Using Meta Learning to Initialize Bayesian Optimization

Albert-Ludwigs-Universität Freiburg

UNI FREIBURG

Matthias Feurer[1] Jost Tobias Springenberg[2] Frank Hutter[1]

[1]Research Group on Learning, Optimization, and Automated Algorithm Design
[2]Machine Learning Lab
Department of Computer Science, University of Freiburg, Germany

Second Workshop on Configuration and Selection of Algorithms, 30 September 2014

Your task: Build an Iris classification system

Your task: Build an Iris classification system

- Choose an algorithm based on dataset characteristics, e.g. for the Iris dataset this could be an SVM

Your task: Build an Iris classification system

- Choose an algorithm based on dataset characteristics, e.g. for the Iris dataset this could be an SVM
- Manual tuning
  -> fiddling with hyperparameters.

Your task: Build an Iris classification system

- Choose an algorithm based on dataset characteristics, e.g. for the Iris dataset this could be an SVM
- Manual tuning
  -> fiddling with hyperparameters.
- Better: Use automated methods like PSO, GA or SMBO

Your task: Build an Iris classification system

- Choose an algorithm based on dataset characteristics, e.g. for the Iris dataset this could be an SVM
- Manual tuning
  -> fiddling with hyperparameters.
- Better: Use automated methods like PSO, GA or SMBO
- Best: AutoWeka

Adding the Iris Barbarta to the dataset

Adding the Iris Barbarta to the dataset

- Manual tuning:
  Use experience and start from the parameters found on the Iris dataset

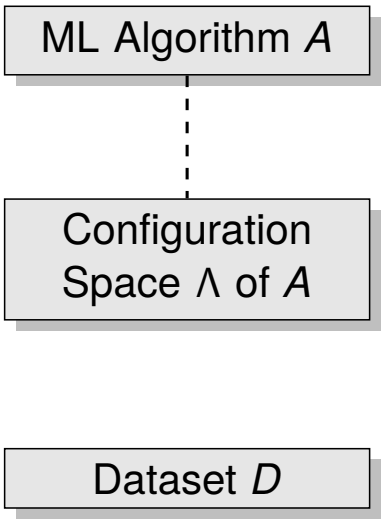
Adding the Iris Barbarta to the dataset

- Manual tuning:
  Use experience and start from the parameters found on the Iris dataset
- Automated methods
  -> start from scratch

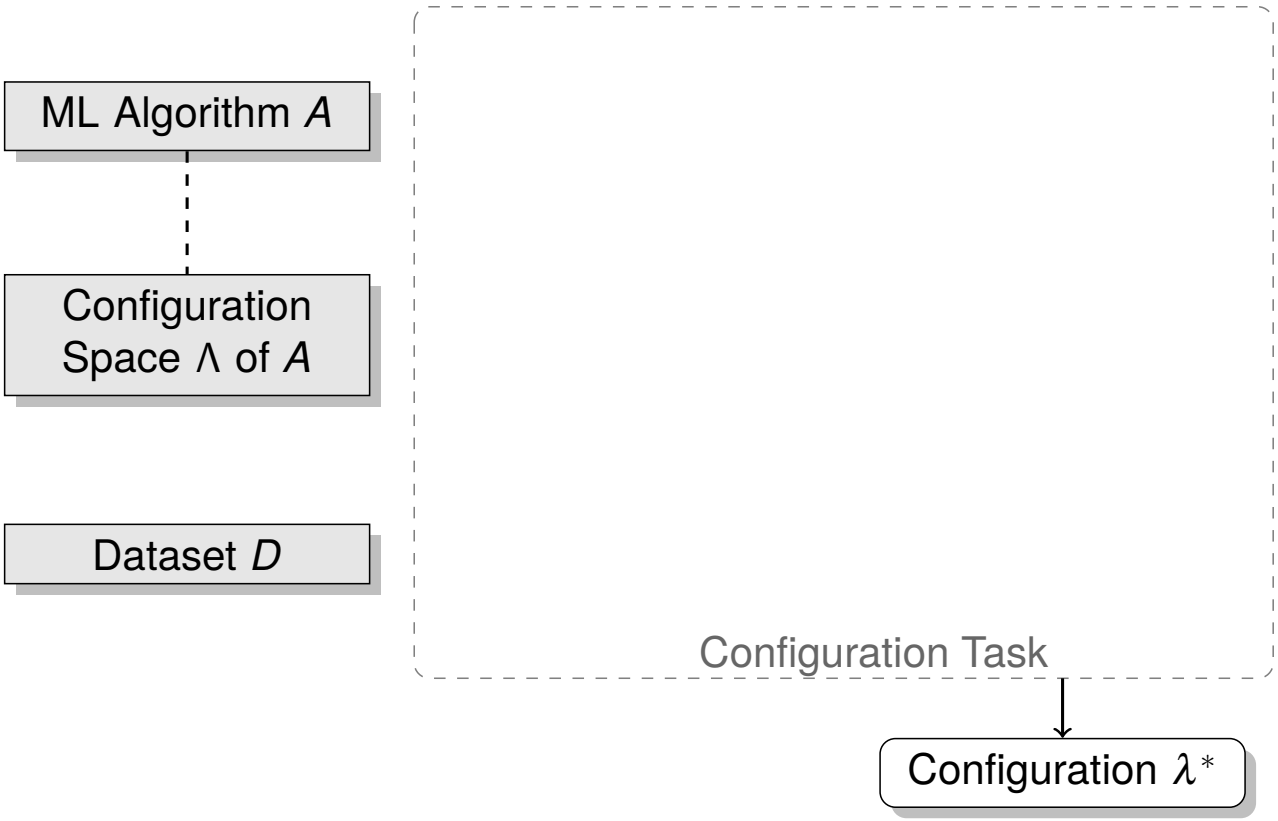
Adding the Iris Barbarta to the dataset

- Manual tuning:
  Use experience and start from the parameters found on the Iris dataset
- Automated methods
  -> start from scratch
- $\rightarrow$ Cast *use experience* into an algorithm.

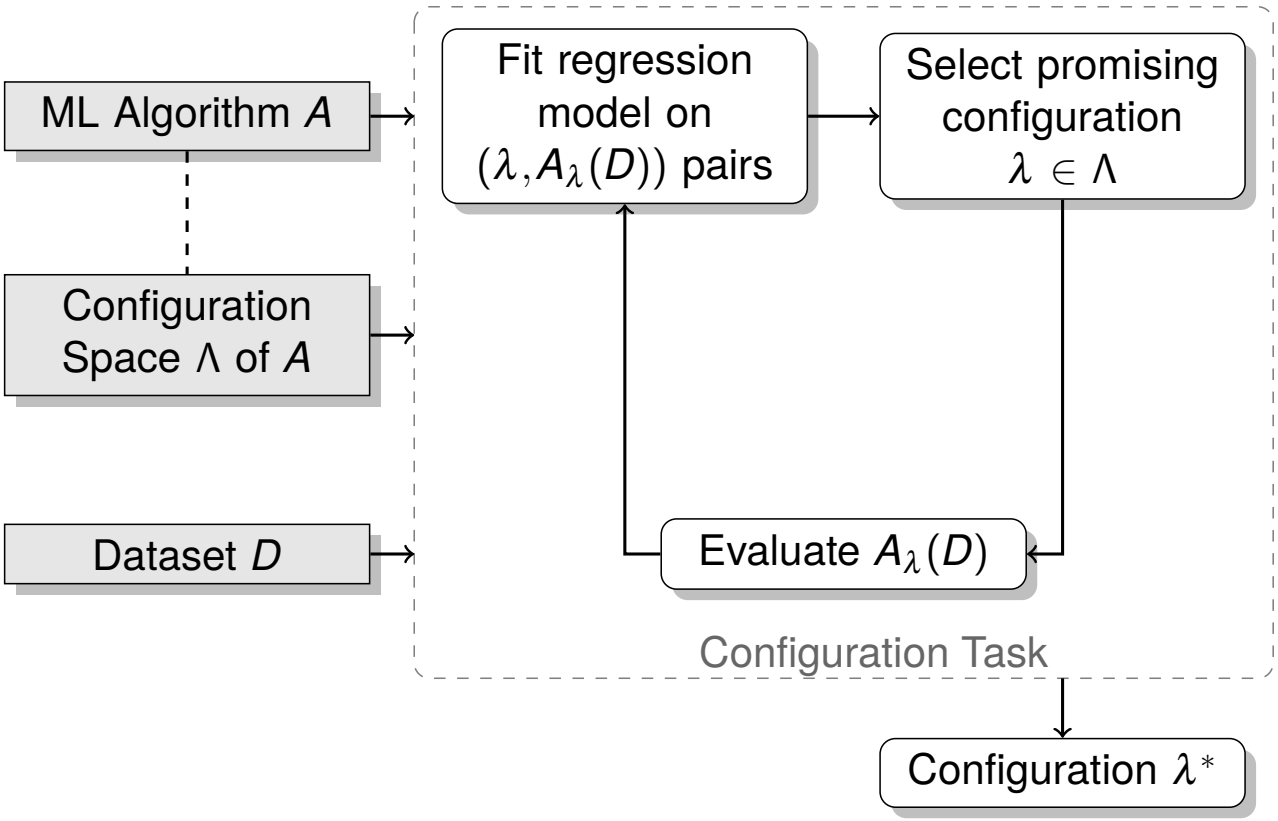
Sequential Model-based Bayesian Optimization (SMBO)



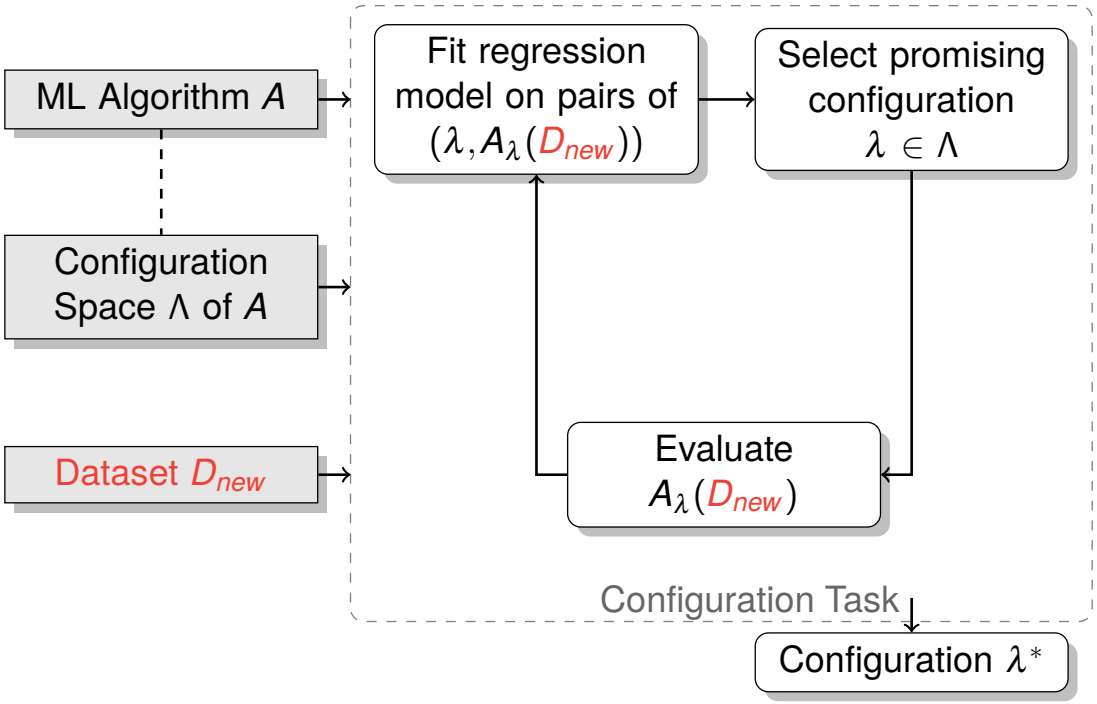
Sequential Model-based Bayesian Optimization (SMBO)



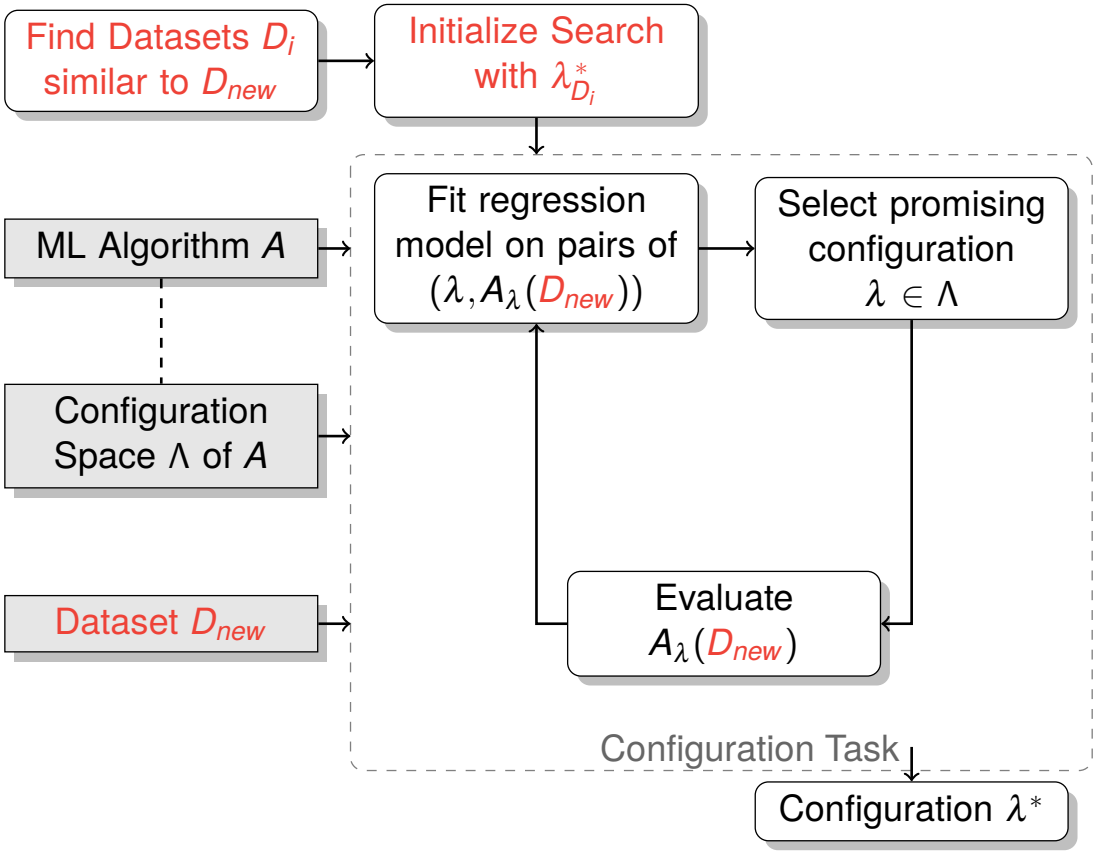
Sequential Model-based Bayesian Optimization (SMBO)



Metalearning-Initialized SMBO (MI-SMBO)



Metalearning-Initialized SMBO (MI-SMBO)



Metafeatures

- # training examples: 150
- # classes: 3
- # features: 4
- # numerical features: 4
- # categorical features: 0
- missing values? No

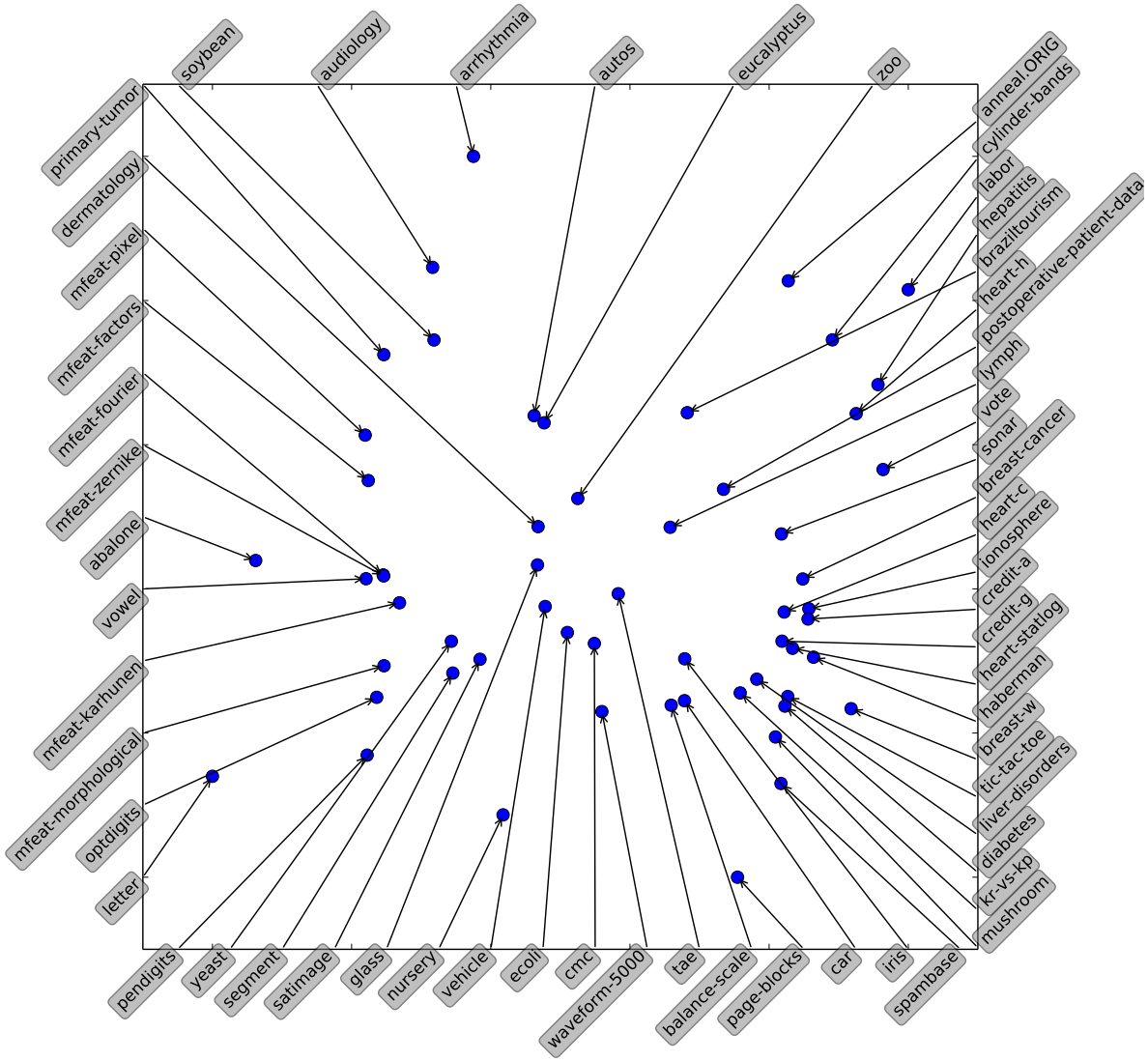
Metalearning-Initialized Bayesian Optimization

UNI FREIBURG

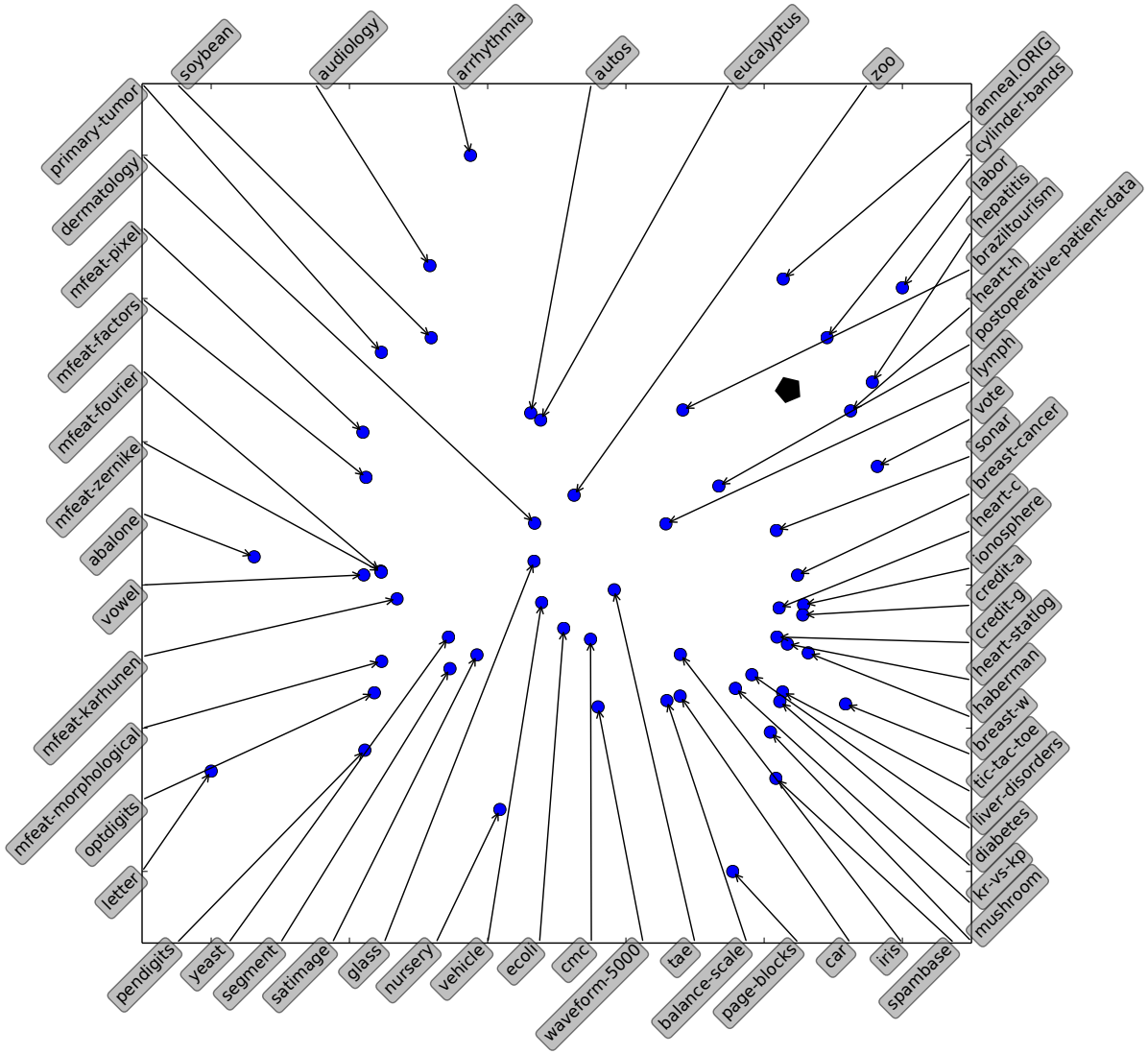
For a new dataset D_{new}:

- Sort known datasets $D_{1:N}$ by distance to D_{new}.
- For each of these datasets, extract the best known hyperparameter configuration $\lambda^*_{D_i}$.
- Initialize SMBO with the first k hyperparameter configurations from the sorted list.

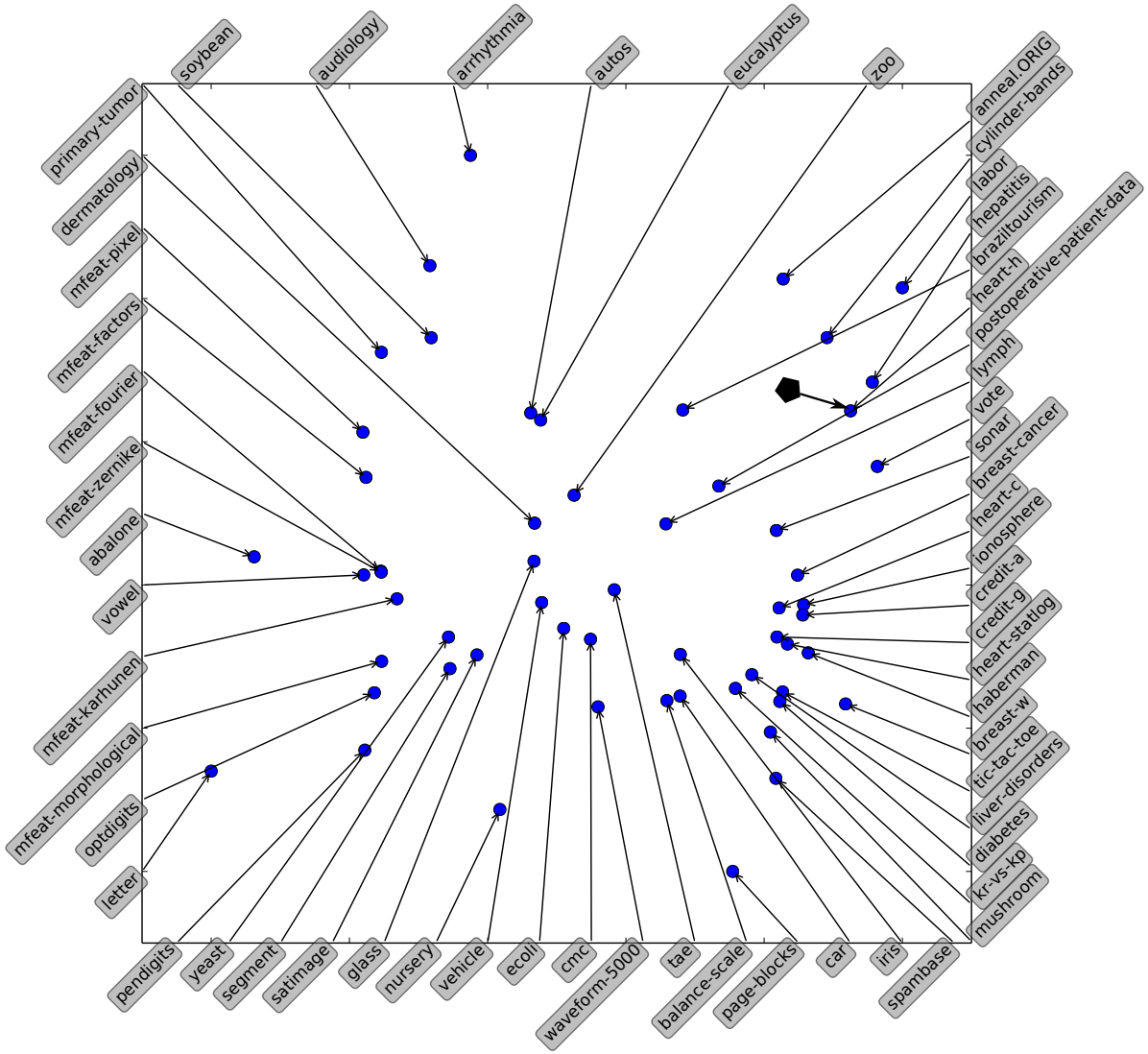
Similarity of Datasets



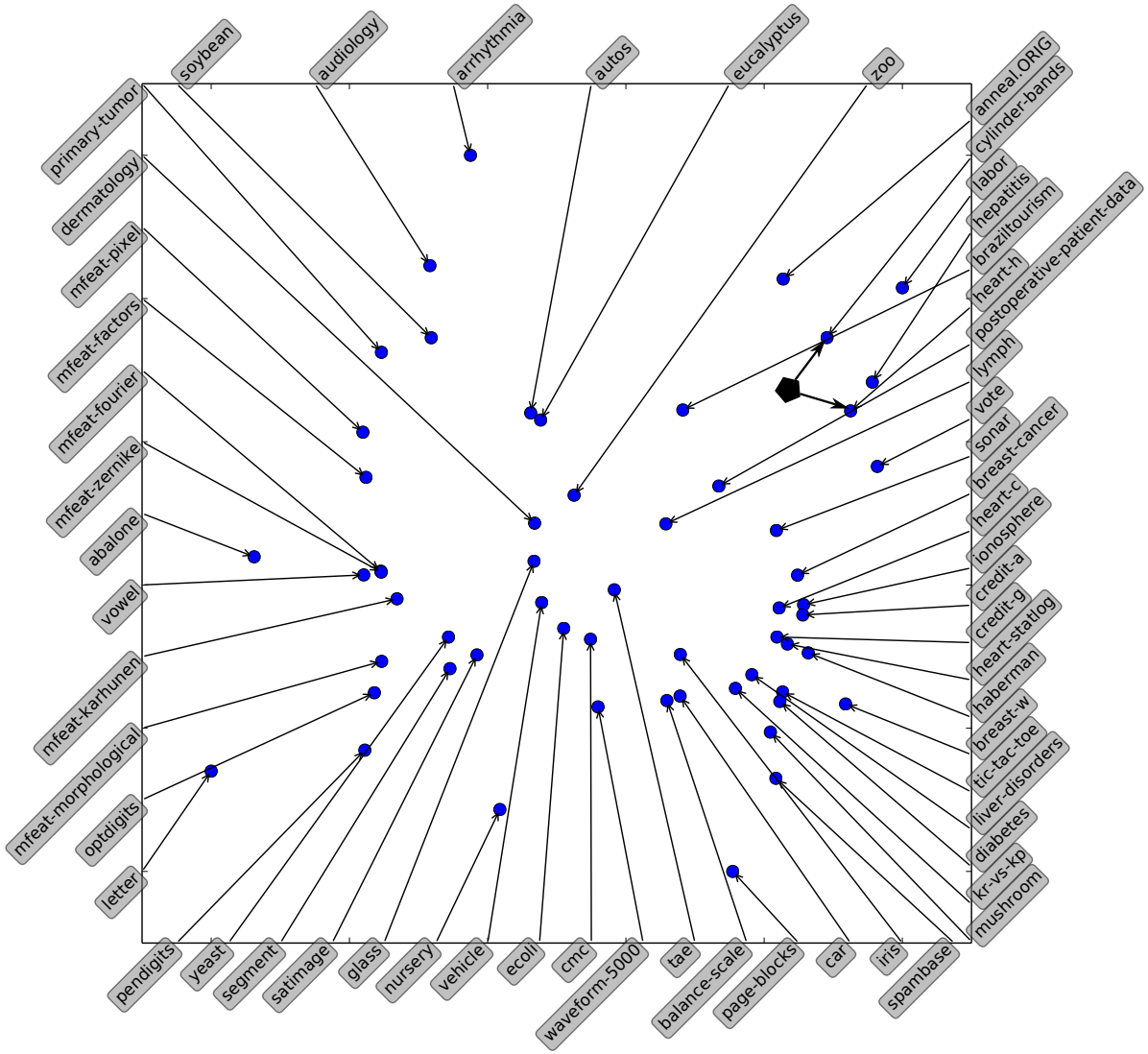
Finding the nearest datasets (1)



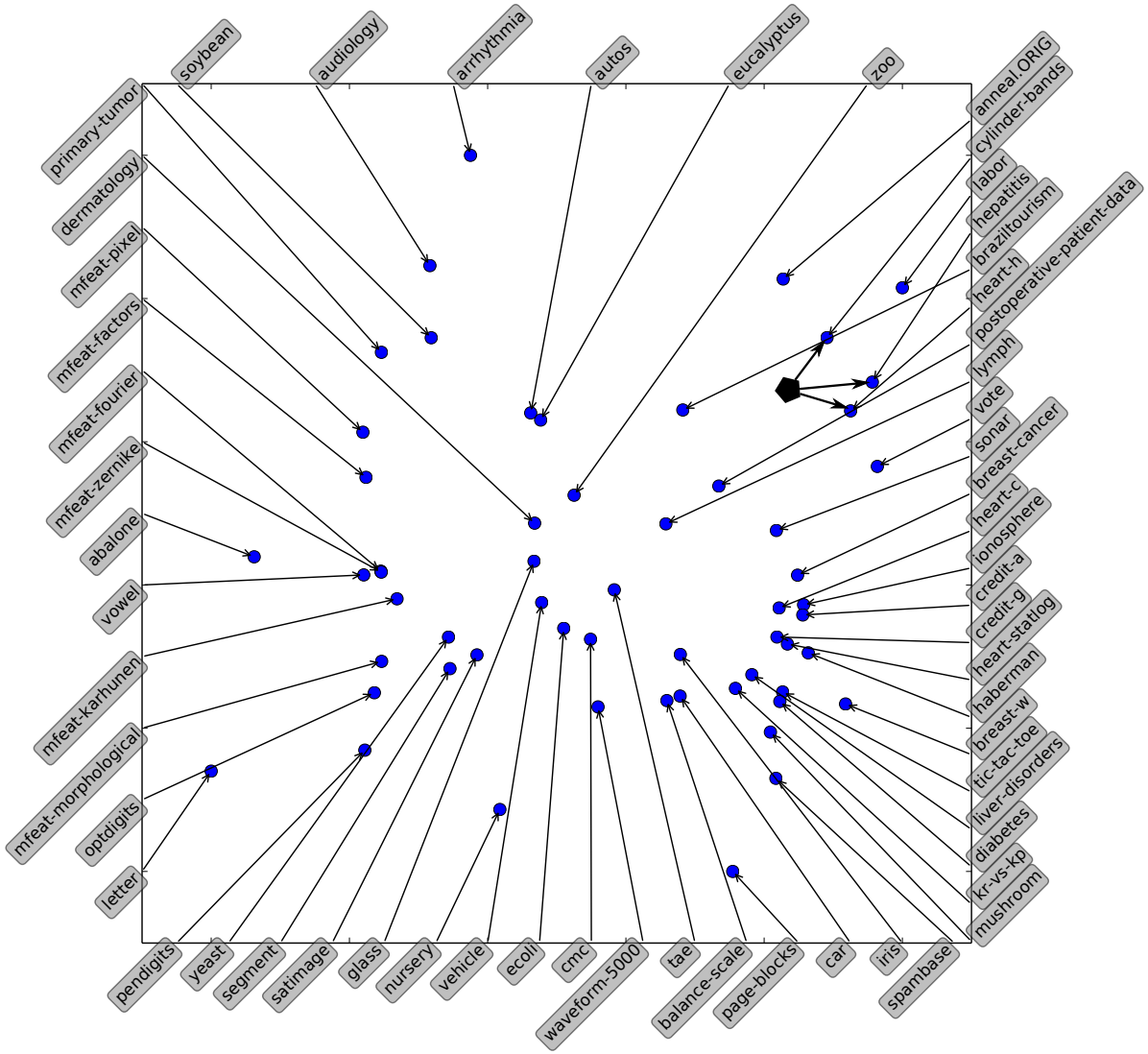
Finding the nearest datasets (2)



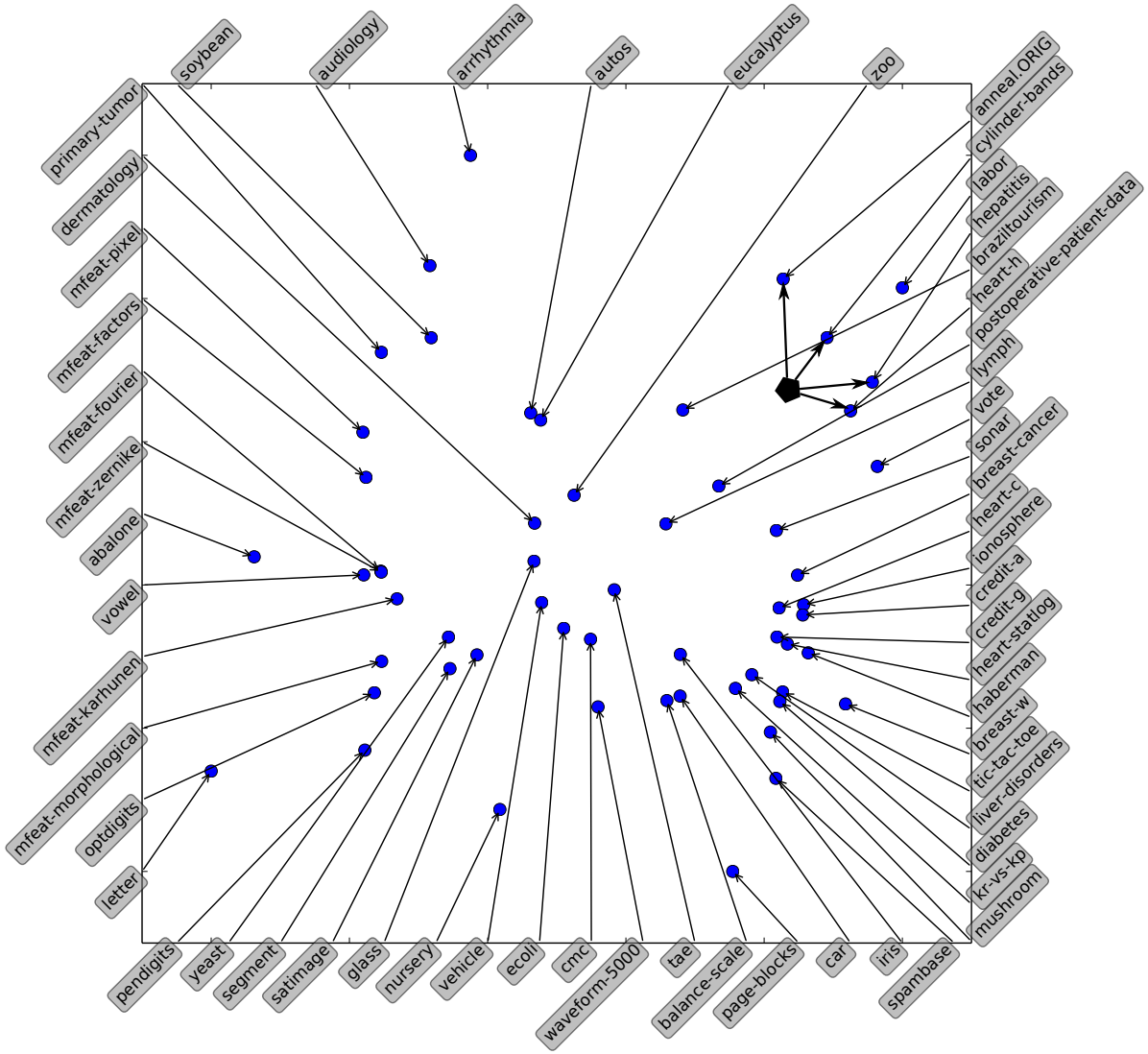
Finding the nearest datasets (3)



Finding the nearest datasets (3)



Finding the nearest datasets (4)



Distance metric (1)

UNI FREIBURG

Commonly used in literature, the L_1 norm:

$$d(D_{\text{new}}, D_j) = \sum_i |m_i^{\text{new}} - m_i^j| \tag{1}$$

Experimental Setup

UNI FREIBURG

- 57 datasets from the OpenML repository

Experimental Setup

UNI FREIBURG

- 57 datasets from the OpenML repository
- 46 metafeatures from the literature:
  - Split into five different subsets, including landmarking
    [Pfahringer et al. 2000]

Experimental Setup

UNI FREIBURG

- 57 datasets from the OpenML repository
- 46 metafeatures from the literature:
  - Split into five different subsets, including landmarking [Pfahringer et al. 2000]
- Two case studies
  - Support Vector Machine with MI-Spearmint [Snoek et al. 2012]
  - AutoSklearn with MI-SMAC [Hutter et al. 2011]

Experimental Setup

- 57 datasets from the OpenML repository
- 46 metafeatures from the literature:
  - Split into five different subsets, including landmarking [Pfahringer et al. 2000]
- Two case studies
  - Support Vector Machine with MI-Spearmint [Snoek et al. 2012]
  - AutoSklearn with MI-SMAC [Hutter et al. 2011]
- Tried 5, 10, 20 and 25 initial configurations

Experimental Setup

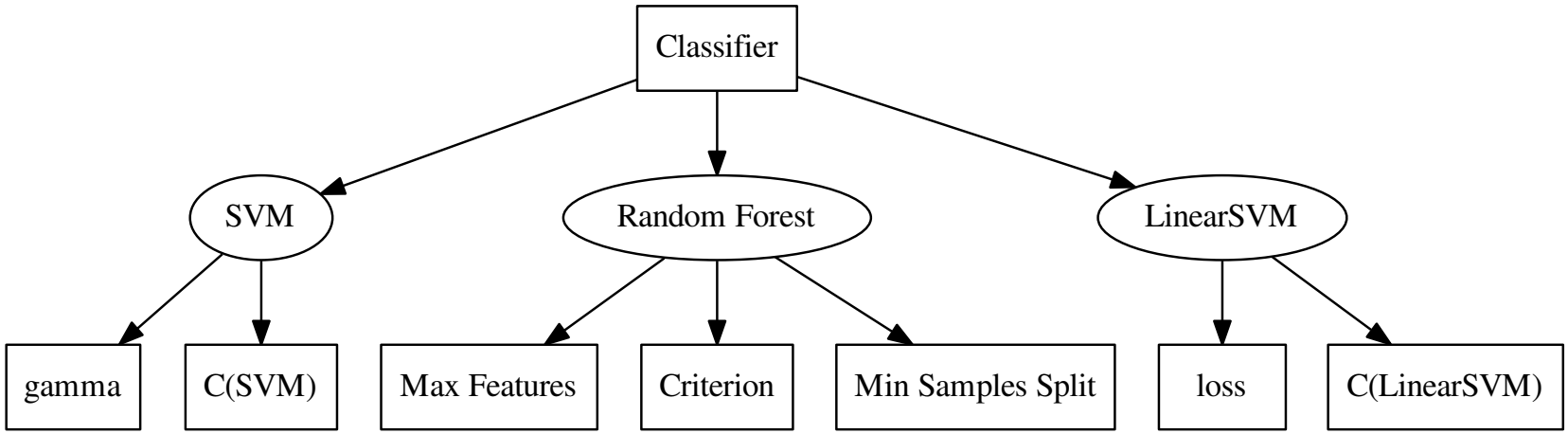
UNI FREIBURG

- 57 datasets from the OpenML repository
- 46 metafeatures from the literature:
  - Split into five different subsets, including landmarking [Pfahringer et al. 2000]
- Two case studies
  - Support Vector Machine with MI-Spearmint [Snoek et al. 2012]
  - AutoSklearn with MI-SMAC [Hutter et al. 2011]
- Tried 5, 10, 20 and 25 initial configurations
- ran each instantiation 10 times on each dataset
  $\rightarrow$ 26220 optimization runs

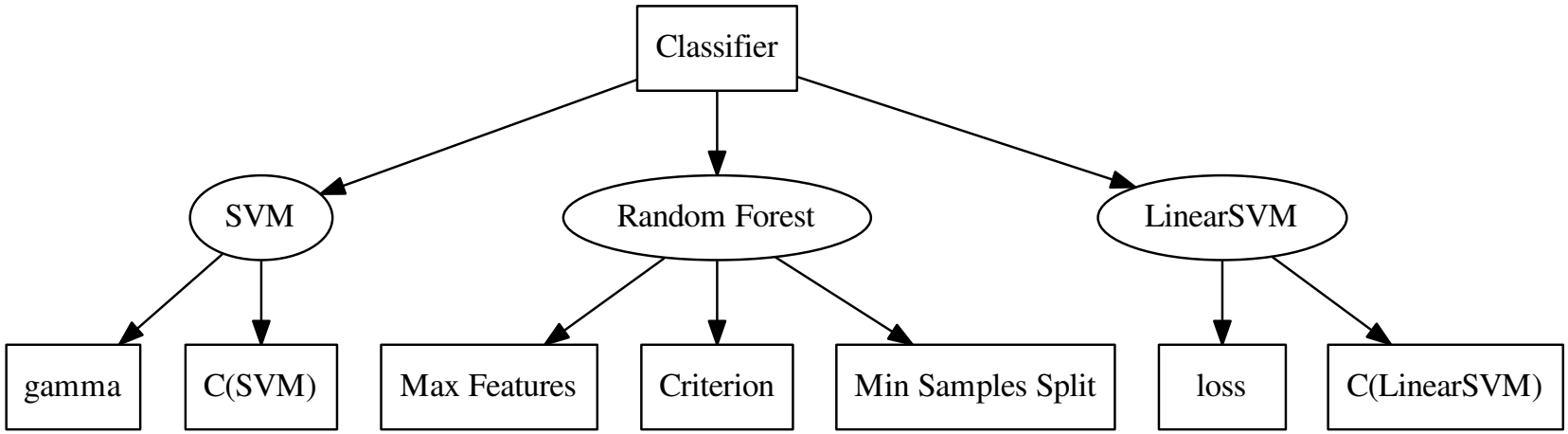
Experimental Setup

- 57 datasets from the OpenML repository
- 46 metafeatures from the literature:
  - Split into five different subsets, including landmarking [Pfahringer et al. 2000]
- Two case studies
  - Support Vector Machine with MI-Spearmint [Snoek et al. 2012]
  - AutoSklearn with MI-SMAC [Hutter et al. 2011]
- Tried 5, 10, 20 and 25 initial configurations
- ran each instantiation 10 times on each dataset
  $\rightarrow$ 26220 optimization runs
- therefore, precomputed a dense grid for every dataset

Combined Algorithm Selection and Hyperparameter Optimization problem (CASH)



Combined Algorithm Selection and Hyperparameter Optimization problem (CASH)



[Auto-WEKA, Thornton et al. 2013]

AutoSklearn: Hyperparameters

UNI FREIBURG

Component	Hyperparameter	# Values
Main	$\lambda_{\text{classifier}}$	3
Main	preprocessing	2
SVM	$\log_2(C)$	21
SVM	$\log_2(\gamma)$	19
LinearSVM	$\log_2(C)$	21
LinearSVM	penalty	2
RF	min splits	5
RF	max features	10
RF	criterion	2
PCA	variance to keep	2

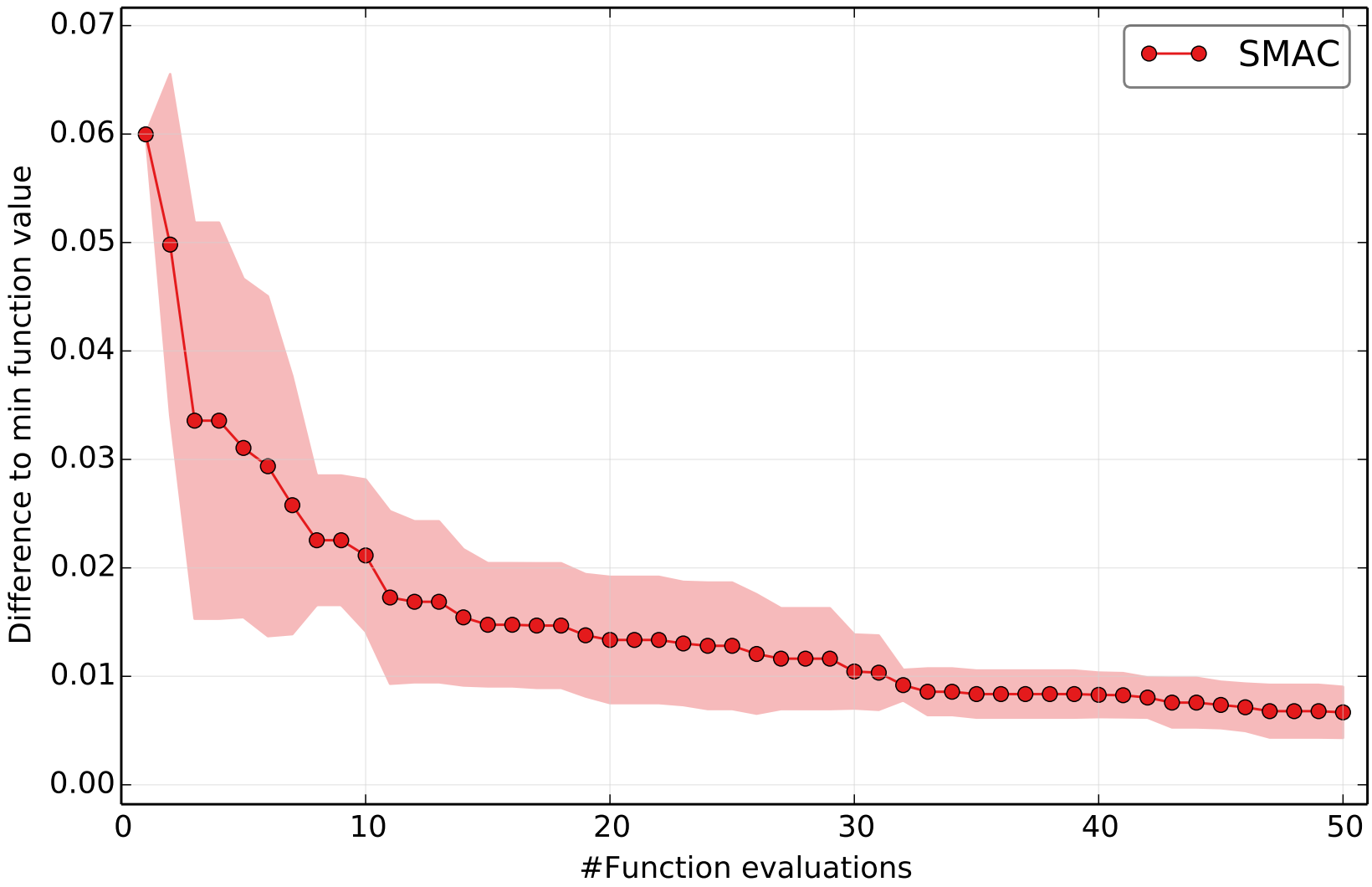
AutoSklearn: Hyperparameters

UNI FREIBURG

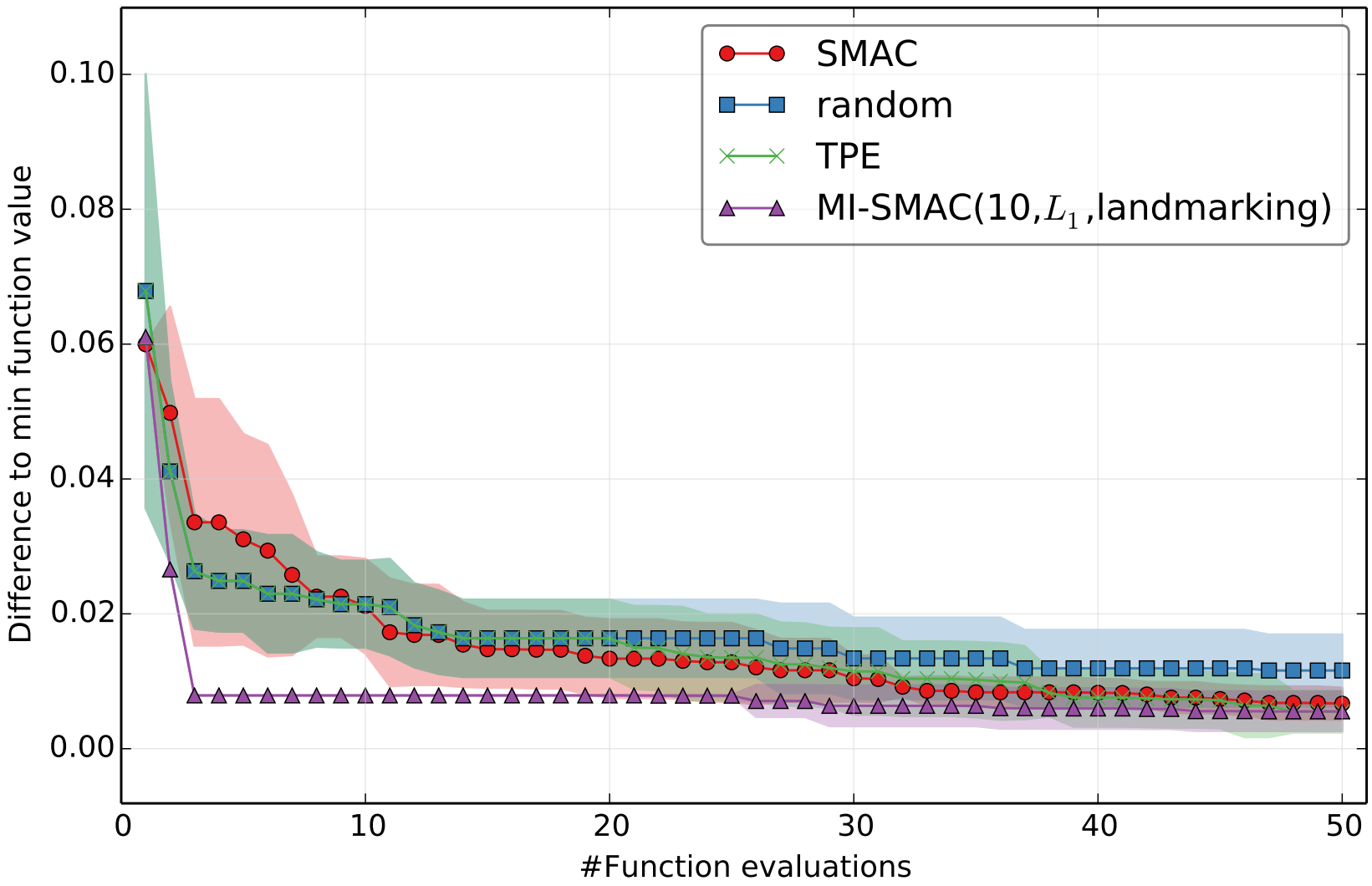
Component	Hyperparameter	# Values
Main	$\lambda_{\text{classifier}}$	3
Main	preprocessing	2
SVM	$\log_2(C)$	21
SVM	$\log_2(\gamma)$	19
LinearSVM	$\log_2(C)$	21
LinearSVM	penalty	2
RF	min splits	5
RF	max features	10
RF	criterion	2
PCA	variance to keep	2

1623 hyperparameter configurations

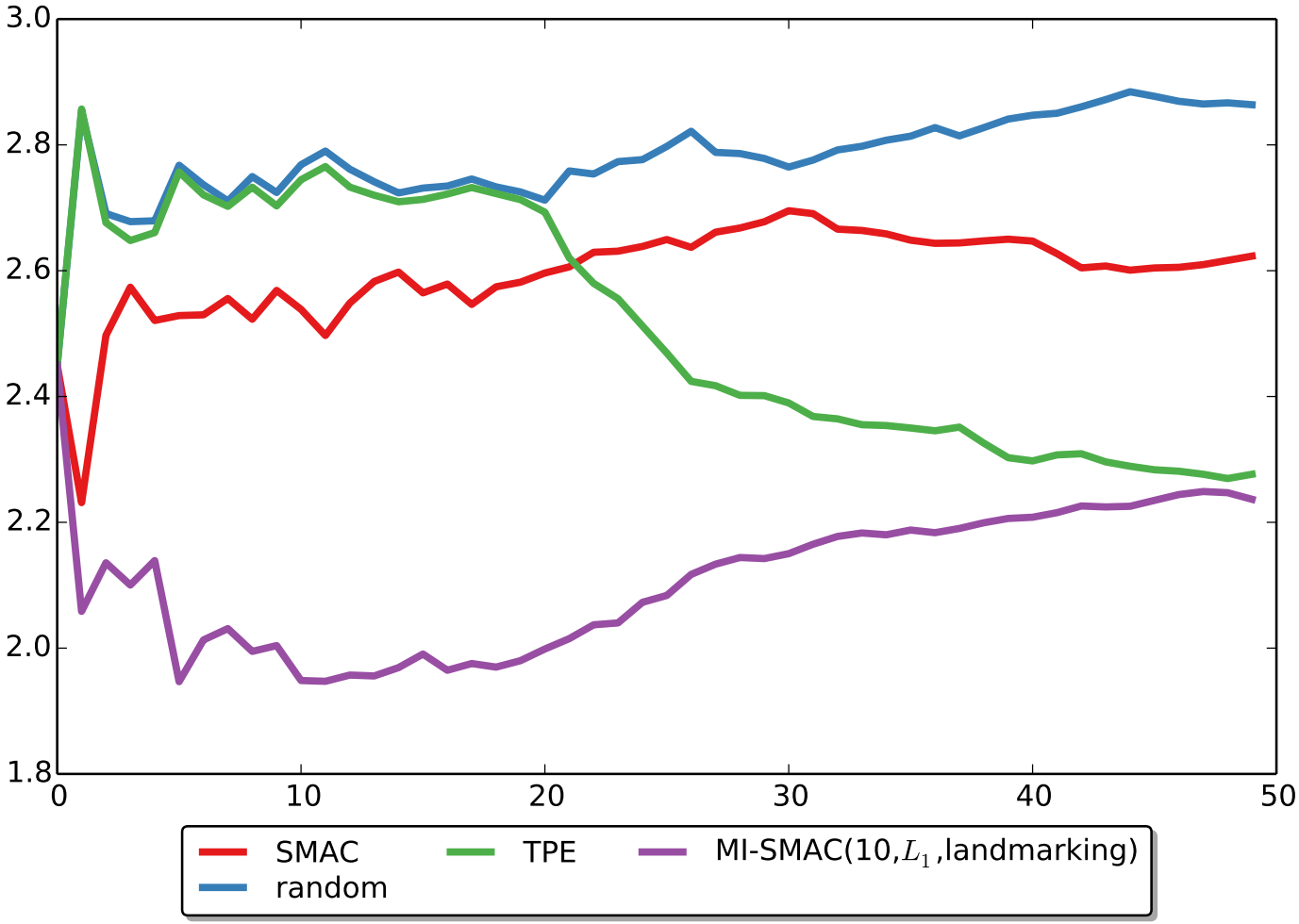
AutoSklearn: Results (1)



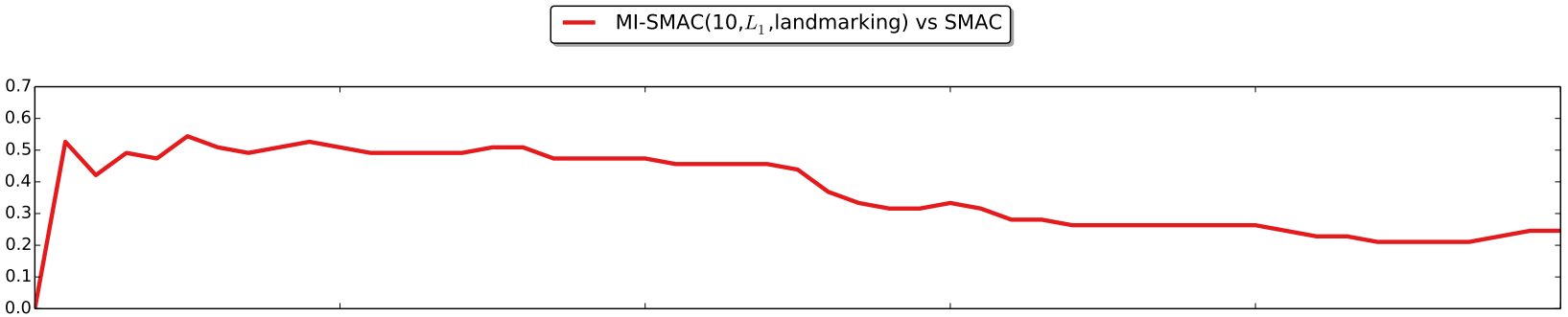
AutoSklearn: Results (1)



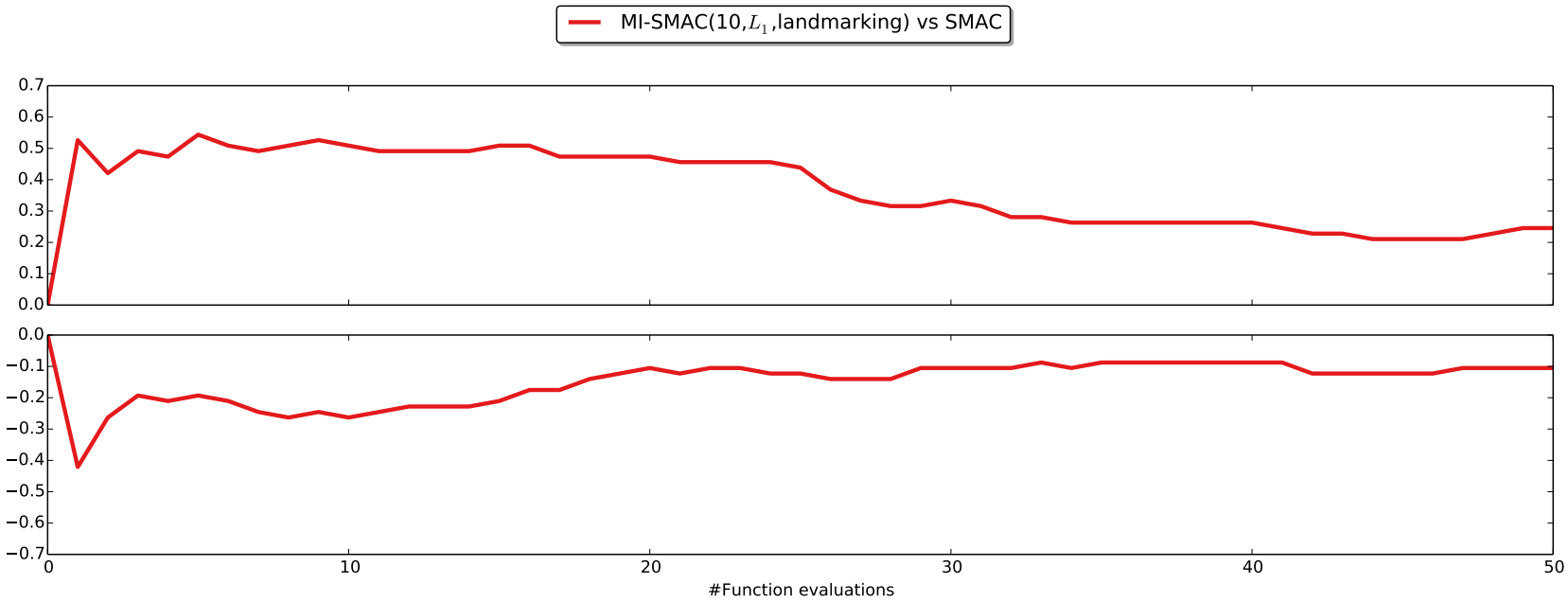
AutoSklearn: Results (2)



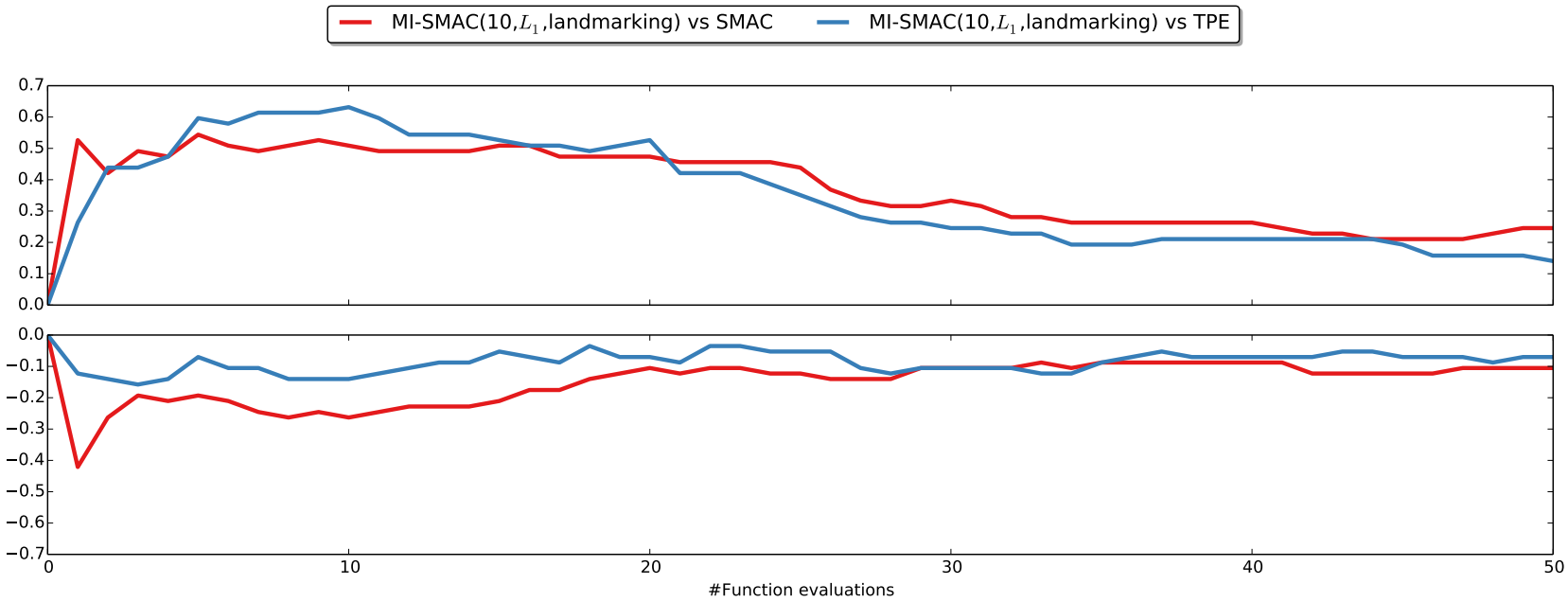
AutoSklearn: Results (3)



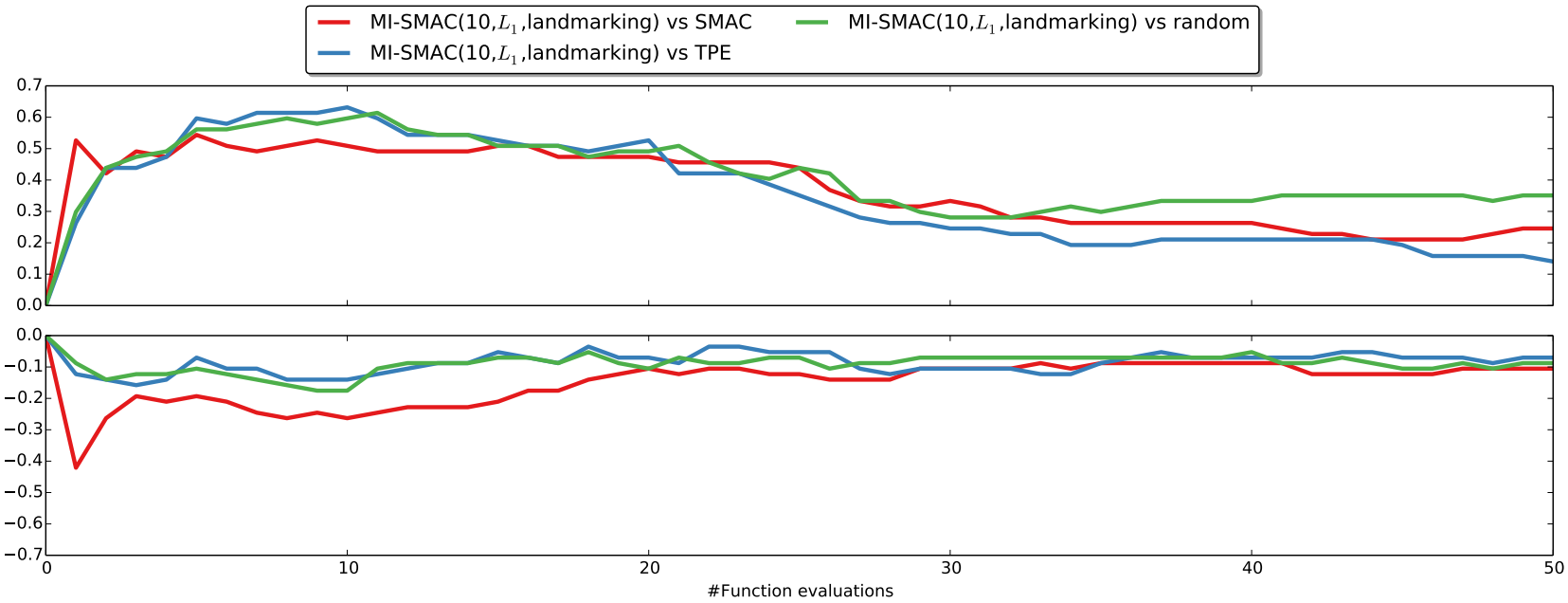
AutoSklearn: Results (3)



AutoSklearn: Results (3)



AutoSklearn: Results (3)



Open questions

UNI FREIBURG

- Does MI-SMBO scale to larger configuration spaces?
- What if gridsearch is too expensive?
- Can the metalearning component be added directly into the SMBO procedure?

Take home messages

UNI FREIBURG

- SMBO can be substantially improved by providing good initial configurations.
- Metalearning provides a sound framework to find these configurations.
- MI-SMAC improves on state-of-the-art methods on a large configuration space, namely AutoSklearn.

The end

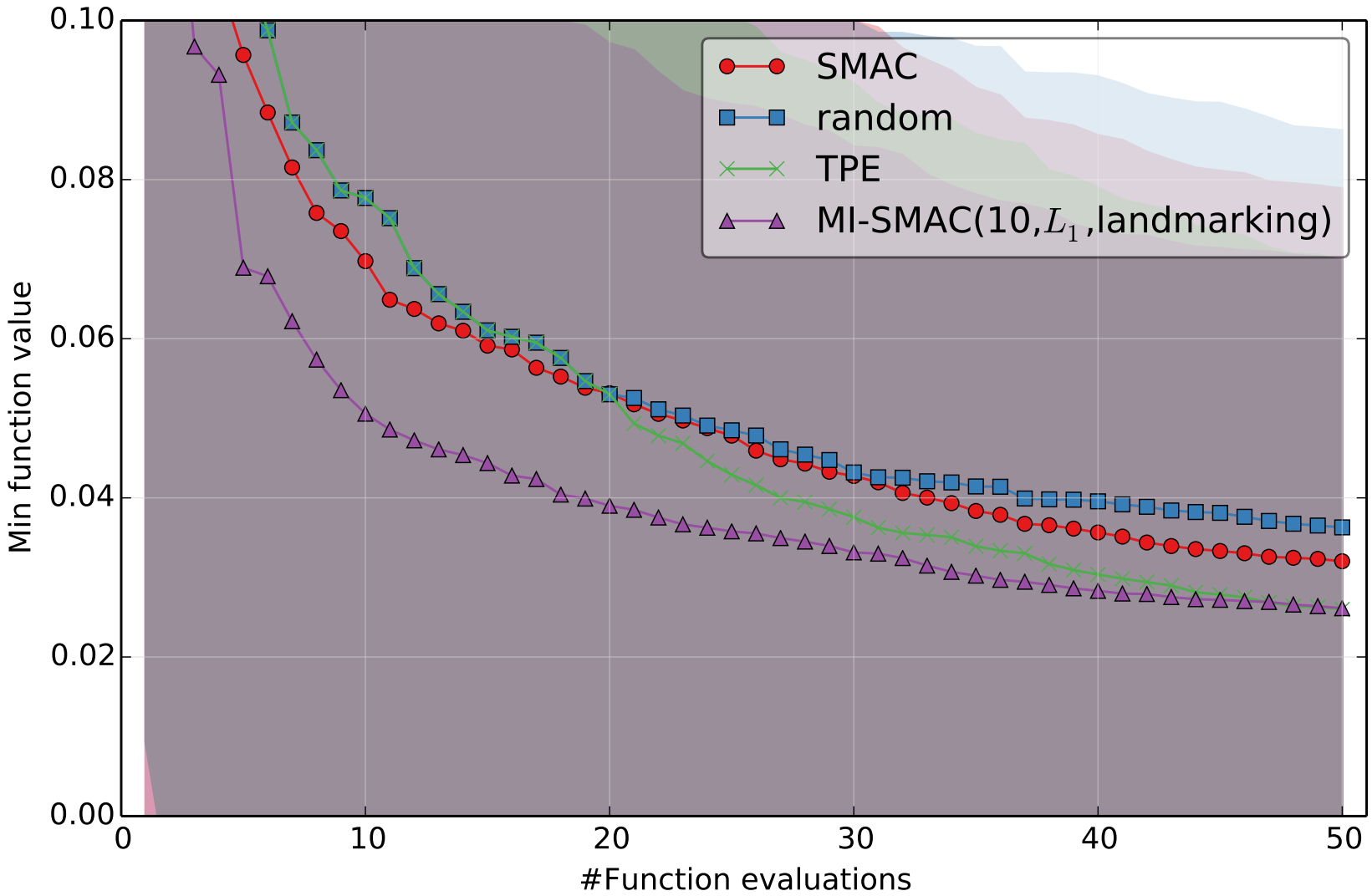
UNI FREIBURG

Thank you for your attention.

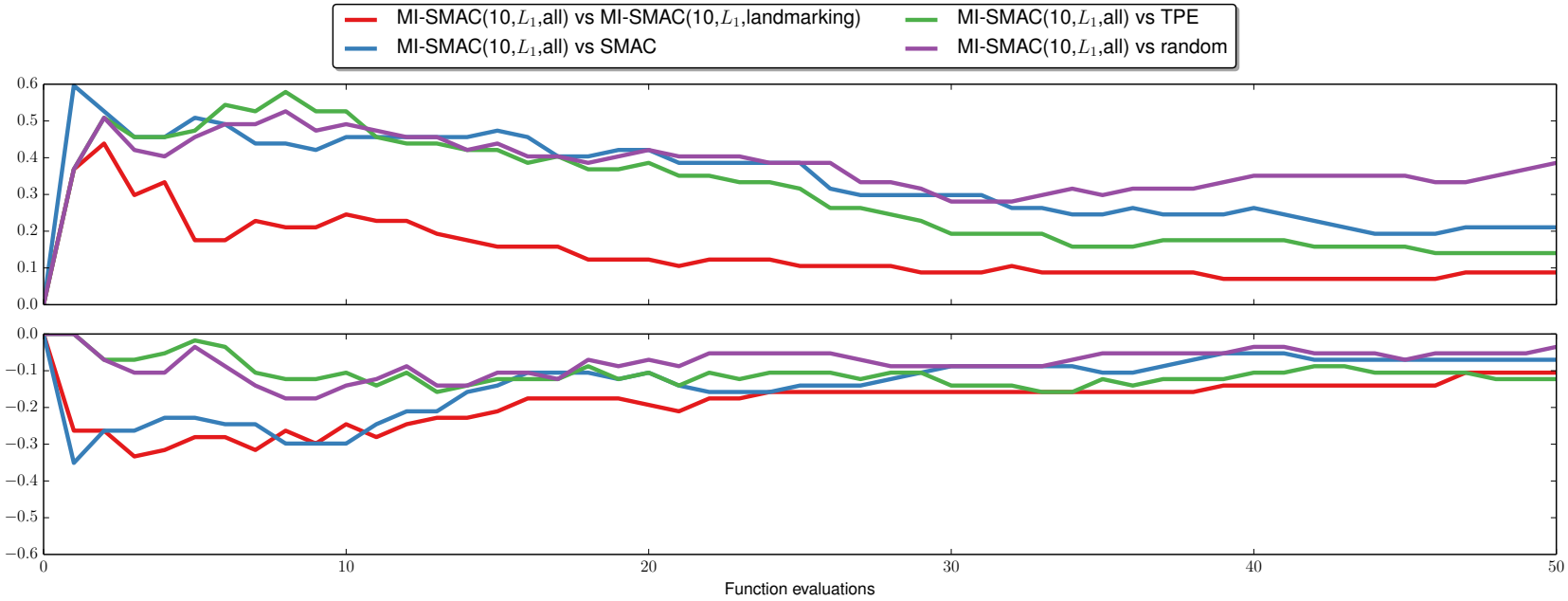
Further questions: `feurerm@cs.uni-freiburg.de`

This presentation was partially supported by an *ECCAI Travel Award* and the *ECCAI sponsors*.

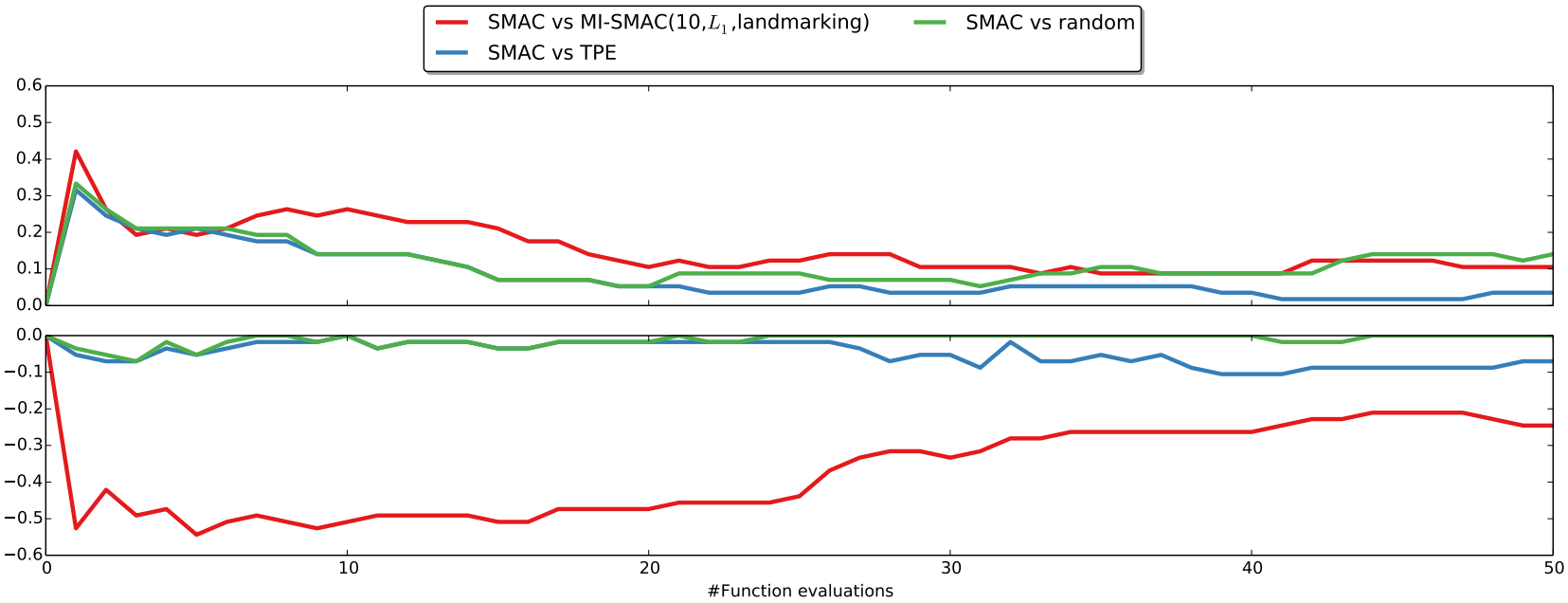
AutoSklearn: Results (5)



AutoSklearn: Results (7)



AutoSklearn: Results (8)



AutoSklearn: Results (9)