

Neural Network Hyperparameter Optimization with Sparse Grids

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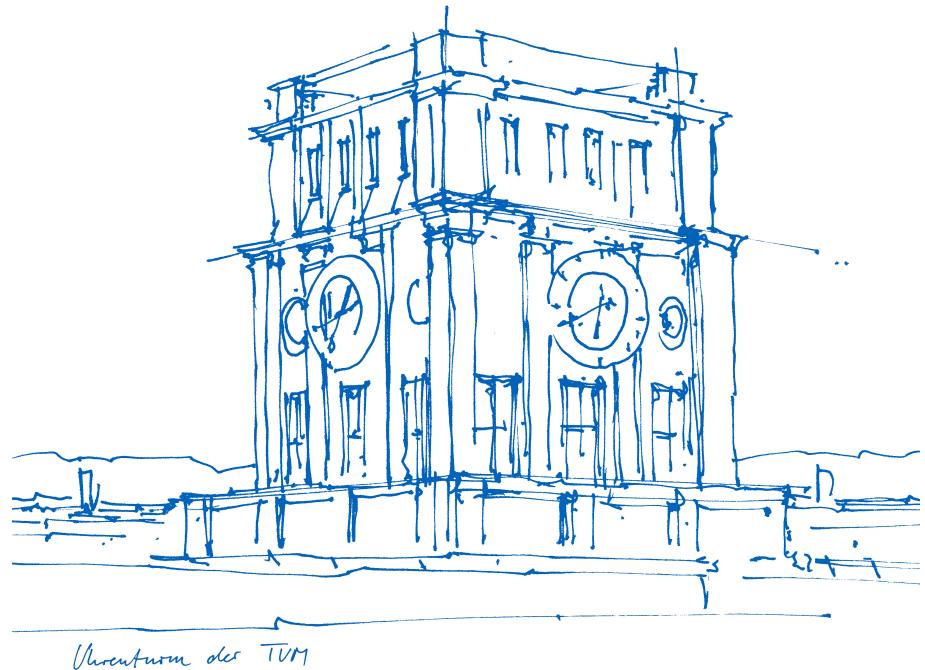
Chair of Scientific Computing

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Department Computer Science

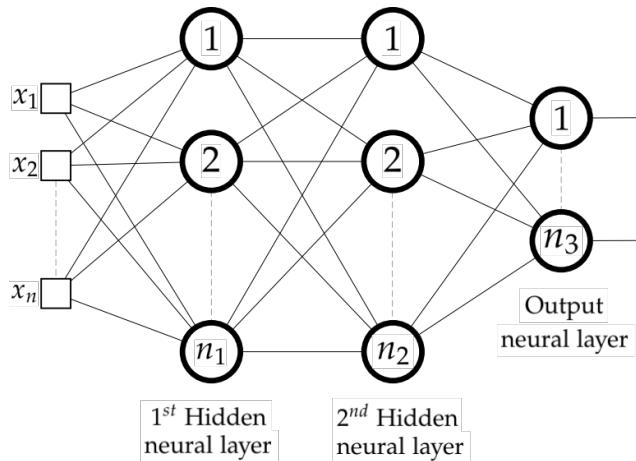
TUM School of Computation, Information
and Technology

Garching, 02. August 2023



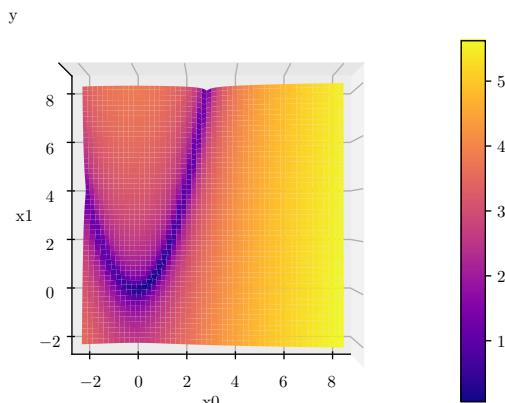
Hyperparameter Optimization

- **Hyperparameters:** Parameters of a ML model that are fixed before training



Number of layers/ neurons, epochs, learning rate, ...

- **Optimization:** finding the optimum of a function

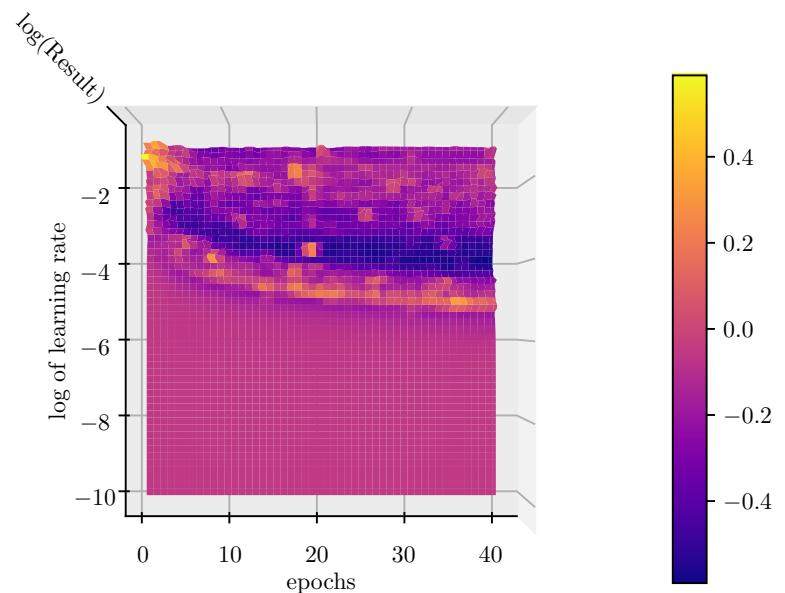


Rosenbrock: Optimum at (1, 1)

Hyperparameter Optimization

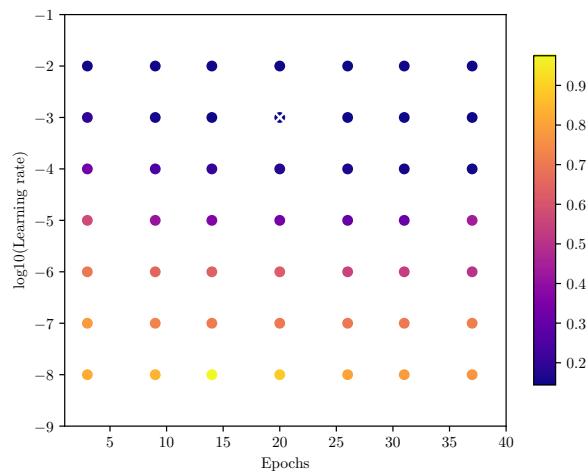
Regression with 2-layer neural network:

- Each function evaluation: 2-fold cross-validation of the network → expensive
- Final value: mean average percentage error on test set (average of 2-fold cross-validation)

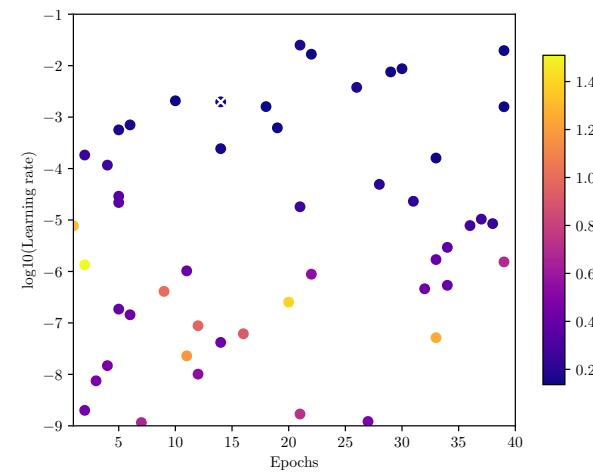


Hyperparameter Optimization – State of the Art

Grid search:



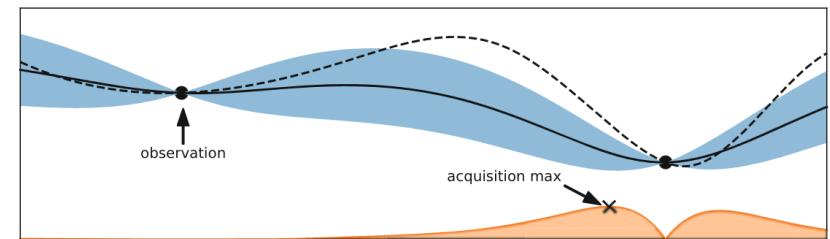
Random search:



Hyperparameter Optimization – State of the Art

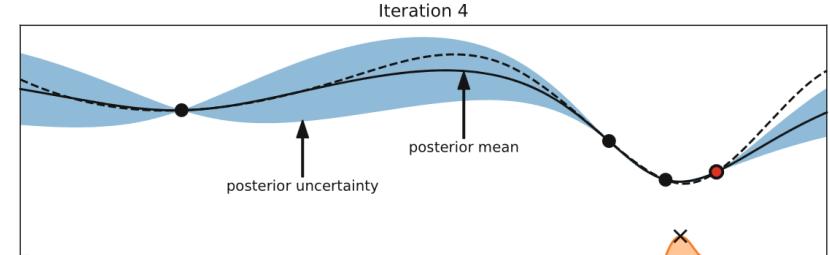
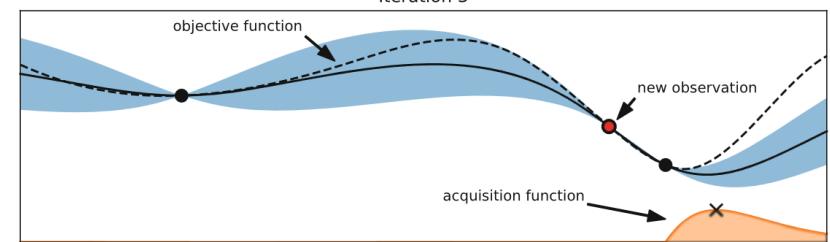
Bayesian optimization:

- **Surrogate model:** approximates the function, e.g. gaussian process, random forest, ...



- **Acquisition function:** finds new candidates for the optimum, e.g. expected improvement:

$$E[I(\lambda)] = E[\max(f_{\min} - y, 0)]$$



λ : configuration
 f_{\min} : best value so far
 y : model prediction

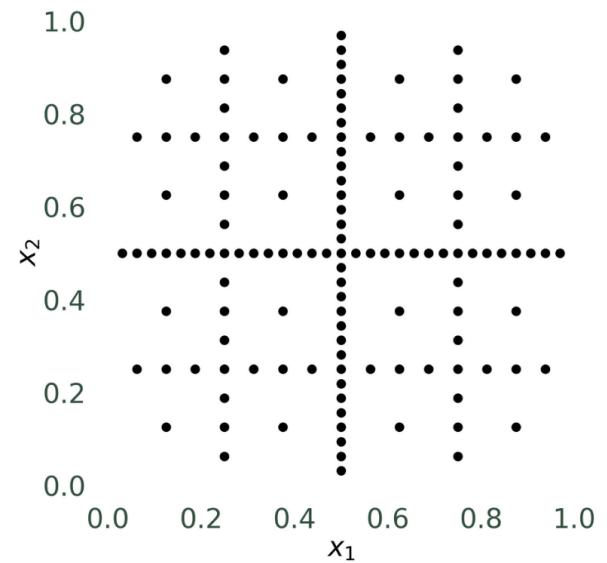
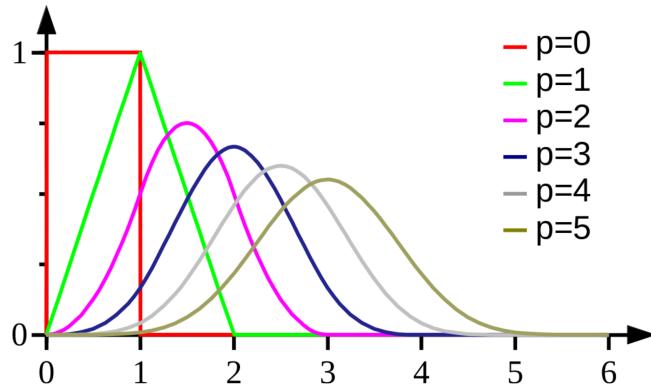
Hyperparameter Optimization with Sparse Grids

Background:

- Efficient way for representing functions:

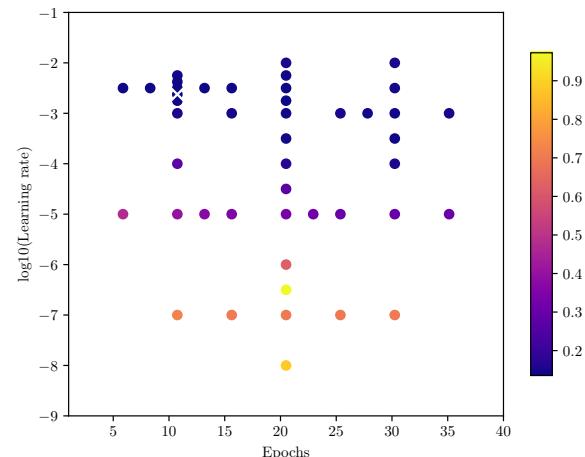
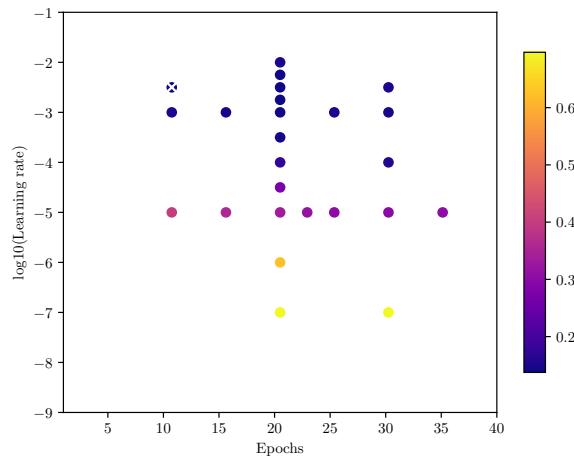
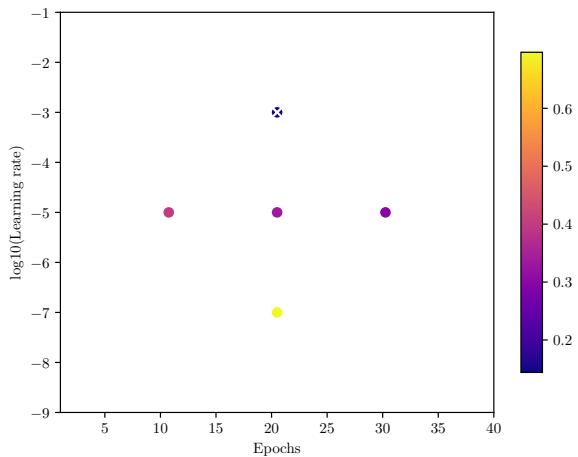
Grid	Number grid points	Error
Full grid	$\mathcal{O}(2^{nd})$	$\mathcal{O}(h_n^2)$
Sparse grid	$\mathcal{O}\left(h_n^{-1} (\log h_n^{-1})^{d-1}\right)$	$\mathcal{O}\left(h_n^2 (\log h_n^{-1})^{d-1}\right)$

- Interpolation with B-splines as basis function:



Sparse Grid Hyperparameter Optimization

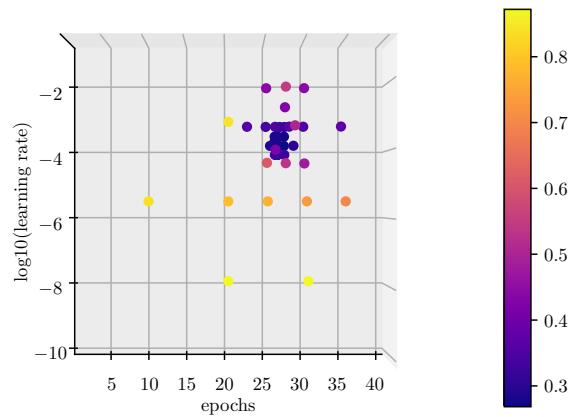
Iterative adaptive grid generation:



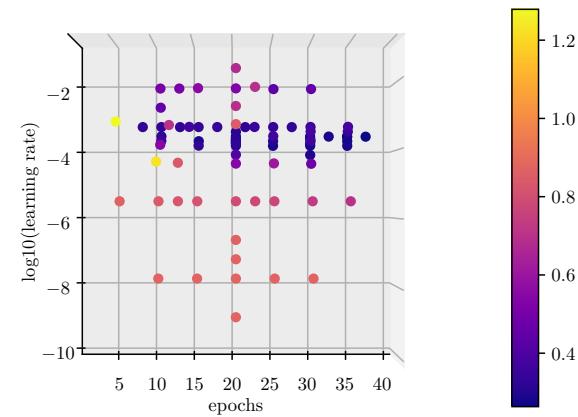
With Novak-Ritter refinement criterion: $(r_{l,i}+1)^{1-\gamma} \cdot (\|l_1\| + d_{l,i} + 1)^\gamma$

Adaptivity Parameter γ

$$\gamma = 0.5$$



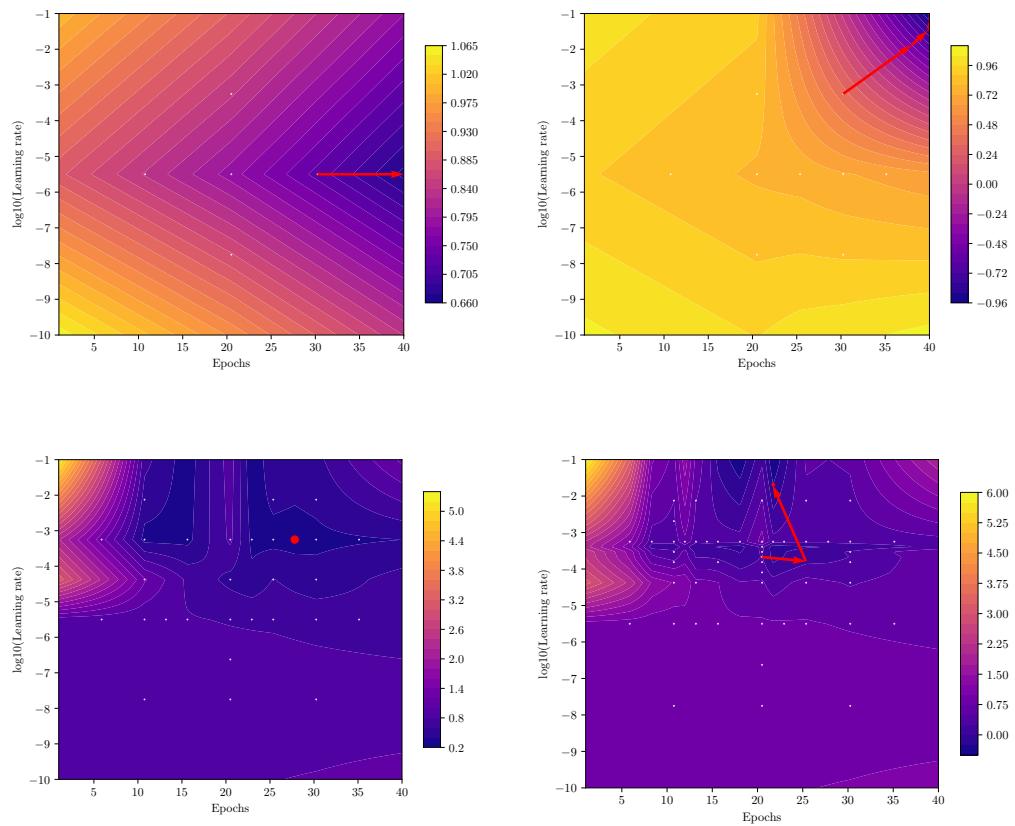
$$\gamma = 0.85$$



With Novak-Ritter refinement criterion: $(r_{l,i}+1)^{1-\gamma} \cdot (\|l_1\| + d_{l,i} + 1)^\gamma$

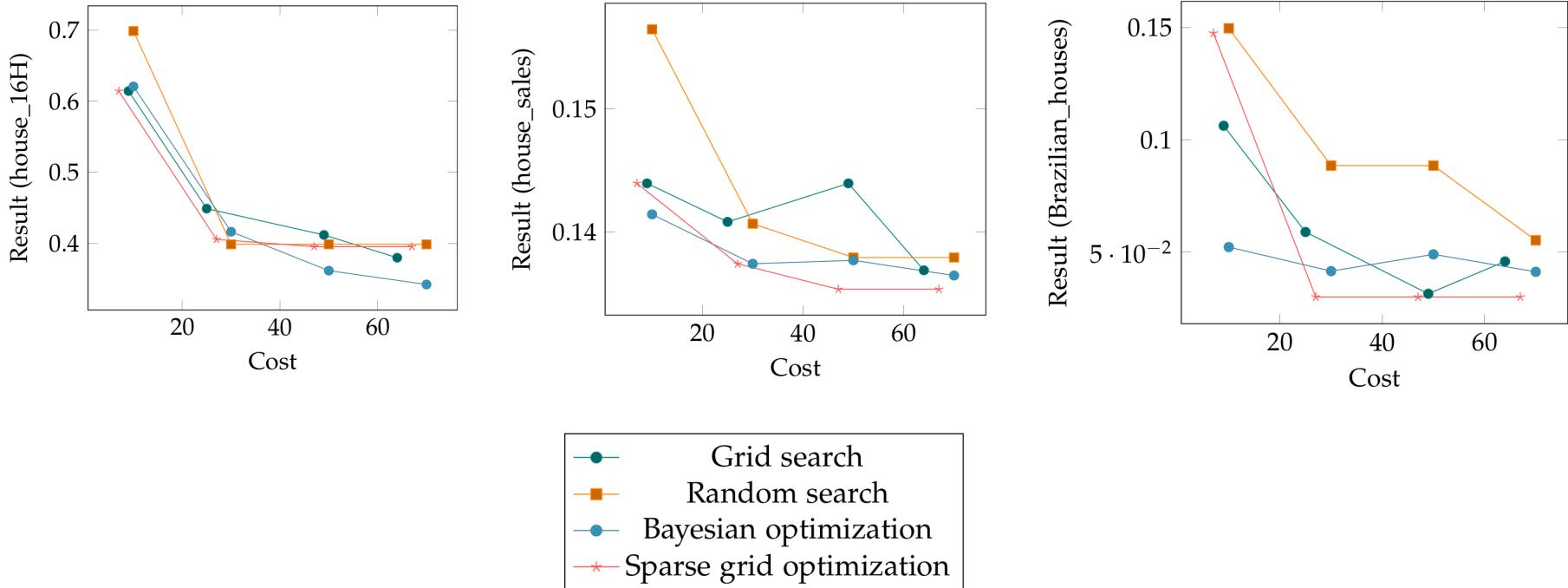
Sparse Grid Hyperparameter Optimization

- **Gradient-free optimizers:**
Nelder Mead, differential evolution, CMA-ES
- **Gradient-based optimizers:**
Gradient descent, NLCG, Newton, Rprop



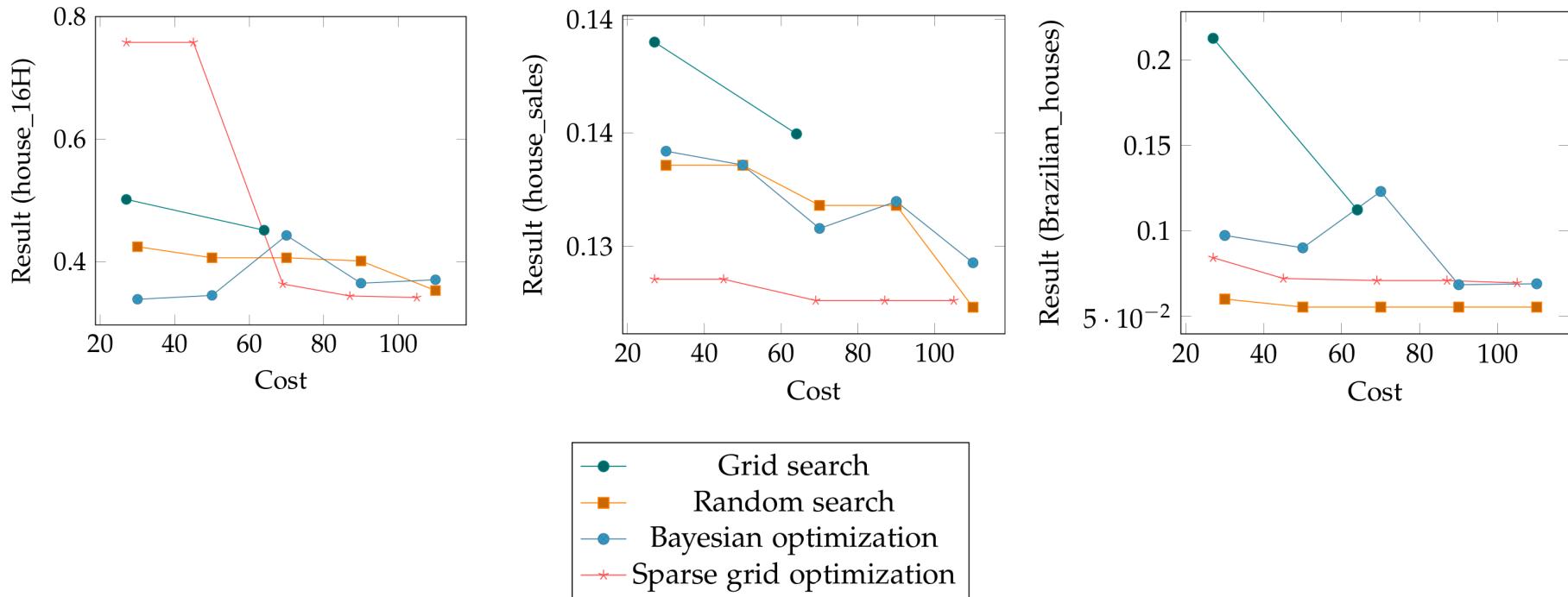
Numerical Results

2D Optimization: Epochs, Learning rate



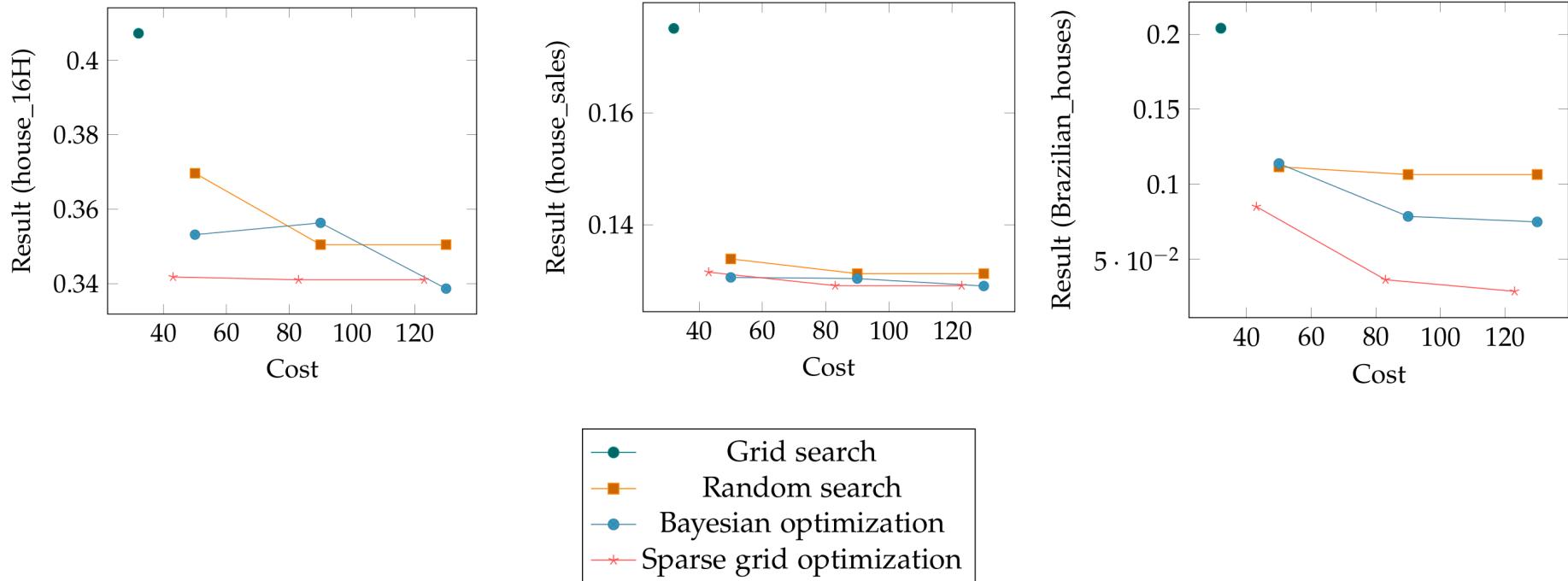
Numerical Results

3D Optimization: Epochs, Learning rate, Batch size



Numerical Results

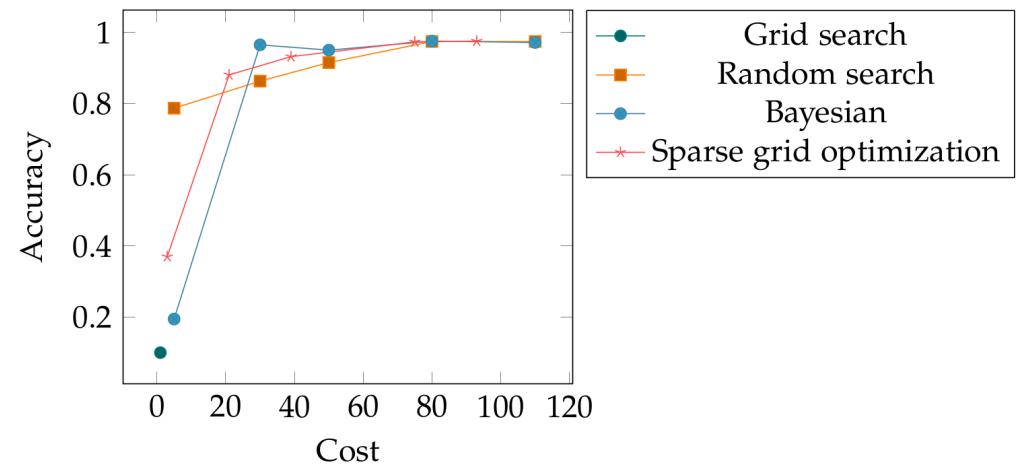
5D Optimization: Epochs, Learning rate, Batch size, Number of layers & neurons per layer



Application: MNIST

9D Optimization:

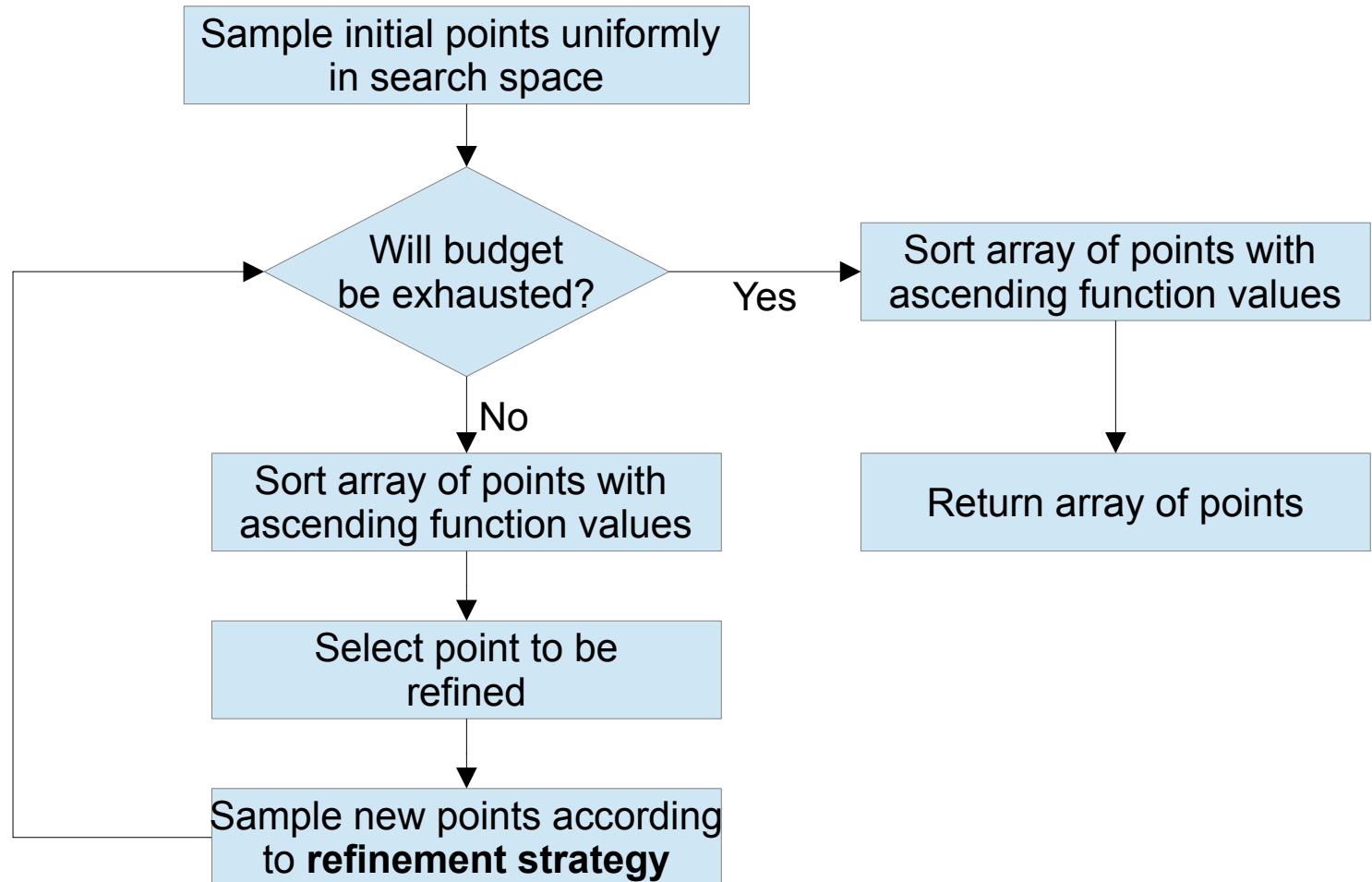
- Epochs
- Batch size
- Learning rate
- Number of convolutional Layers
- Number of fully connected layers
- Kernel size
- Pool size
- Neurons per fully connected
- Dropout probability



Algorithm	Configuration	Accuracy	Cost
GS	(5, 600, 10^{-6} , 2, 2, 2, 2, 4, 0.5)	10.1%	1
RS	(9, 975, 0.0173, 2, 1, 3, 1, 6, 0.619)	97.4%	80
BO	(6, 584, $10^{-2.17}$, 2, 1, 3, 1, 5, 0.281)	97.5%	80
SG	(7, 400, 10^{-2} , 2, 2, 2, 2, 5, 0.5)	97.5%	93

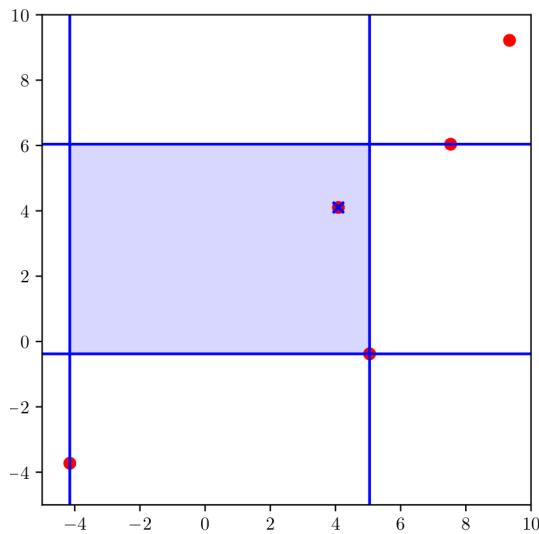
Iterative Adaptive Random Search

Algorithm:

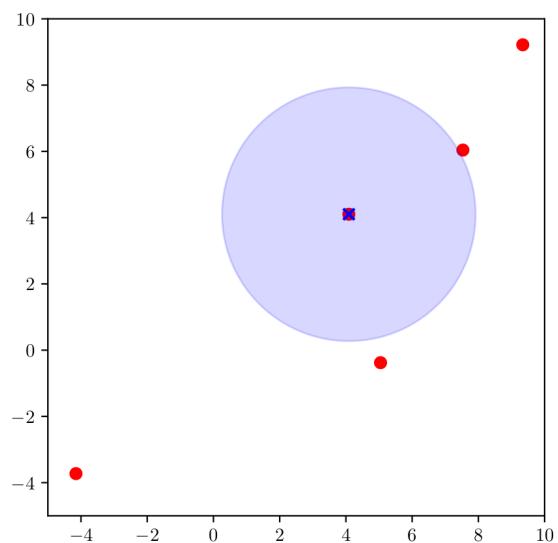


Refinement Strategies

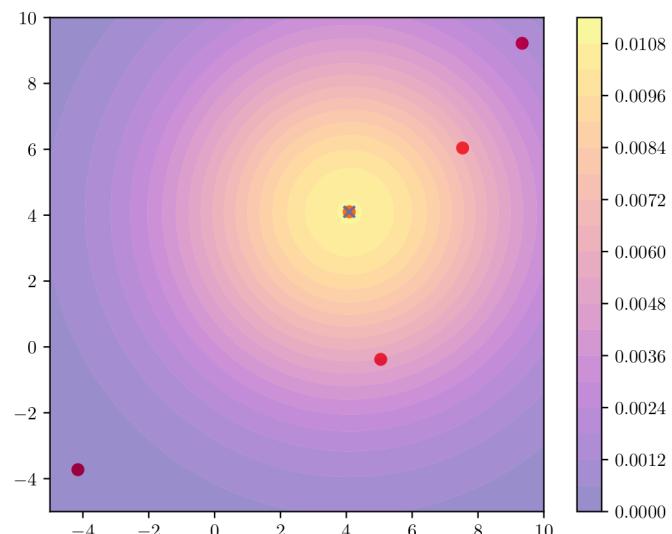
Interval based refinement



Uniform d-ball sampling



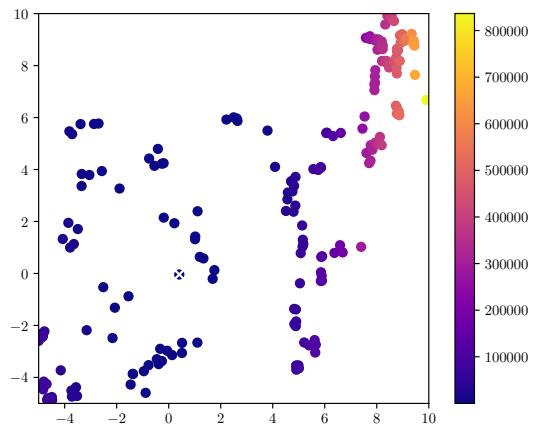
Normal distribution sampling



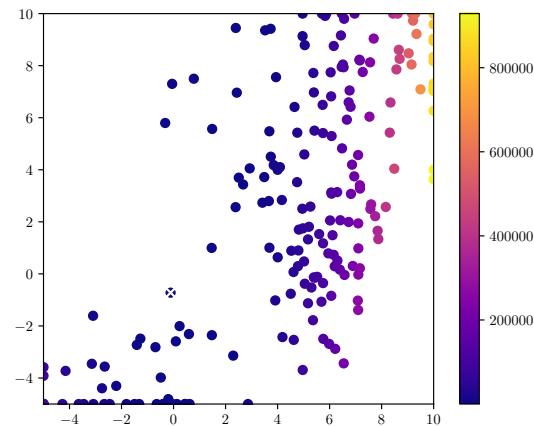
Refinement criterion: $(rank_i + 1)^{1-\gamma} \cdot (level_i + refinements_i + 1)^\gamma$

Adaptivity parameter $\gamma = 1.0$

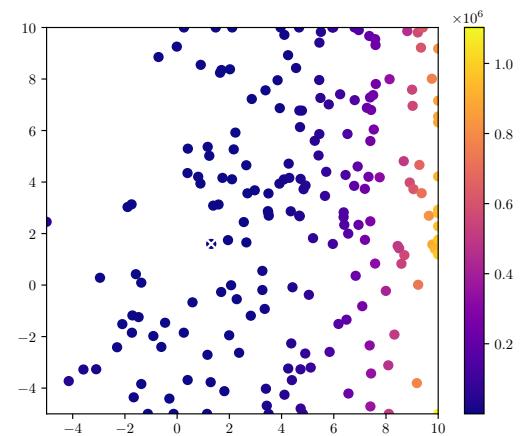
Interval based refinement



Uniform d-ball sampling



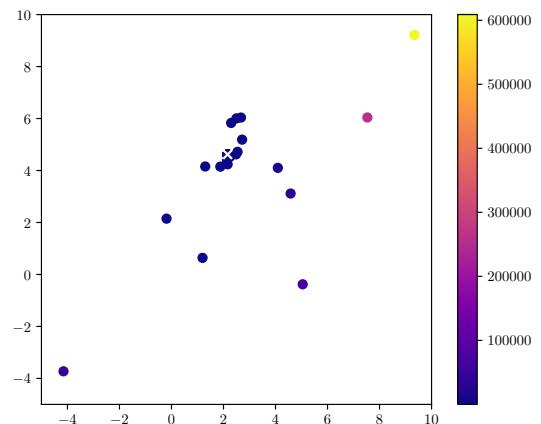
Normal distribution sampling



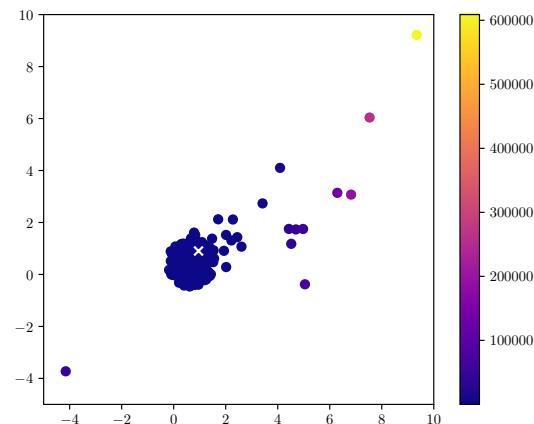
Refinement criterion: $\underbrace{(rank_i + 1)^{1-\gamma} \cdot (level_i + refinements_i + 1)^\gamma}_1$

Adaptivity parameter $\gamma = 0.0$

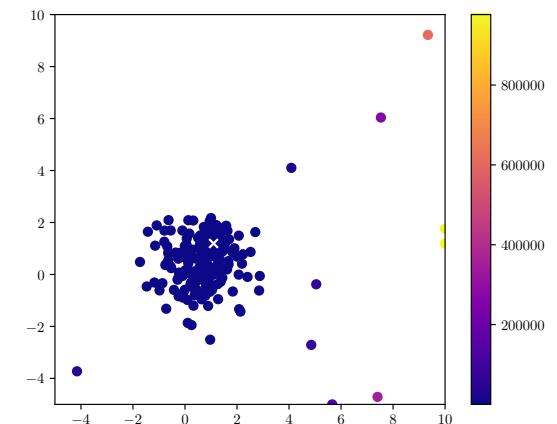
Interval based refinement



Uniform d-ball sampling



Normal distribution sampling

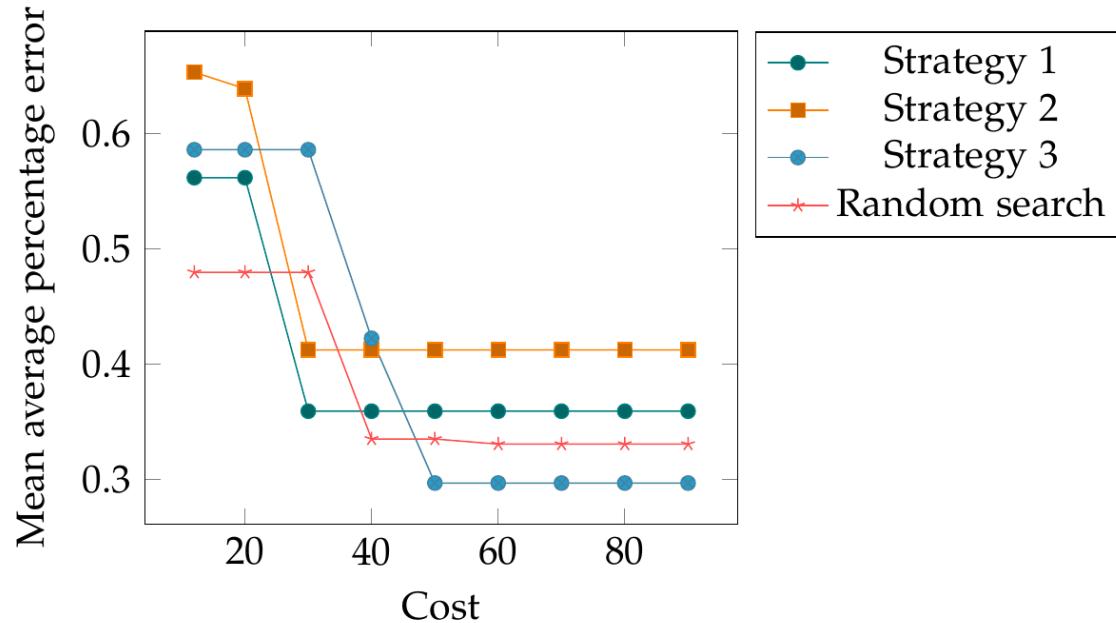


Refinement criterion: $(rank_i + 1)^{1-\gamma} \cdot \underbrace{(level_i + refinements_i + 1)^\gamma}_1$

1

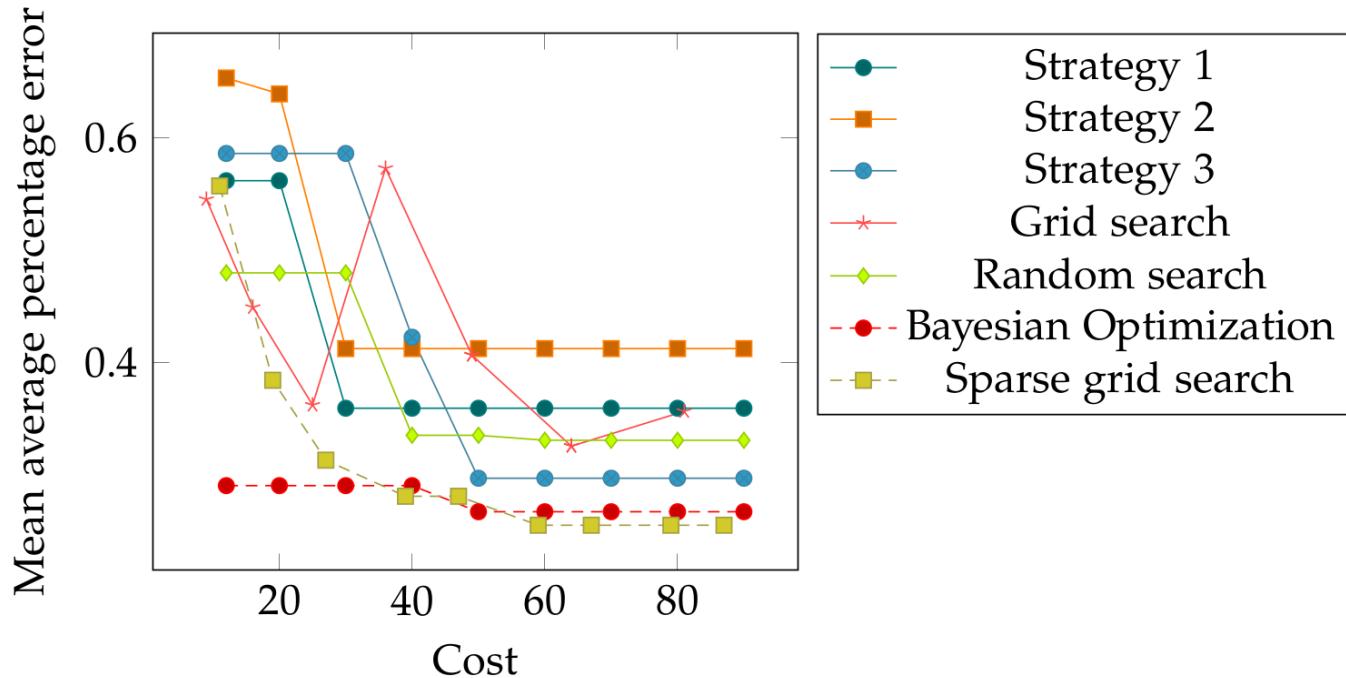
Comparison of Optimization Algorithms

2D Optimization: Epochs & Learning rate



Comparison of Optimization Algorithms

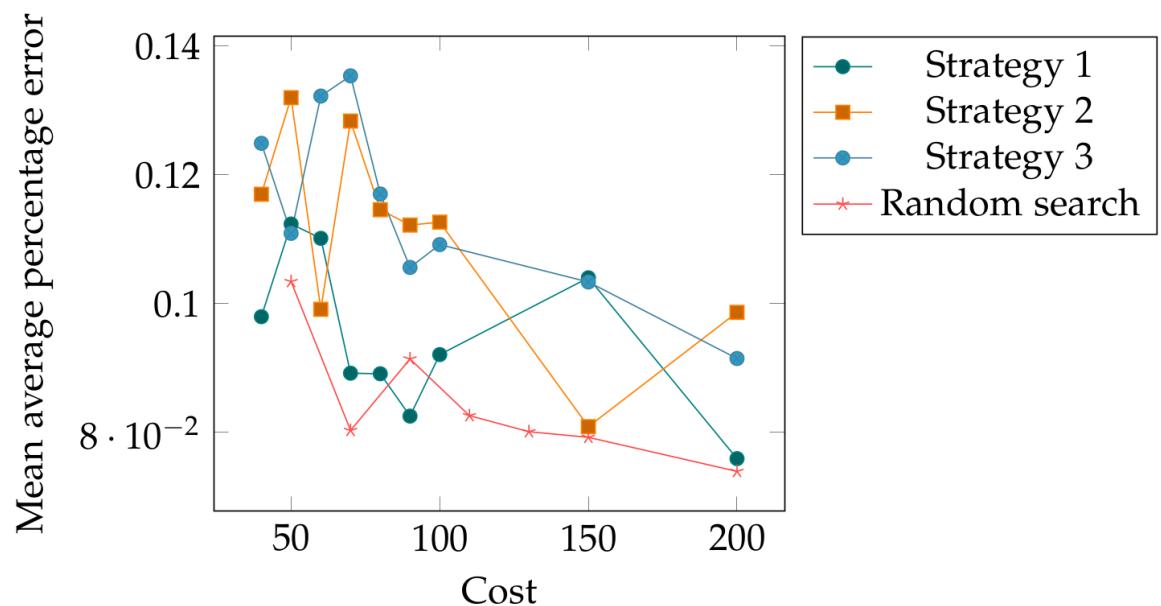
2D Optimization: Epochs & Learning rate



Comparison of Optimization Algorithms

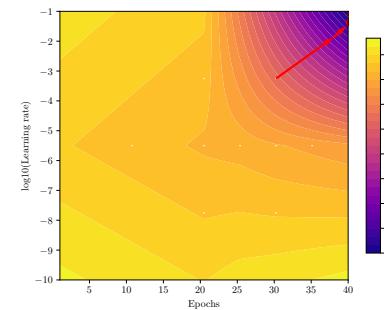
6D Optimization:

- Epochs
- Batch size
- Learning rate
- Number of layers
- Neurons per layer
- Dropout probability

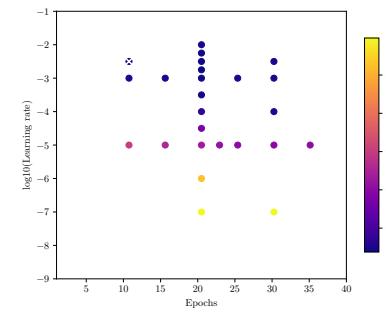


Discussion – Sparse Grid Hyperparameter Optimization

- **Often not enough grid points for optimizer**
→ apply global and local optimizer and compare with the best grid point



- **Problem if optimum at the boundary**
→ optimizer can sometimes help or use sparse grid with boundary points



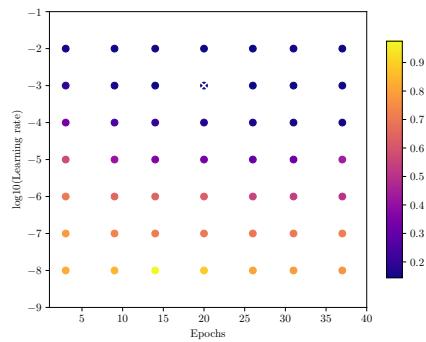
- **BUT: time to solution most important**
- Good results especially in higher dimensions

Discussion – Iterative Adaptive Random Search

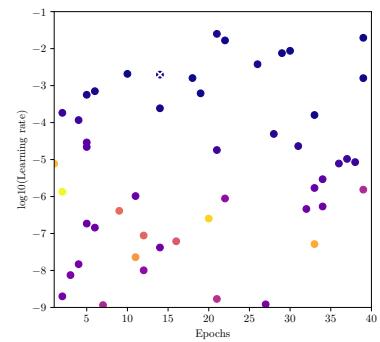
- Promising results in small dimension
- **Problem:** Volume of d-ball compared to d-hypercube decreases rapidly for increasing d
→ worse performance than conventional random search for higher dimensions
- More analysis:
 - Convergence?
 - Adapt algorithm?
 - Other search radius?
 - Change refinement criterion (e.g. include function value)?
 - Other refinement strategy?

Conclusion

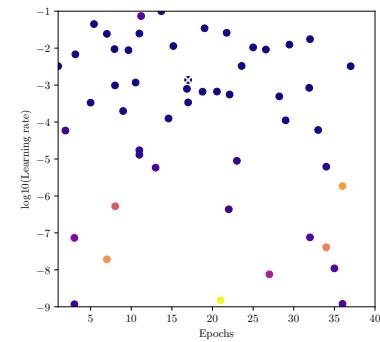
Grid search:



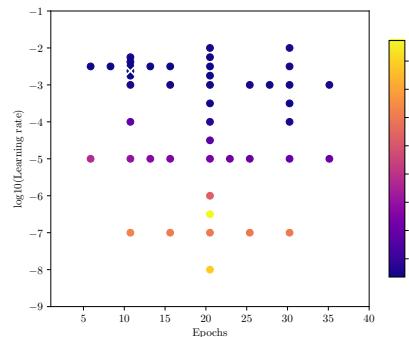
Random search:



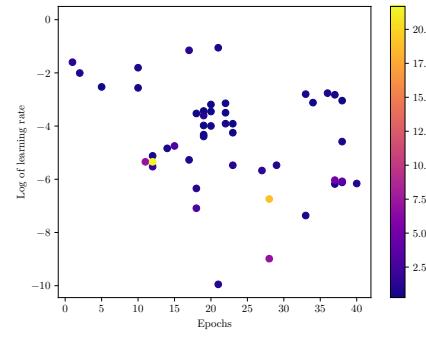
Bayesian optimization:



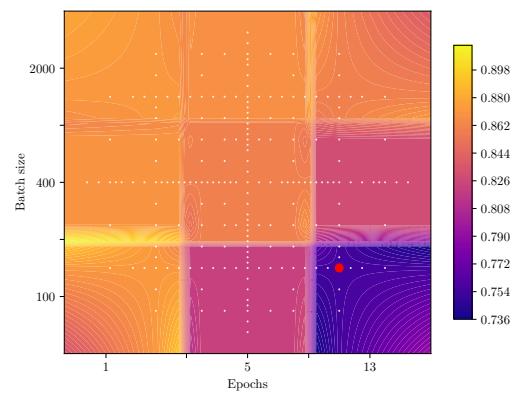
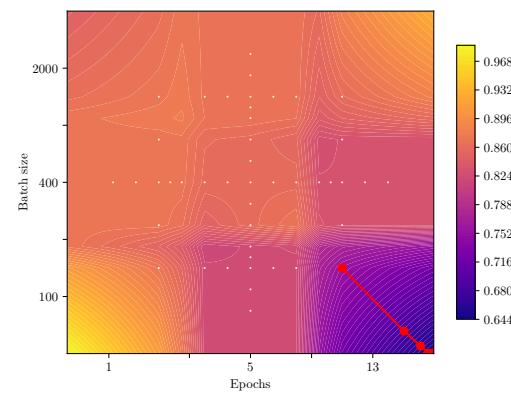
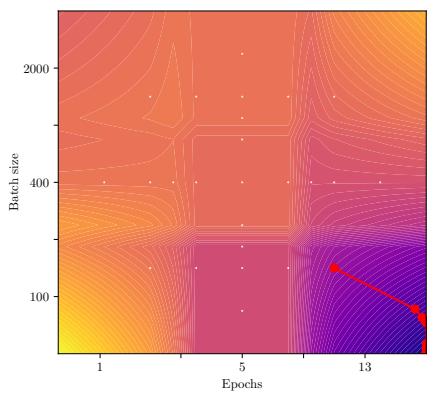
Sparse grid optimization:



Iterative adaptive grid search:



Optimization – Categorical Hyperparameters



Examples: choice of optimizer as hyperparameter, rounding to integers