Surrogate Model Based Optimization of the Substrate Feed Mixture of a Biogas Plant

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Overview

- Presented work is based on a collaboration with Daniel Gaida and Thomas Bartz-Beielstein [Zaefferer et al., 2016]

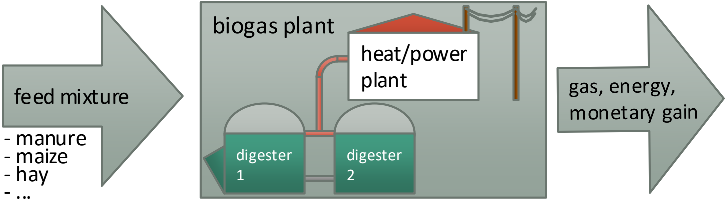
1. Problem: Feed Mixture Optimization
2. Surrogate Model-Based-Optimization
3. Integration of Expert Knowledge
4. Case Study: Model Quality
5. Case Study: Optimization Performance
6. Summary and Outlook

Problem: Feed Mixture Optimization

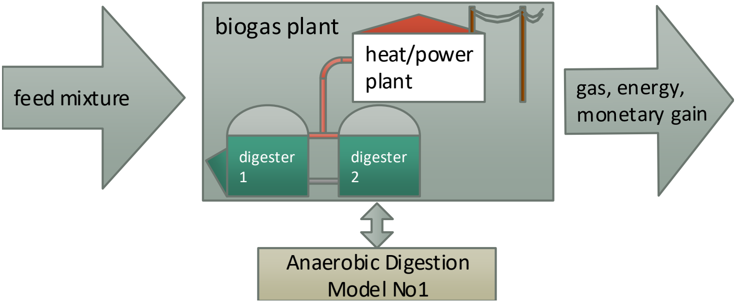
- Goal: maximize monetary gain of biogas plants
- Gain depends on feed mixture

$$\max_{\boldsymbol{x} \in \mathcal{X}} y = f(\boldsymbol{x}),$$

  - y: gain
  - $\boldsymbol{x}$: feed mixture
  - $\mathcal{X} \subseteq \mathbb{R}^{+n}$: Search space, respecting bounds on availability of material

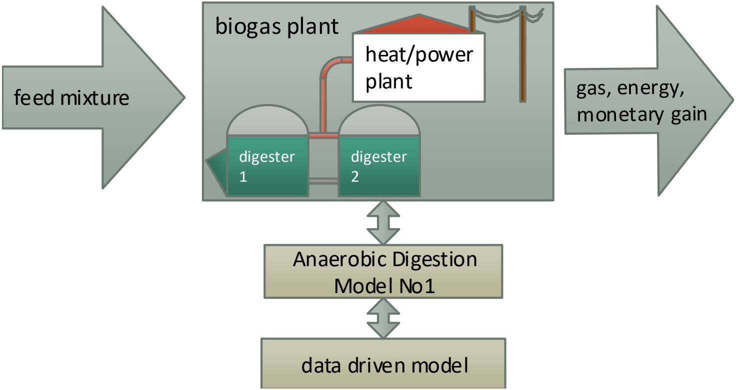


- Slow biochemical processes
  - Direct optimization infeasible
  - Need for simulation models, e.g.:
    - Computational Fluid Dynamics (CFD)
    - Anaerobic Digestion Model No1 (ADM1) [Batstone et al., 2002]



Surrogate Model-Based-Optimization

- Simulation still time consuming
- Need for data-driven surrogate models



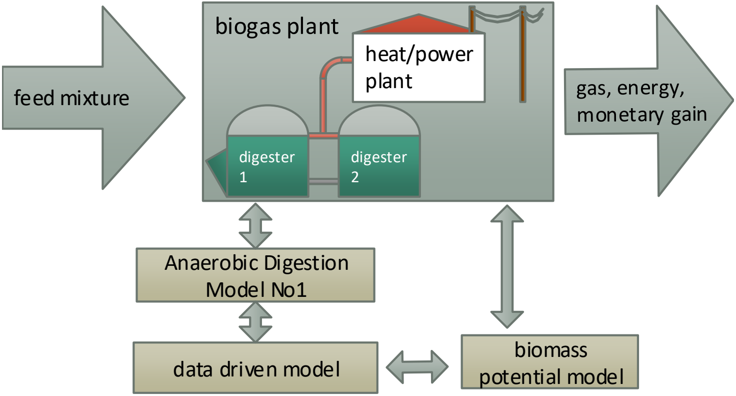
Surrogate Model-Based-Optimization

- Algorithm
  1. Initial design $\mathbf{X} = \{\mathbf{x}_1, ...\mathbf{x}_n\}$
  2. Evaluate with simulation (here: ADM1) $y_i = f_f(\mathbf{x}_i)$
  3. Train data-driven surrogate model with $\mathbf{X}$ and $\boldsymbol{y}$, yielding $\hat{f}_f(\mathbf{x})$
  4. Optimize surrogate $\mathbf{x}_{n+1} = max_{\mathbf{x}} \hat{f}_f(\mathbf{x})$
- Repeat 2-4 until budget exhausted
- Model: Kriging / Gaussian process regression [Forrester et al., 2008]

Integration of Expert Knowledge

Available expert knowledge

- Not a pure-black box problem
- Coarse grained guess: biomass potential (BMP)
  - Cheap to compute
  - But inaccurate
- Also: knowledge about gain changes, e.g., manure bonus



Use of expert knowledge

- i) Improve initial design: include optimum of BMP model $f_c(\mathbf{x})$
- ii) Improve surrogate model of ADM1 $f_f(\mathbf{x})$ via BMP model $f_c(\mathbf{x})$
- iii) Improve surrogate model: avoid discontinuities (manure bonus)

Multi-fidelity approaches

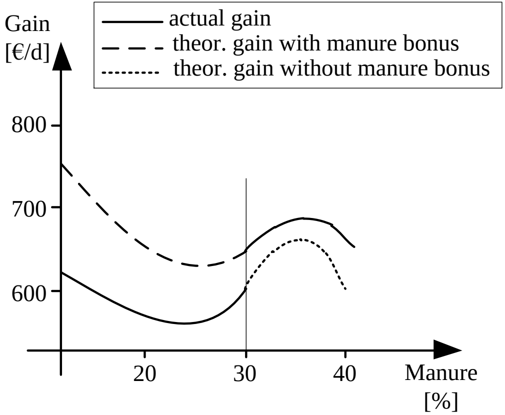
- Model the differences between the coarse BMP and the fine ADM1 function $\hat{f}_f(\mathbf{x}) = \hat{f}_{diff}(\mathbf{x}) + f_c(\mathbf{x})$
- Use the BMP model output as an input to the surrogate model $\hat{f}_f(\mathbf{x}) = \hat{f}_{input}(\mathbf{x}, f_c(\mathbf{x}))$
- Model correlation between BMP and ADM1 explicitly via multi-output Gaussian processes / co-Kriging [Forrester et al., 2007]

$$\hat{f}_f(\mathbf{x}) = \hat{\mu} + \mathbf{c}^T \mathbf{C}^{-1}(\mathbf{y} - \mathbf{1}\hat{\mu}),$$

- $\mathbf{C}$: Matrix of covariances of the training data (coarse-coarse, fine-coarse, fine-fine)
- $\mathbf{c}$: vector of covariances of new sample $\mathbf{x}$ and training data (coarse and fine)

Avoiding discontinuity

- Problem: discontinuity in the target function landscape
- May deteriorate Kriging model
- Location and reason of discontinuity is known a priori: manure bonus



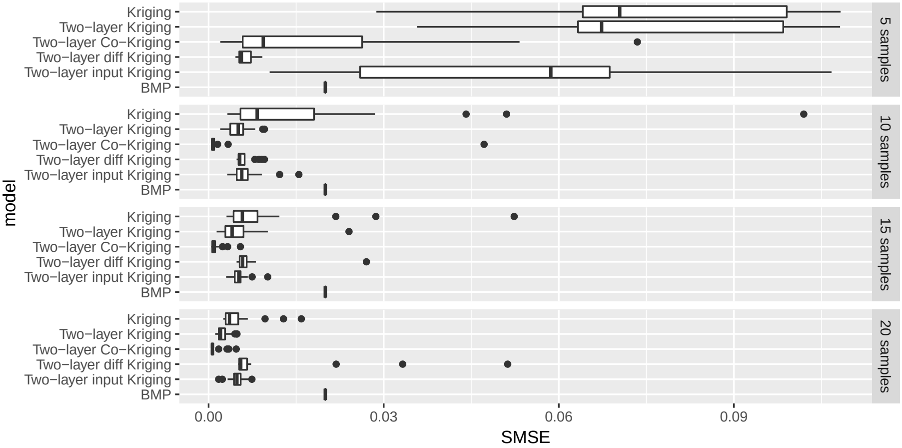
- Solution: train two models, with and without manure bonus. Switch between them.

Case Study: Model Quality

Setup:

- 2D case: mixture of pig manure and maize
- 5, 10, 15 and 20 evaluations of the ADM1 / fine model
- 100 evaluations of the BMP / coarse model
- Latin hypercube sampling (LHS)
- Error measure: SMSE [Keijzer, 2004]

Model Quality



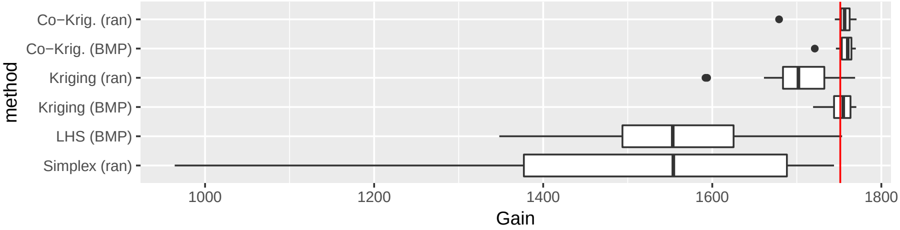
Optimization Performance

Setup:

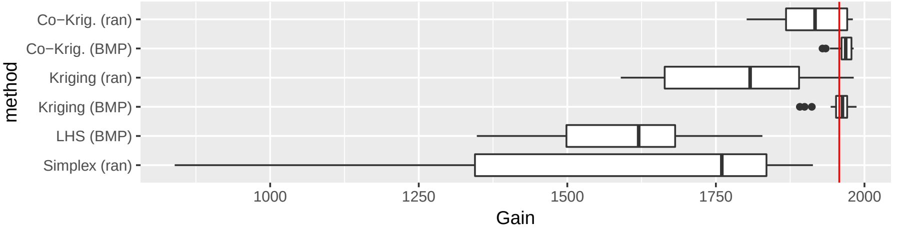
- 2D: pig manure and maize
- 5D: pig manure, maize, grass, corncob, cow manure
- Models:
  - 2-layer Kriging
  - 2-layer co-Kriging
- Initial design (fine): 3 x dimension
- Initial design (coarse): 50 x dimension
- Budget: 5 x dimension
- Surrogate budget: 500 x dimension
- Simulation failure: penalty / imputation
- Initialization: LHS with or without BMP optimum

Optimization Results

- 2D case, after 10 evaluations



- 5D case, after 25 evaluations



Optimization Results

method	dim	gain [eur/d]	gross time [s]	net time [s]	failures
Simplex (ran)	2	1554	898.24	0.37	1
Simplex (BMP)	2	1751	1451.61	0.41	0
LHS (BMP)	2	1553	975.49	**0.32**	1
Kriging (ran)	2	1702	909.30	10.68	2
Kriging (BMP)	2	1755	895.94	10.66	0
Co-Krig. (ran)	2	1757	861.50	15.20	2
Co-Krig. (BMP)	2	**1760**	**805.76**	15.08	0
Simplex (ran)	5	1760	2779.87	0.92	7
Simplex (BMP)	5	1958	**1594.88**	0.98	0
LHS (BMP)	5	1620	3156.73	**0.88**	0
Kriging (ran)	5	1808	2763.89	53.16	2
Kriging (BMP)	5	1963	2615.60	53.51	4
Co-Krig. (ran)	5	1917	2980.53	293.60	4
Co-Krig. (BMP)	5	**1968**	2877.09	288.97	1

Summary and Outlook

Summary

- Pros:
  - Two-layer model approach improves accuracy
  - Multi-fidelity information improves accuracy and performance
  - BMP initialization improves performance
- Cons:
  - Co-Kriging: computational cost may impede benefits
  - Comparison to (deterministic) downhill simplex problematic
  - Generalization?

Open Issues

- Integration in online control (dynamic optimization)
- Larger set of test cases
- More accurate/expensive models, e.g., CFD-based
- Additional objectives or constraints

Thanks for Listening

- Questions?

References I

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Overall best solutions found

	2D	5D
gain [€/ d]	1,770	1,987
maize [m^3/d]	22.85	5.22
pig manure [m^3/d]	11.85	11.48
grass silage [m^3/d]	0	18.98
corn-cob-mix [m^3/d]	0	0.01
cow manure [m^3/d]	0	0.08
manure bonus	yes	yes
ammonia digester [mg/l]	163.4	216.6
ammonia post-digester [mg/l]	291.0	464.2

Scaled MSE

$$\mathsf{SMSE}(\mathbf{y}, \hat{\mathbf{y}}) \; = \; \mathsf{MSE}(\mathbf{y}, \mathbf{1}a + b\hat{\mathbf{y}}) =$$

$$= \frac{1}{n} \sum_{i=1}^{n} (y_i - (a + b\hat{y}_i))^2$$

$$\text{where} \quad b \; = \; \frac{\mathsf{cov}(\mathbf{y}, \hat{\mathbf{y}})}{\mathsf{var}(\hat{\mathbf{y}})} \quad \text{and} \quad a = \bar{\hat{\mathbf{y}}} - b\bar{\mathbf{y}}$$