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

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ACM SIGSIM PADS

24-26 May 2017, NTU, Singapore
Motivation

- 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

\[(MOP) \min F(x) = (f_1(x), f_2(x), \ldots, f_p(x)) \quad x \in X\]
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

[Diagrams and images related to the text content]
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

High-dimensional input space
\[ a_i, ..., a_j \]
\[ b_k, ..., b_n \]
\[ x_p, ..., x_q \]
\[ t_0, ..., t_m \]

Three-dimensional input space
\[ a_i, ..., a_j \]
\[ t_0, ..., t_m \]
\[ x_p, ..., x_q \]
\[ t_0, ..., t_m \]

Spline-based time slicing in 2D

Feasible design space approximation

Objective function approximation

Motivation  Related Work  Our Approach  Evaluation  Conclusion
Relationship Approximation

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

**Unknown objective function**

**Objective space O**

**Parameter space C**

**Simulation time T**

**Spline at \( t_k \)**

**Spline at \( t_n \)**

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

\[ F_i(x) = a_i + b_i x + c_i x^2 + d_i x^3 \]
Relationship Approximation

Control point, obtained via density clustering

Unknown objective function

B-Spline surface approximation of objective function

Objective space $O$

Parameter space $C$

Simulation time $T$
Overview

High-dimensional input space

\[ a_i, ..., a_j \]
\[ b_k, ..., b_n \]
... 
\[ x_p, ..., x_q \]
\[ t_0, ..., t_m \]

Three-dimensional input space

\[ a_i, ..., a_j \]
\[ t_0, ..., t_m \]
... 
\[ x_p, ..., x_q \]
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Spline-based time slicing in 2D

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Motivation
Related Work
Our Approach
Evaluation
Conclusion
Density Clustering

Objective space \( O \)

Unknown objective function

Approximated noise behavior

Noise behavior

Parameter space \( C \)

- Noise outliers
- Core points
- Centre point

Motivation
Related Work
Our Approach
Evaluation
Conclusion
Density Clustering

Motivation

Related Work

Our Approach

Evaluation

Conclusion
Density Clustering
Gradient based Sampling

Objective space $O$

Intermediate spline approximation

Unknown objective function

Parameter space $C$

Current sampling points

Next sampling point choices

Spline uncertainty
Overview

High-dimensional input space

\[ a_i, \ldots, a_j \]
\[ b_k, \ldots, b_n \]
\[ \ldots \]
\[ x_p, \ldots, x_q \]
\[ t_0, \ldots, t_m \]

Three-dimensional input space

\[ a_i, \ldots, a_j \]
\[ t_0, \ldots, t_m \]
\[ \ldots \]
\[ x_p, \ldots, x_q \]
\[ t_0, \ldots, t_m \]

Spline-based time slicing in 2D

Feasible design space approximation

Objective function approximation

Motivation Related Work Our Approach Evaluation Conclusion
Feasible Design Space Approximation

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

\[ \omega_i(c, t) = \frac{1}{n} \sum_{p=0}^{p=k} \Theta_p \cdot \left| \frac{O}{n} - s_p(c, t) \cdot \frac{O}{\sum_{q=0}^{q=k} |t_q - s_q(c, t)|} \right| \]
Multi-Agent System based Optimization

Multi Agent System

Agent organization
Simulation objective $\alpha$
Negotiation agent
Objective agent $a$

Agent organization
Simulation objective $\beta$
Negotiation agent
Objective agent $b$

Agent organization
Simulation objective $\gamma$
Negotiation agent
Objective agent $c$

Parameter space: B-Spline surface approximations

Motivation
Related Work
Our Approach
Evaluation
Conclusion
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
Evaluation

![Sampling Rate Chart](image)

- Uniform / No clustering
- Uniform / DBScan
- Uniform / K-Means
- Random / No clustering
- Random / DBScan
- Random / K-Means
- Gradient / No clustering
- Gradient / DBScan
- Gradient / K-Means

**Sampling Rate**

- %
- 0 10 20 30 40 50 60 70 80

Conclusion
**Evaluation**

![Graph showing Required Dbscan samples vs Amount of samples for Dbscan]

- **Approximation error [%]**
- **Amount of samples for Dbscan**

The graph illustrates the relationship between the amount of samples for Dbscan and the approximation error in percentage. As the amount of samples increases, the approximation error decreases, indicating improved accuracy with more samples.
## Evaluation Overview

<table>
<thead>
<tr>
<th>Sampling:</th>
<th>Uniform</th>
<th>Random</th>
<th>Gradient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clustering:</td>
<td>Det. $c_p$</td>
<td>Det. $c_p$</td>
<td>Det. $c_p$</td>
</tr>
<tr>
<td></td>
<td>$c_g$</td>
<td>$c_g$</td>
<td>$c_g$</td>
</tr>
<tr>
<td>Binominal, $t = 9.0, p = 0.5$</td>
<td>15.8</td>
<td>15.9</td>
<td>10.71</td>
</tr>
<tr>
<td>Geometric, $k = 0.3$</td>
<td>15.66</td>
<td>15.71</td>
<td>10.61</td>
</tr>
<tr>
<td>Pascal, $k = 3.0, p = 0.5$</td>
<td>15.6</td>
<td>15.72</td>
<td>10.58</td>
</tr>
<tr>
<td>Uniform, $a = 0.1, b = 9.0$</td>
<td>15.33</td>
<td>15.56</td>
<td>10.29</td>
</tr>
<tr>
<td>Poisson, $\mu = 0.1$</td>
<td>15.59</td>
<td>15.81</td>
<td>10.54</td>
</tr>
<tr>
<td>Cauchy, $a = 5.0, b = 1.0$</td>
<td>15.1</td>
<td>15.3</td>
<td>10.44</td>
</tr>
<tr>
<td>Chi-squared, $n = 3.0$</td>
<td>15.7</td>
<td>15.9</td>
<td>10.61</td>
</tr>
<tr>
<td>Fisher-F, $m = 2.0, n = 2.0$</td>
<td>15.35</td>
<td>15.51</td>
<td>10.84</td>
</tr>
<tr>
<td>Normal, $\mu = 5.0, \sigma = 2.0$</td>
<td>15.56</td>
<td>15.62</td>
<td>10.55</td>
</tr>
<tr>
<td>Exponential, $\lambda = 3.5$</td>
<td>15.65</td>
<td>15.7</td>
<td>10.62</td>
</tr>
</tbody>
</table>
Evaluation

- Optimization problem

\[
\begin{align*}
  f_1(x, y) &= 4x^2 + 4y^2 + N \\
  f_2(x, y) &= (x - 5)^2 + (y - 5)^2 + N \\
  \text{s.t.} \\
  g_1(x, y) &= (x - 5)^2 + y^2 \leq 25 \\
  g_2(x, y) &= (x - 8)^2 + (y + 3)^2 \geq 7.7
\end{align*}
\]

(Binh/Korn’99)
**Evaluation**

**MAS-based Optimization**

- **Initial configuration from agents**
- **Optimal configuration from agents after two negotiations**

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Motivation | Related Work | Our Approach | Evaluation | Conclusion
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

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