Neural Network Hyperparameter Optimization with Sparse Grids

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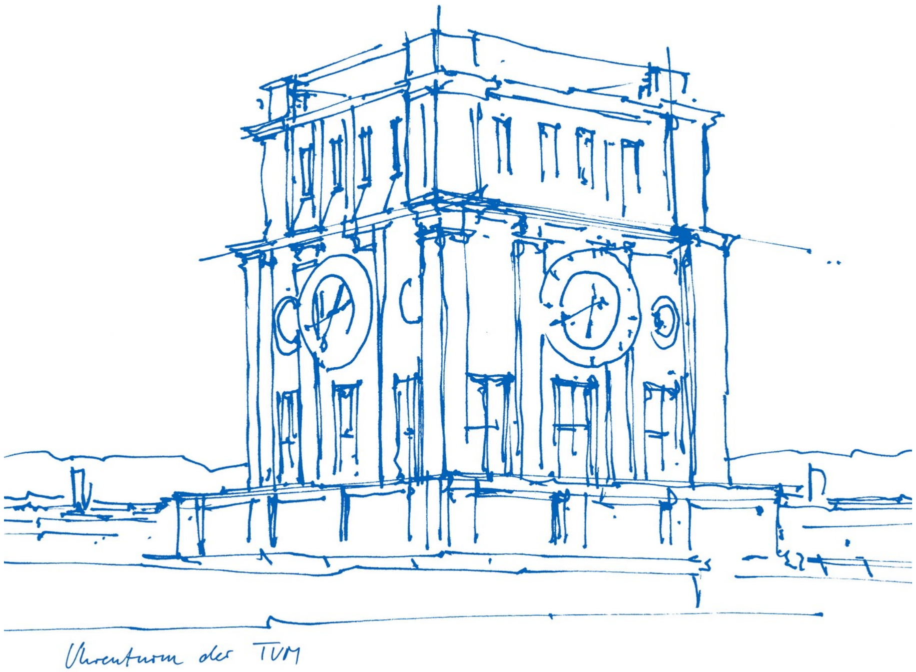
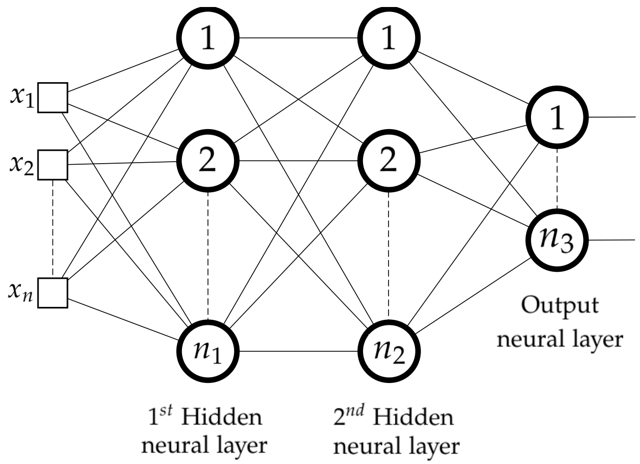


Outline

- Introduction
  - Def. Hyperparameters
  - Overview over techniques from literature
  - Overview over new techniques
- Sparse Grid Search
  - Implementation
  - Analysis
  - Numerical results (and comparison with other techniques)
- Iterative adaptive random search
  - Implementation
  - Analysis
  - Numerical results
- Discussion & Conclusion
- Outlook

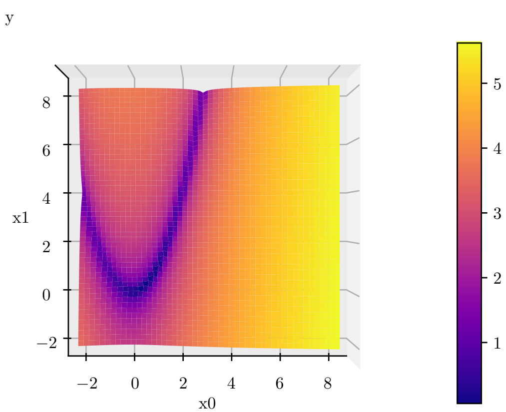
Hyperparameter Optimization

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



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

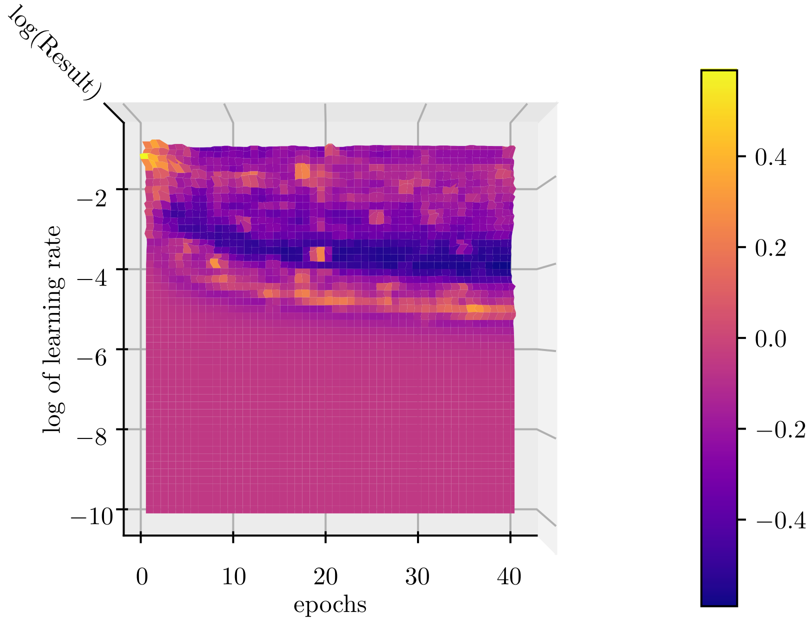
- **Optimization:** finding the optimum of a function



Rosenbrock: Optimum at (1, 1)

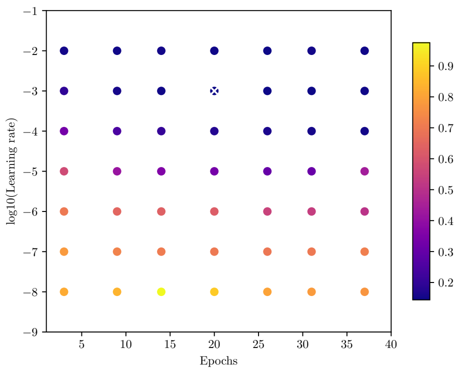
Hyperparameter Optimization

- **Regression of 2-layer neural network:**

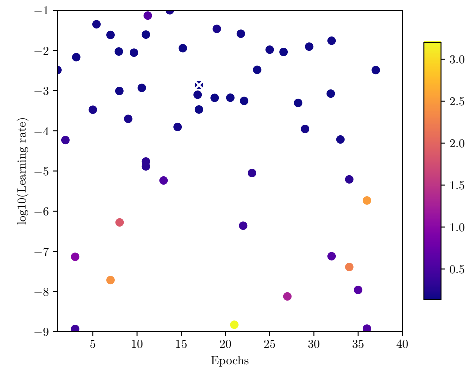


Hyperparameter Optimization

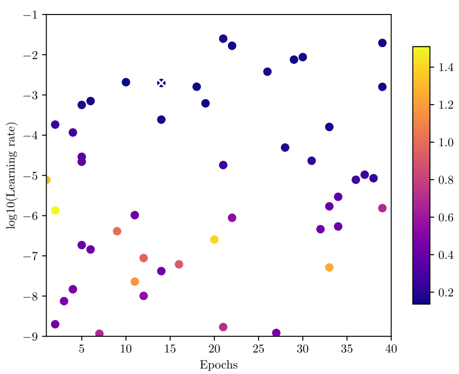
Grid search:



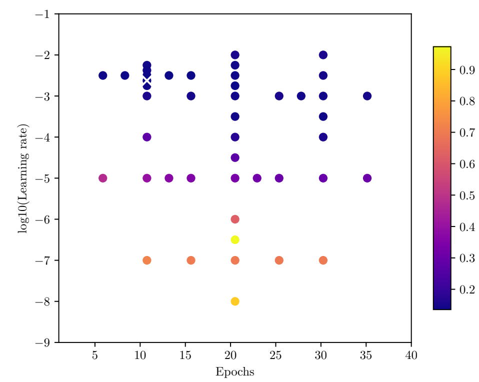
Bayesian optimization:



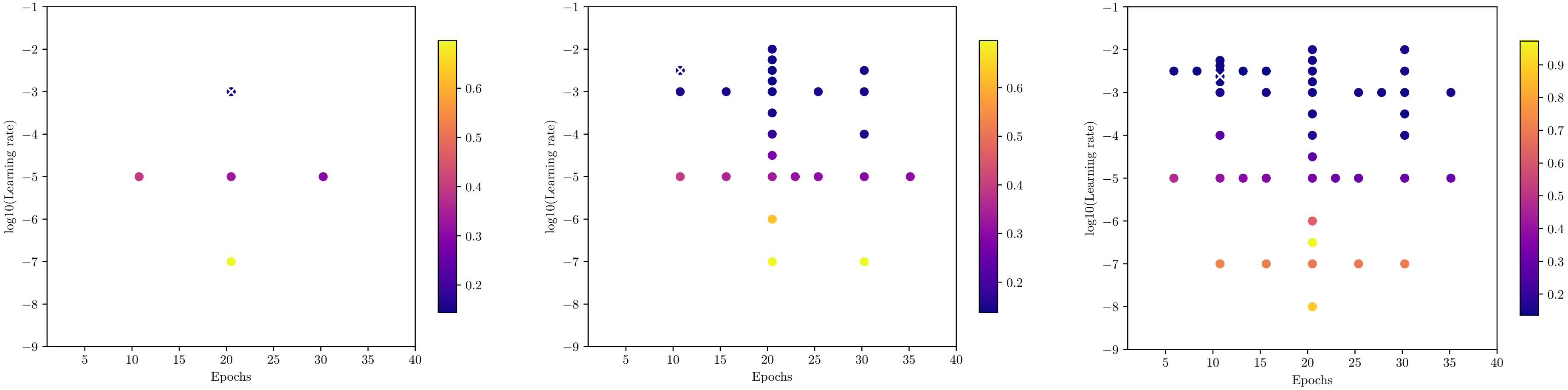
Random search:



Sparse grid search:



Sparse Grid Hyperparameter Optimization



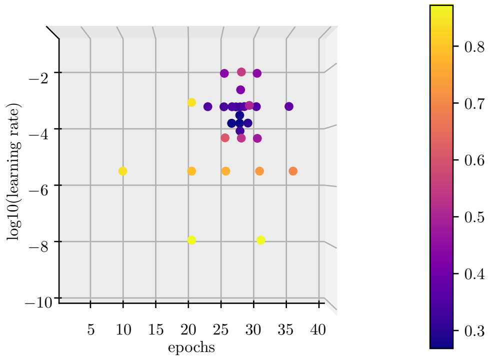
With Novak-Ritter refinement criterion: $\left(r_{l,i}+1\right)^{1-\gamma}\cdot\left(\|l_1\|+d_{l,i}+1\right)^{\gamma}$

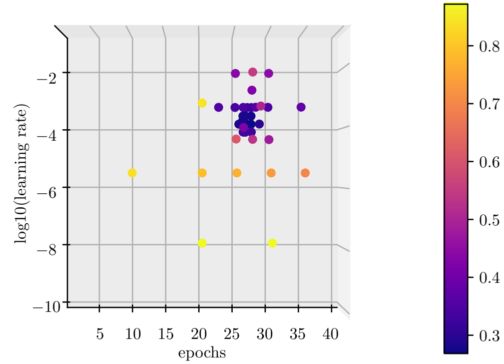
Adaptivity Parameter γ

Budget = 30

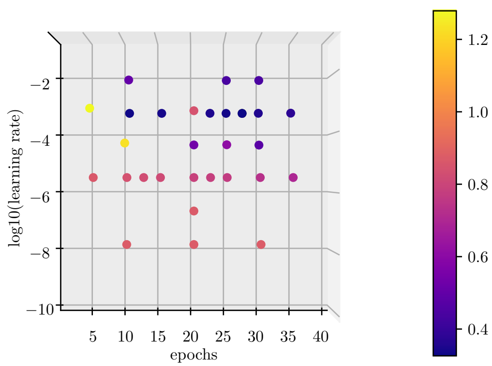
Budget = 50

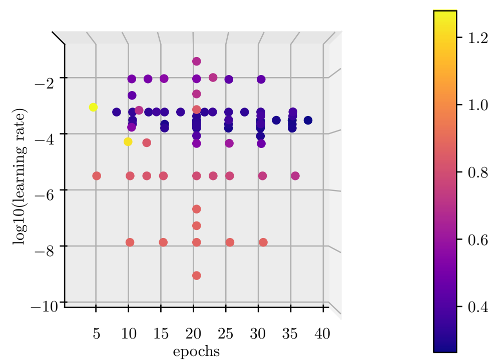
γ = 0.5





γ = 0.85

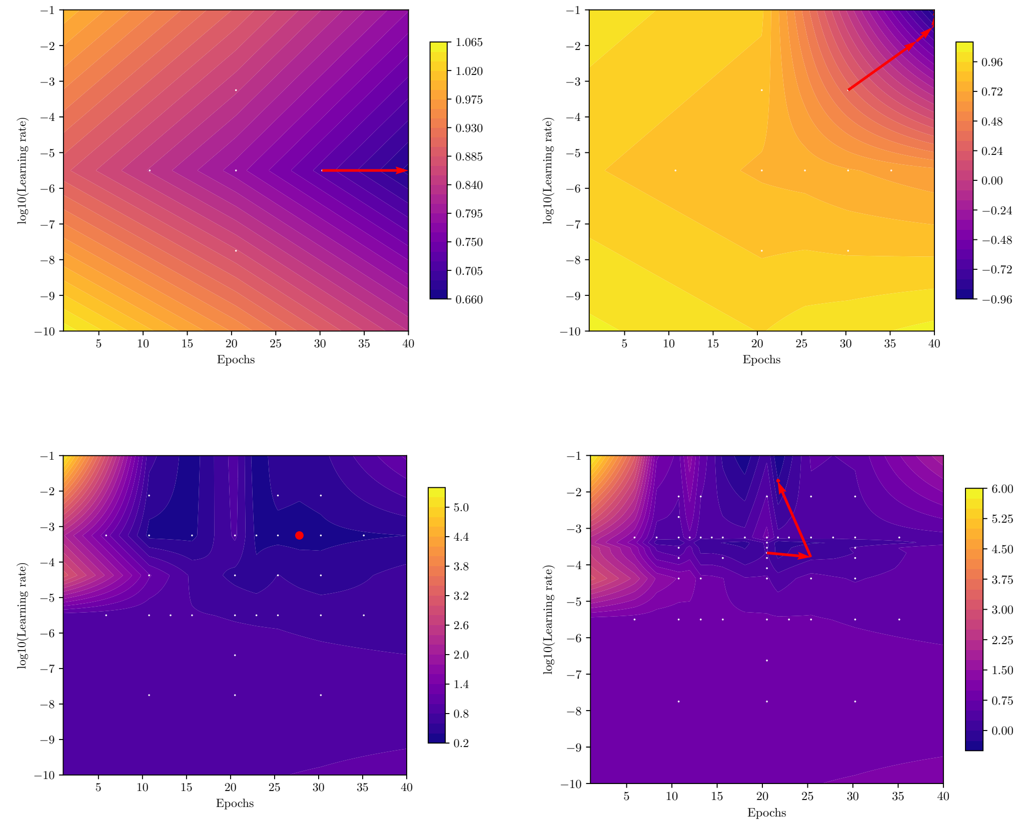




Sparse Grid Hyperparameter Optimization

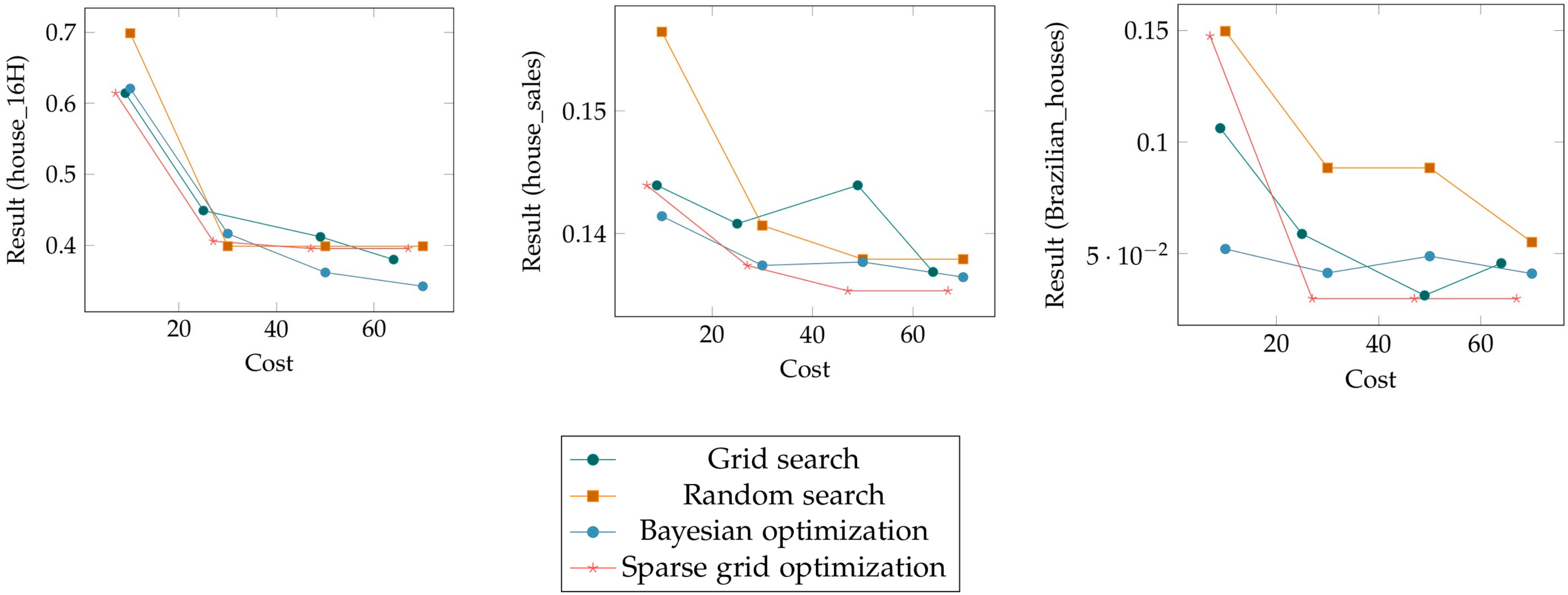
- **Gradient-free optimizers:**
  Nelder Mead, differential evolution, CMA-ES

- **Gradient-based optimizers:**
  <u>Gradient descent</u>**,** NLCG, Newton, Rprop



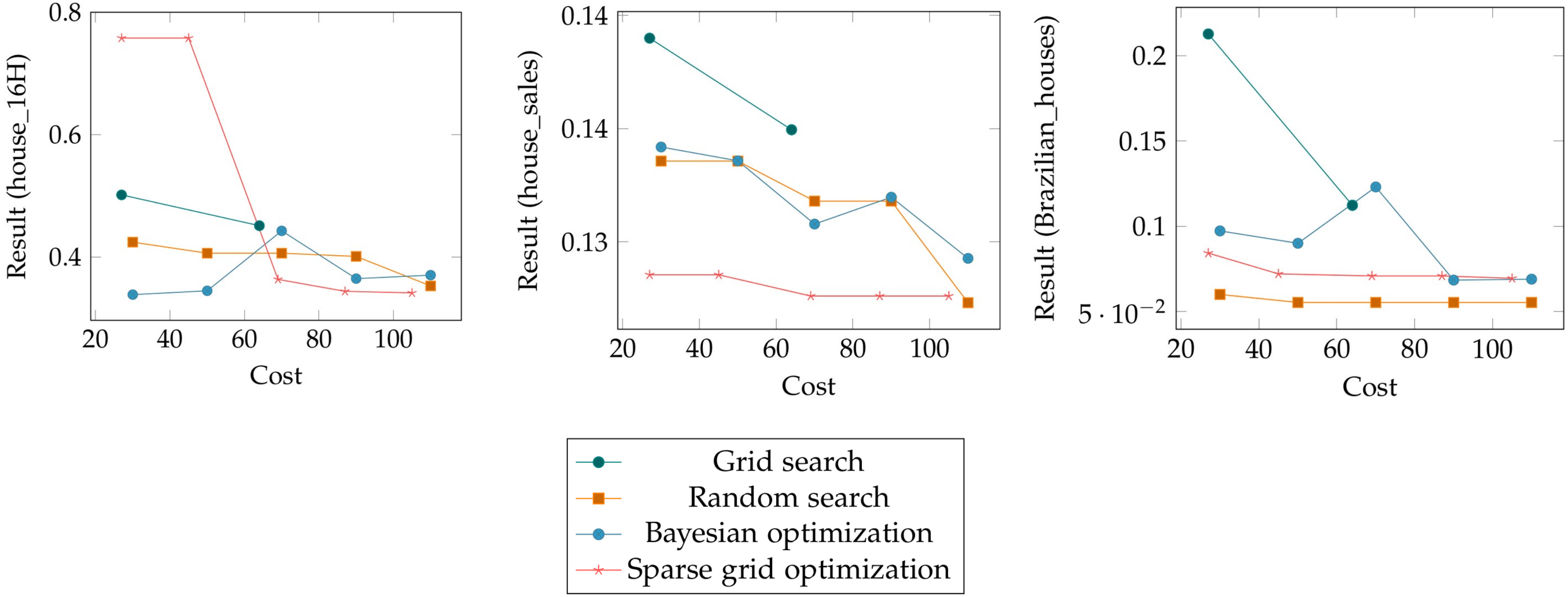
Numerical Results

2D Optimization: Epochs, Learning rate



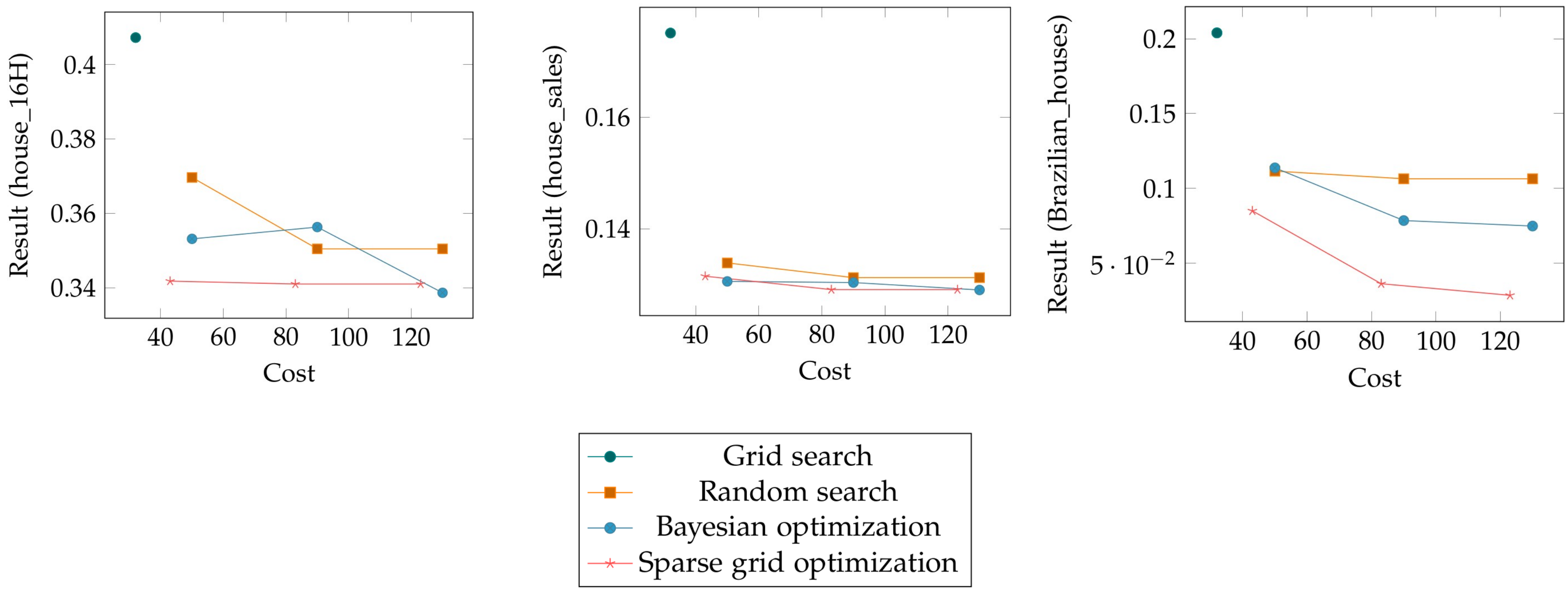
Numerical Results

3D Optimization: Epochs, Learning rate, Batch size



Numerical Results

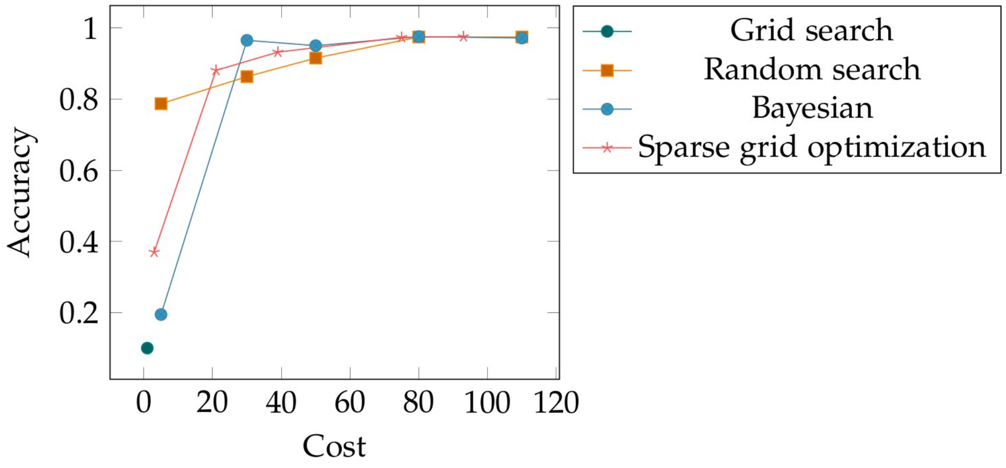
5D Optimization: Epochs, Learning rate, Batch size, Number of layers & neurons per layer



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

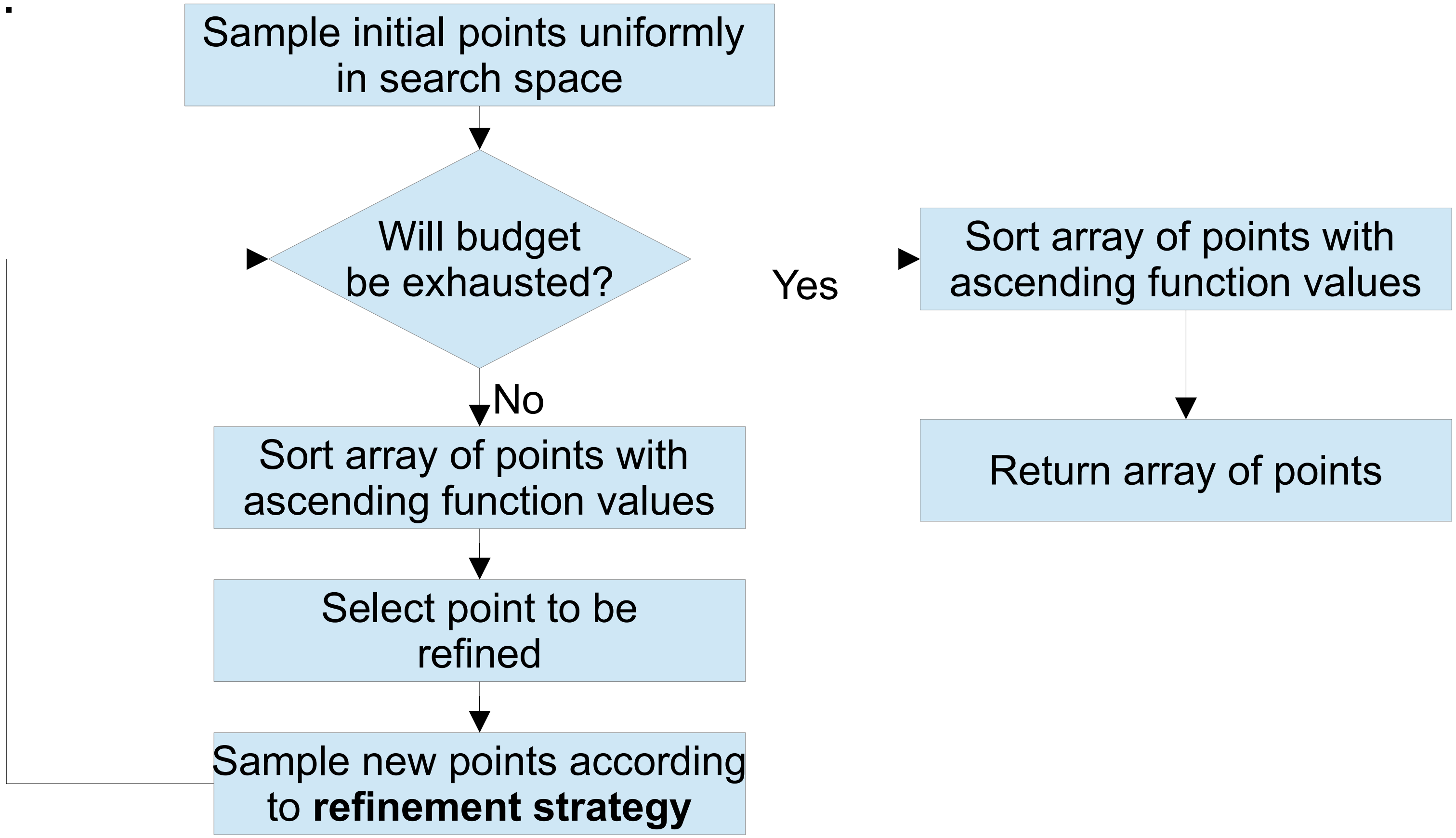


Algorithm	Configuration	Accuracy	Cost
GS	$(5, 600, 10^{-6}, 2, 2, 2, 2, 4, 0.5)$	10.1%	1
RS	$(9, 975, 0.0173, 2, 1, 3, 1, 6, 0.619)$	97.4%	80
BO	$(6, 584, 10^{-2.17}, 2, 1, 3, 1, 5, 0.281)$	97.5%	80
SG	$(7, 400, 10^{-2}, 2, 2, 2, 2, 5, 0.5)$	97.5%	93

Improvement of Random Search

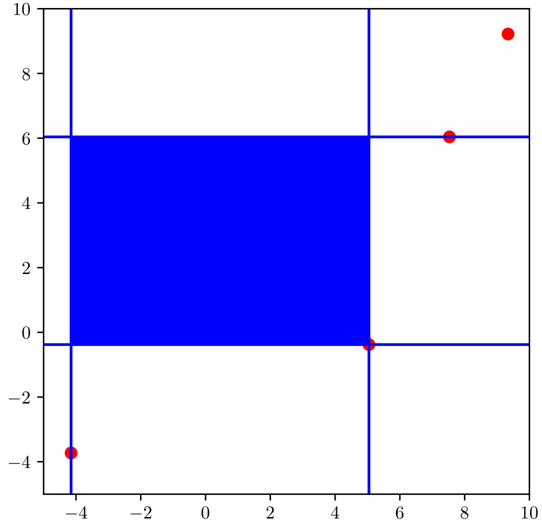
Idea: Combine advantages of random search and iterative optimization algorithm

Algorithm:

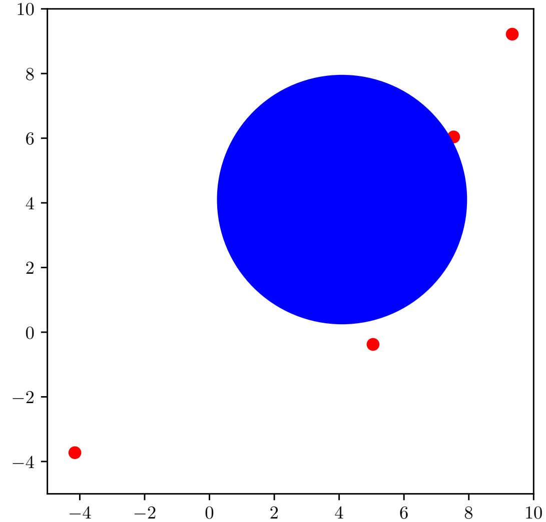


Refinement Strategies

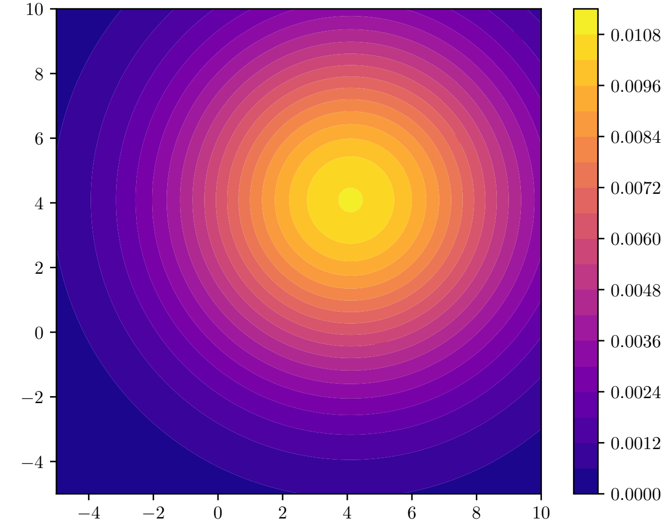
Interval based refinement



Uniform d-ball sampling



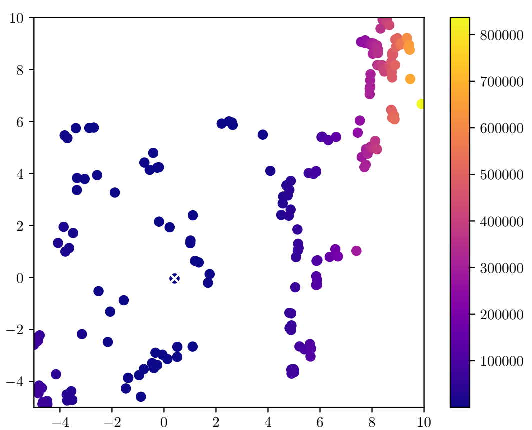
Normal distribution sampling



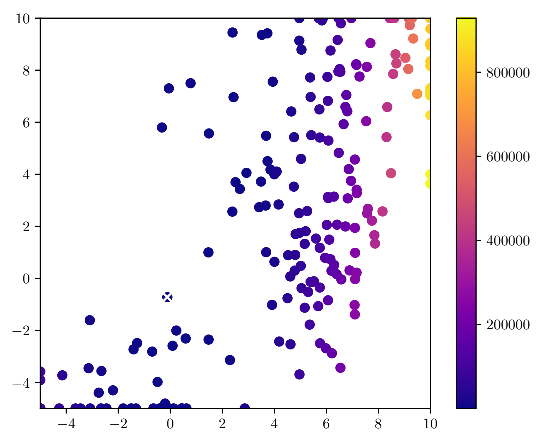
Refinement criterion: $(rank_i+1)^{1-\gamma}\cdot(level_i+refinements_i+1)^{\gamma}$

Adaptivity parameter γ = 1.0

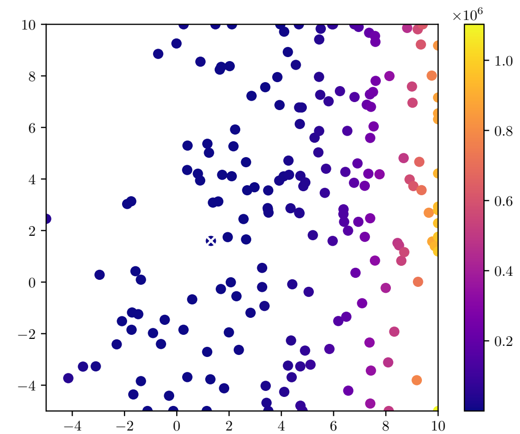
Interval based refinement



Uniform d-ball sampling

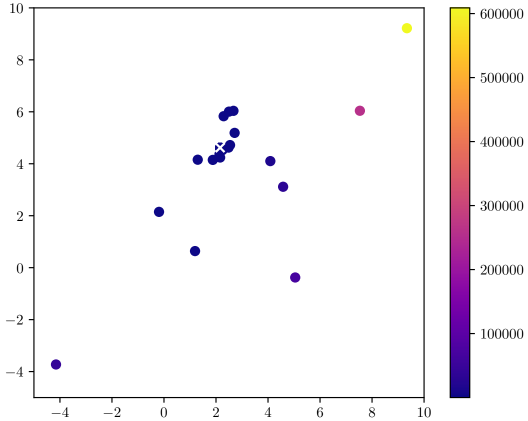
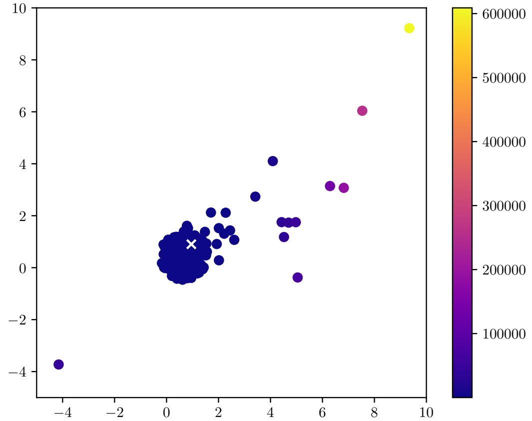
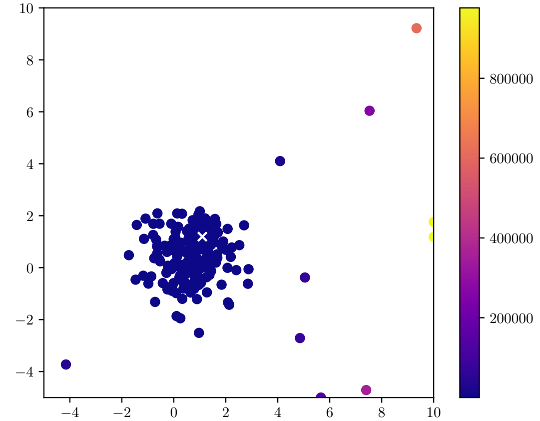


Normal distribution sampling



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

Adaptivity parameter γ = 0.0

Interval based refinement	Uniform d-ball sampling	Normal distribution sampling
		

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