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Multi-objective simulation optimization of the adhesive bonding process of materials

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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 break 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

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Objective

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

- Uncertain performance
- Constrained optimization (feasibility)

Burned sample

Adhesive failure

Substrate failure

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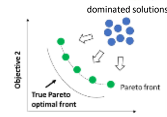
Multi-objective optimization

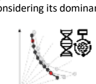
Minimizing all the objectives, the dominance of two configurations λ_1, λ_2 refers to:

- $\lambda_1 \prec \lambda_2$, λ_1 dominates λ_2 iff $f_i(\lambda_1) \le f_i(\lambda_2), \forall\, i \in \{1, \dots, m\}$, and $\exists\, i \in \{1, \dots, m\}$ such that $f_i(\lambda_1) < f_i(\lambda_2)$
- $\lambda_1 \prec\prec \lambda_2$ when λ_1 strictly dominates λ_2 iff $f_i(\lambda_1) < f_i(\lambda_2), \forall\, i \in \{1, \dots, m\}$



How to solve multi-objective problems?

1. Optimize all the objectives at the same time, considering its dominance relation



NSGA-II

2. Transform the problem (scalarization functions)

Augmented Tchebycheff scalarization function

$$\underbrace{\max_{j=1,\dots,m} \lambda_j}_{\text{Weight for objective } j}\big(f_j(x) - \underbrace{z_j^*}_{\text{Ideal value}}\big) + \underbrace{\rho}_{\text{Small positive value}} \sum_{j=1}^{m} \lambda_j\big(f_j(x) - z_j^*\big)$$

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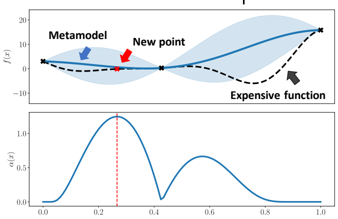
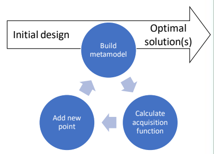
Metamodel-based optimization



Goal:
- **Assuming minimization**



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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:

predictor

Spatial correlation among the new point and the observed points

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

Observed response of the *n points*

Covariance matrix of the *n* observed points

Noise estimation for the *n* points

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

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

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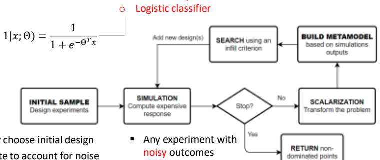
Approach

- Smartly choose next design point(s) for expensive observation
- Infill criterion: Modified Expected Improvement * Probability feasibility
  - Particle Swarm Optimization
    - Logistic classifier

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

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



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

- Any experiment with noisy outcomes
- Simulator provided by JMLab

- Augmented Tchebycheff scalarization
- Dynamically assignment of weights

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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

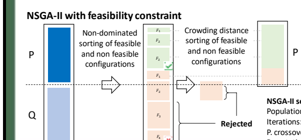
Acquisition function optimization: PSO

Swarm size: 30
Function tolerance: $1e^{-6}$
Iterations: 1800
Max stall iterations: 10

MO-GP setting:

Covariance function: Gaussian
Initial design size: 30 (LHS)
Iterations: 180

NSGA-II with feasibility constraint



Expensive evaluations for NSGA-II and GP (budget): **210**
Comparison metric: Hypervolume indicator

NSGA-II setting:
Population size: 10
Iterations: 20
P. crossover: 0.9
P. mutation: 0.5

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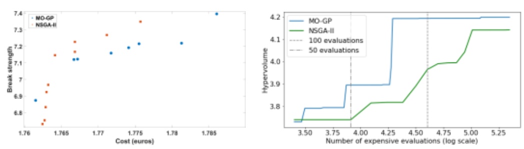
Results



MO-GP converges to a hypervolume that is superior to the one obtained with NSGA-II, requiring only a fraction of the allowed function evaluations

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Conclusions and future work

- Machine Learning techniques allows to obtain high-quality solutions within a smaller number of experiments, compared with a popular and well-known algorithm such as NSGA-II.
- 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 development of an interactive software tool, allowing lab experts to validate the results generated by the algorithm in a real-life test environment, and to apply this type of algorithm also to other process optimization problems.

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