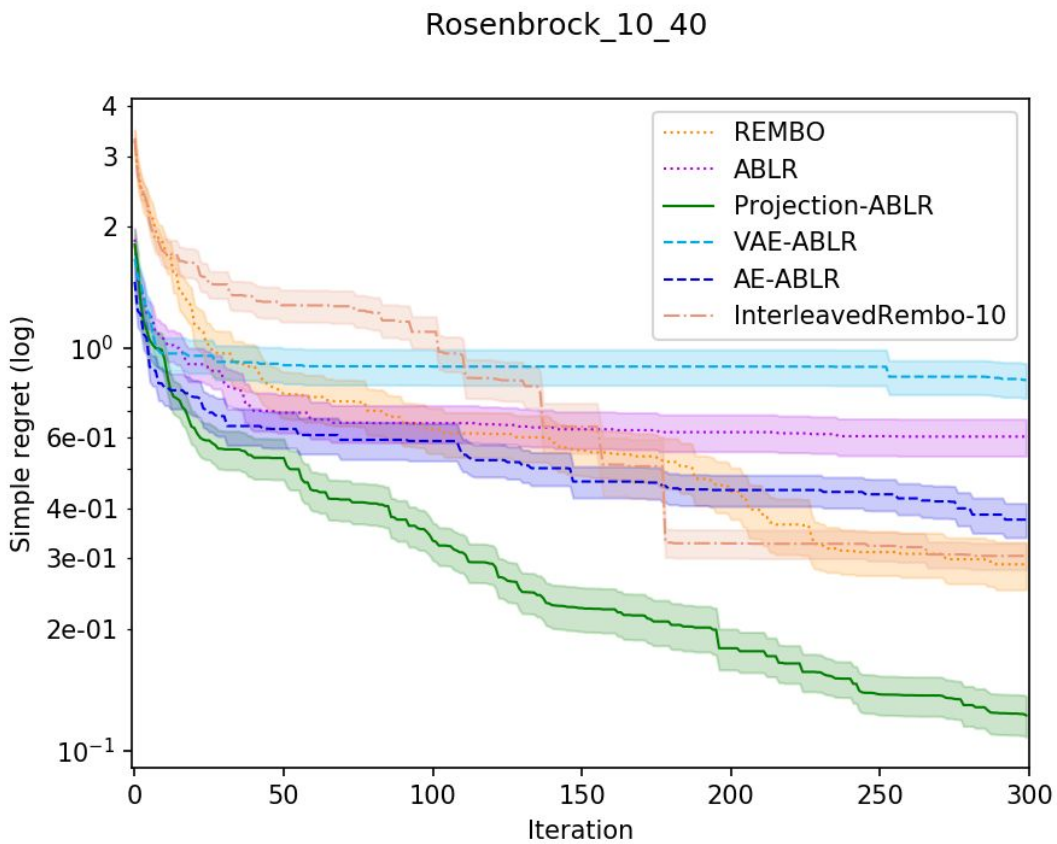
Results -

High Dimensional BO - with Transfer Learning





HD-BO with Transfer Learning models trained using metadata (30 tasks 10 points per task)

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Summary

- Method which jointly learns low dimensional latent space mappings and multi-task ABLR model
- In the Transfer Learning setting, *Projection-MT-ABLR* achieves lower regret than other baselines
- Increasing metadata - Scales linearly with number of tasks and points per task
  - our model learn tasks better when points per task are moderate

Open challenges:

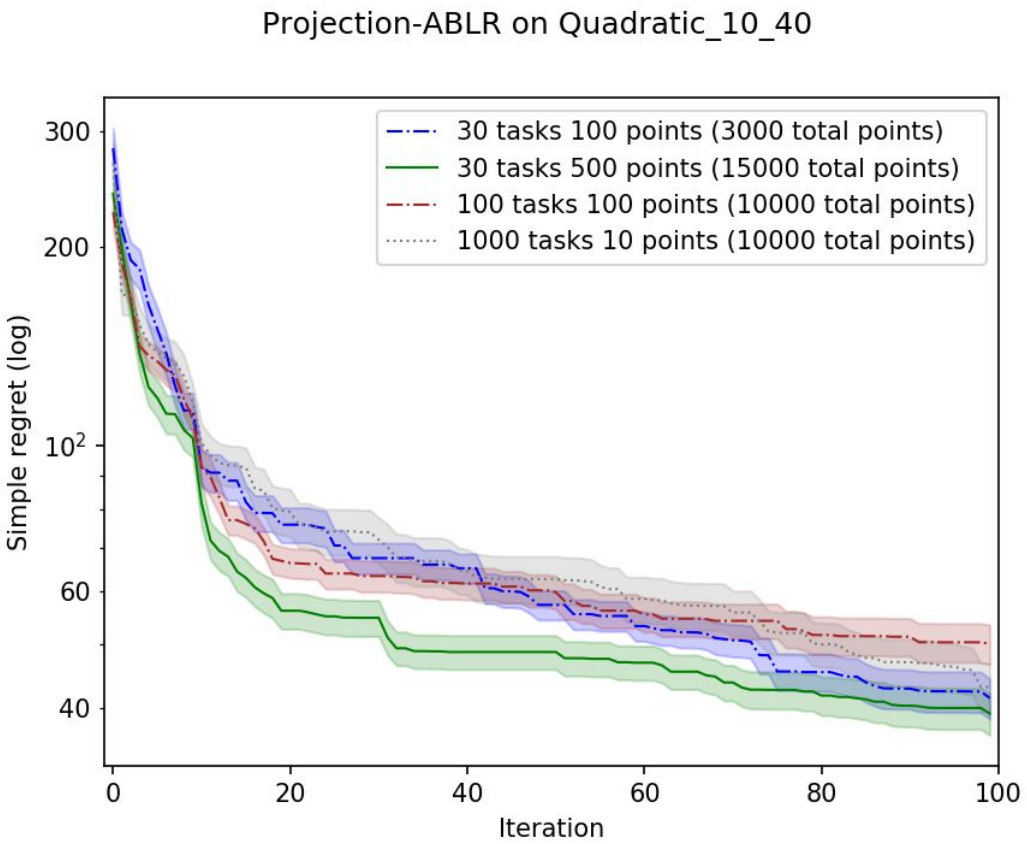
- Estimating intrinsic dimensionality from metadata
  - Tried out cross validation on multiple latent models with varying latent space dimension

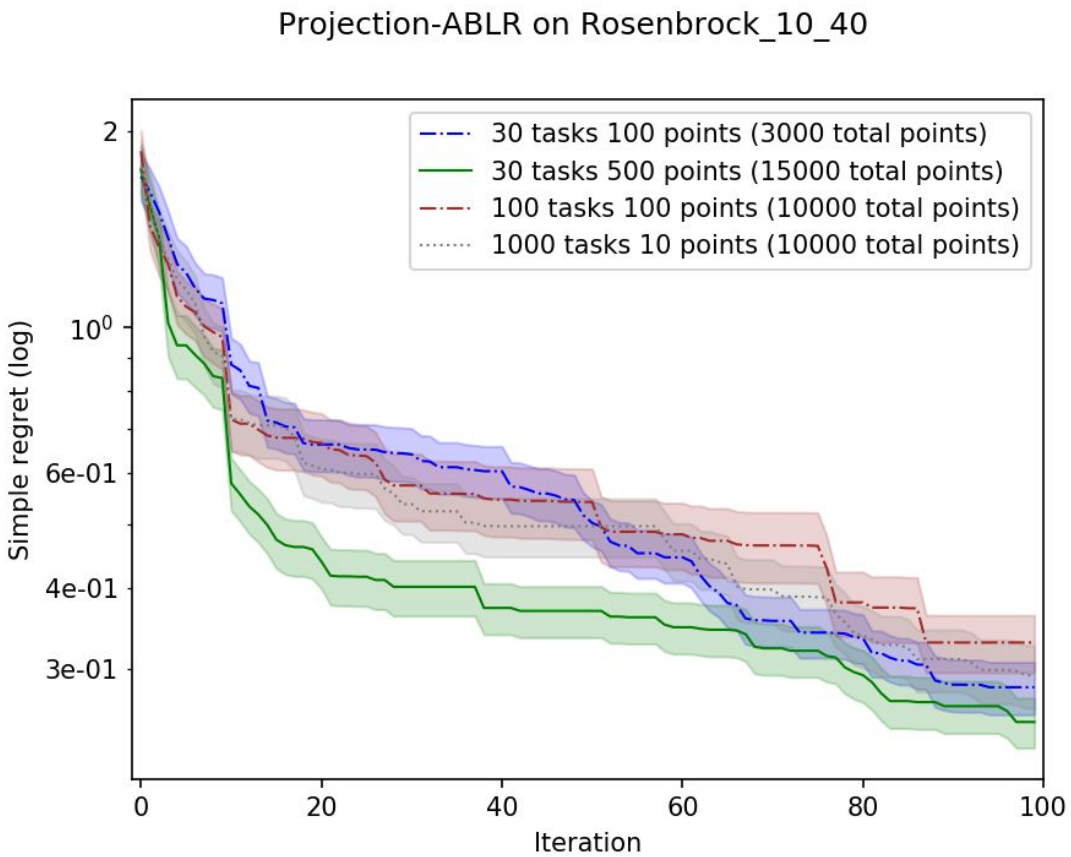
Thank you!
Questions?

Additional slides

Results -

Increasing metadata





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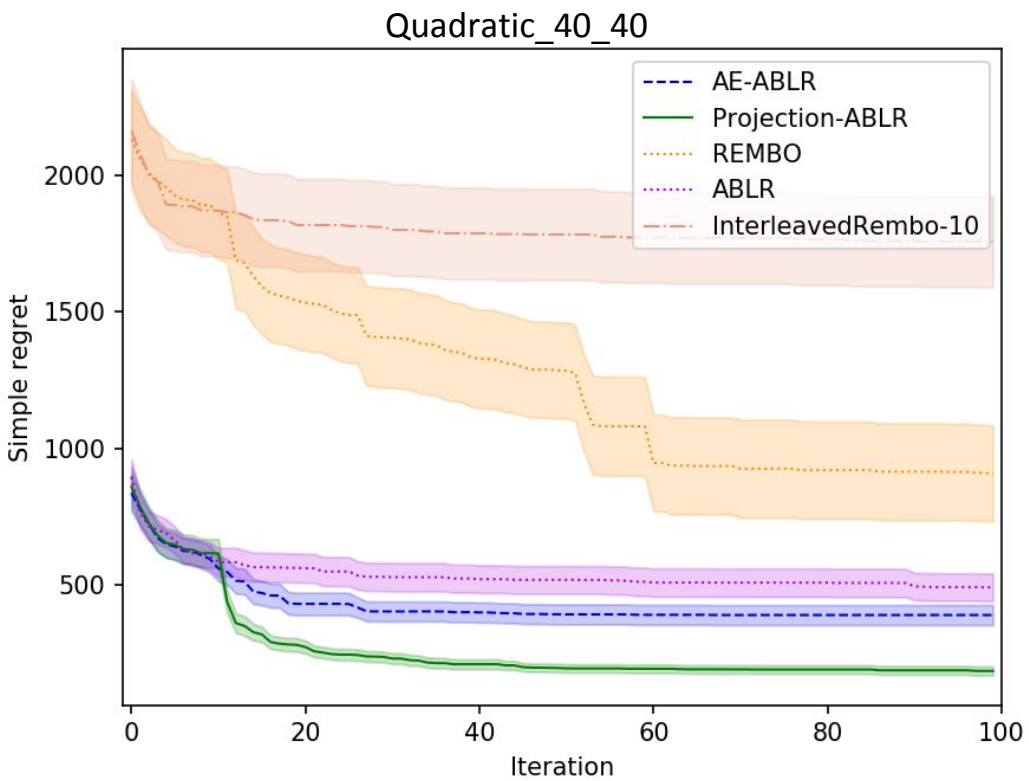
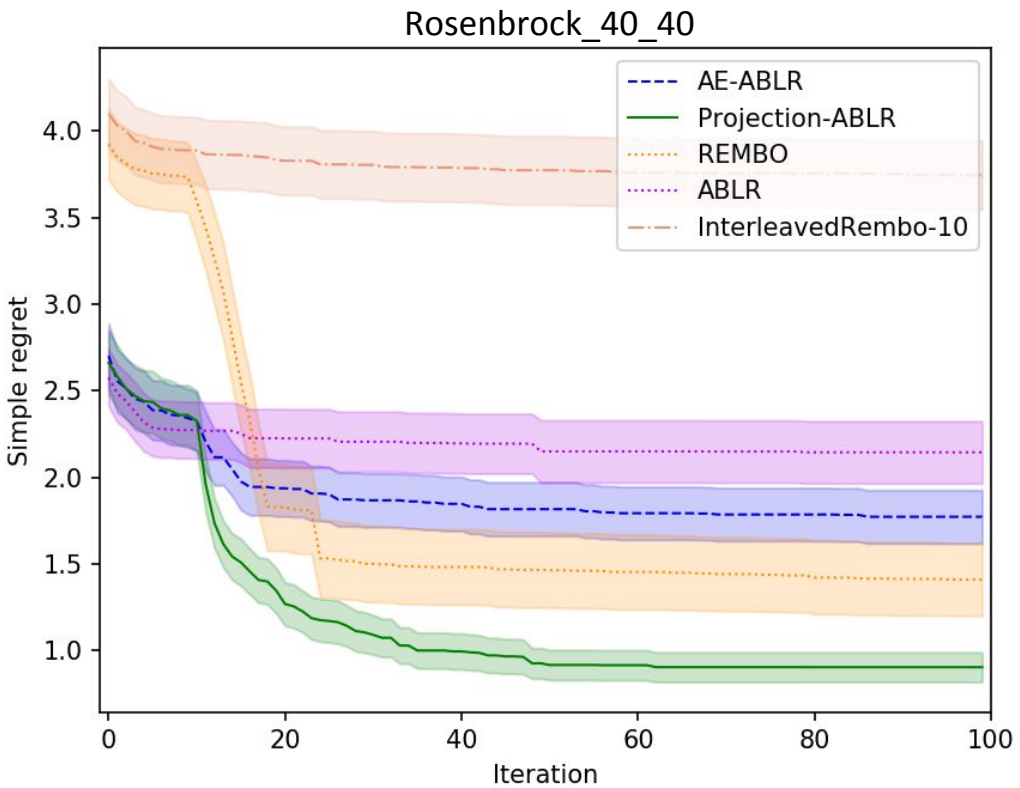
Results -

High Dimensional BO - without intrinsic structure

with Transfer Learning:





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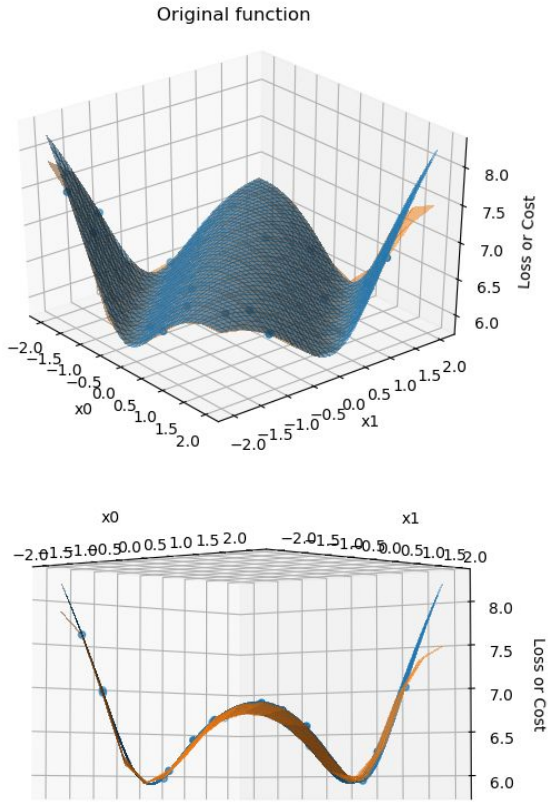
Experiments -

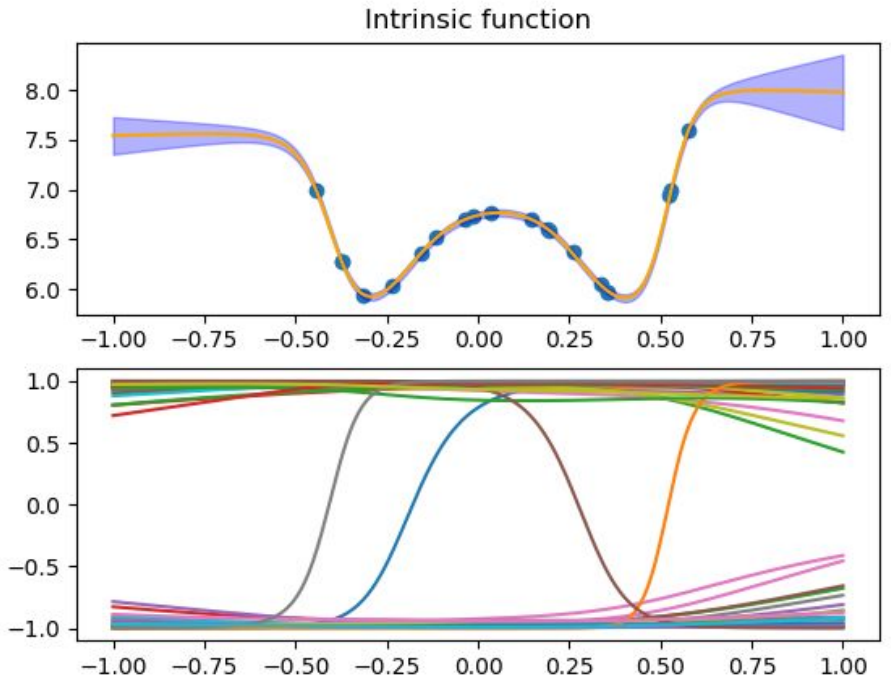
Models used in experiments

Model	Modeling space	Based on	Transfer Learning
REMBO, InterleavedRembo	Latent space $\mathbb{R}^d$	GP	No
MultiTaskABLR	Original space $\mathbb{R}^{\mathbb{D}}$	BLR	Yes
Projection-ABLR, AE-ABLR, VAE-ABLR	Latent space $\mathbb{R}^d$	BLR	Yes

Results -

Learning the intrinsic function





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