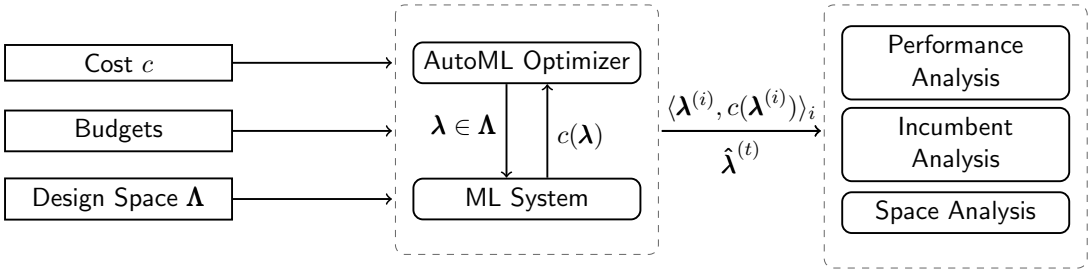
# AutoML: Interpretability

## Studying the AutoML Optimization Process

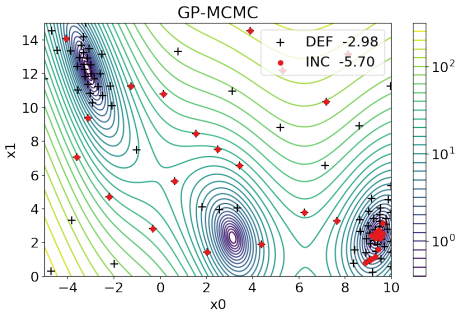
Bernd Bischl  Frank Hutter  Lars Kotthoff
Marius Lindauer  Joaquin Vanschoren

# Idea




$\rightsquigarrow$ focus on how the AutoML optimizer samples from the design space $\mathbf{\Lambda}$

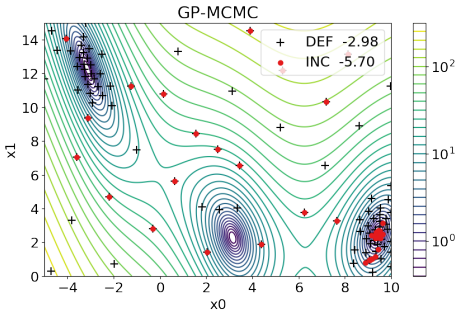
# Analyzing the Sampling Behavior




Source: [Lindauer et al. 2019]

- Plot of a 1D or 2D function

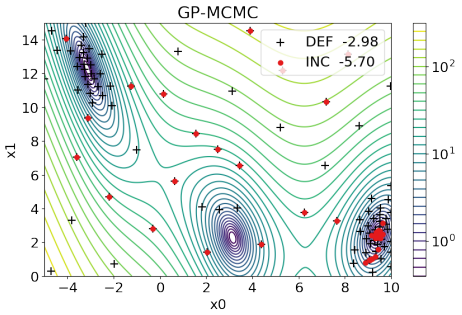
# Analyzing the Sampling Behavior




Source: [Lindauer et al. 2019]

- Plot of a 1D or 2D function
- Background shows the ground truth (real function values)

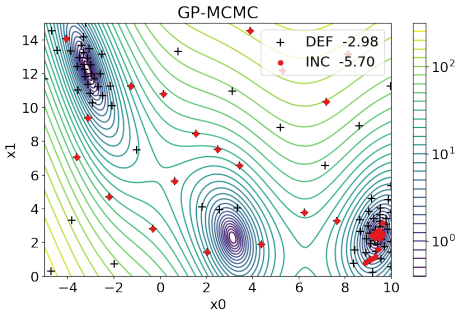
# Analyzing the Sampling Behavior




Source: [Lindauer et al. 2019]

- Plot of a 1D or 2D function
- Background shows the ground truth (real function values)
- Dots are sampled points in the search space

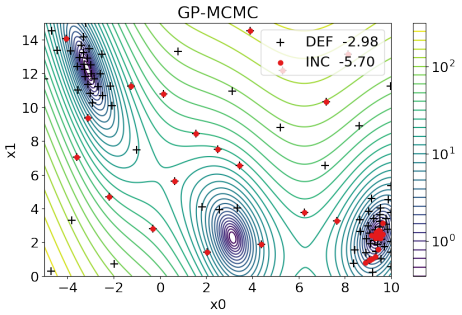
# Analyzing the Sampling Behavior




Source: [Lindauer et al. 2019]

- Plot of a 1D or 2D function
- Background shows the ground truth (real function values)
- Dots are sampled points in the search space
- Typical approach in Bayesian Optimization community

# Analyzing the Sampling Behavior

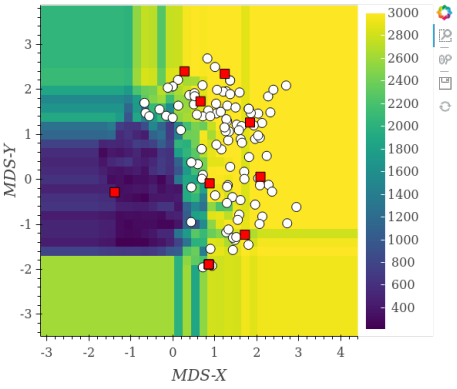



Source: [Lindauer et al. 2019]

- Plot of a 1D or 2D function
- Background shows the ground truth (real function values)
- Dots are sampled points in the search space
- Typical approach in Bayesian Optimization community

$\rightsquigarrow$ Impossible for higher dimensional problems?

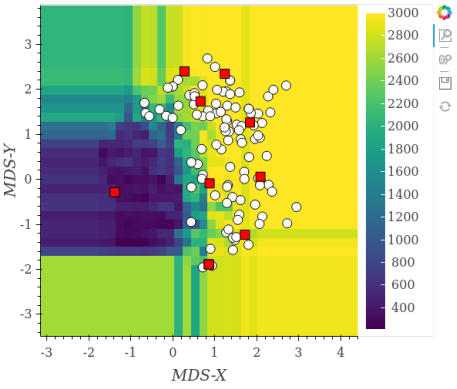
# Analyzing the Sampling Behavior in $N$-D




Source: [Lindauer et al. 2019]

- Same idea as before
  but we have to project $N$-D into 2-D

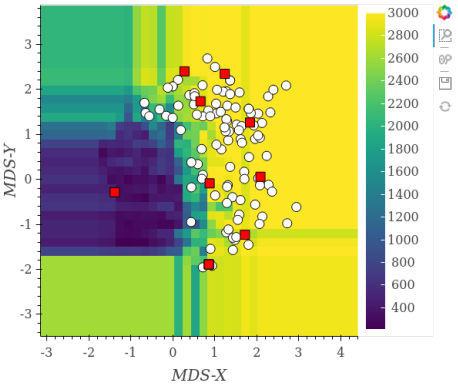
# Analyzing the Sampling Behavior in $N$-D




Source: [Lindauer et al. 2019]

- Same idea as before
  but we have to project $N$-D into 2-D
  1. Use an MDS to project down to 2-D

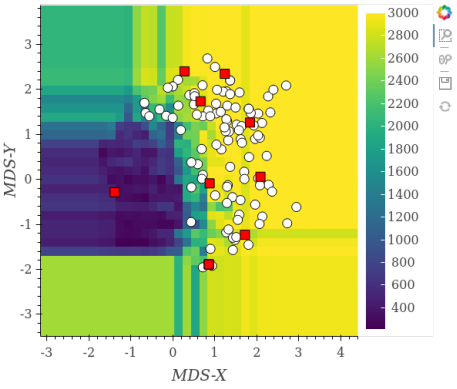
# Analyzing the Sampling Behavior in $N$-D




Source: [Lindauer et al. 2019]

- Same idea as before
  but we have to project $N$-D into 2-D
  1. Use an MDS to project down to 2-D
  2. Each dot is single hyperparameter configuration

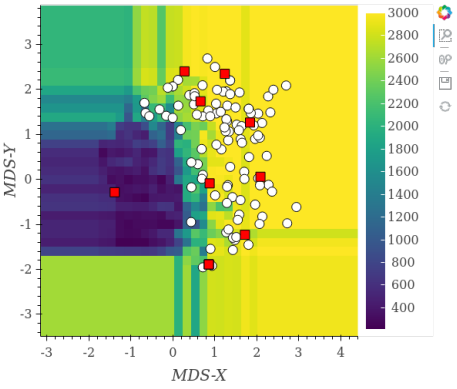
# Analyzing the Sampling Behavior in $N$-D




Source: [Lindauer et al. 2019]

- Same idea as before
  but we have to project $N$-D into 2-D
  1. Use an MDS to project down to 2-D
  2. Each dot is single hyperparameter configuration
  3. Red squares are intermediate incumbents

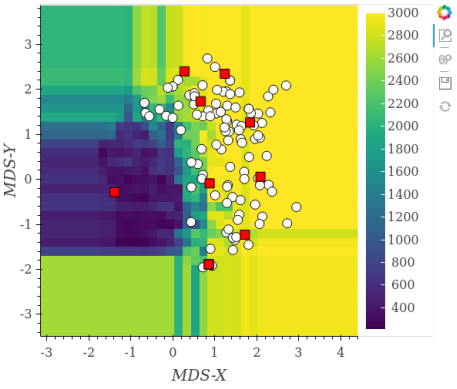
# Analyzing the Sampling Behavior in $N$-D




Source: [Lindauer et al. 2019]

- Same idea as before
  but we have to project $N$-D into 2-D
  1. Use an MDS to project down to 2-D
  2. Each dot is single hyperparameter configuration
  3. Red squares are intermediate incumbents
  4. The background is colored wrt a performance-estimate
     (e.g., reusing model fitted during BO)

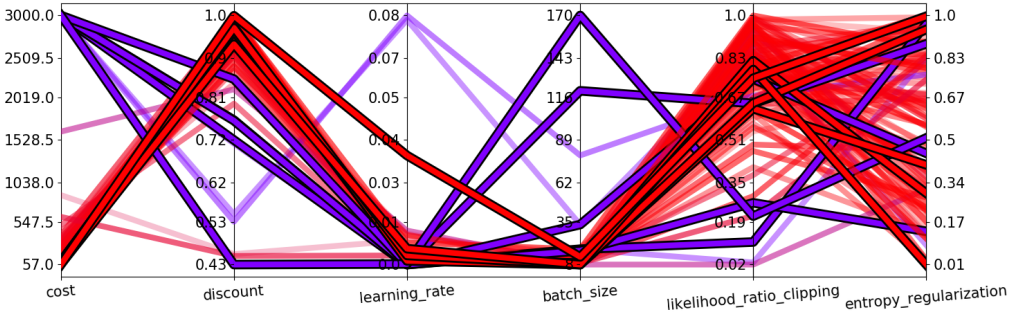
# Analyzing the Sampling Behavior in $N$-D




Source: [Lindauer et al. 2019]

- Same idea as before
  but we have to project $N$-D into 2-D
  1. Use an MDS to project down to 2-D
  2. Each dot is single hyperparameter configuration
  3. Red squares are intermediate incumbents
  4. The background is colored wrt a performance-estimate (e.g., reusing model fitted during BO)
  5. Extension: Animation by showing how points get added over time

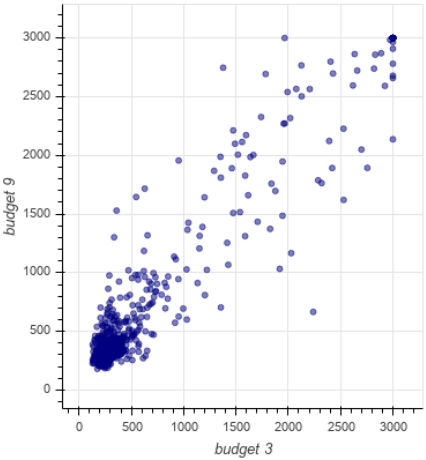
# Parallel Coordinate Plot [Golovin et al. 2017]




Source: [Lindauer et al. 2019]

- Each coordinate is one hyperparameter;
- Except the most left one: cost or loss

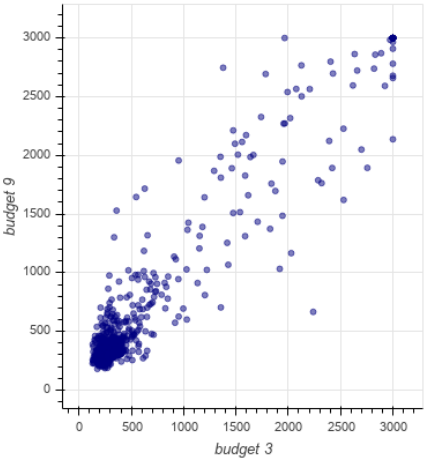
# Multi-Fidelity Checks




Source: [Lindauer et al. 2019]

- Challenge of multi-fidelity approaches:
  - How to choose the fidelities (a.k.a. budgets)

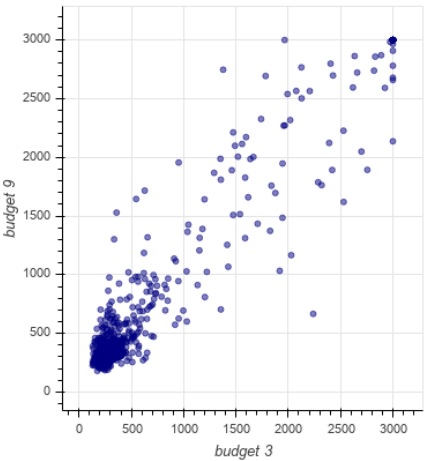
# Multi-Fidelity Checks




Source: [Lindauer et al. 2019]

- Challenge of multi-fidelity approaches:
  - How to choose the fidelities (a.k.a. budgets)
- Important Property:
  - Decisions on small budgets should be reasonable for higher budgets

# Multi-Fidelity Checks




Source: [Lindauer et al. 2019]

- Challenge of multi-fidelity approaches:
  - How to choose the fidelities (a.k.a. budgets)
- Important Property:
  - Decisions on small budgets should be reasonable for higher budgets
- Analysis:
  1. Scatter plot of performance on Budget X vs. Budget Y
  2. Each dot is sampled hyperparameter configuration
  3. Compute rank correlation (here: 0.69)