Multi-objective optimization of adhesive bonding process in constrained and noisy settings

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1

Motivation

Need for better fuel efficiency

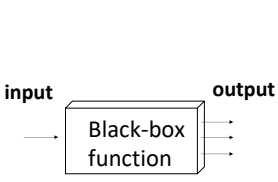
Results in lighter bodies, new materials

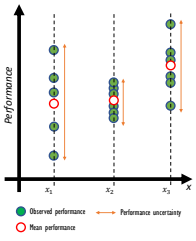
Which tend to be more fragile, more difficult to join

The right bonding process will improve strength

- Multi-objective optimization
  - Minimize cost **VS.** Maximize tensile strength
- Real experimentation is **expensive** and yield **noisy outputs**
  - The same process configuration generates different break strength/type of failure
- Different types of failure
  - Adhesive, cohesive, or substrate failure

2





3

Efficiently find good process parameters with a minimal set of experiments, and considering the **trade-off** between tensile strength and production cost

- Gaussian Process Regression (GPR) to account for the heterogeneous noise
- Acquisition function to sequentially (one-by-one) suggest new process parameter configurations to be evaluated.
  - GPR model and feasibility prediction)

Tensile strength — Production cost

$$\min\ [-TS(x),\ PC(x)]$$
$$\text{s.t. } 0.5 - Pf(x) \leq 0$$

probability that a process configuration x is feasible

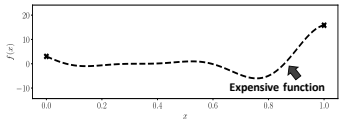
☒ Burned sample

☒ Adhesive failure

☑ Substrate failure

4

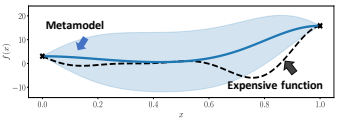
Metamodel-based optimization



Goal:
- **Assuming minimization**

5

Metamodel-based optimization



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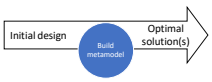
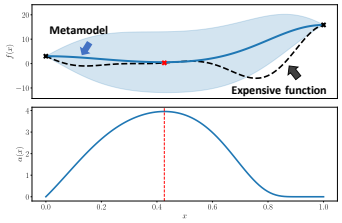


6

Metamodel-based optimization



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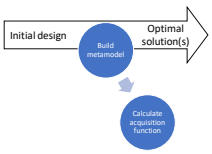
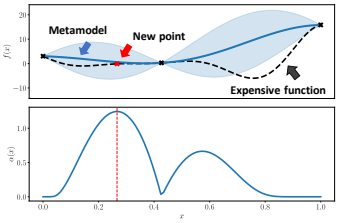


7

Metamodel-based optimization



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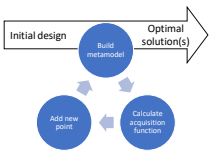
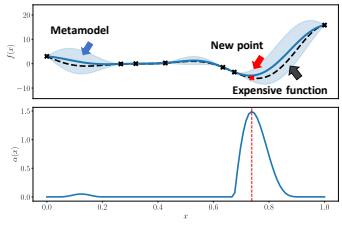


8

Metamodel-based optimization



9

Gaussian Process with heteroscedastic noise

Function representation:

$$f(x) = m(x) + M(x) + \epsilon_r(x)$$

Mean of the process; Noise observed in replication r; unknown response function; Realization of a Gaussian random field with mean zero (covariance function)

$$Cov(y_i, y_j) = k(x_i, x_j)$$

Predictor and uncertainty estimator:

$$\hat{y}(x_*) = k_* \left[\boldsymbol{K_n} + \boldsymbol{\Sigma_\epsilon}\right]^{-1} \boldsymbol{Y}$$

predictor; Spatial correlation among the new point and the observed points; Observed response of the n points; Covariance matrix of the n observed points; Noise estimation for the n points

$$\Sigma_e = Diag\left\{\frac{Var(f(x_i))}{r_i}\right\}, i \in \{1, \dots, n\}$$

Uncertainty estimator

$$\hat{s}^2(x_*) = k_{**} - k_* \left[\boldsymbol{K_n} + \boldsymbol{\Sigma_\epsilon}\right]^{-1} \boldsymbol{k_*^T}$$

Covariance function applied to the new point and itself

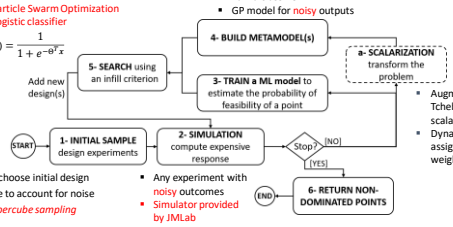
10

Proposed approach

- Smartly choose next design point(s) for expensive observation
  - Particle Swarm Optimization
  - Logistic classifier

$$P(y = 1|x; \Theta) = \frac{1}{1 + e^{-\theta^T x}}$$

- Outcome prediction at non-observed points
- Uncertainty estimate of outcomes
- Train a classifier
- GP model for noisy outputs



- Augmented Tchebycheff scalarization
- Dynamically assignment of weights

- Smartly choose initial design
- Replicate to account for noise
- *Latin hypercube sampling*

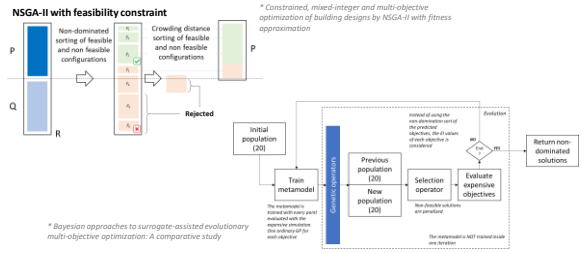
- Any experiment with noisy outcomes
- Simulator provided by JMLab

11

Experiment design

NSGA-II with feasibility constraint

** Constrained, mixed-integer and multi-objective optimization of building designs by NSGA-II with fitness approximation*



** Bayesian approaches to surrogate-assisted evolutionary multi-objective optimization: A comparative study*

12

Experiment design

Process parameters	Min	Max
Pre-processing	0	1
Plasma power	300	500
Plasma speed	5	250
Distance	0.2	2
Number of passes	1	50
Real time	1	120

Summary of the parameters of the optimization approaches

Setting	MO-GP	cNSGA-II	GP-cNSGA-II
Size of initial design		LHS: $N = 20$	
Crossover probability	-	$c_p = 0.9$	
Mutation probability	-	$m_p = 0.1$	
Replications		$r = 5$	
Iterations/Generations	100	5	
Acquisition function	CMEI	-	EI
Acquisition function optimization	PSO[7]	-	
Kernel	Gaussian	-	Gaussian

Acquisition function

Probability of being feasible

$$CMEI(x_*) = MEI(x_*) * P(y = 1|x)$$

GP prediction — Root square of the uncertainty prediction

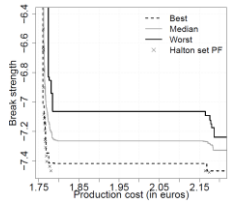
$$MEI(x_*) = \left(\hat{f}(y_{min}) - \hat{f}(x_*)\right)\Phi\left(\frac{\hat{f}(y_{min}) - \hat{f}(x_*)}{\hat{s}(x_*)}\right) + \hat{s}(x_*)\phi\left(\frac{\hat{f}(y_{min}) - \hat{f}(x_*)}{\hat{s}(x_*)}\right)$$

GP prediction of the best observed function value so far

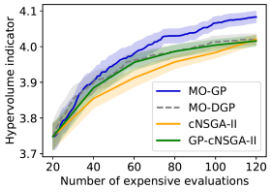
Φ –standard normal distribution
ϕ –standard normal density

13

Results



Best, median and worst Pareto front obtained for MO-GP.



The evolution of the hypervolume indicator ($mean \pm \frac{std}{\sqrt{50}}$ of 50 macro-replications

14

Results

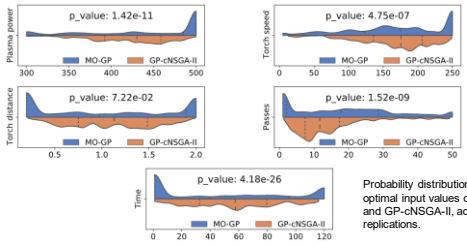
Wilcoxon's rank sum test shows a significant p value (α = 0.05) for differences between MO-GP and the other algorithms:

GP-cNSGA-II: 0,
MO-DGP: 1.0e-05,
cNSGA-II: 0

GP-cNSGA-II: 0.012,
MO-DGP: 1.8e-04,
cNSGA-II: 0.0144)

15

Results



Probability distributions of the Pareto-optimal input values obtained by MO-GP and GP-cNSGA-II, across 50 macro-replications.

16

Conclusions and future work

- The use of machine learning techniques holds great promise in solving complex and expensive optimization problems, as it allows to obtain high-quality solutions within a smaller number of experiments, compared with evolutionary algorithms
- The use of the infill criterion allows the algorithm to efficiently search for the Pareto-optimal process settings, exploiting the information that has been learned from the already observed process settings (through the GPR and LRC models)

❑ Future research will focus on the inclusion of a third objective (minimization of the debonding break strength), account for the uncertainty in the feasibility, and the deployment of an interactive tool for real lab experiments.

17

Thanks
Q & A

18