Model-Based Optimization for Expensive Black-Box Problems and Hyperparameter Optimization

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Sequential model-based optimization

Parallel batch proposals

Multicriteria SMBO

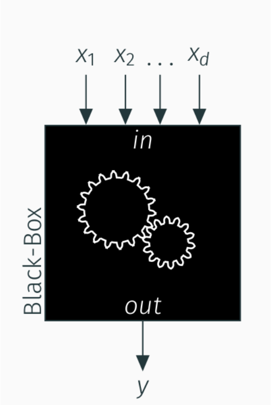
Interesting Challenges

ML Model Selection and Hyperparameter Optimization

Section 1

Sequential model-based optimization

Expensive Black-Box Optimization



$$y = f(\boldsymbol{x}) \;, \quad f : \mathbb{X} \to \mathbb{R} \tag{1}$$

$$\boldsymbol{x}^* = \arg\min_{\boldsymbol{x} \in \mathbb{X}} f(\boldsymbol{x}) \tag{2}$$

- y, target value
- $\boldsymbol{x} \in \mathbb{X} \subset \mathbb{R}^d$, domain
- $f(\boldsymbol{x})$ function with considerably long runtime
- Goal: Find optimum $\boldsymbol{x}^*$

Sequential model-based optimization

- Setting: Expensive black-box problem $f : x \to \mathbb{R} = min$!
- Classical problem: Computer simulation with a bunch of control parameters and performance output; or algorithmic performance on 1 or more problem instances; we often optimize ML pipelines
- Idea: Let's approximate f via regression!

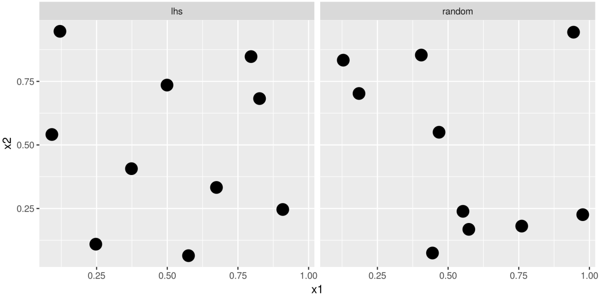
Generic MBO Pseudo Code

- Create initial space filling design and evaluate with f
- In each iteration:
  - Fit regression model on all evaluated points to predict $\hat{f}(\mathbf{x})$ and uncertainty $\hat{s}(\mathbf{x})$
  - Propose point via infill criterion

$$\mathrm{EI}(x) \uparrow \iff \hat{f}(\mathbf{x}) \downarrow \wedge \hat{s}(\mathbf{x}) \uparrow$$

  - Evaluate proposed point and add to design
  - EGO proposes kriging (aka Gaussian Process) and EI
    Jones 1998, Efficient Global Opt. of Exp. Black-Box Functions

Latin Hypercube Designs

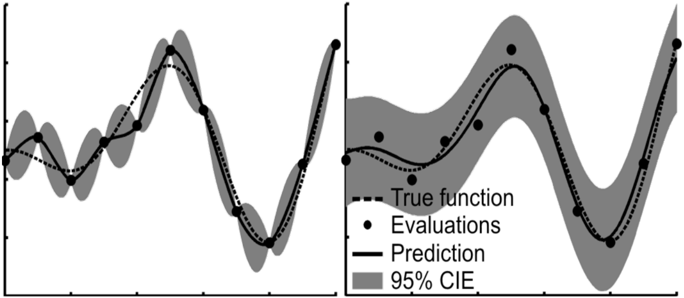


- Initial design to train first regression model
- Not too small, not too large
- LHS / maximin designs: Min dist between points is maximized
- But: Type of design usually has not the largest effect on MBO, and unequal distances between points could even be beneficial

Kriging and local uncertainty prediction

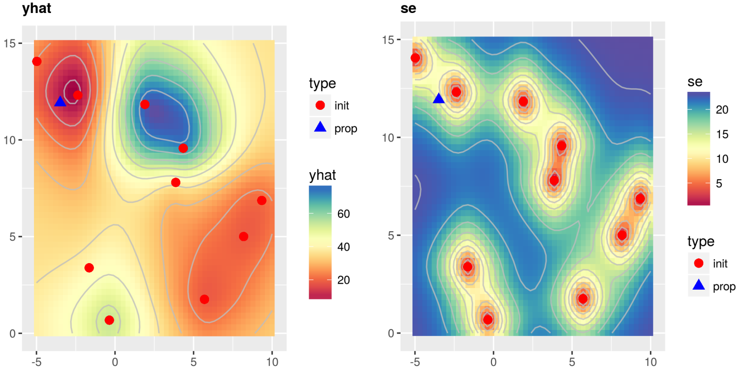
Model: Zero-mean GP $Y(x)$ with const. trend and cov. kernel $k_\theta(x_1, x_2)$.

- $\boldsymbol{y} = (y_1, \ldots, y_n)^T$, $\boldsymbol{K} = (k(\boldsymbol{x}_i, \boldsymbol{x}_j))_{i,j=1,\ldots,n}$
- $\boldsymbol{k}_*(\boldsymbol{x}) = (k(\boldsymbol{x}_1, \boldsymbol{x}), \ldots, k(\boldsymbol{x}_n, \boldsymbol{x}))^T$
- $\hat{\mu} = \mathbf{1}^T \boldsymbol{K}^{-1} \boldsymbol{y} / \mathbf{1}^T \boldsymbol{K}^{-1} \mathbf{1}$ (BLUE)
- Prediction: $\hat{f}(\boldsymbol{x}) = E[Y(x)|Y(x_i) = y_i, i = 1, \ldots, n] =$
  $\hat{\mu} + \mathbf{k}_n(x)^T K^{-1}(\mathbf{y} - \hat{\mu}\mathbf{1})$
- Uncertainty: $\hat{s}^2(\boldsymbol{x}) = Var[Y(x)|Y(x_i) = y_i, i = 1, \ldots, n] =$
  $\sigma^2 - \mathbf{k}_n^T(x) K^{-1} \mathbf{k}_n(x) + \frac{(1 - \mathbf{1}^T K^{-1} \mathbf{k}_n^T(x))^2}{\mathbf{1}^T K^{-1} \mathbf{1}}$



Kriging / GP is a spatial model

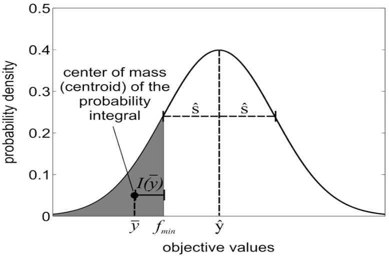
- Correlation between outcomes (y_1, y_2) depends on dist of x_1, x_2
  E.g. Gaussian covar kernel $k(x_1, x_2) = exp(\frac{-||x_1 - x_2||}{2\sigma})$
- Useful smoothness assumption for optimization
- Posterior uncertainty at new x increases with dist to design points
- Allows to enforce exploration

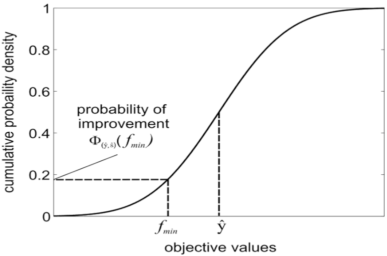


Infill Criteria: Expected Improvement

- Define improvement at x over best visited point with $y = f_{min}$ as random variable $I(x) = |f_{min} - Y(x)|^+$
- For kriging $Y(x) \sim N(\hat{f}(\boldsymbol{x}), \hat{s}^2(\boldsymbol{x}))$ (given $x = x$)
- Now define $EI(x) = E[I(x)|x = x]$
- Expectation is integral over normal density starting at f_{min}
- Alternative: Lower confidence bound (LCB) $\hat{f}(\boldsymbol{x}) - \lambda \hat{s}(\boldsymbol{x})$

Result: $EI(x) = \left(f_{min} - \hat{f}(\boldsymbol{x})\right) \Phi\left(\frac{f_{min} - \hat{f}(\boldsymbol{x}))}{\hat{s}(\boldsymbol{x})}\right) + \hat{s}(\boldsymbol{x}) \phi\left(\frac{f_{min} - \hat{f}(\boldsymbol{x})}{\hat{s}(\boldsymbol{x})}\right)$

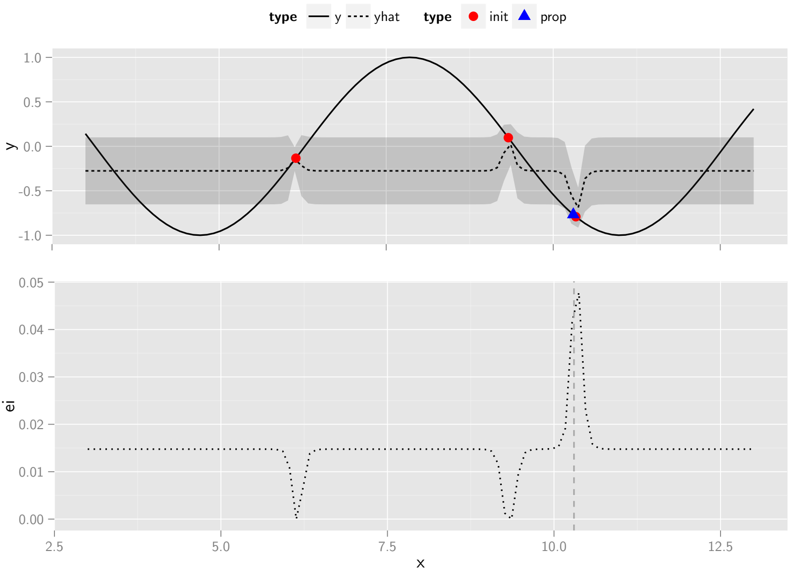


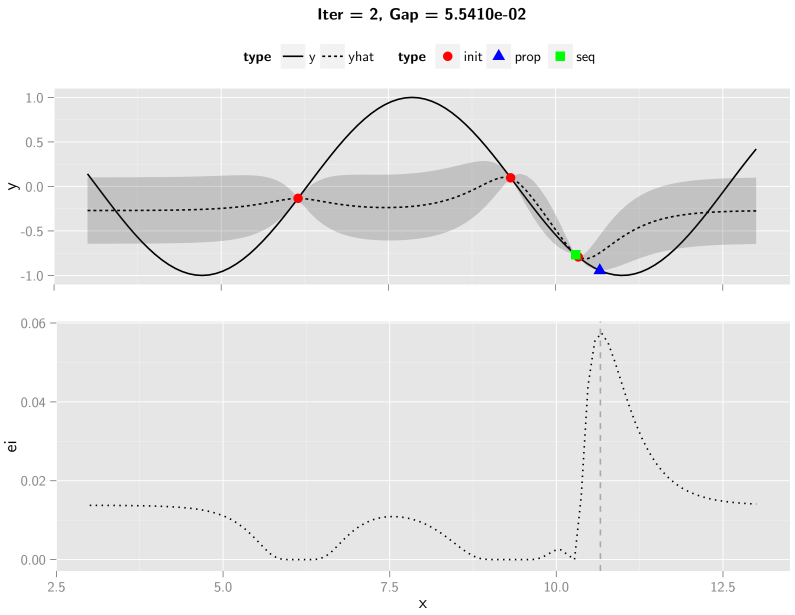


FOCUSSEARCH

- EI optimization is multimodal and not that simple
- But objective is now cheap to evaluate
- Many different algorithms exist, from gradient-based methods with restarts to evolutionary algorithms
- We use an iterated, focusing random search coined "focus search"
- In each iteration a random search is performed
- We then shrink the constraints of the feasible region towards the best point in the current iteration (focusing) and iterate, to enforce local convergence
- Whole process is restarted a few times
- Works also for categorical and hierarchical params

Iter = 1, Gap = 2.0795e-01

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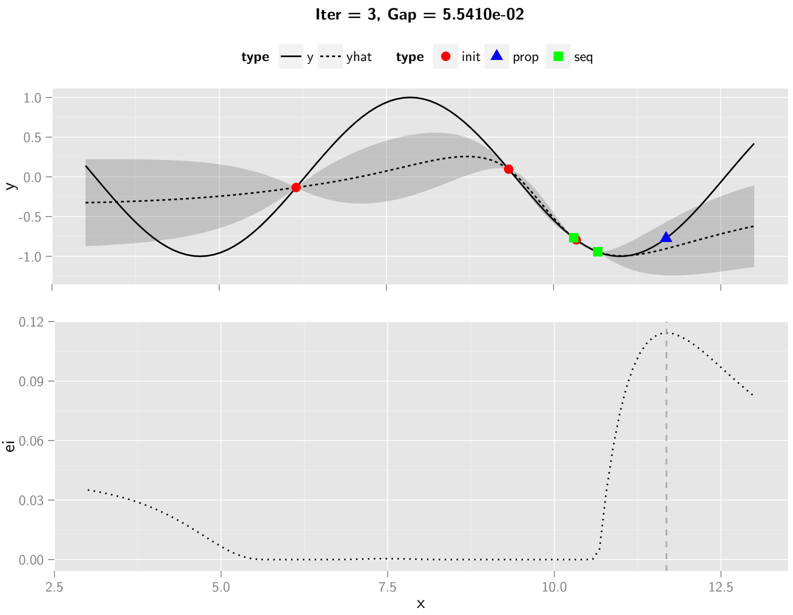
type
y
yhat
type
init
prop
seq
y
1.0
0.5
0.0
-0.5
-1.0
ei
0.06
0.04
0.02
0.00
2.5
5.0
7.5
10.0
12.5
x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y
yhat
type
init
prop
seq
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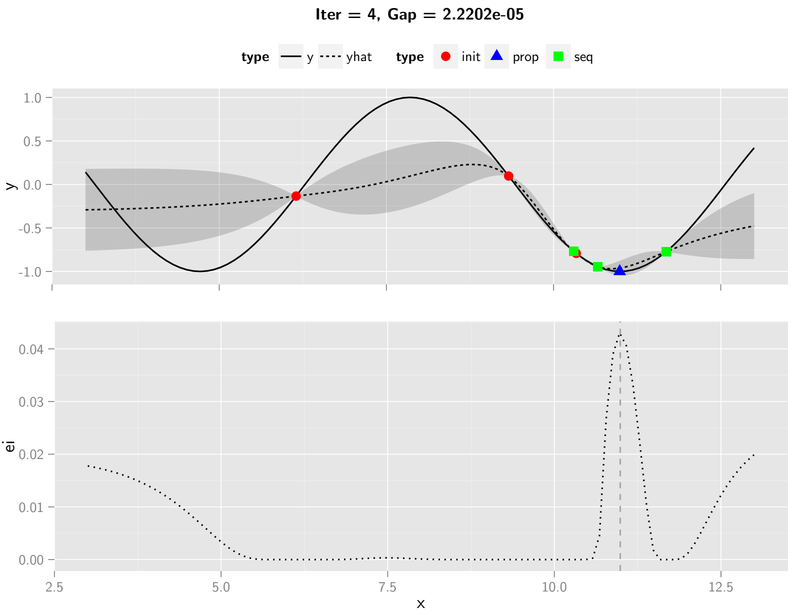
0.0
-0.5
-1.0
y
0.12
0.09
0.06
0.03
0.00
ei
2.5
5.0
7.5
10.0
12.5
x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y
yhat
type
init
prop
seq
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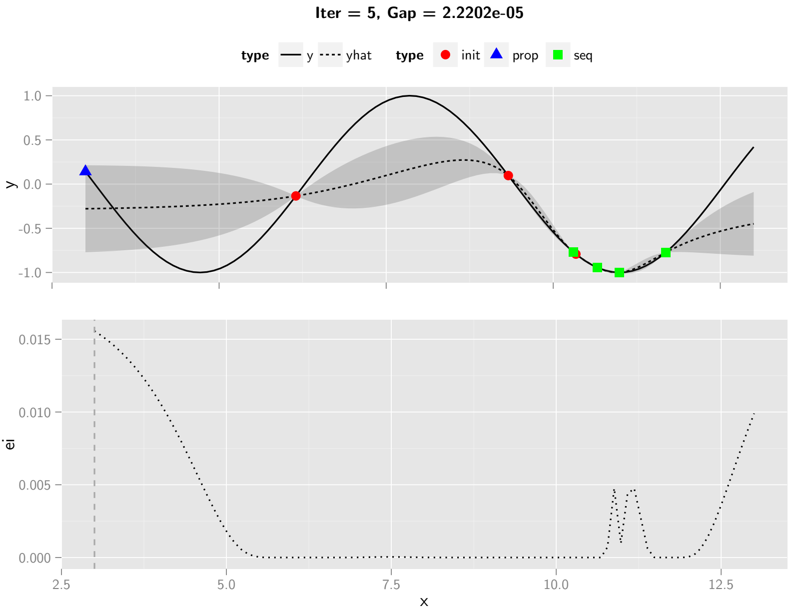
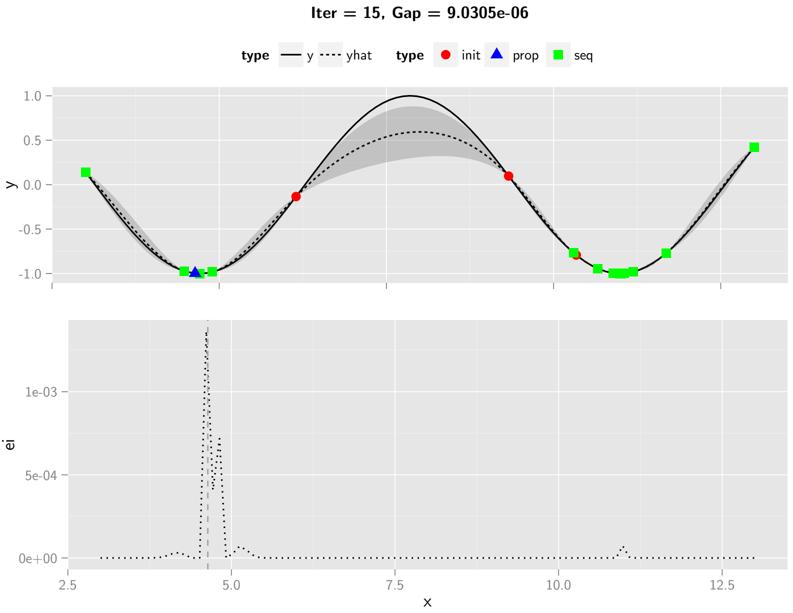
0.0
-0.5
-1.0
y
0.04
0.03
0.02
0.01
0.00
ei
2.5
5.0
7.5
10.0
12.5
x

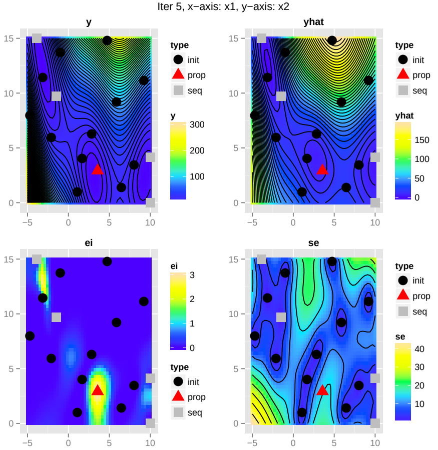


Iter = 5, Gap = 2.2202e-05
type
y
yhat
type
init
prop
seq
1.0
0.5
0.0
-0.5
-1.0
y
0.015
0.010
0.005
0.000
ei
2.5
5.0
7.5
10.0
12.5
x


Iter = 15, Gap = 9.0305e-06
type
y
yhat
type
init
prop
seq
1.0
0.5
0.0
-0.5
-1.0
y
1e-03
5e-04
0e+00
ei
2.5
5.0
7.5
10.0
12.5
x

mlrMBO: Model-Based Optimization Toolbox

- Any regression from mlr
- Arbtritrary infill
- Single - or multi-crit
- Multi-point proposal
- Via parallelMap and batchtools runs on many parallel backends and clusters
- Algorithm configuration
- Active research

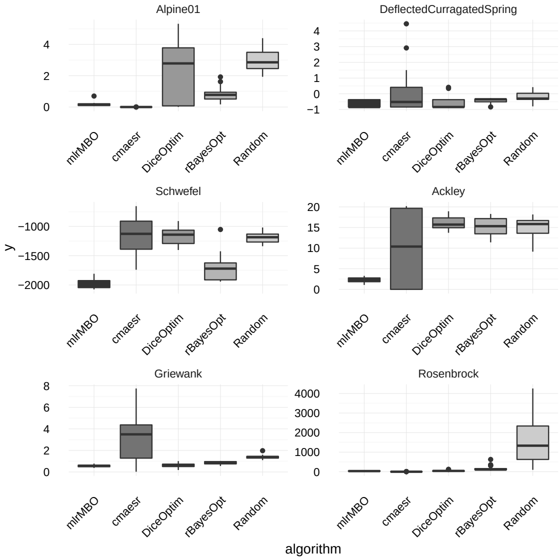


- mlr: `https://github.com/mlr-org/mlr`
- mlrMBO: `https://github.com/mlr-org/mlrMBO`
- mlrMBO Paper on arXiv (under review) `https://arxiv.org/abs/1703.03373`

Benchmark MBO on artificial test functions

- Comparison of mlrMBO on multiple different test functions
  - Multimodal
  - Smooth
  - Fully numeric
  - *Well known*
- We use GPs with
  - LCB with $\lambda = 1$
  - Focussearch
  - 200 iterations
  - 25 point initial design, created by LHS sampling
- Comparison with
  - Random search
  - CMAES
  - other MBO implementations in R

MBO GP vs. competitors in 5D



Section 2

Parallel batch proposals

Motivation for batch proposal

- Function evaluations expensive
- Often many cores available on a cluster
- Underlying f can in many cases not be easily parallelized
- Natural to consider batch proposal
- Parallel MBO: suggest q promising points to evaluate: $\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_q^*$
- We need to balance exploration and exploitation
- Non-trivial to construct infill criterion for this

Review of parallel MBO strategies

- **Constant liar**: (Ginsbourger et al., 2010)
  - Fit kriging model based on real data and find $\boldsymbol{x}_1^*$ according to EI-criterion.
  - "Guess" $f(\boldsymbol{x}_{i-1}^*)$, update the model and find $\boldsymbol{x}_i^*$, $i = 2, ..., q$
  - Use f_{min} for "guessing"

- q-**LCB**: (Hutter et al., 2012)
  - q times: sample λ from $Exp(1)$ and optimize single LCB criterion
  - $\boldsymbol{x}^* = \arg\min_{\boldsymbol{x}\in\mathcal{X}} \mathrm{LCB}(\boldsymbol{x}) = \arg\min_{\boldsymbol{x}\in\mathcal{X}} \; \hat{f}(\boldsymbol{x}) - \lambda\hat{s}(\boldsymbol{x})\,.$

Multiobjectivization and proposed idea

- **Multiobjectivization**
  - Originates from multi-modal optimization
  - Add distance to neighbors for current set as artificial objective
  - Use multiobjective optimization
  - Select by hypervolume or first objective or ...

- **Our approach**
  - Decouple $\hat{f}(\boldsymbol{x})$ and $\hat{s}(\boldsymbol{x})$ as objectives – instead of EI – to have different exploration / exploitation trade-offs
  - Consider distance measure as potential extra objective
  - Run multiobjective EA to select q well-performing, diverse points
  - Distance is possible alternative if no or bad $\hat{s}(\boldsymbol{x})$ estimator
  - Decoupling $y(\boldsymbol{x})$, $\hat{s}(\boldsymbol{x})$ potential alternative when *EI* derivation does not hold for other model classes

Bischl, Wessing et al:*MOI-MBO: Multiobjective infill for parallel model-based optimization*, LION 2014

Experimental setup

Problem Instances

- All 24 test functions of the black-box optimization benchmark (BBOB) noise-free test suite
- Dimensions $d \in \{5, 10\}$

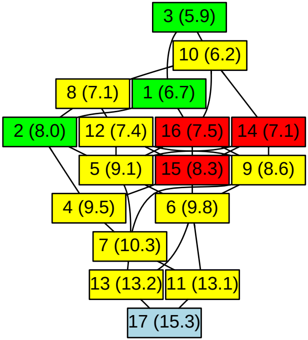
Budget

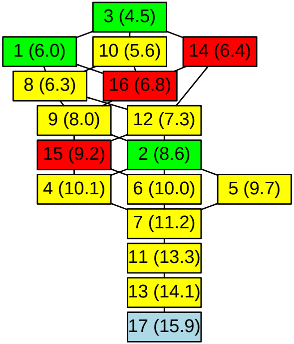
- For every function 10 initial designs of size $5 \cdot d$
  $\Rightarrow$ 10 statistical replications for each problem instance
- $40 \cdot d$ function evaluations on top of the initial design
- Parallel optimization: batches of size $q = 5$

Visualization: Preference relation graph

- Each node represents an approach (mean rank in braces)
- Two nodes are connected with an edge if one approach (the upper) is significantly better than the other (the lower) according to the sign test

Result Graphs





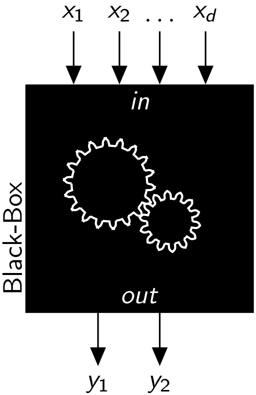
- 01: ego
- 02: ego_ea_ei
- 03: ego_ea_mean
- 04: moi_ei.dist_nb_first
- 05: moi_ei.dist_nb_hv
- 06: moi_ei.dist_nn_first
- 07: moi_ei.dist_nn_hv
- 08: moi_mean.se.dist_nb_first
- 09: moi_mean.se.dist_nb_hv

- 10: moi_mean.se.dist_nn_first
- 11: moi_mean.se.dist_nn_hv
- 12: moi_mean.se_nn_first
- 13: moi_mean.se_nn_hv
- 14: par_cl
- 15: par_cl_ea
- 16: par_lcb
- 17: random_search

Section 3

Multicriteria SMBO

Model-based multi-objective optimization



$$\min_{\boldsymbol{x} \in \mathbb{X}} \mathbf{f}(\boldsymbol{x}) = \boldsymbol{y} = (y_1, ..., y_m) \text{ with } \mathbf{f} : \mathbb{R}^d \to \mathbb{R}^m$$

- $\boldsymbol{y}$ *dominates* $\tilde{\boldsymbol{y}}$ if (3)

$$\forall i \in \{1, ..., m\} : y_i \leq \tilde{y}_i \quad (4)$$

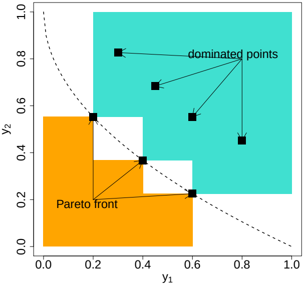
$$\text{and } \exists i \in \{1, ..., m\} : y_i < \tilde{y}_i \quad (5)$$

- Set of non-dominated solutions:

  $\mathcal{X}^* := \{\mathbf{x} \in \mathcal{X} | \nexists \tilde{\mathbf{x}} \in \mathcal{X} : \mathbf{f}(\tilde{\mathbf{x}}) \text{ dominates } \mathbf{f}(\mathbf{x})\}$

- Pareto set $\mathcal{X}^*$, Pareto front $\mathbf{f}(\mathcal{X}^*)$
- Goal: Find $\hat{\mathcal{X}}^*$ of non-dominated points that estimates the true set $\mathcal{X}^*$

Model-based multi-objective optimization



$$\min_{\boldsymbol{x} \in \mathbb{X}} \mathbf{f}(\boldsymbol{x}) = \boldsymbol{y} = (y_1, \ldots, y_m) \text{ with } \mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$$

- $\boldsymbol{y}$ *dominates* $\tilde{\boldsymbol{y}}$ if (6)

$$\forall i \in \{1, \ldots, m\} : y_i \leq \tilde{y}_i \tag{7}$$

$$\text{and } \exists i \in \{1, \ldots, m\} : y_i < \tilde{y}_i \tag{8}$$

- Set of non-dominated solutions:

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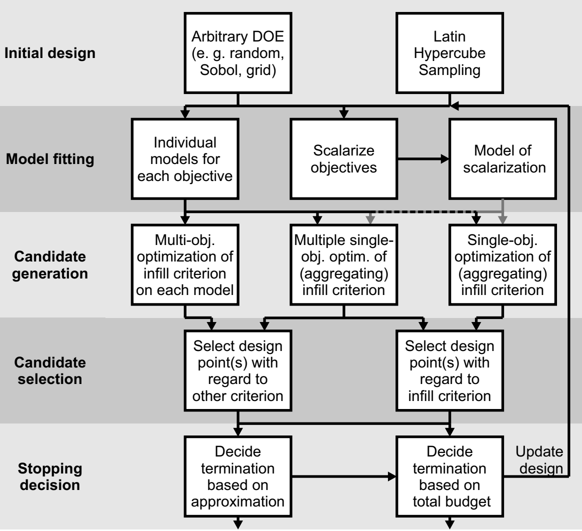
Taxonomy



Horn, Wagner, Bischl et al:*Model-based multi-objective optimization: Taxonomy, multi-point proposal, toolbox and benchmark*, EMO 2014

Batch Proposal

- Most MBMO lack way to propose $N > 1$ points (batch evaluation)
- Batch evaluations are essential for distributed computing
- We integrated such mechanism(s) for arbitrary MBMO
- Replaced single phases of the taxonomy

ParEGO

1. Scalarize objectives using the augmented Tchebycheff norm

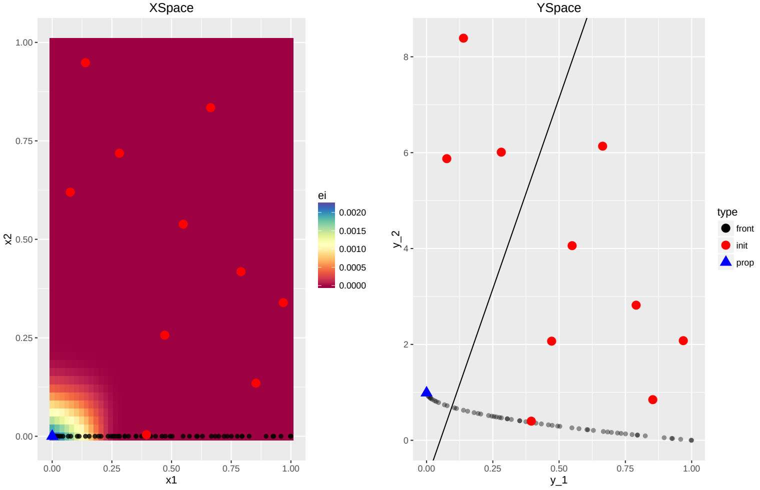
$$\max_{i=1,\ldots,d} [w_i f_i(\mathbf{x})] + \rho \sum_{i=1}^{d} w_i f_i(\mathbf{x})$$

   with uniformly distributed weight vector $\mathbf{w}$ ($\sum w_i = 1$) and fit surrogate model to the respective scalarization.
2. Single-objective optimization of EI (or LCB?)

Batch proposal: **Increase the number and diversity of randomly drawn weight vectors**

- If N points are desired, cN ($c > 1$) weight vectors are considered
- Greedily reduce set of weight vectors by excluding one vector of the pair with minimum distance
- Scalarizations implied by each weight vector are computed
- Fit and optimize models for each scalarization
- Optima of each model build the batch to be evaluated

Animation of ParEGO



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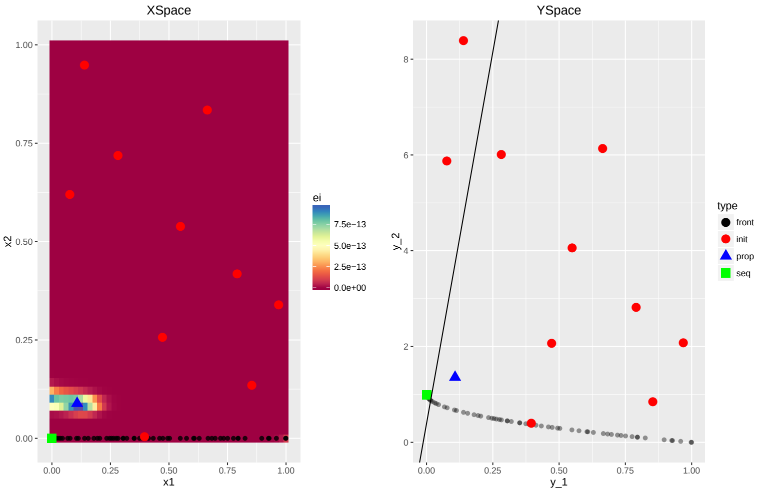
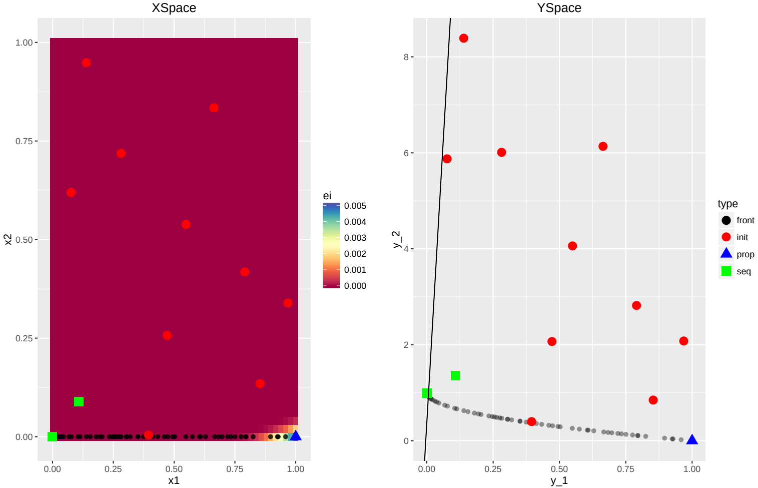
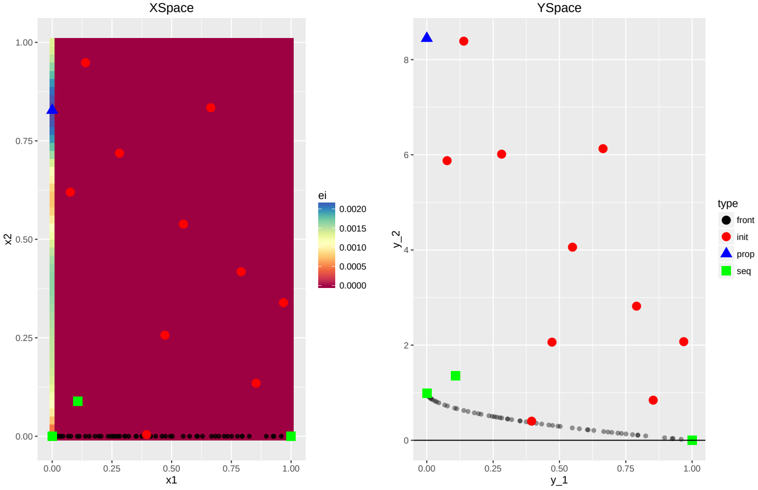


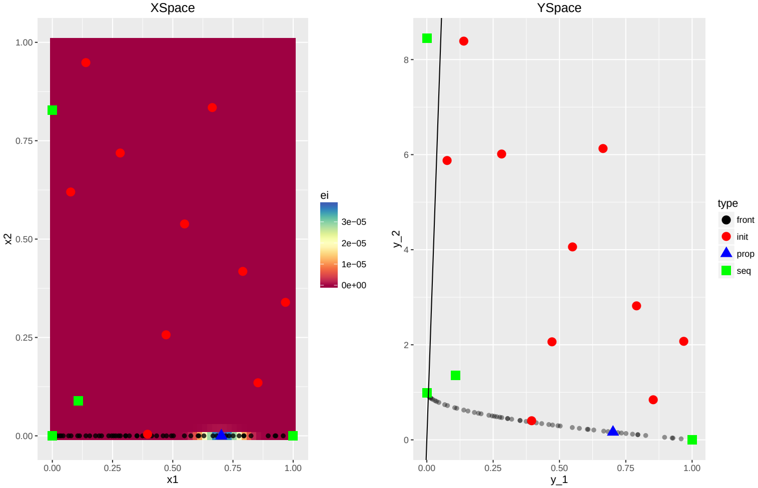
Animation of ParEGO



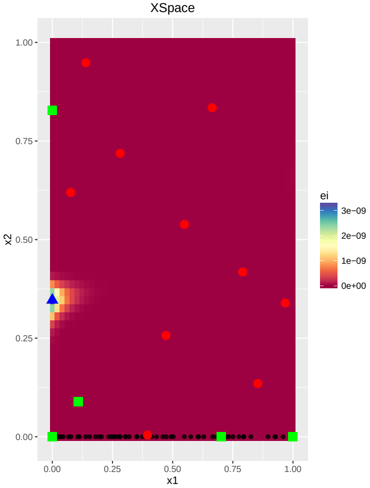
Animation of ParEGO

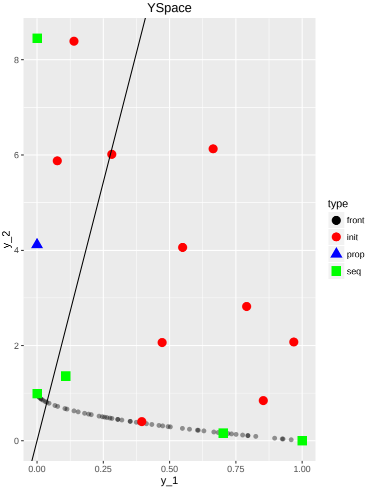


Animation of ParEGO

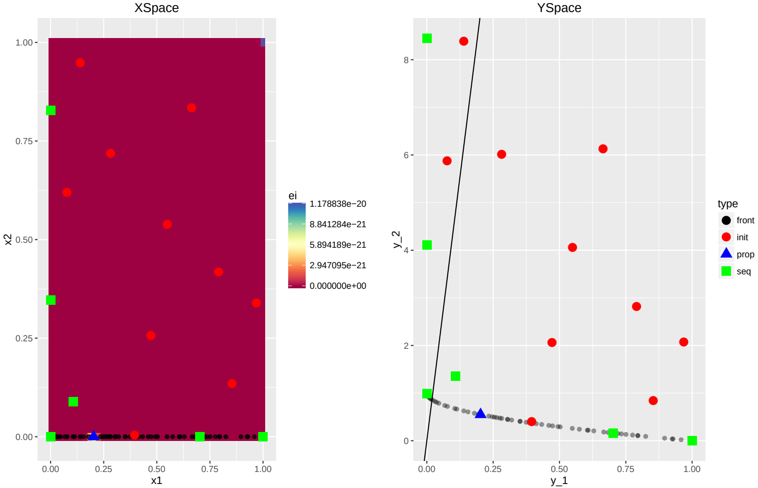


Animation of ParEGO

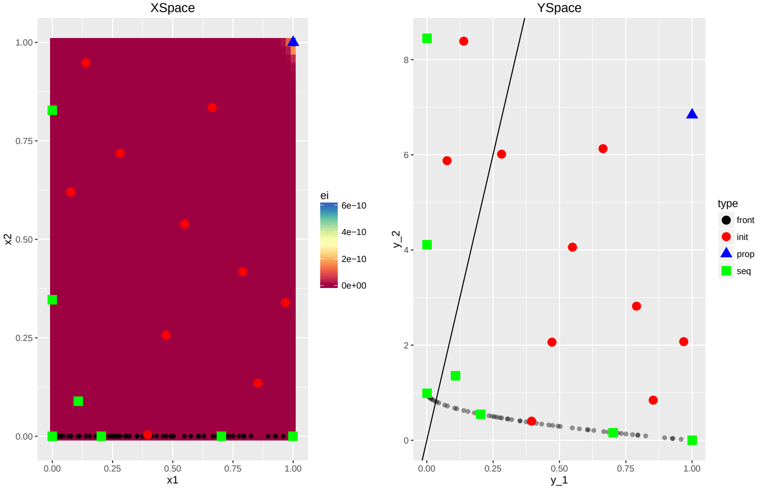




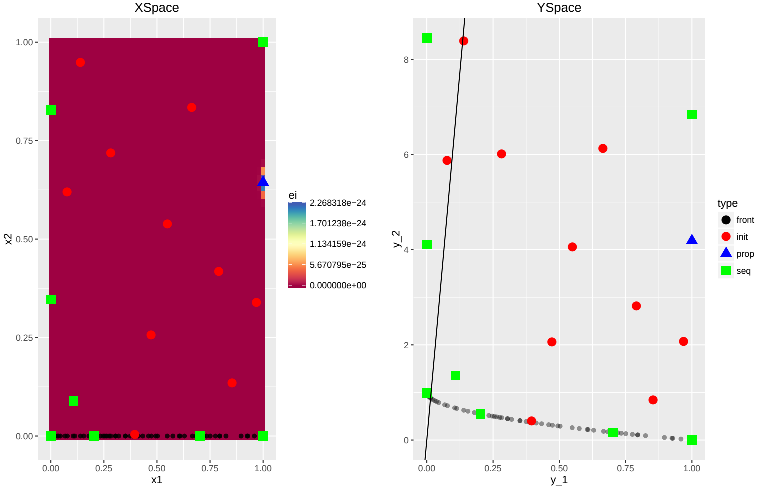
Animation of ParEGO



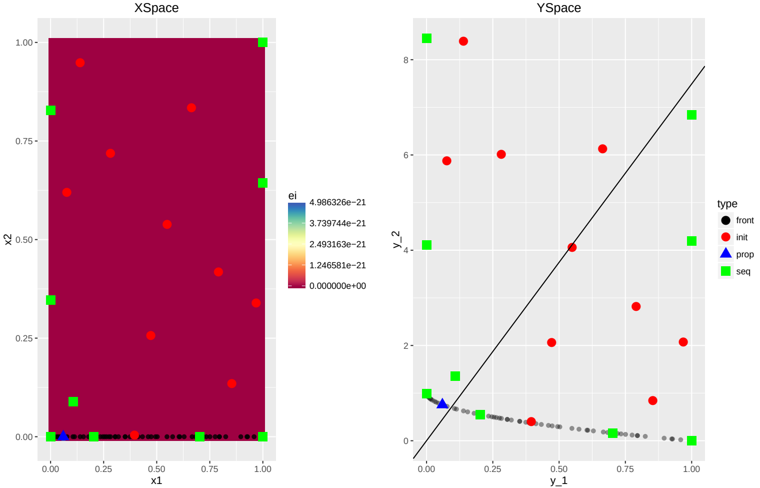
Animation of ParEGO



Animation of ParEGO



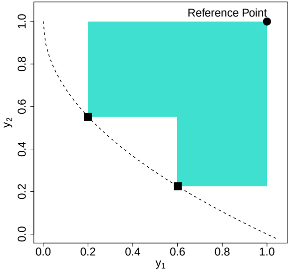
Animation of ParEGO



SMS-EGO

- Individual models for each objective
- Single-objective optimization of aggregating infill criterion: Calculate contribution of the confidence bound of representative solution to the current front approximation

- Calculate LCB for each objective
- Measure contribution with regard to the hypervolume indicator
- For ε-dominated ($\preceq_\varepsilon$) solutions, a penalty $\Psi(\mathbf{x}) = -1 + \prod_{j=1}^{m} \left(1 + (l(\mathbf{x}) - y_j^{(i)})\right)$ is added (Actually not needed for Focussearch.)



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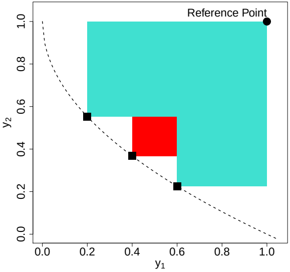

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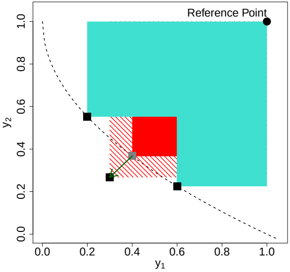


SMS-EGO: Batch proposal

Modification of phase candidate generation: **Use simulated evaluations for candidate generation**

- The proposed point $\vec{x}^*$ is not directly evaluated, but the LCB $l(\vec{x}^*)$ is added to the current approximation without refitting the model
- Repeat until N points for a batch evaluation have been found

Approximative RBF-SVM Training Algorithms

SVM solver	Description
Pegasos	Stochastic Gradient Descent
BSGD	Budgeted Stochastic Gradient Descent
LLSVM	Low-rank kernel approximation + linear solver
LIBSVM	"Exact" SMO solver
LASVM	Online variant of SMO solver
LIBBVM/CVM	Minimum Enclosing Ball (only squared hinge loss)
SVMperf	Cutting Plane Algorithm

- What is the trade-off between training time and prediction error?
- Most solvers have 2 additional parameters on top of C and γ
- Optimizing 2 expensive objectives in a 4-dim parameter space.
- Replace grid search with more sophisticated PAREGO-algorithm.

Approximative SVM Training Algorithms

- **We expect:** Every solver has a trade-off between training time and prediction error: Given more time a solver (should) reach a better solution.
- **Our goal:** Analyze this trade-off! Solve the multi-criteria optimization problem with respect to the two objectives error and training time by varying the parameters.
- **The challenge:** Optimizing 2 expensive objectives in a 4-dimensional parameter space.
- **Our approach:** Replace standard grid search with more sophisticated PAREGO-algorithm.

Approximative SVM Training Algorithms

The parameters (C, γ) of the SVM itself were optimized over $2^{[-15,15]}$ respectively. Every solver has further approximation parameters:

SVM solver	Parameters	Optimization Space
Pegasos	#Epochs	$2^{[0,7]}$
BGSD	Budget size, #Epochs	$2^{[4,11]}$, $2^{[0,7]}$
LLSVM	Matrix rank	$2^{[4,11]}$
LIBSVM	ϵ (Accuracy)	$2^{[-13,-1]}$
LASVM	ϵ (Accuracy), #Epochs	$2^{[-13,-1]}$, $2^{[0,7]}$
LIBBVM/CVM	ϵ (Accuracy)	$2^{[-19,-1]}$
SVMperf	ϵ (Accuracy), #Cutting planes	$2^{[-13,-1]}$, $2^{[4,11]}$

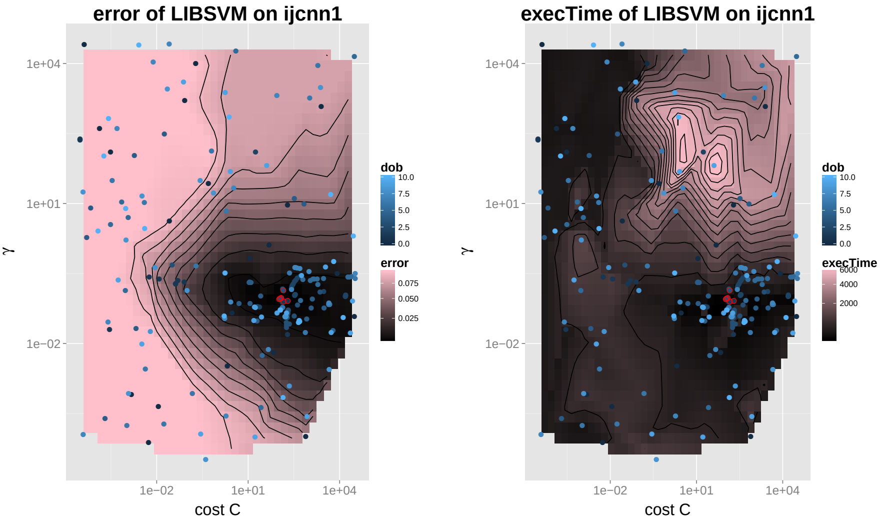
Additional parameters set to default values.

Datasets

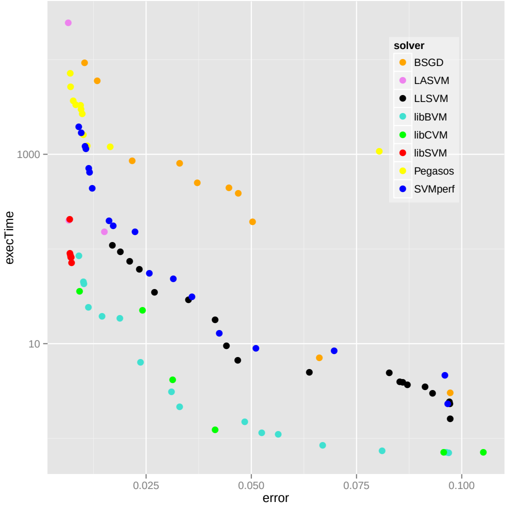
data set	# points	# features	class ratio	sparsity
wXa	34 780	300	34.45	95.19 %
aXa	36 974	123	3.17	88.72 %
protein	42 153	357	1.16	71.46 %
mnist	70 000	780	0.96	80.76 %
vehicle	98 528	100	1.00	0 %
shuttle	101 500	9	0.27	0.23 %
spektren	175 090	22	0.80	0 %
ijcnn1	176 691	22	9.41	40.91 %
arthrosis	262 142	178	1.19	0.01 %
cod-rna	488 565	8	2.00	0.02 %
covtype	581 012	54	1.05	78 %
poker	1 025 010	10	1.00	0 %

Table: Overview of the data sets.

Test error landscape (LIBSVM)



All Pareto fronts for ijcnn1 dataset



- 176 691 samples
  22 features
  9.41 class ratio
- Wee see:
  LIBSVM: exact but slow
  LIBBVM/CVM: good front - speed increase with small accuracy loss
  SVMperf / LLSVM / BSGD: can be really fast, but higher accuracy loss
  LASVM / Pegasos: less exact and even slower as LIBSVM

Section 4

Interesting Challenges

Challenge: The correct surrogate?

- GPs are very much tailored to what we want to do, due to their spatial structure in the kernel and the uncertainty estimator.
- But GPs are rather slow. And (fortunately) due to parallization (or speed-up tricks like subsampling) we have more design points to train on.
- Categorical features are also a problem in GPs (although methods exist, usually by changing the kernel)
- Random Forests handle categorical features nicely, are much faster. But they don't rely on a spatial kernel and the uncertainty estimation is much more heuristic / may not represent what we want.

Challenge: Time Heterogeneity

- Complex configuration spaces across many algorithms results in vastly different runtimes in design points.
- Actually just the RBF-SVM tuning can result in very different runtimes.
- We don't care how many points we evaluate, we care about total walltime of the configuration.
- The option to subsample further complicates things.
- Parallelization further complicates things.
- Option: Estimate runtime as well with a surrogate, integrate it into acquisition function.

Section 5

ML Model Selection and Hyperparameter Optimization

Automatic Model Selection

Prior approaches:

- Looking for the silver bullet model
  $\rightsquigarrow$ Failure
- Exhaustive benchmarking / search
  $\rightsquigarrow$ Very expensive, often contradicting results
- Meta-Learning:
  $\rightsquigarrow$ Good meta-features are hard to construct
  $\rightsquigarrow$ IMHO: Gets more interesting when combined with SMBO

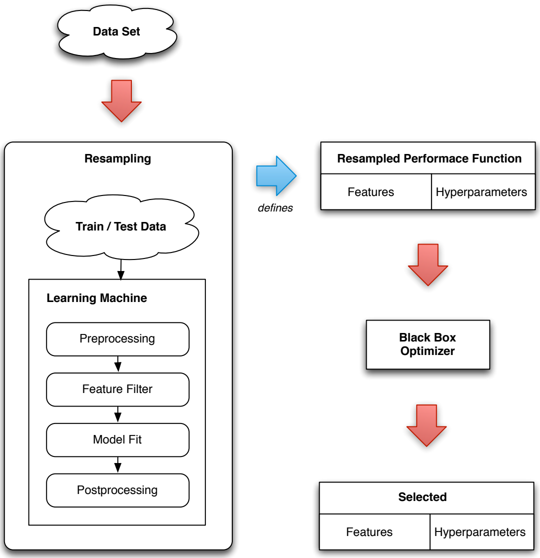
Goal for AutoML:

- Data dependent
- Automatic
- Include every relevant modeling decision
- Efficient
- Learn on the model-settings level!

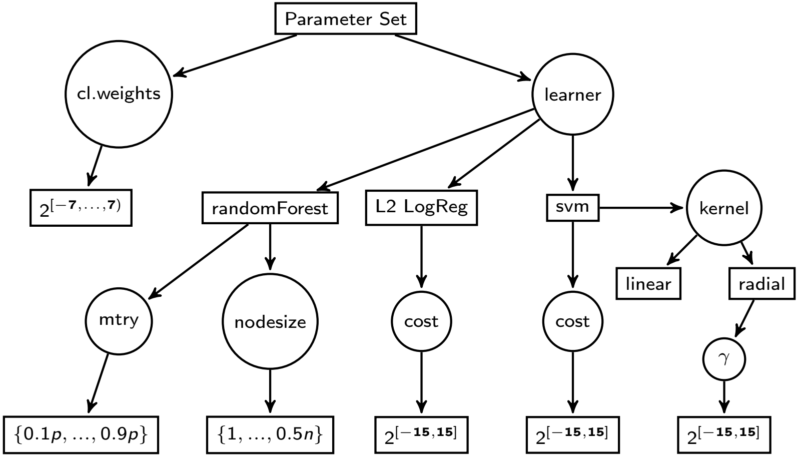
From Normal SMBO to Hyperarameter Tuning

- Objective function is resampled performance measure
- Parameter space $\theta \in \Theta$
  might be discrete and dependent / hierarchical
- No derivative for $f(\cdot, \theta)$, black-box
- Objective is stochastic / noisy
- Objective is expensive to evaluate
- In general we face a problem of algorithm configuration:
- $\rightsquigarrow$ Usual approaches: racing or model-based / bayesian optimization

From Normal SMBO to Hyperarameter Tuning



Complex Parameter Space



From Normal SMBO to Hyperarameter Tuning

- Initial design: LHS principle can be extended, or just use random
- Focus search: Can be (easily) extended, as it is based on random search. To zoom in for categorical parameters we randomly drop a category for each param which is not present in the currently best configuration.

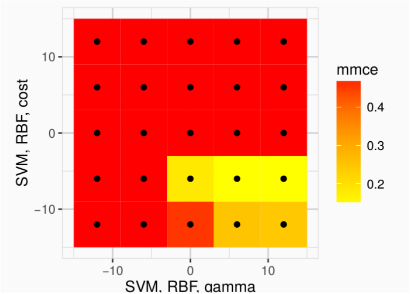
- Few approaches for GPs with categorical params exist (usually with new covar kernels), not very established
- Alternative: Random regression forest (mlrMBO, SMAC)
- Estimate uncertainty / confidence interval for mean response by efficient bootstrap technique[1], or jackknife, so we can define $EI(x)$ for the RF
- Dependent params in mlrMBO: Imputation:
- Many of the current techniques to handle these problems are (from a theoretical standpoint) somewhat crude

[1]Sexton et al, "Standard errors for bagged and random forest estimators, 2009."

Hyperparameter Tuning

- Still common practice: grid seach
  For a SVM it might look like:
  - $C \in (2^{-12}, 2^{-10}, 2^{-8}, \ldots, 2^{8}, 2^{10}, 2^{12})$
  - $\gamma \in (2^{-12}, 2^{-10}, 2^{-8}, \ldots, 2^{8}, 2^{10}, 2^{12})$
  - Evaluate all $13^2 = 169$ combinations $C \times \gamma$
- Bad beacause:
  - optimum might be "off the grid"
  - lots of evaluations in bad areas
  - lots of costy evaluations
- How bad?

Hyperparameter Tuning

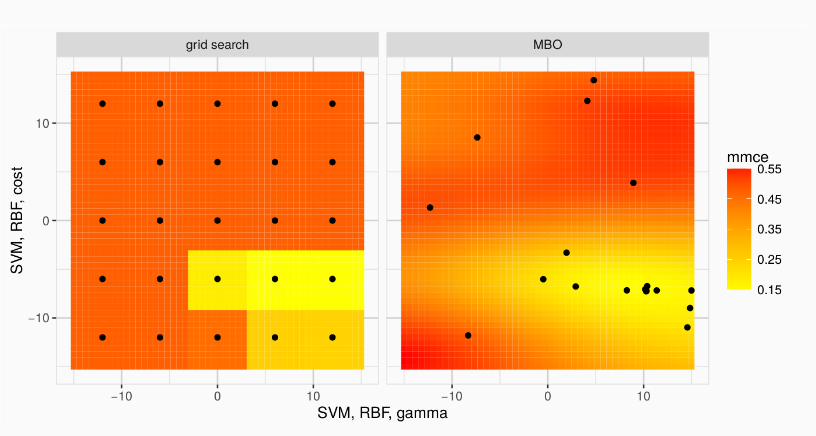


- Because of budget restrictions grid might even be smaller!
- Unpromising area quite big!
- Lots of costly evaluations!

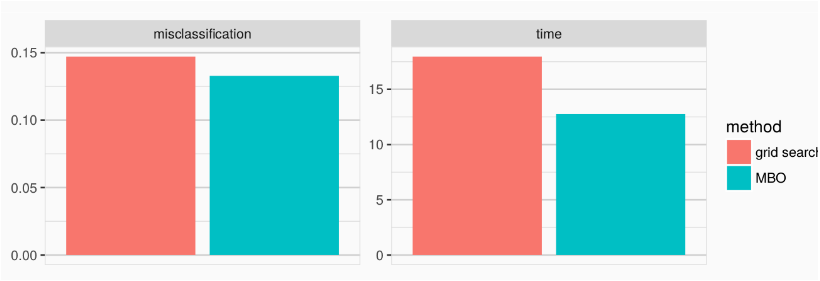
With **mlrMBO** it is not hard to do it better!
More interesting applications to time-series regression and cost-sensitive classification[2]

[2] Koch, Bischl et al: *Tuning and evolution of support vector kernels*, EI 2012

Hyperparameter Tuning



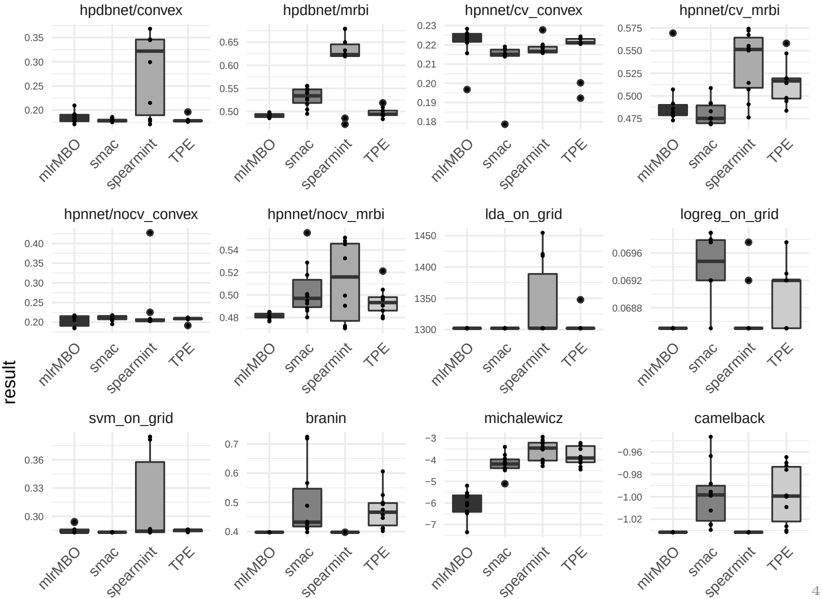
Hyperparameter Tuning



HPOlib

- HPOlib is a set of standard benchmarks for hyperparameter optimizer
- Allows comparison with
  - Spearmint
  - SMAC
  - Hyperopt (TPE)
- Benchmarks:
  - Numeric test functions (similar to the ones we've seen bevor)
  - Numeric machine learning problems (lda, SVM, logistic regression)
  - Deep neural networks and deep belief networks with 15 and 35 parameters.
- For benchmarks with discrete and dependent parameters (hpnnet, hpdbnet) a random forest with standard error estimation is used.

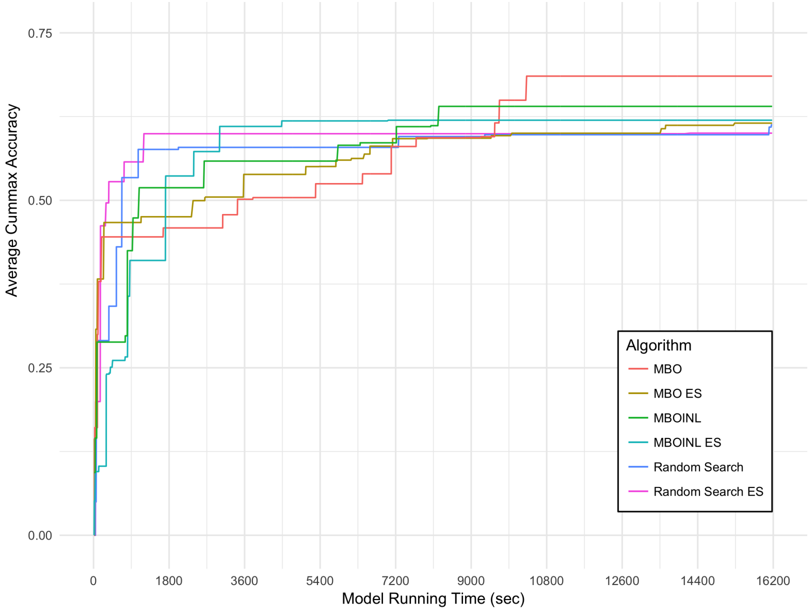
MBO: HPOLIB


result
hpdbnet/convex
hpdbnet/mrbi
hpnnet/cv_convex
hpnnet/cv_mrbi
hpnnet/nocv_convex
hpnnet/nocv_mrbi
lda_on_grid
logreg_on_grid
svm_on_grid
branin
michalewicz
camelback
mlrMBO
smac
spearmint
TPE

Deep Learning Configuration Example

- Dataset: CIFAR-10 (60000 32x32 images with 3 color channels; 10 classes)
- Configuration of a deep neural network (mxnet)
- Size of parameter set: 30, including number of hidden layers, activation functions, regularization, convolution layer setting, etc.
- Split: 2/3 training set, 1/6 test set, 1/6 validation set
- Time budget per tuning run: 4.5h (16200 sec)
- Surrogate: Random forest
- Acquisition: LCB with $\lambda = 2$

Deep Learning Configuration Example



Thanks! Any comments or questions?