Neural Network Hyperparameter Optimization with Sparse Grids

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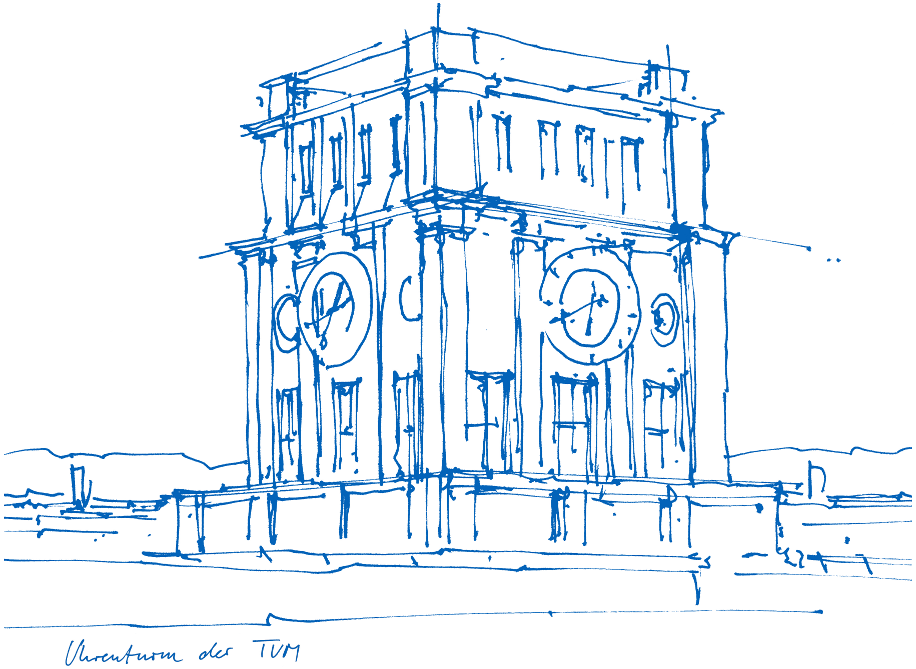
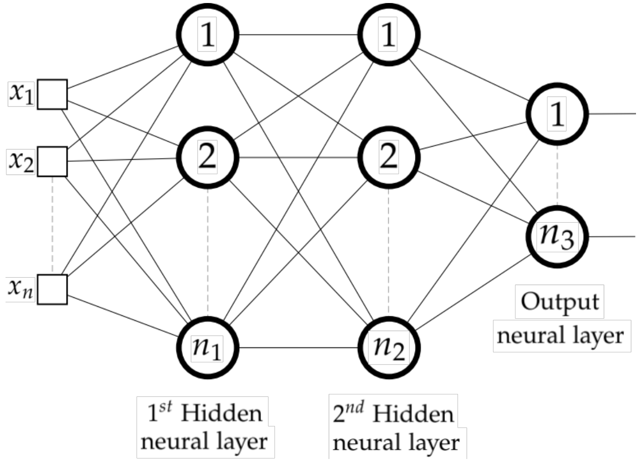


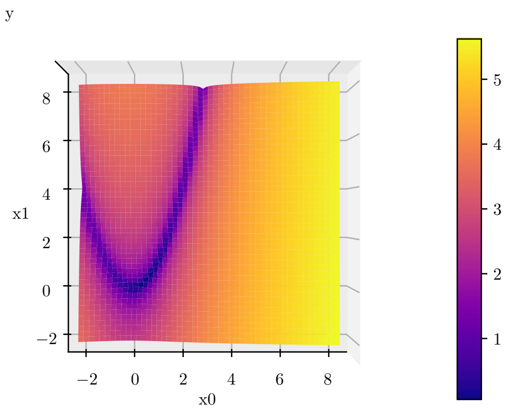
Hyperparameter Optimization

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



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

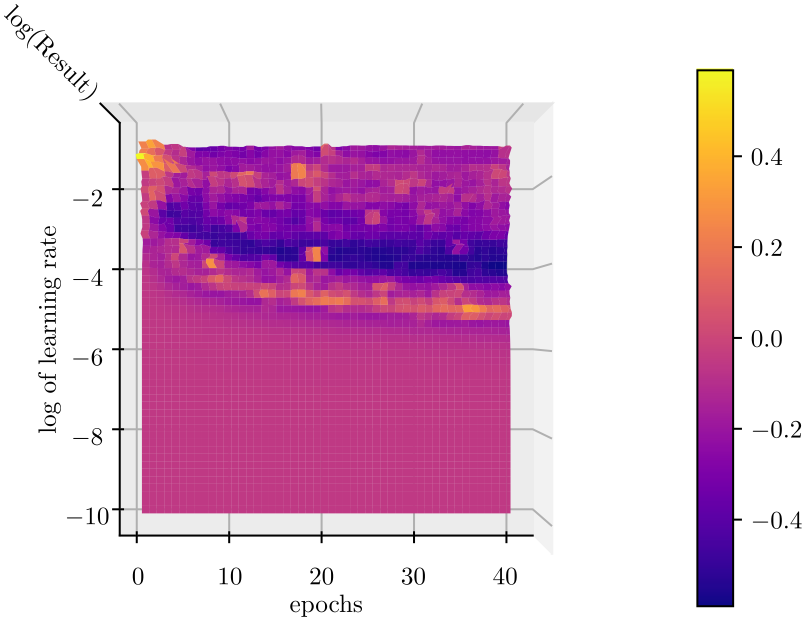
- **Optimization:** finding the optimum of a function



Rosenbrock: Optimum at (1, 1)

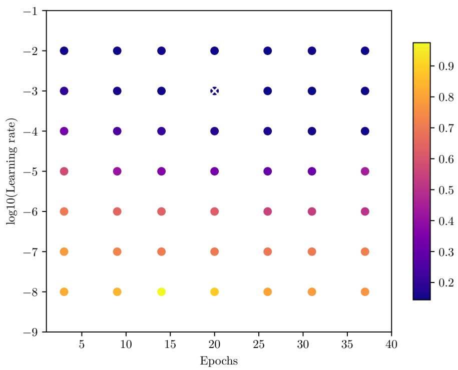
Hyperparameter Optimization

Regression of 2-layer neural network:

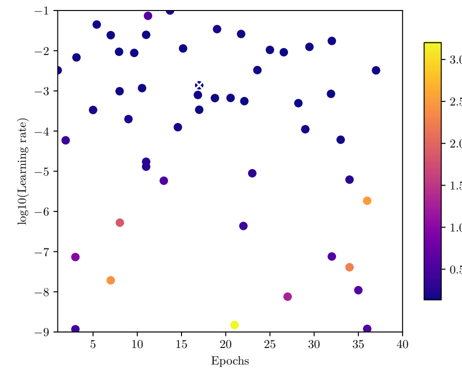


Hyperparameter Optimization

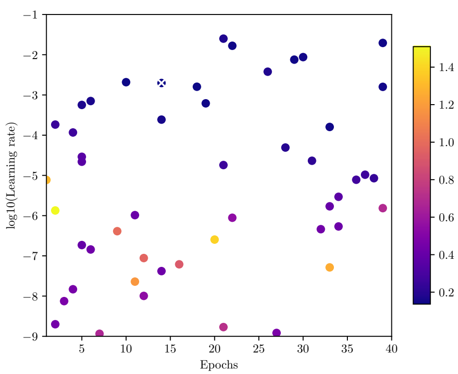
Grid search:



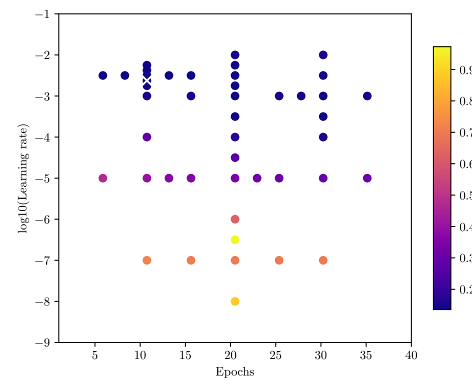
Bayesian optimization:



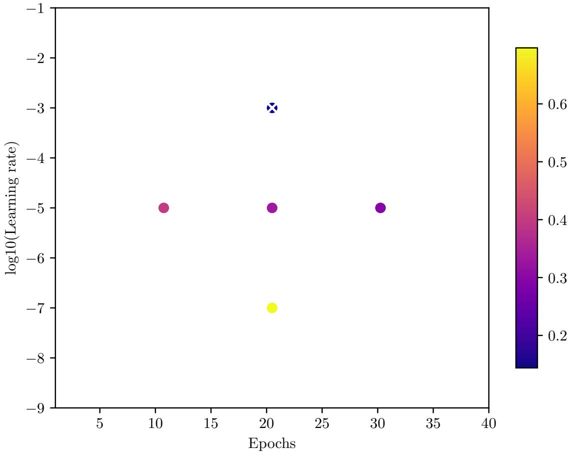
Random search:

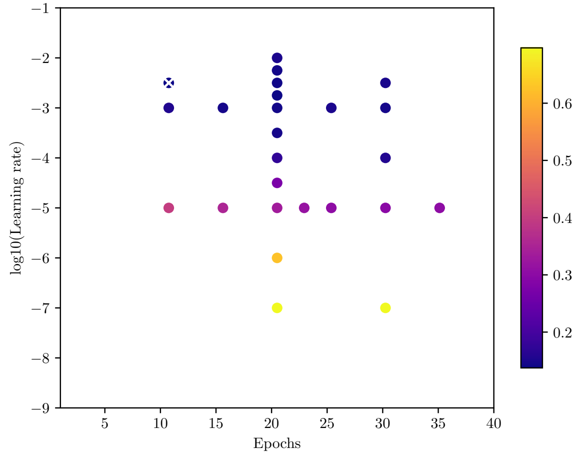


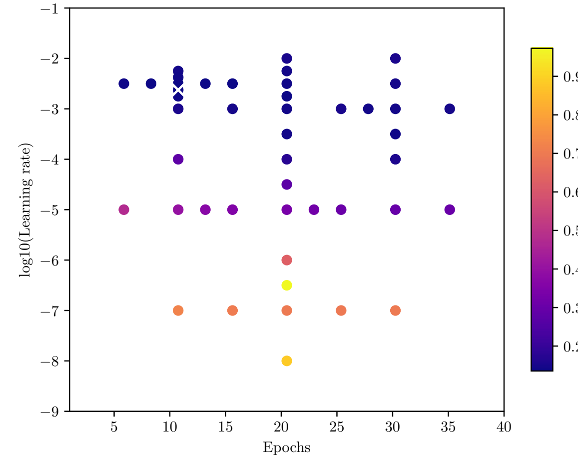
Sparse grid search:



Sparse Grid Hyperparameter Optimization







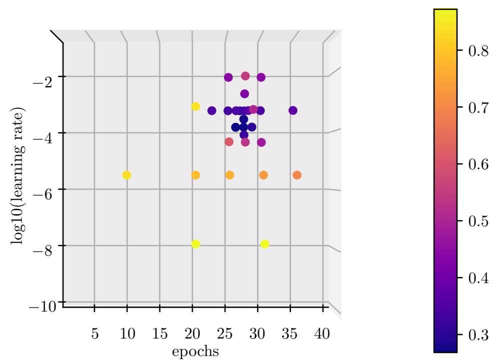
With Novak-Ritter refinement criterion: $\left(r_{l,i}+1\right)^{1-\gamma}\cdot\left(\|l_1\|+d_{l,i}+1\right)^{\gamma}$

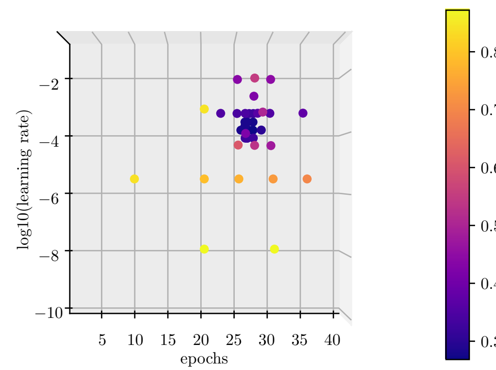
Adaptivity Parameter γ

Budget = 30

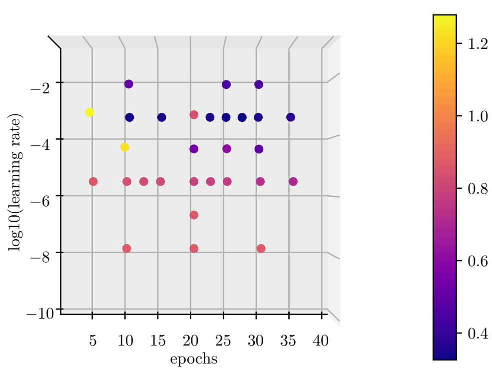
Budget = 50

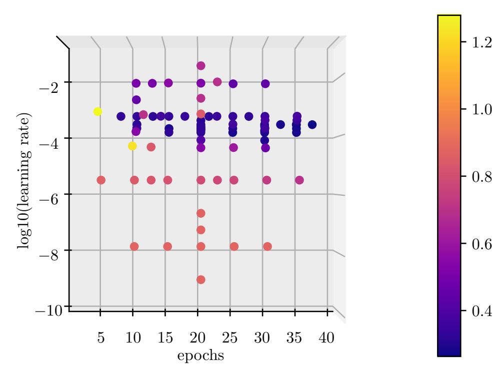
γ = 0.5





γ = 0.85

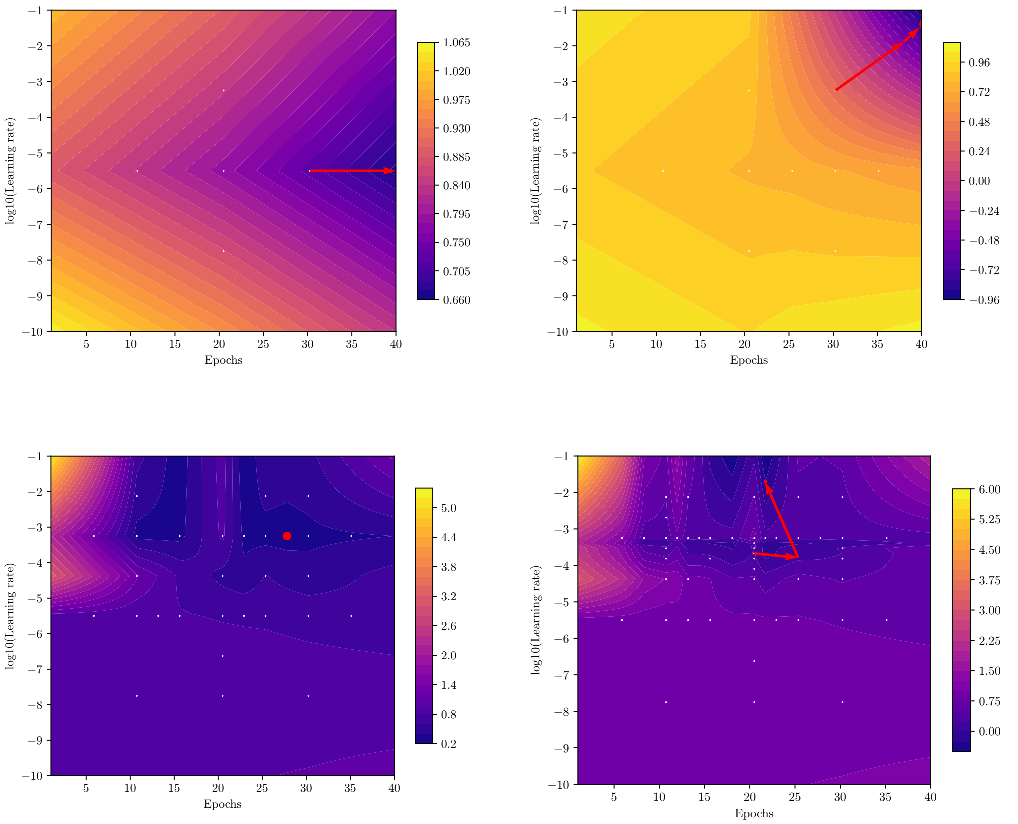




Sparse Grid Hyperparameter Optimization

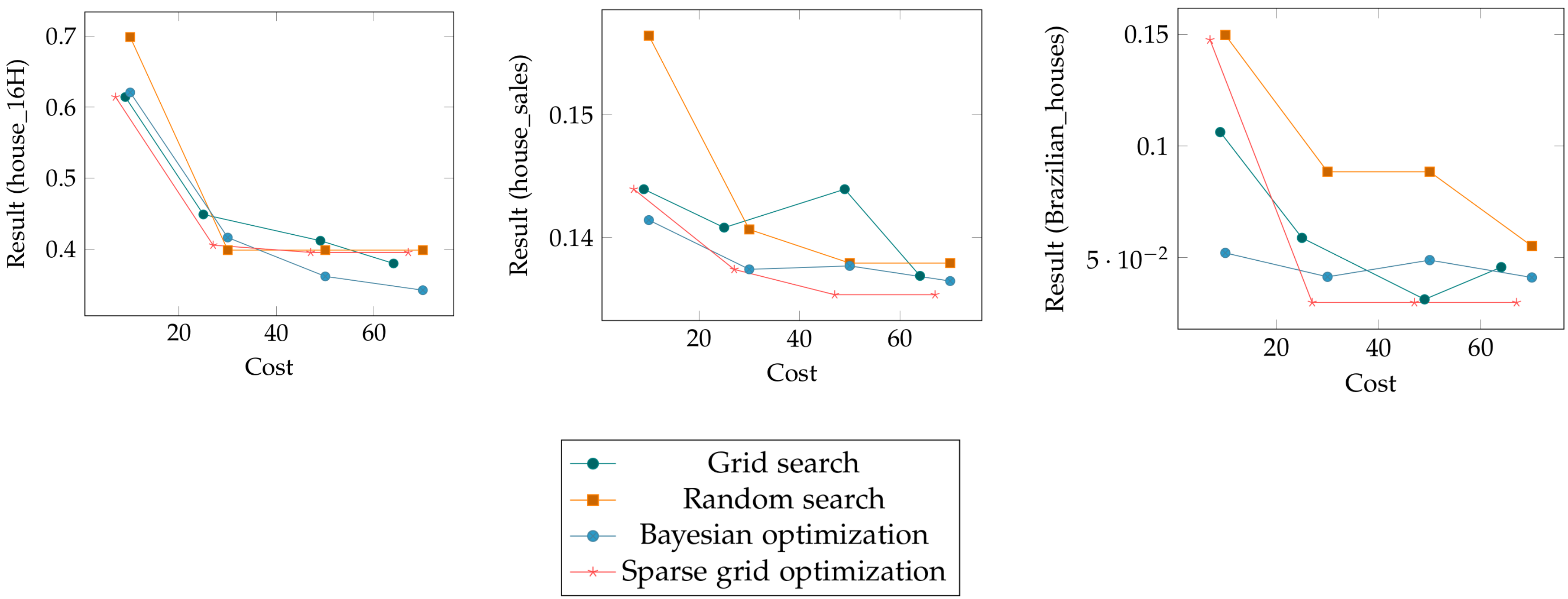
- **Gradient-free optimizers:** Nelder Mead, differential evolution, CMA-ES

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



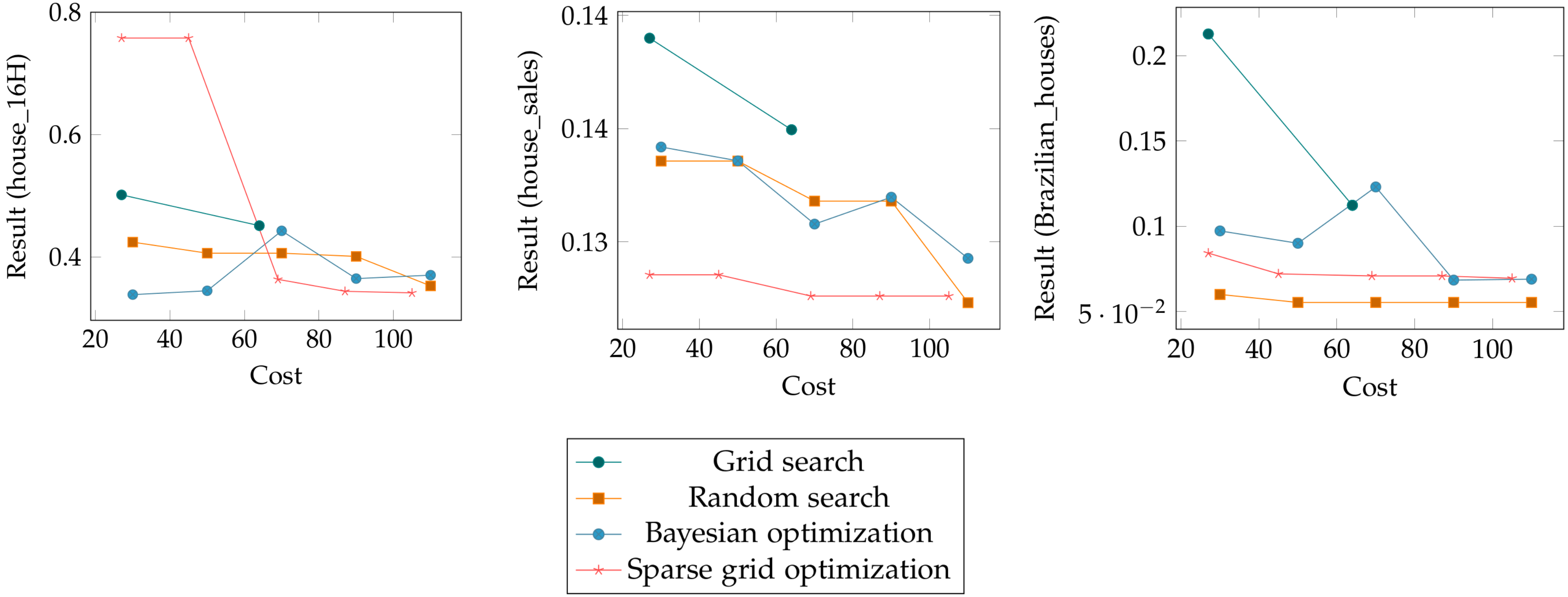
Numerical Results

2D Optimization: Epochs, Learning rate



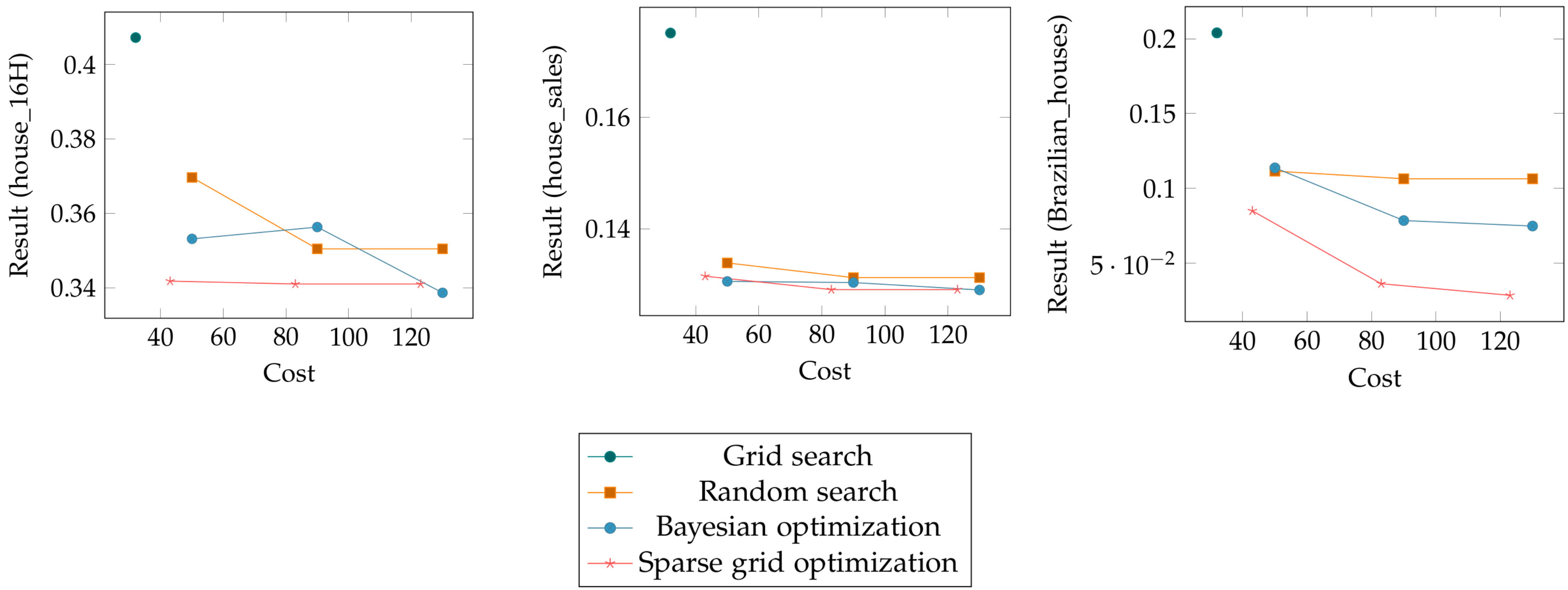
Numerical Results

3D Optimization: Epochs, Learning rate, Batch size



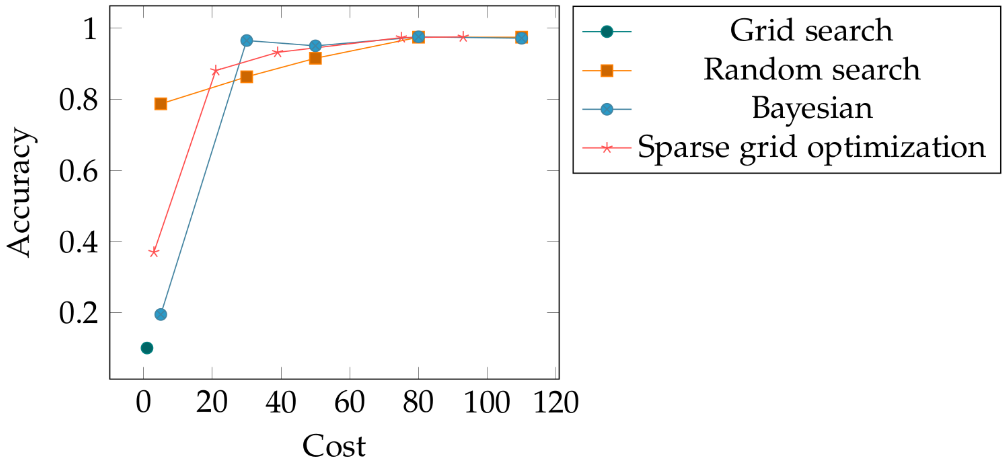
Numerical Results

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



Application: MNIST

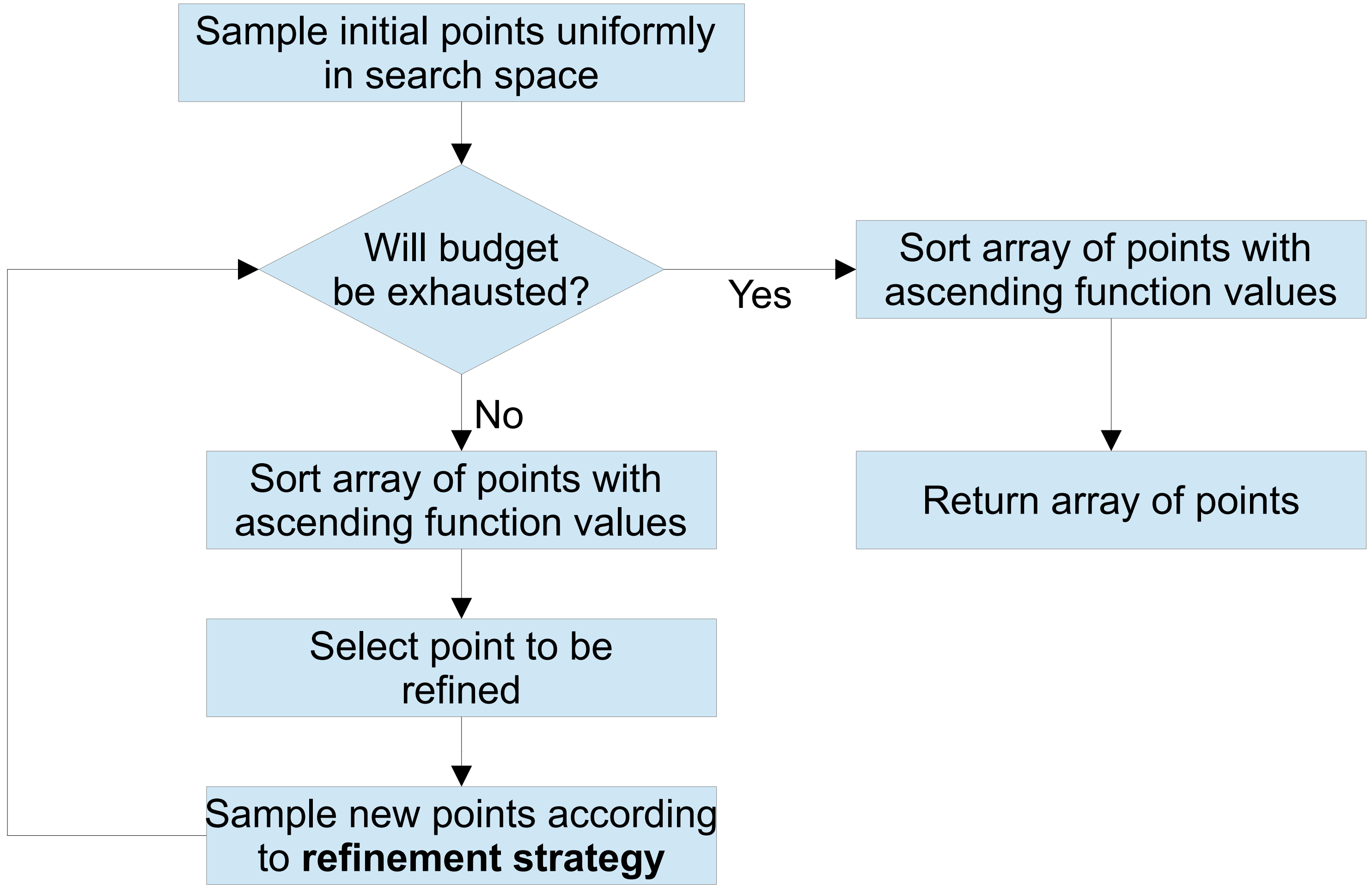
9D Optimization:
- Epochs
- Batch size
- Learning rate
- Number of convolutional Layers
- Number of fully connected layers
- Kernel size
- Pool size
- Neurons per fully connected
- Dropout probability



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

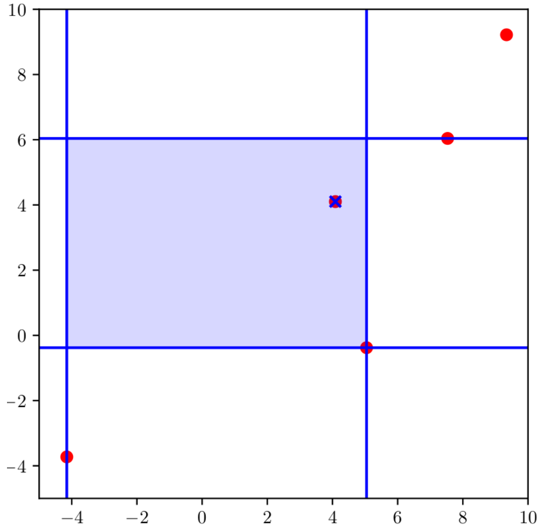
Iterative Adaptive Random Search

Algorithm:

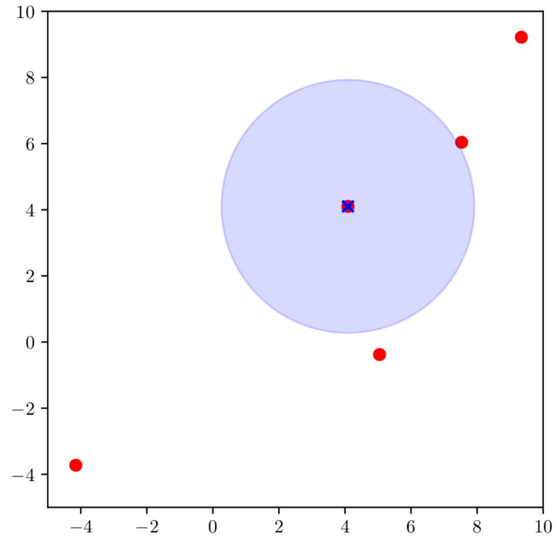


Refinement Strategies

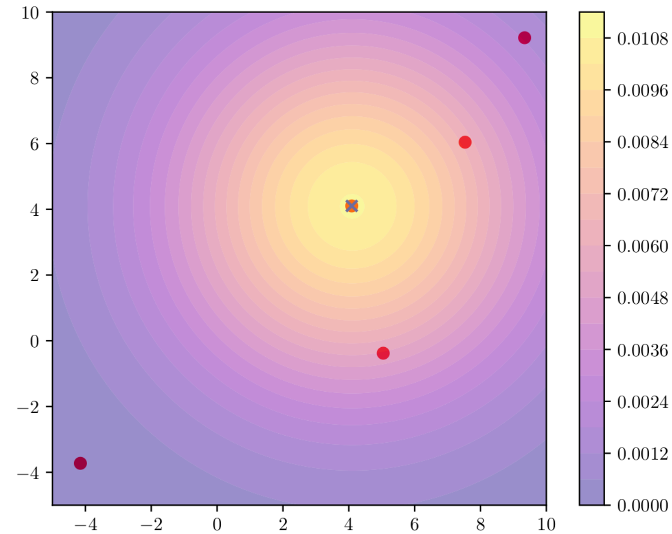
Interval based refinement



Uniform d-ball sampling



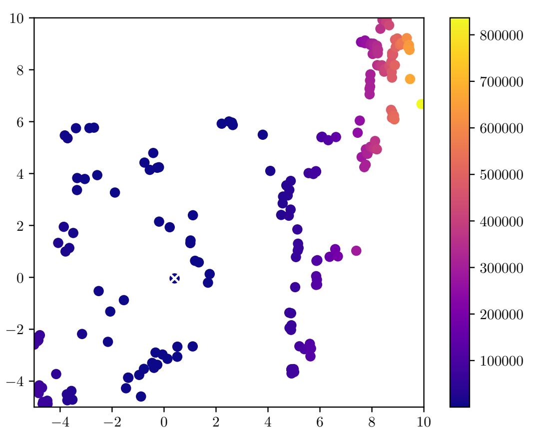
Normal distribution sampling



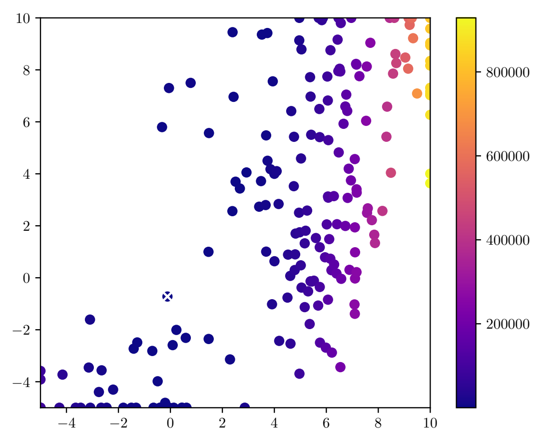
Refinement criterion: $(rank_i+1)^{1-\gamma}\cdot(level_i+refinements_i+1)^{\gamma}$

Adaptivity parameter γ = 1.0

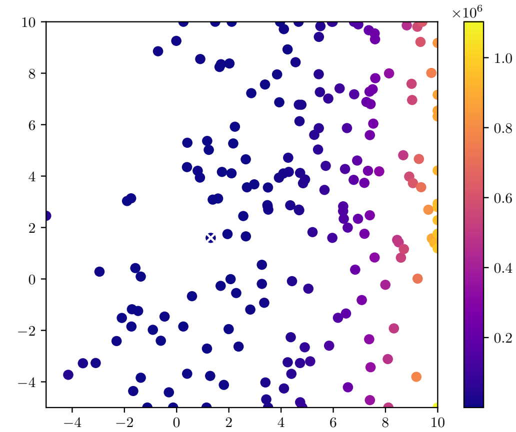
Interval based refinement



Uniform d-ball sampling



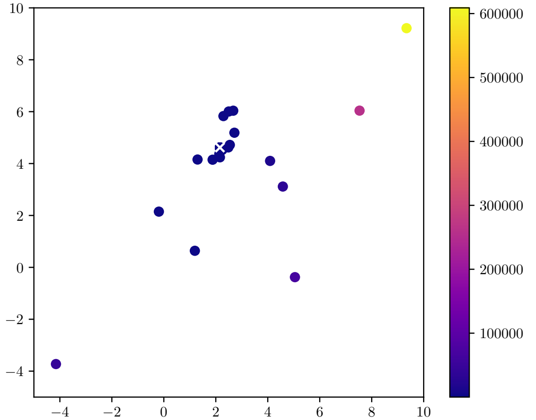
Normal distribution sampling



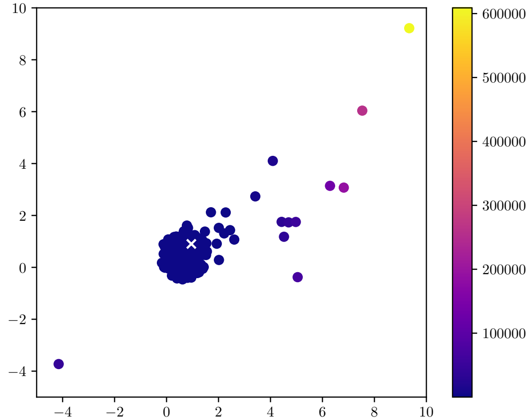
Refinement criterion: $$\underbrace{(rank_i+1)^{1-\gamma}}_{1} \cdot (level_i + refinements_i + 1)^{\gamma}$$

Adaptivity parameter γ = 0.0

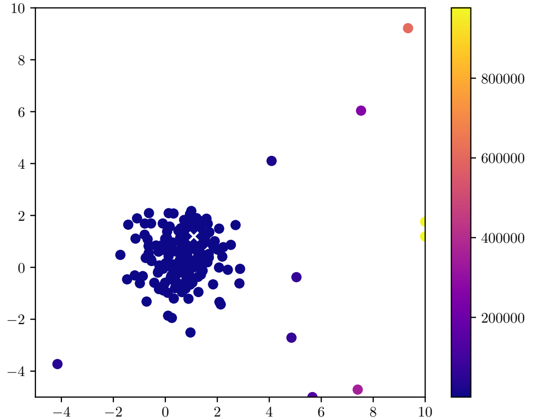
Interval based refinement



Uniform d-ball sampling



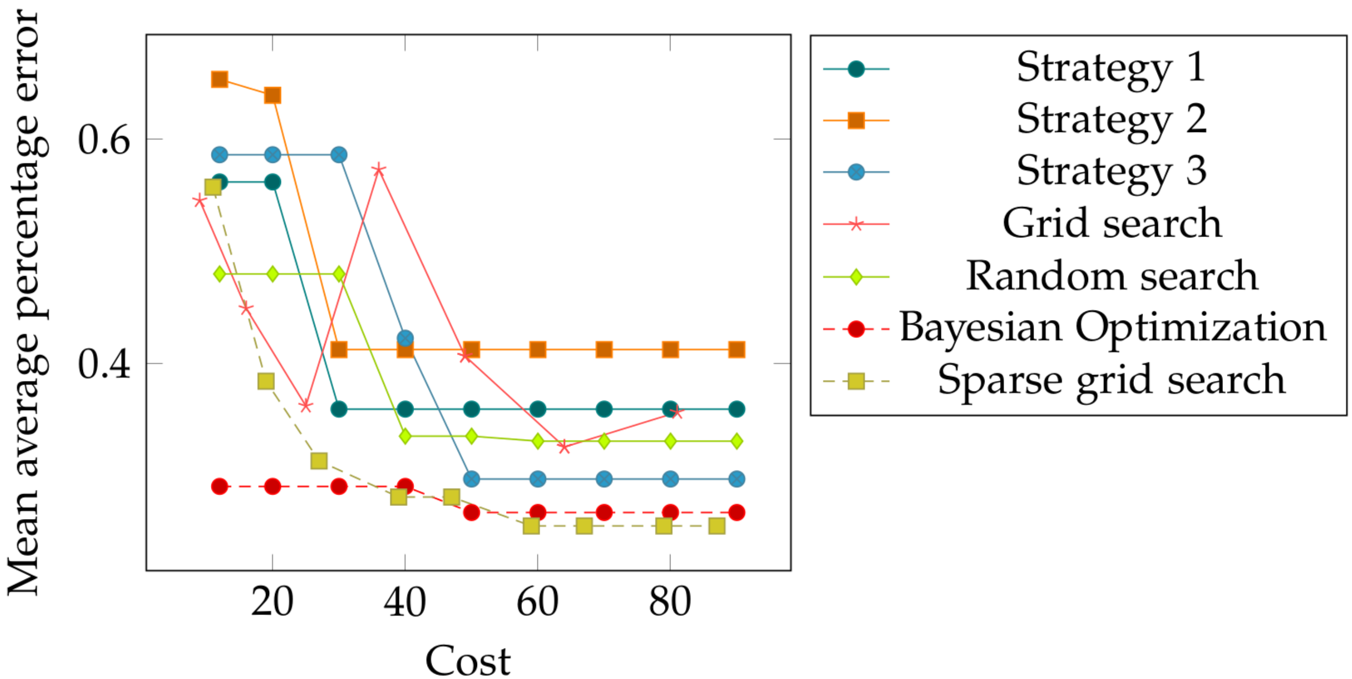
Normal distribution sampling



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

Comparison of Optimization Algorithms

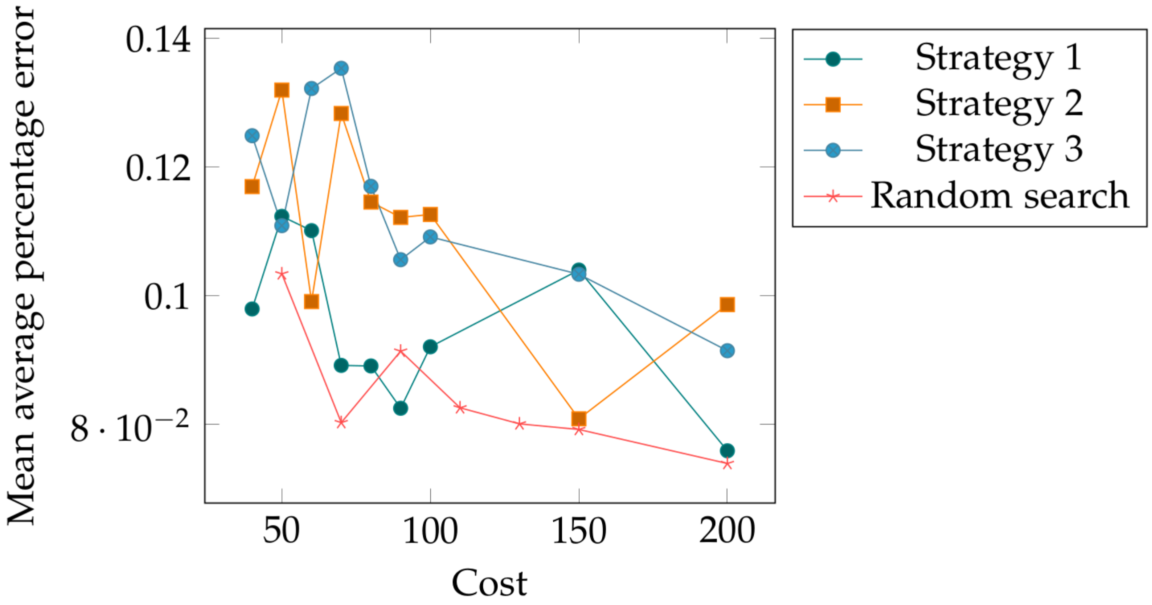
2D Optimization: Epochs & Learning rate



Comparison of Optimization Algorithms

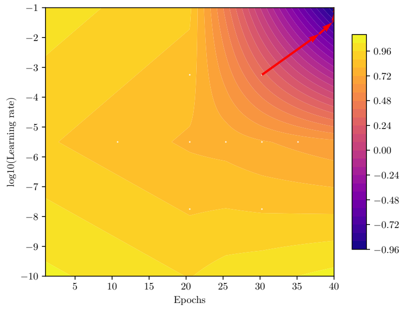
6D Optimization:

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

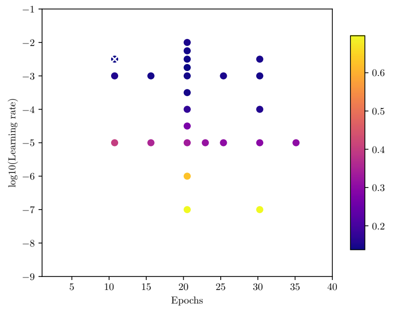


Discussion – Sparse Grid Hyperparameter Optimization

- **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

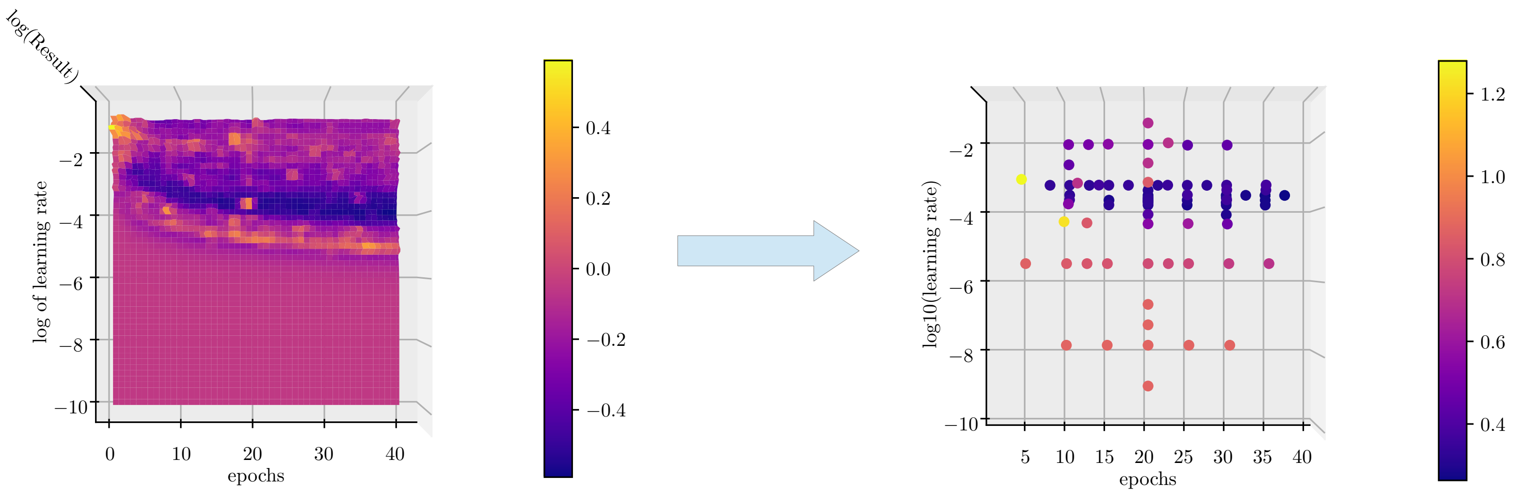


- **BUT: time to solution most important**

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. add function value)?
  - Other refinement strategy?

Conclusion


log(Result)
log of learning rate
−2
−4
−6
−8
−10
0
10
20
30
40
epochs
0.4
0.2
0.0
−0.2
−0.4
log10(learning rate)
−2
−4
−6
−8
−10
5
10
15
20
25
30
35
40
epochs
1.2
1.0
0.8
0.6
0.4