Bremen

GDS: Gradient based Density Spline Surfaces for Multiobjective Optimization in Arbitrary Simulations

Patrick Lange, Rene Weller, Gabriel Zachmann

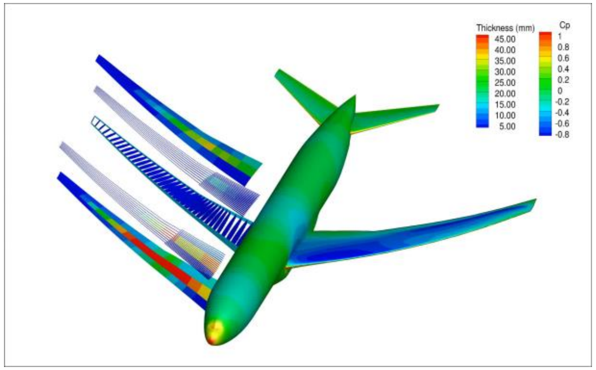
University of Bremen, Germany

cgvr.informatik.uni-bremen.de

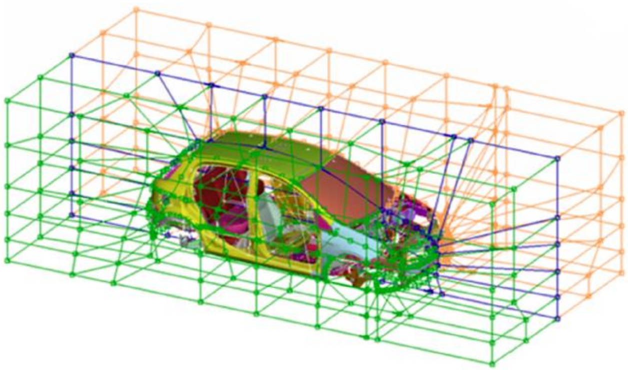
ACM SIGSIM PADS

24-26 May 2017, NTU, Singapore

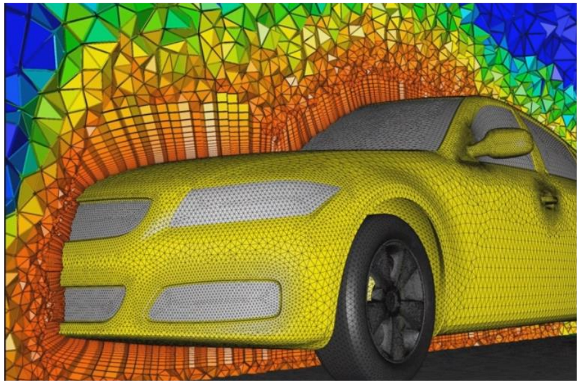
Motivation



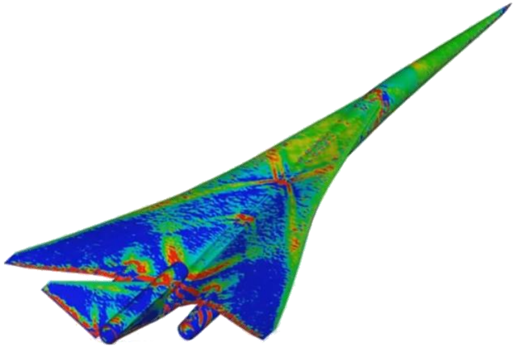
[Lyu'14]



(MDO Laboratory, http://mdolab.engin.umich.edu/)



(Pointwise, http://www.pointwise.com/index.shtml)

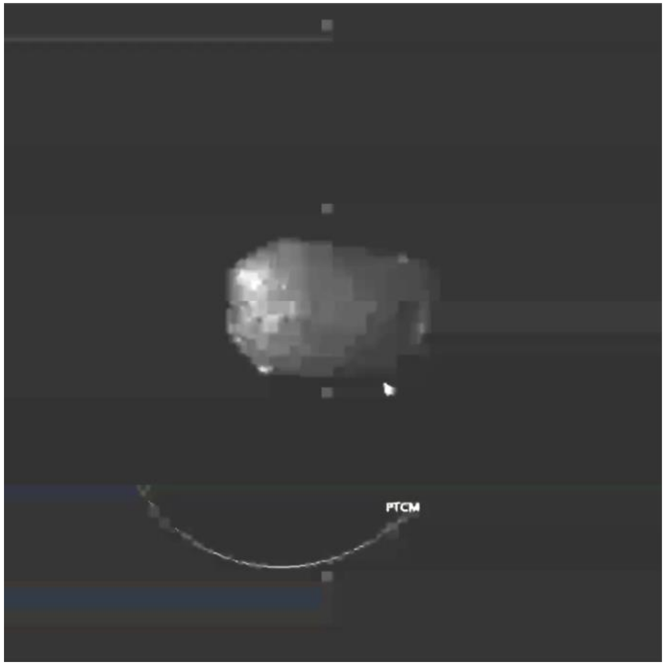


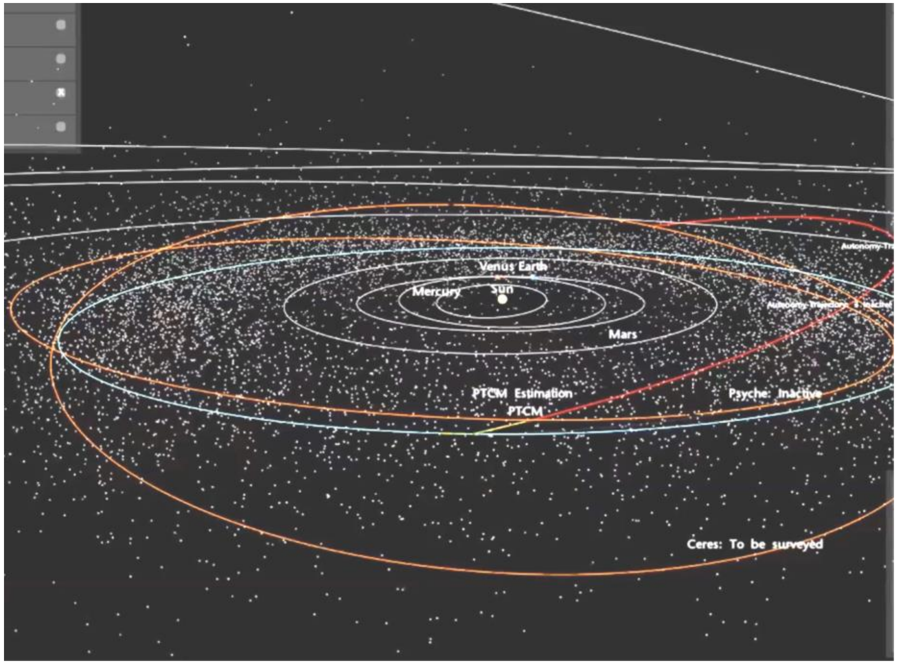
(MDO Laboratory, http://mdolab.engin.umich.edu/)

- Known objective functions
- Fast simulation execution

Motivation

- Feasibility studies
- Blackbox simulation leads to unknown objective functions
- Computational expensive (stochastic) simulation

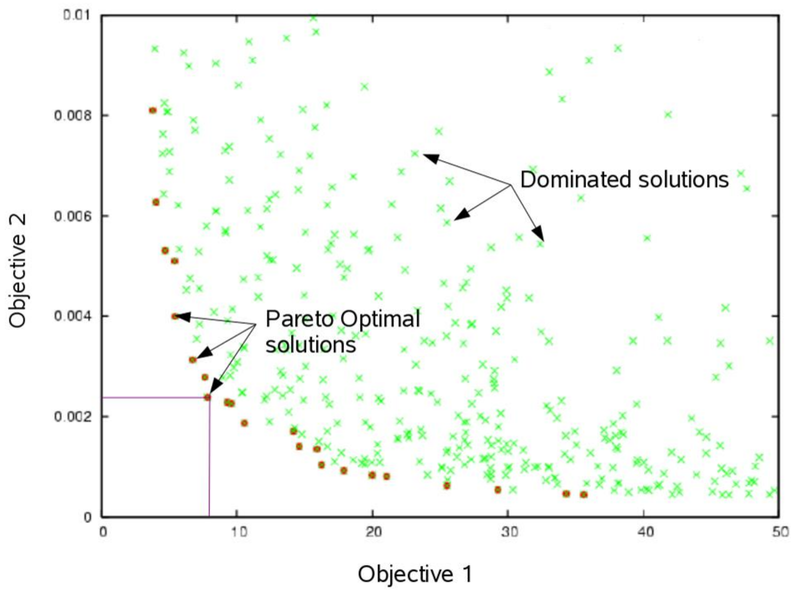




Simulation-based Optimization

- Multidisciplinary design attempts to satisfy multiple, possibly conflicting, objectives at once

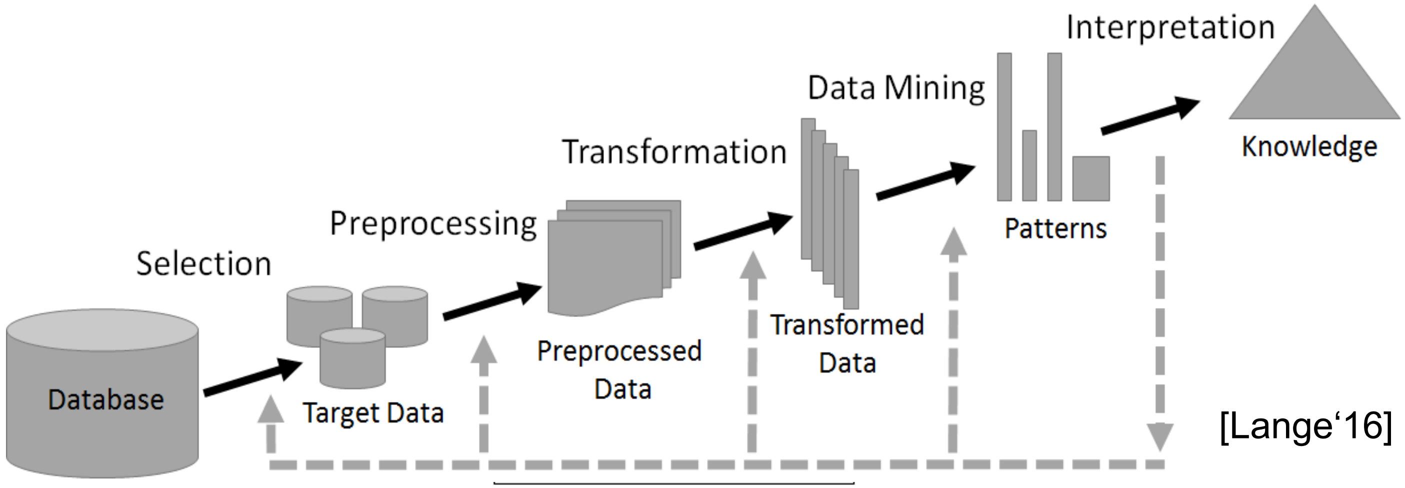
$$(MOP)\ \min_{x \in X} F(x) = (f_1(x), f_2(x), \dots, f_p(x))$$



(From: Cenaero http://www.cenaero.be/Page.asp?docid=27103&)

Our Approach

- Precise approximation of unknown objective functions and feasible design space
- Approximation allows (multiobjective-)optimization
- Deterministic and stochastic blackbox simulations for SOP and MOP



[Lange'16]

Previous Work

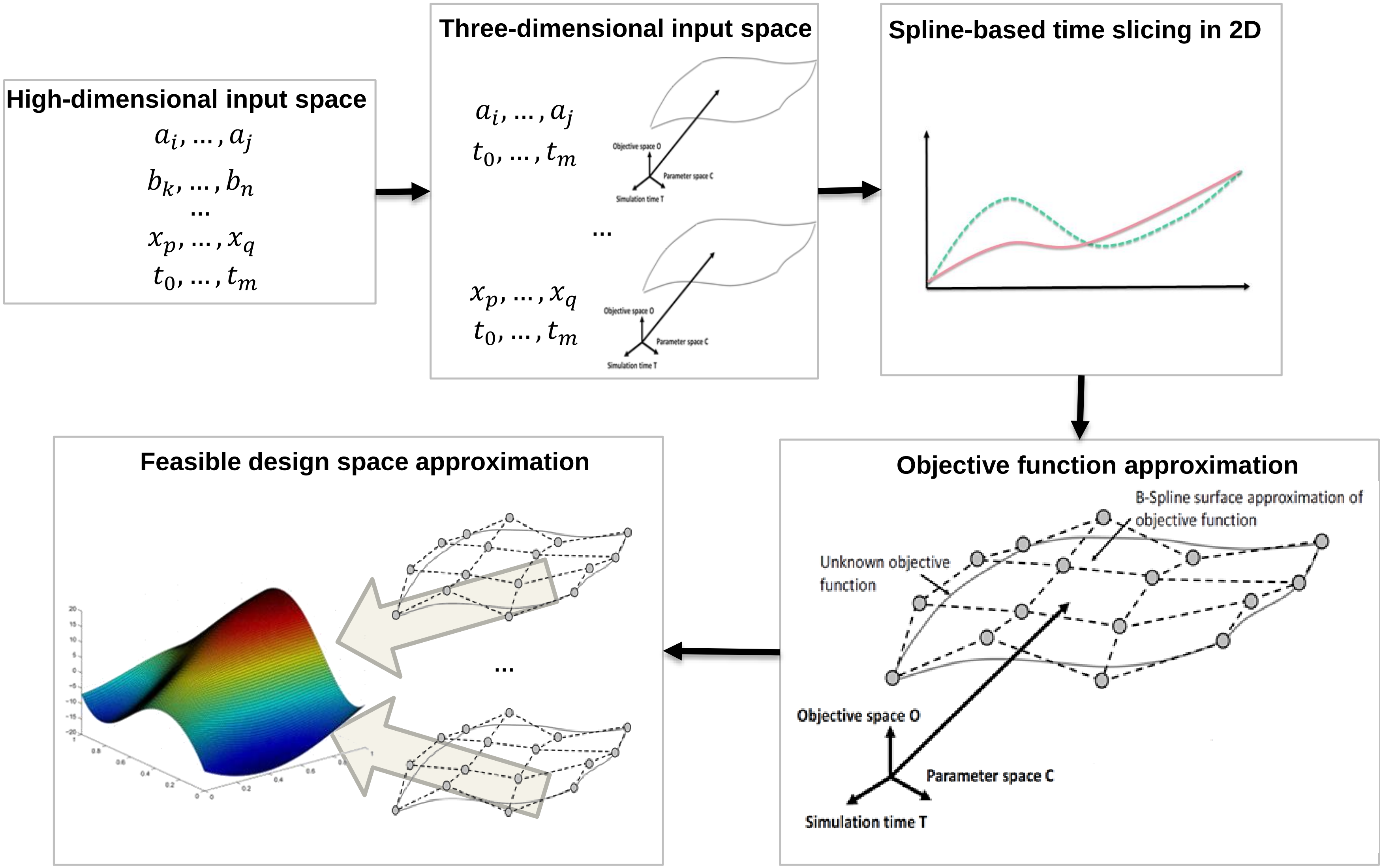
- Knowledge discovery in (deterministic) simulation (based optimization)
- Single objective optimization
  - Landscape characterization problem exploration via support vector machines [Burl‘06]
  - Determination of adaptation strategies for linear relationships [Lattner‘11]
  - Linear regression of input parameters and classification [Painter‘06]
  - Visual analytics [Feldkamp’15]
- Multi objective optimization
  - Analysis of existing Pareto solutions [Bandaru‘10,Sugimura‘07,Liebscher‘09,Dudas‘15]

Remaining Challenges

- Automatic approximation and optimization
- Consider computationally expensive simulations
- Consider stochastic simulations

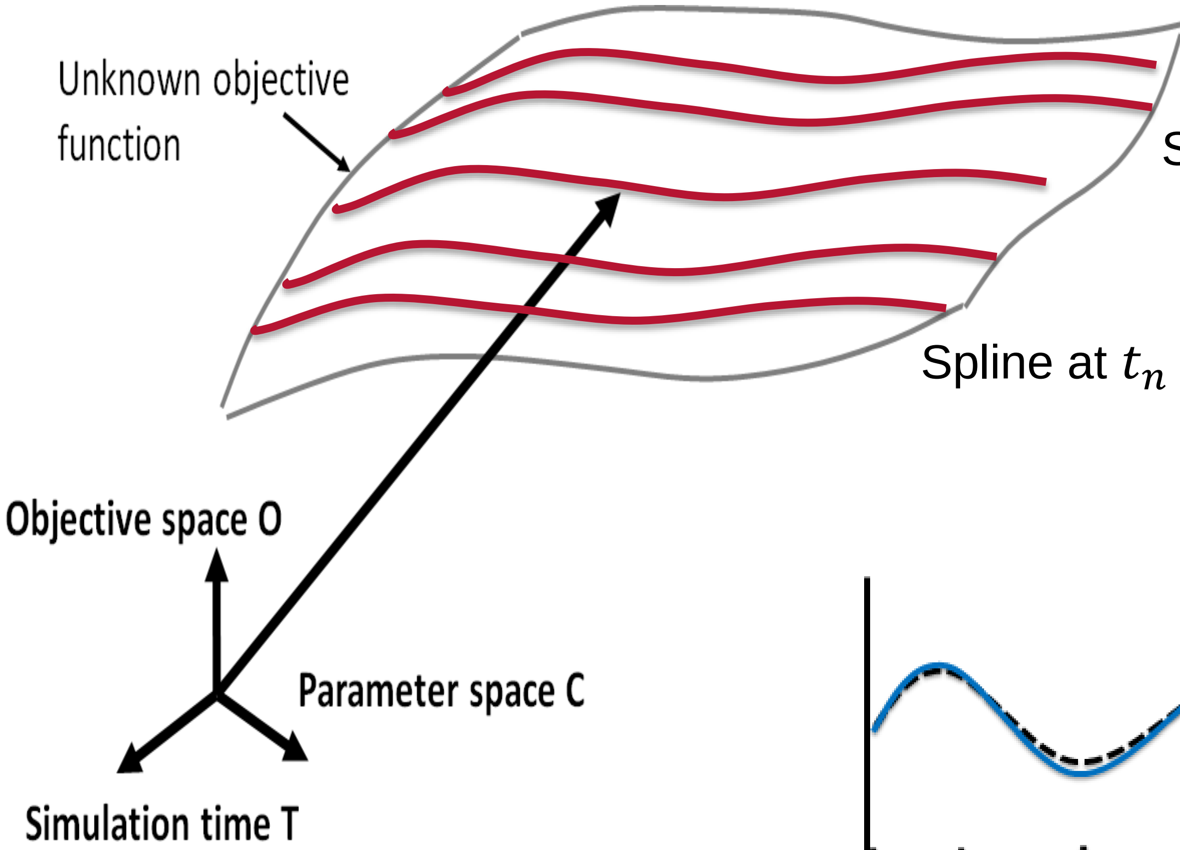
- Within the context of knowledge discovery process
  - What are suitable data mining methods in order to achieve above?

Overview of Approach



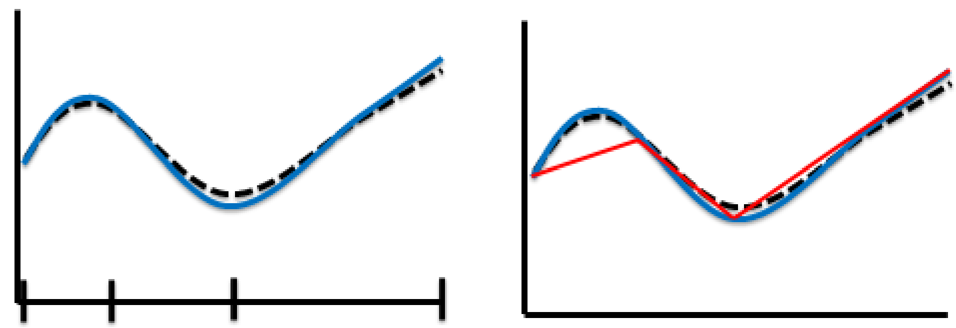
Relationship Approximation

$$f: C, T \rightarrow O = f(c,t) \rightarrow o_i$$

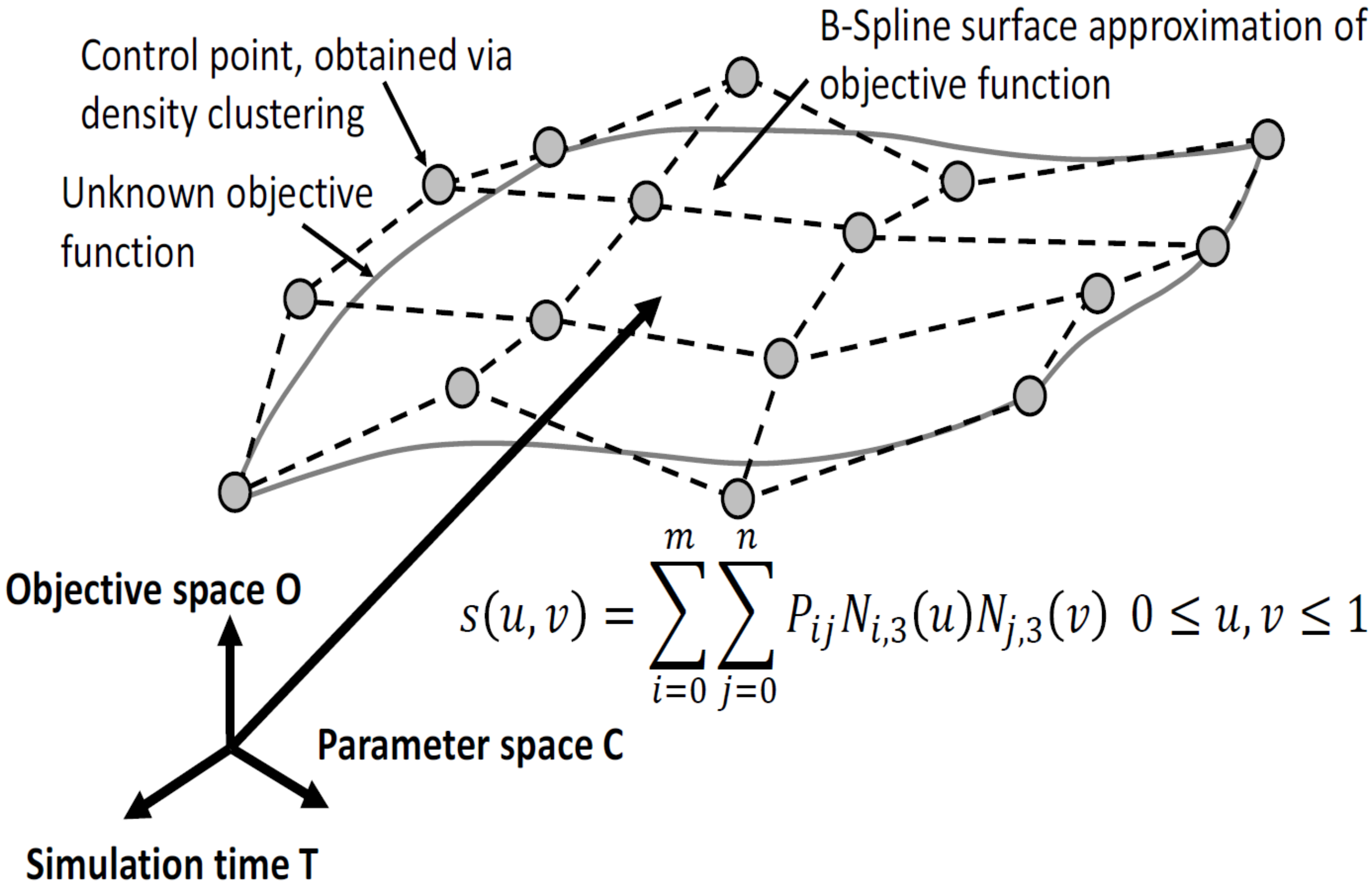


$$S(x) = \begin{cases} F_1(x), x_0 \leq x \leq x_1 \\ F_i(x), x_{i-1} \leq x \leq x_i \\ F_n(x), x_{n-1} \leq x \leq x_n \end{cases}$$

$$F_i(x) = a_i + b_i x + c_i x^2 + d_i x^3$$

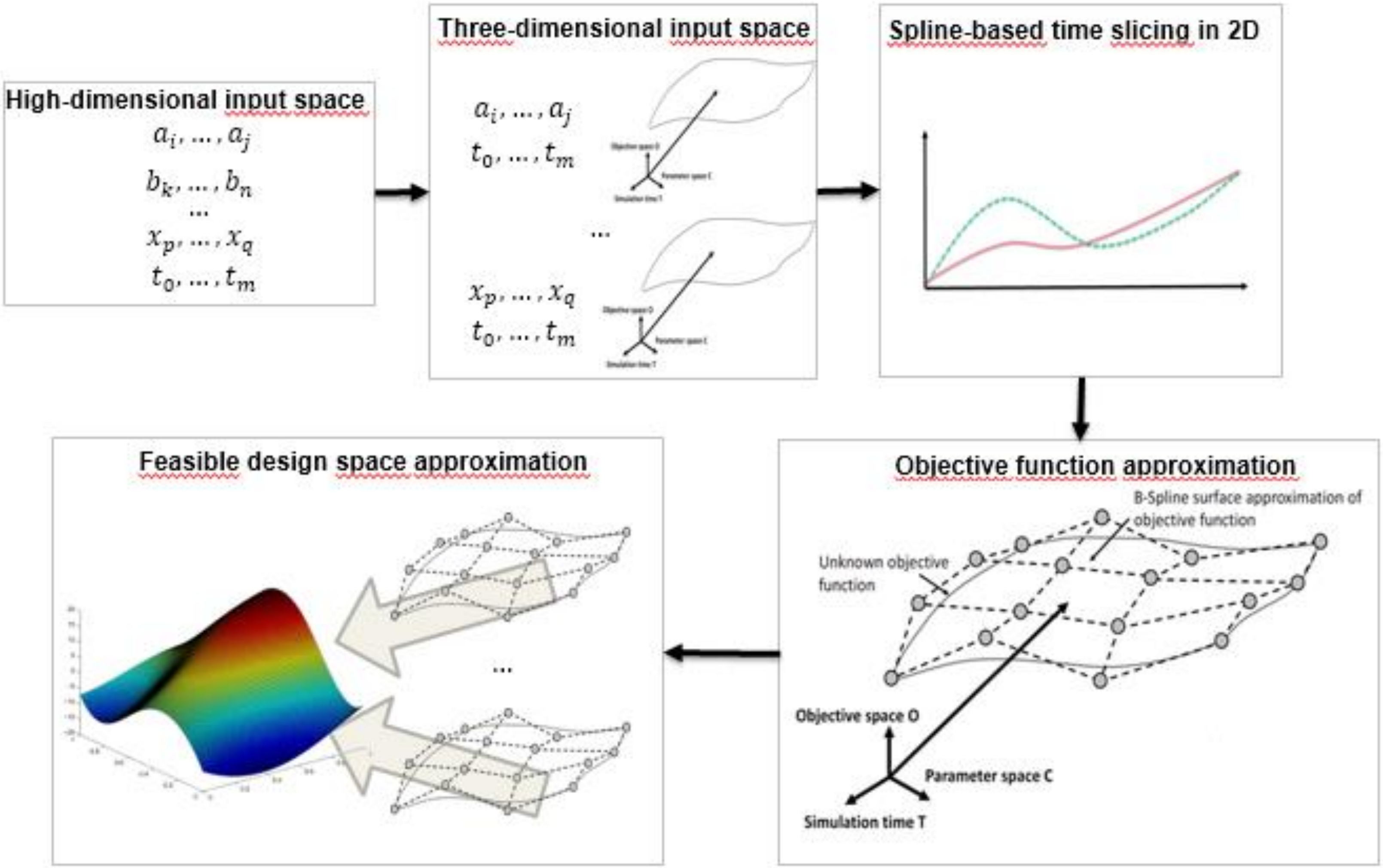


Relationship Approximation



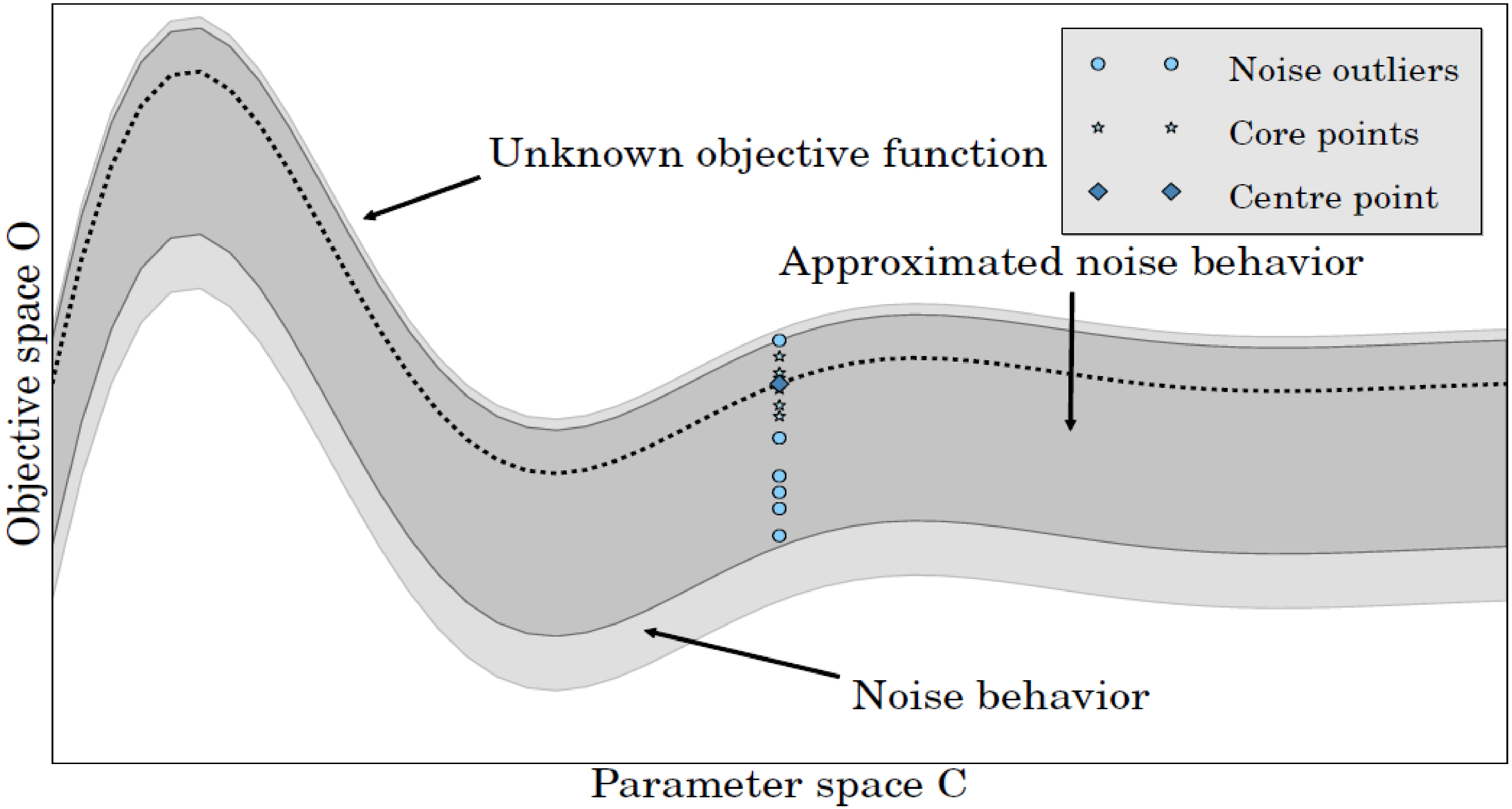
$$s(u,v) = \sum_{i=0}^{m} \sum_{j=0}^{n} P_{ij} N_{i,3}(u) N_{j,3}(v) \quad 0 \leq u,v \leq 1$$

Overview

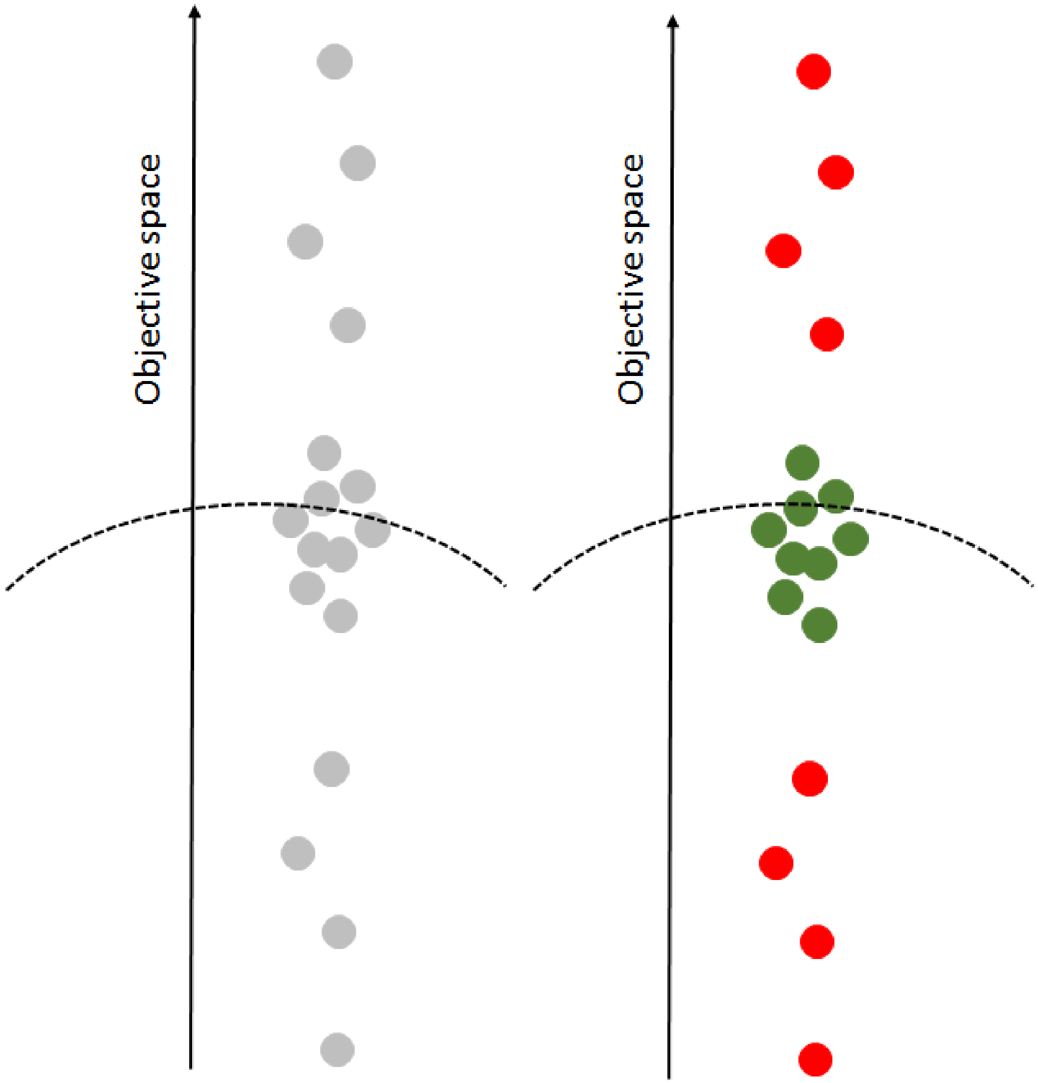


High-dimensional input space
$a_i, \ldots, a_j$
$b_k, \ldots, b_n$
...
$x_p, \ldots, x_q$
$t_0, \ldots, t_m$
Three-dimensional input space
$a_i, \ldots, a_j$
$t_0, \ldots, t_m$
...
$x_p, \ldots, x_q$
$t_0, \ldots, t_m$
Spline-based time slicing in 2D
Objective function approximation
B-Spline surface approximation of objective function
Unknown objective function
Objective space O
Parameter space C
Simulation time T
Feasible design space approximation
...

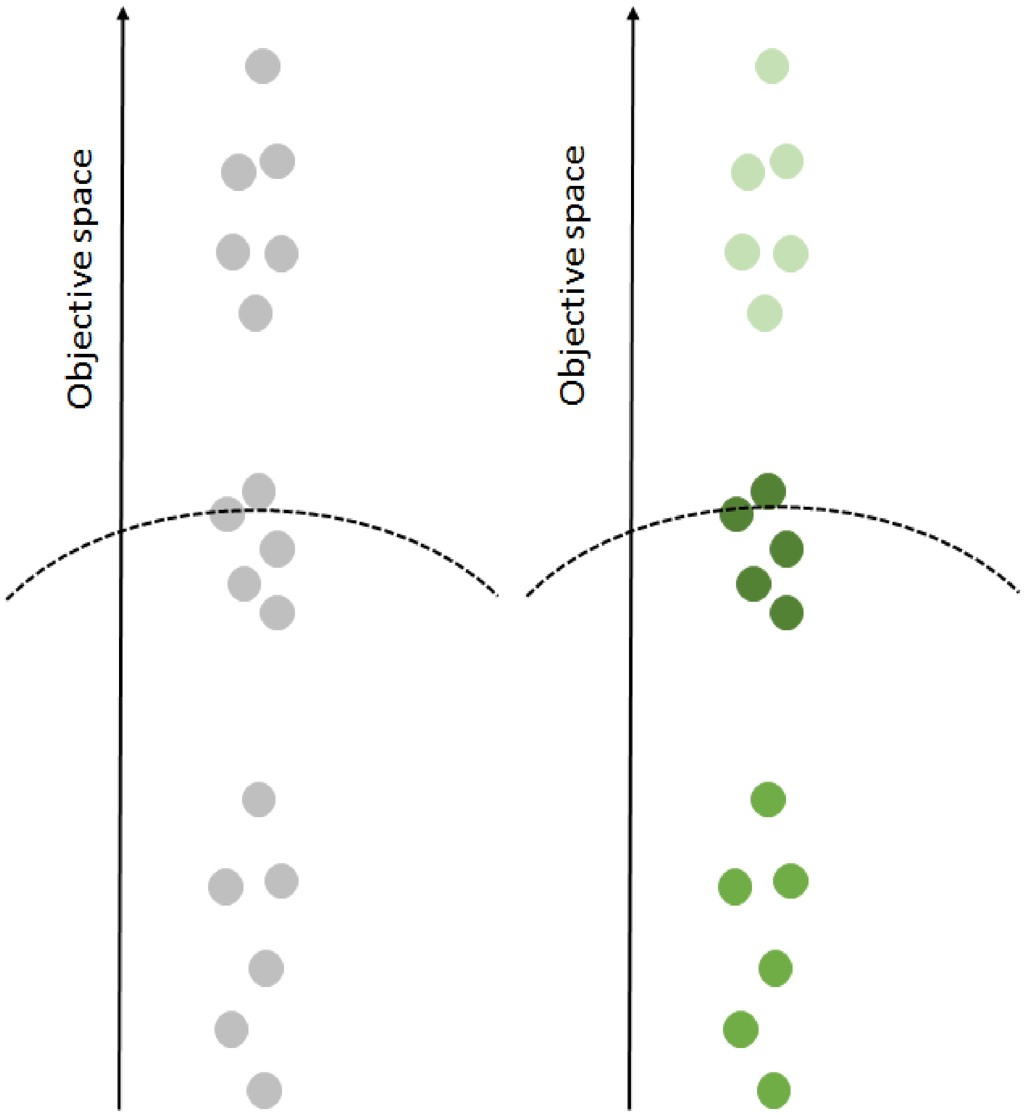
Density Clustering



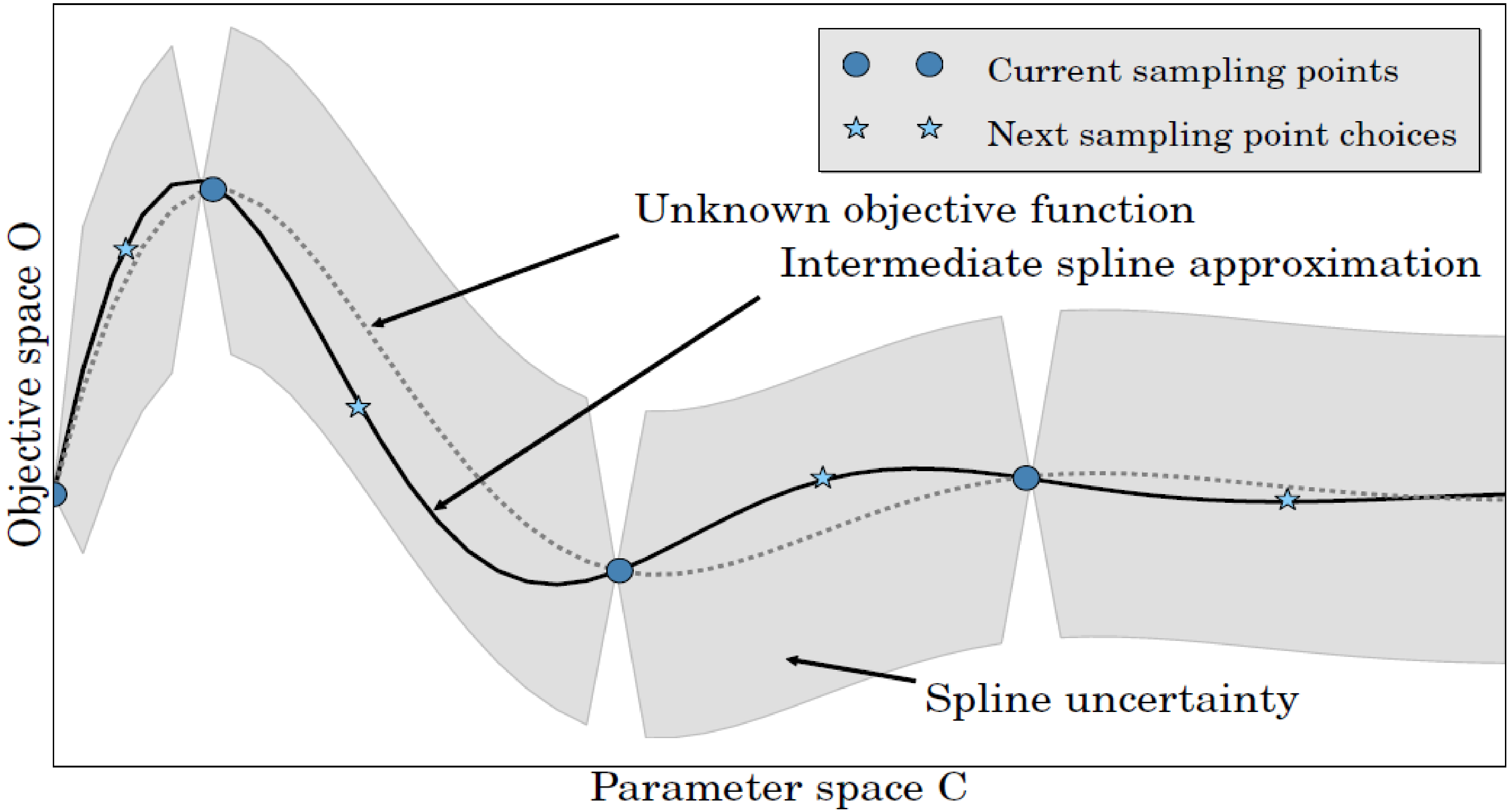
Density Clustering



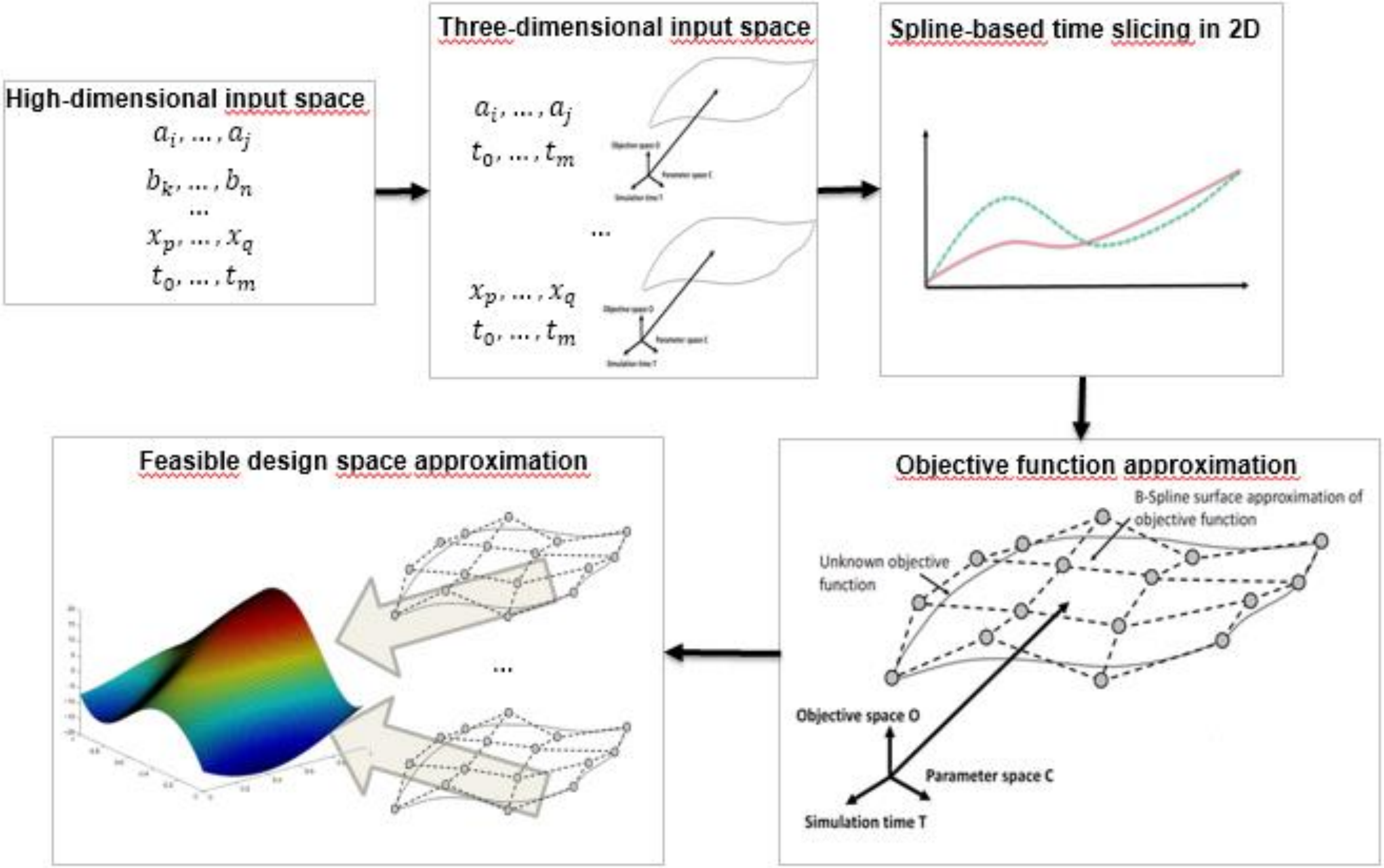
Density Clustering



Gradient based Sampling



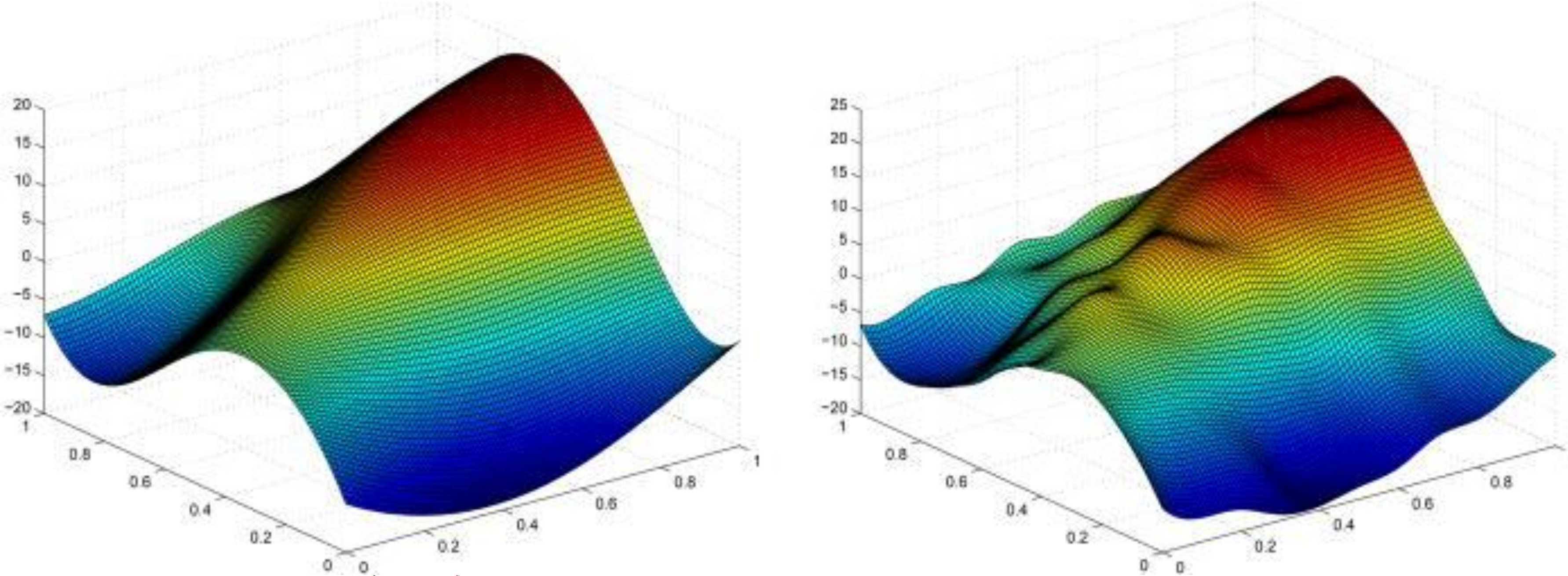
Overview


High-dimensional input space
$a_i, \ldots, a_j$
$b_k, \ldots, b_n$
...
$x_p, \ldots, x_q$
$t_0, \ldots, t_m$
Three-dimensional input space
$a_i, \ldots, a_j$
$t_0, \ldots, t_m$
...
$x_p, \ldots, x_q$
$t_0, \ldots, t_m$
Spline-based time slicing in 2D
Objective function approximation
B-Spline surface approximation of objective function
Unknown objective function
Objective space O
Parameter space C
Simulation time T
Feasible design space approximation
...

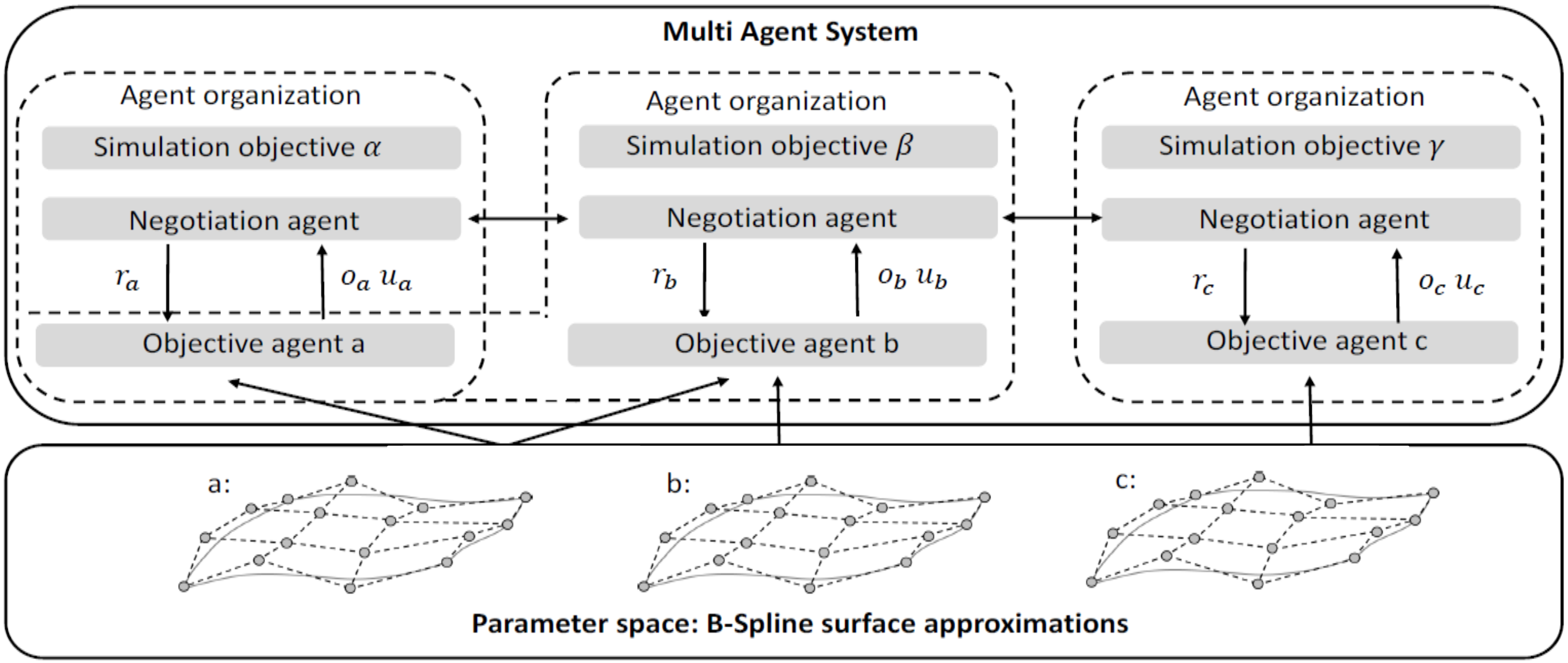
Feasible Design Space Approximation

- Re-formulation of MOP based on B-spline surface approximations

$$\omega_i(c,t) = \sum_{p=0}^{p=k} \Theta_p \cdot \left| \frac{o}{n} - s_p(c,t) \cdot \frac{o}{\sum_{q=0}^{q=k} |t_q - s_q(c,t)|} \right|$$



Multi-Agent System based Optimization



Evaluation

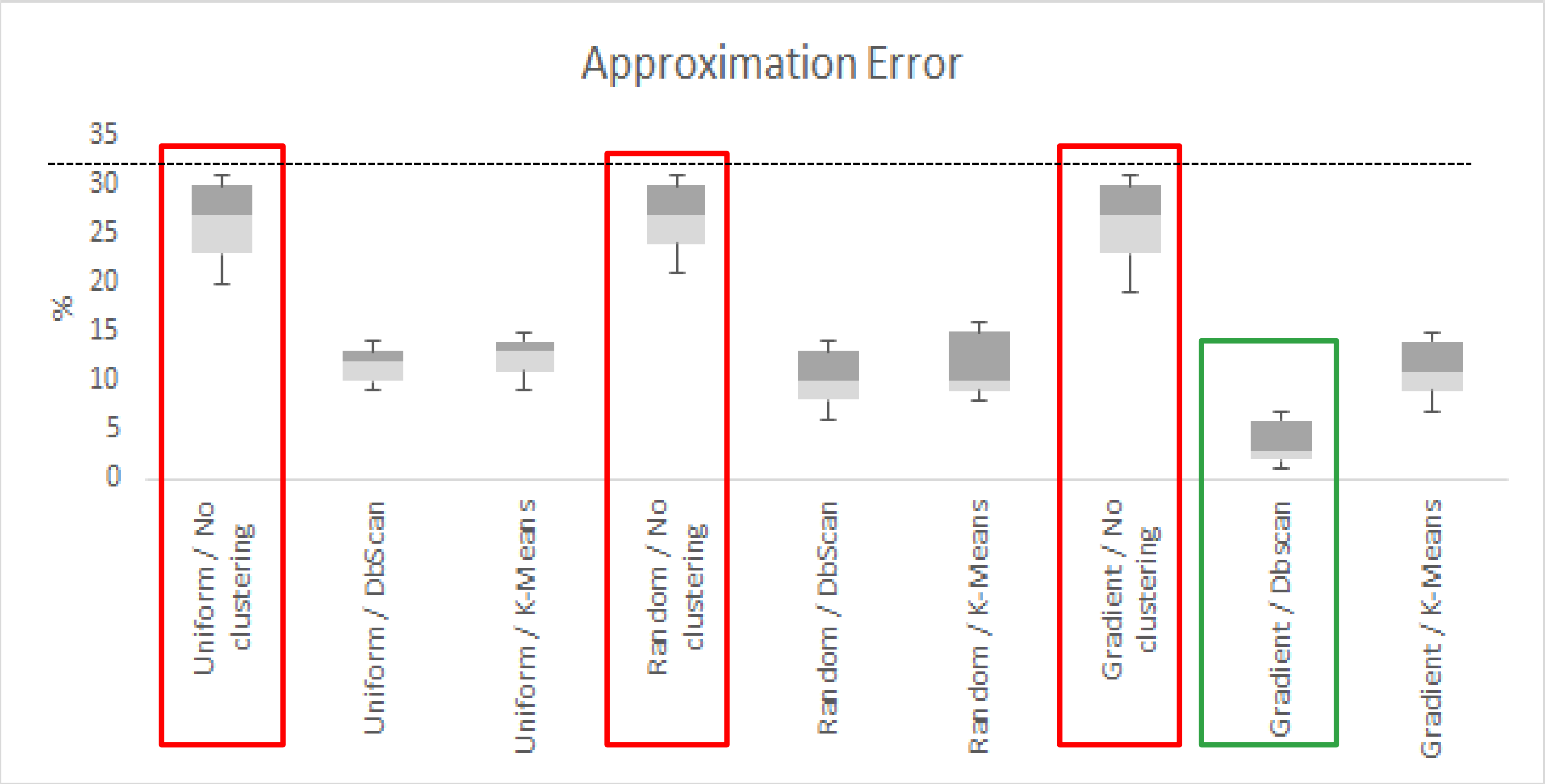
- Windows, C and C++/14
- Nine competitors
  - Three sampling strategies
  - Three clustering approaches

- Synthetic functions

$$f_p(c,t) = \sum_{i=0}^{n} a_i (c-p)^i + \sum_{j=0}^{m} b_j (t-q)^j + N$$

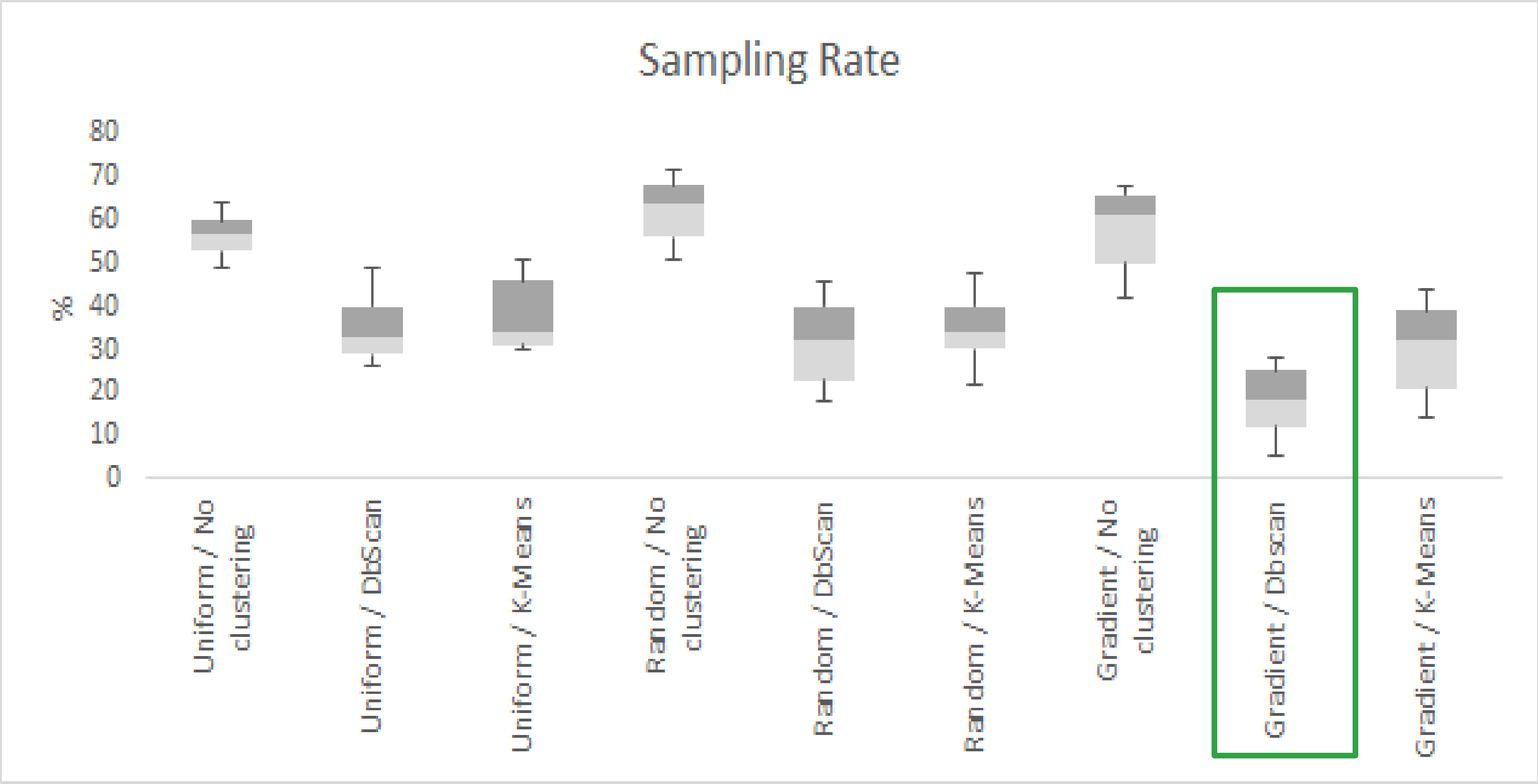
$$f_g(c,t) = \sum_{i=0}^{n} a_i e^{-\frac{(c-b_i)^2}{2c_i^2}} + \sum_{j=0}^{m} b_j e^{\frac{(t-b_j)^2}{2c_j^2}} + N$$

Evaluation



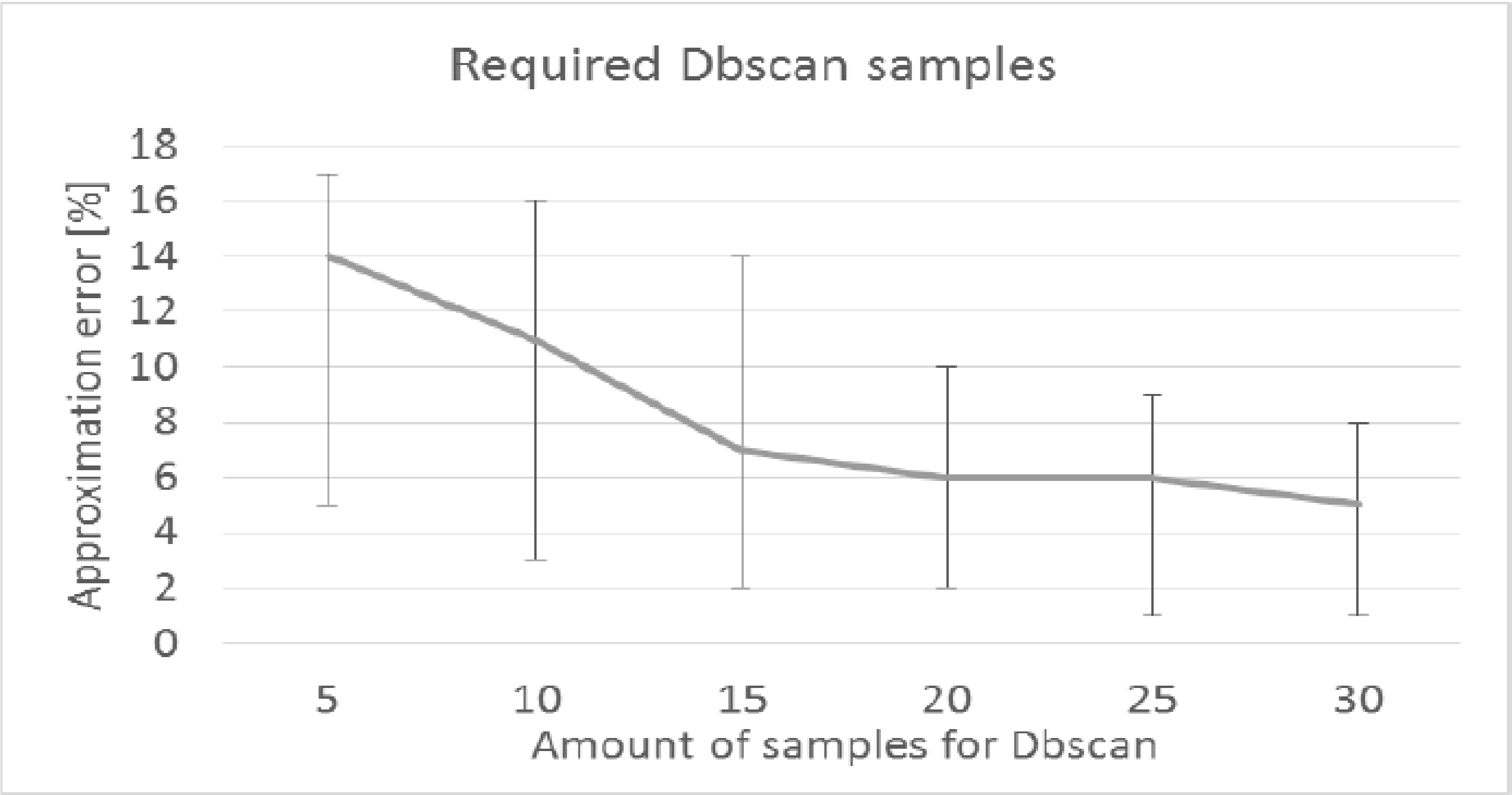
Approximation Error
35
30
25
20
15
10
5
0
%
Uniform / No clustering
Uniform / DbScan
Uniform / K-Means
Random / No clustering
Random / DbScan
Random / K-Means
Gradient / No clustering
Gradient / Dbscan
Gradient / K-Means

Evaluation



Sampling Rate
80
70
60
50
40
30
20
10
0
%
Uniform / No clustering
Uniform / DbScan
Uniform / K-Means
Random / No clustering
Random / DbScan
Random / K-Means
Gradient / No clustering
Gradient / Dbscan
Gradient / K-Means

Evaluation



Required Dbscan samples
Approximation error [%]
18
16
14
12
10
8
6
4
2
0
5
10
15
20
25
30
Amount of samples for Dbscan

Bremen

Evaluation Overview

Sampling:	Uniform						Random						Gradient					
Clustering:	Det.		Dbscan		K-Means		Det.		Dbscan		K-Means		Det.		Dbscan		K-Means	
	$\bar{e_p}$	$\bar{e_g}$	$\bar{e_p}$	$\bar{e_g}$	$\bar{e_p}$	$\bar{e_g}$	$\bar{e_p}$	$\bar{e_g}$	$\bar{e_p}$	$\bar{e_g}$	$\bar{e_p}$	$\bar{e_g}$	$\bar{e_p}$	$\bar{e_g}$	$\bar{e_p}$	$\bar{e_g}$	$\bar{e_p}$	$\bar{e_g}$
Probability mass functions																		
Binominal, $t = 9.0, p = 0.5$ $P(i\|t,p) = \binom{t}{i} \cdot p^i \cdot (1-p)^{t-i}$	15.8	15.9	10.71	10.8	13.86	13.96	16.68	16.71	10.55	10.59	13.42	13.56	15.65	15.72	8.67	8.71	11.34	11.41
Geometric, $k = 0.3$ $p(i\|k) = k \cdot (1-k)^i$	15.66	15.71	10.61	10.67	13.34	13.58	16.54	16.68	10.33	10.4	13.23	13.32	15.52	15.76	8.62	8.69	11.56	11.63
Pascal, $k = 3.0, p = 0.5$ $p(i\|k,p) = \binom{k+i-1}{i} \cdot p^k \cdot (1-p)^i$	15.6	15.72	10.58	10.61	12.26	13.37	16.27	16.32	10.32	10.4	13.67	13.7	15.65	15.86	8.53	8.6	11.23	11.38
Uniform, $a = 0.1, b = 9.0$ $p(x\|a,b) = \frac{1}{b-a}$	15.33	15.56	10.29	10.41	13.44	13.49	16.02	16.1	10.07	10.12	13.72	13.79	15.3	15.53	8.32	8.45	11.67	11.75
Poisson, $\mu = 0.1$ $p(x\|\mu) = \frac{\mu^i}{i!} e^{-\mu}$	15.59	15.81	10.54	10.61	12.19	12.55	16.42	16.51	10.3	10.38	13.21	13.32	15.56	15.62	8.56	8.61	11.85	11.93
Probability density functions																		
Cauchy, $a = 5.0, b = 1.0$ $p(x\|a,b) = \frac{1}{\pi \cdot b \cdot [1+(\frac{x-a}{b})^2]}$	15.1	15.3	10.44	10.48	12.42	12.56	16.24	16.28	10.25	10.3	13.33	13.42	15.15	15.25	8.47	8.52	11.24	11.4
Chi-squared, $n = 3.0$ $p(x\|n) = \frac{1}{\Gamma(\frac{n}{2}) \cdot 2^{\frac{n}{2}}} \cdot x^{\frac{n}{2}-1} \cdot e^{-\frac{x}{2}}$	15.7	15.9	10.61	10.63	12.11	12.46	16.28	16.43	10.4	10.48	13.56	13.61	15.7	15.78	8.62	8.7	10.87	10.96
Fisher-F, $m = 2.0, n = 2.0$ $p(x\|m,n) = \frac{\Gamma(\frac{m+n}{2})}{\Gamma(\frac{m}{2}) \cdot \Gamma(\frac{n}{2})} \cdot \frac{\frac{mx}{n}^{\frac{m}{2}}}{x \cdot (1+\frac{mx}{n})^{\frac{m+n}{2}}}$	15.35	15.51	10.84	10.88	12.71	12.83	16.35	16.48	10.73	10.79	13.56	13.6	15.13	15.31	8.75	8.81	11.74	11.83
Normal, $\mu = 5.0, \sigma = 2.0$ $p(x\|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \cdot e^{-\frac{(x-\mu)^2}{2\sigma^2}}$	15.56	15.62	10.55	10.63	11.98	12.68	16.4	16.53	10.39	10.44	13.67	13.72	15.52	15.59	8.48	8.54	11.52	11.6
Exponential, $\lambda = 3.5$ $p(x\|\lambda) = \lambda e^{-\lambda x}$	15.65	15.7	10.62	10.67	13.46	13.66	16.36	16.48	10.34	10.41	13.73	13.78	15.6	15.72	8.63	8.78	11.64	11.67

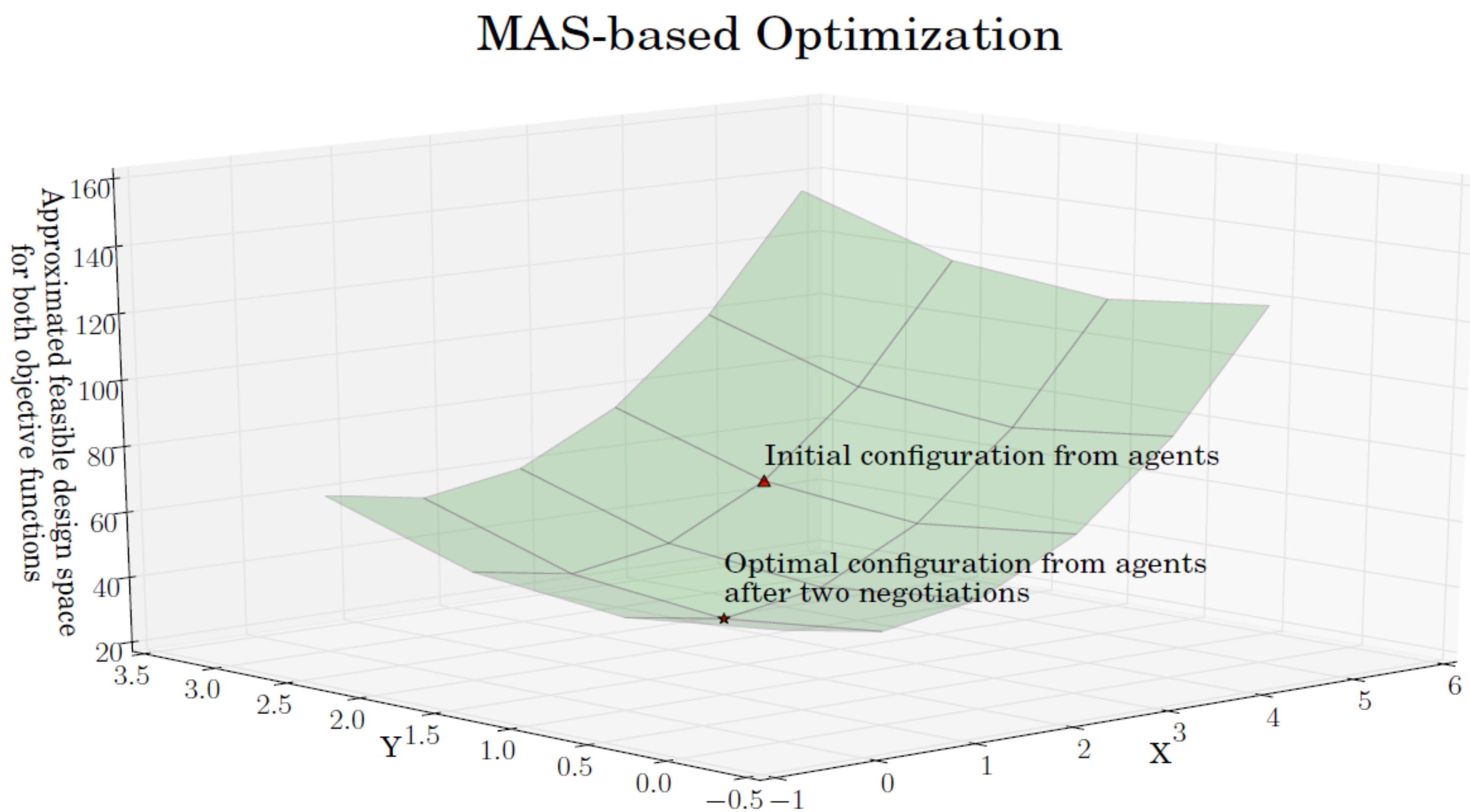
Evaluation

- Optimization problem

$$f_1(x,y) = 4x^2 + 4y^2 + N$$
$$f_2(x,y) = (x-5)^2 + (y-5)^2 + N$$
$$s.t.$$
$$g_1(x,y) = (x-5)^2 + y^2 \leq 25$$
$$g_2(x,y) = (x-8)^2 + (y+3)^2 \geq 7.7$$

(Binh/Korn'99)

Evaluation

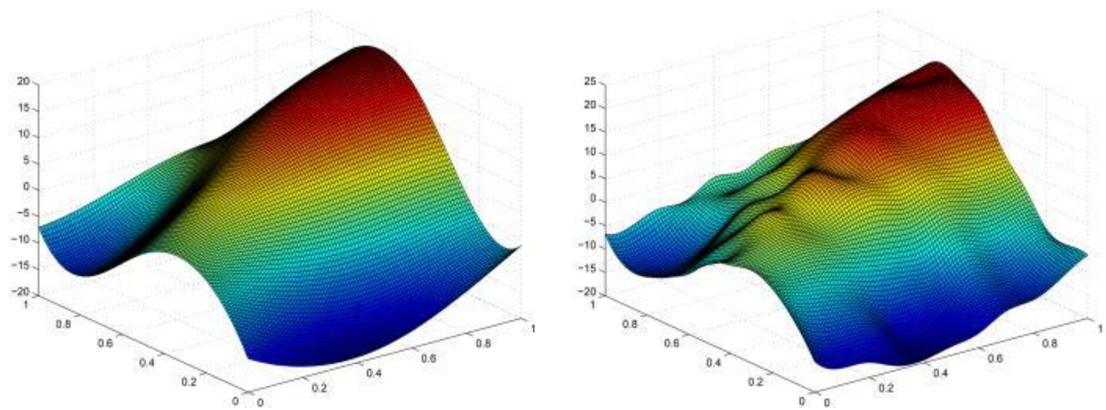


MAS-based Optimization
Approximated feasible design space for both objective functions
160
140
120
100
80
60
40
20
Y
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
X
−1
0
1
2
3
4
5
6
Initial configuration from agents
Optimal configuration from agents after two negotiations

Conclusion

- Approximation of objective functions and the feasible design space
  - Minimizes amount of required samples
  - Arbitrary deterministic and stochastic blackbox simulations
- Computation of Pareto solution via multi-agent system approach
  - Converges fast and solutions are close to Pareto front
- Approximation can replace costly simulation runs
- Requires knowledge discovery process [Lange‘16]

Thank you for your attention



Patrick Lange, Rene Weller, Gabriel Zachmann
{lange,weller,zach}@cs.uni-bremen.de

This research is based upon the project KaNaRiA, supported by German Aerospace Center (DLR) with funds of German Federal Ministry of Economics and Technoloy (BMWi) grant *50NA1318*