Surrogate Model for Mixed-Variables Evolutionary Optimization based on GLM and RBF Networks

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Optimization of empirical functions

optimization:

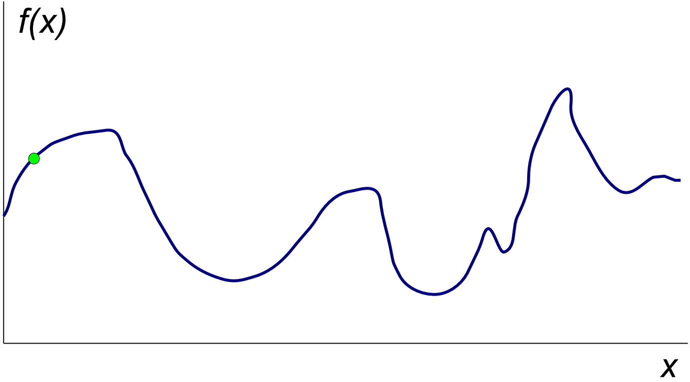
- S – set of feasible solutions, $f(x)$ – objective function
- **optimization** (minimization) is finding such $x^\star \in S$ that

$$f(x^\star) = \min_{\forall x \in S} f(x)$$

empirical objective functions:

- costly and/or time demanding evaluation of suggested solutions
- **cost** of the whole optimization measured by the resources spent on evaluations (time, money,...)
- discrete and continuous variables expected: $S = (\mathbf{S}^{(\mathrm{D})}, \mathbf{S}^{(\mathrm{C})})$

Optimization of empirical functions



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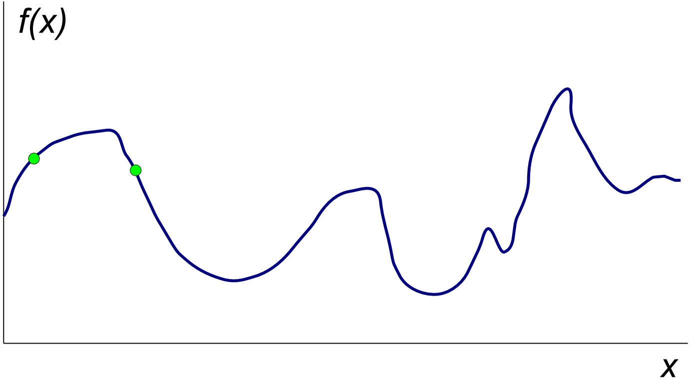

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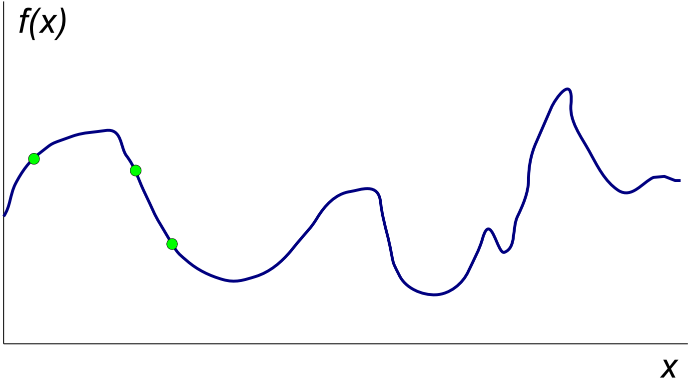

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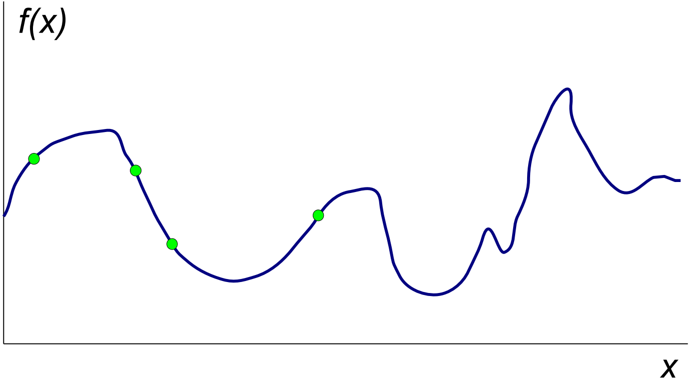

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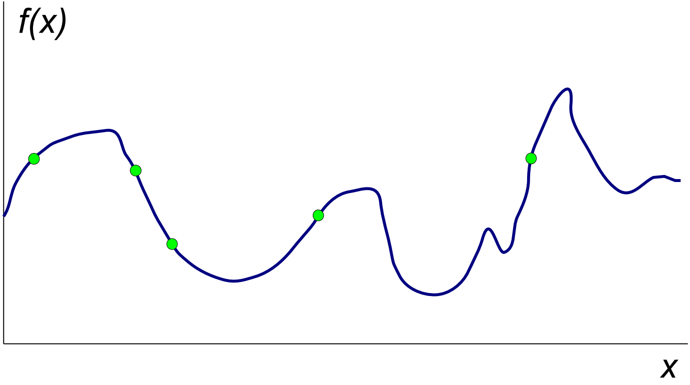

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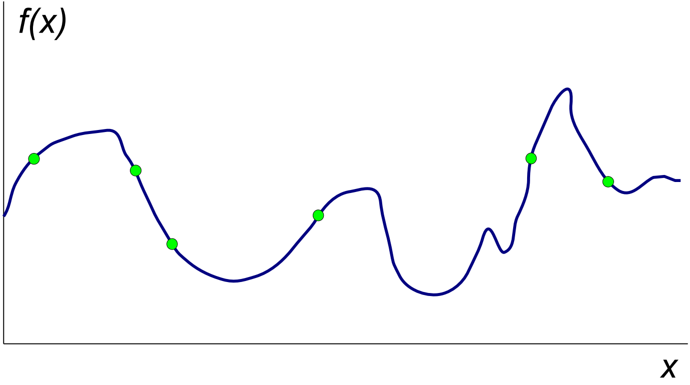

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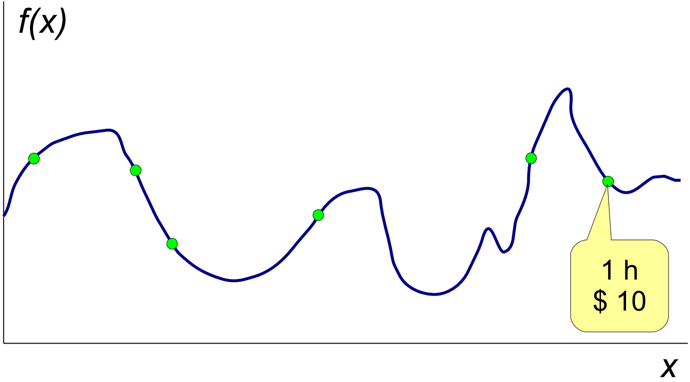

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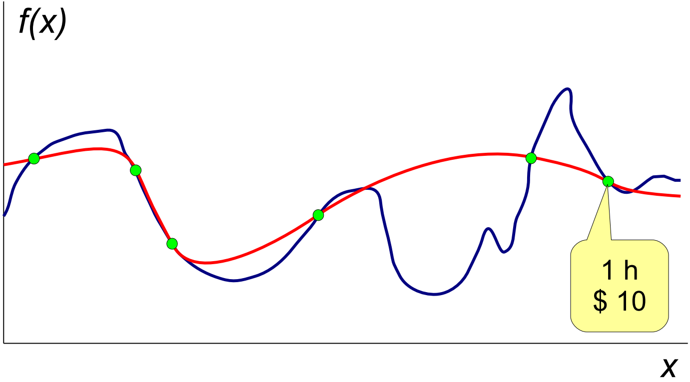

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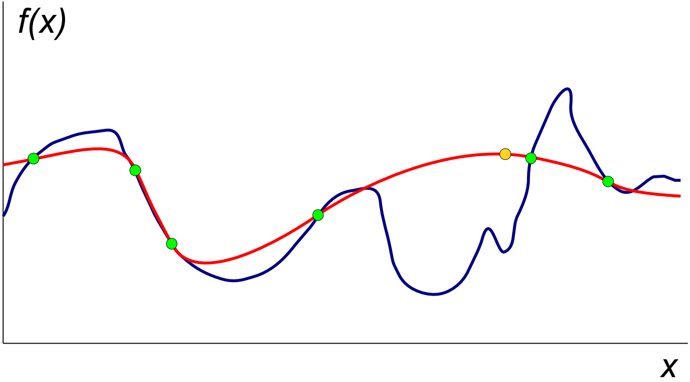

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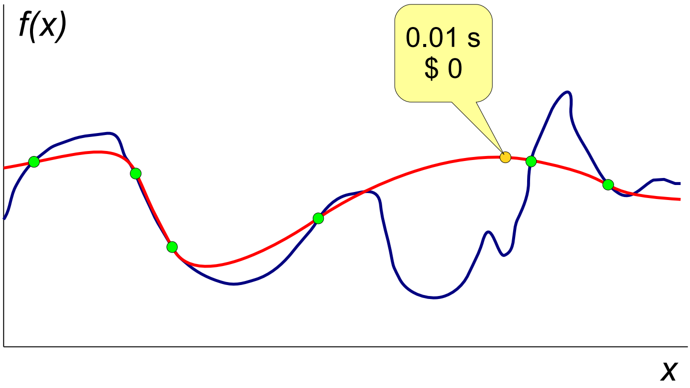

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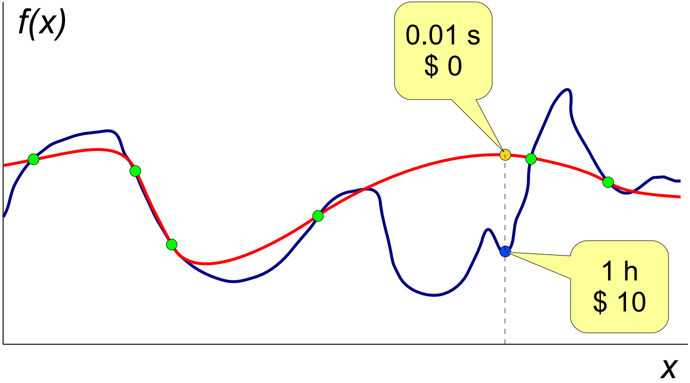

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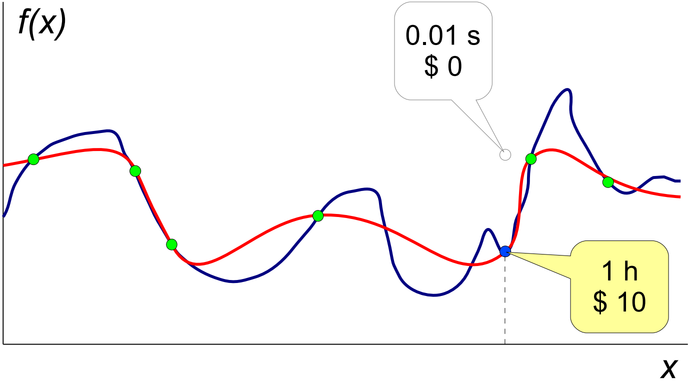


Surrogate models of objective functions

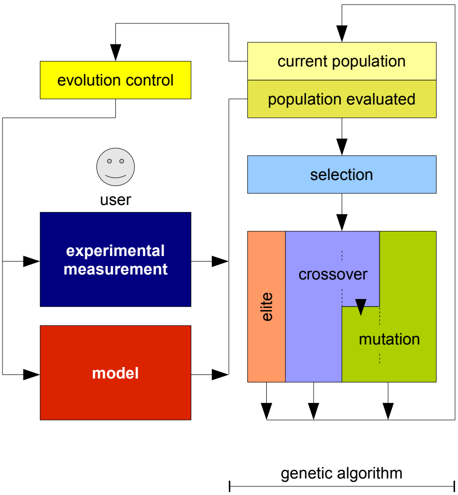
General idea

- usually evaluate suggested solutions with a cheap regression model
- use the original measurements to focus the search and ensure the true evaluation of the best found solution

- $(-)$ surrogate model is an approximation of the original fitness – almost always more or less **inaccurate**
- $(+)$ very fast and **cheap**
- **learning** from new measured results of experiments

Genetic algorithm and surrogate model

- genetic algorithm used as an optimization technique
- two kinds of fitness evaluation
  - experimental measurement (blue)
  - model fitness (red)



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Regression model

requirement: both for continuous ($\mathbf{S}^{(\mathrm{D})}$) and discrete ($\mathbf{S}^{(\mathrm{D})}$) variables

- **continuous variables**: RBF network(s)
- **discrete variables**: GLM

RBF networks

RBF network

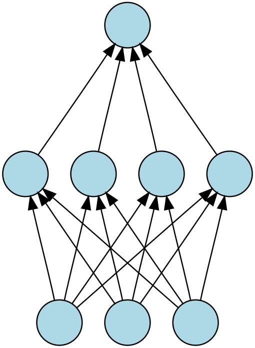
$$f(\mathbf{x}) = \sum_{i=1}^{g} \pi_i f_i(||\mathbf{x} - \mathbf{c}_i||)$$

composed of

- g Gaussian radial components $f_1, \ldots, f_g$ with variable widths w_i

$$f_i(||\mathbf{x} - \mathbf{c}_i||) = \mathrm{e}^{||w_i(\mathbf{x} - \mathbf{c}_i)||}$$

- variable centers $\mathbf{c}_i \in \mathbb{R}^n$
- components' weights $\pi_1, \ldots, \pi_g$



(Generalized) Linear Models

GLM

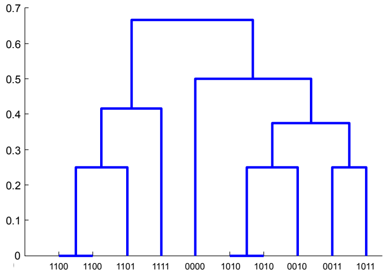
$$\hat{y} = g^{-1}\left(\sum_{j=0}^{d} x_j \beta_j\right)$$

- independent observed values Y;
  assumed from an exponential-family distribution
- explanatory variables $(x_1, x_2, \ldots, x_d)$ transformed through a linear model with parameters $\beta_1, \ldots, \beta_d$
- link function g connects the random and systematic component, depends on the distribution

Model construction – (1) clustering

clustering of the discrete data (in $\mathbf{S}^{(\mathrm{D})}$)

- similar discrete combinations are grouped into the same cluster
- hierarchical clustering with guaranteed minimal size
- m – the number of clusters



Model construction – (2) RBF networks

RBF networks

- trained on continuous parts of each such a cluster
- for $k = 1, \ldots, m$

$$\hat{f}^{(k)}_{\mathrm{DSCL}} : \mathbf{S}^{(\mathrm{C})} \to \mathbf{R}$$

- the best number of components $g^\star$ chosen by cross-validation
- for evaluation on a new $\mathbf{x}$
  - the nearest cluster $k^\star$ is identified (from discrete part)
  - its RBF network's value is computed (from continuous part):

$$\hat{f}^{(k^\star)}_{\mathrm{DSCL}}(\mathbf{x}^{(\mathrm{C})}) = \sum_{i=1}^{g^\star} \pi_{k^\star,i} f_{k^\star,i}(||\mathbf{x}^{(\mathrm{C})} - \mathbf{c}_{k^\star,i}||)$$

Model construction – (3) GLM model

GLM model

- model of the residuals

$$\hat{f}_{\mathrm{GLM}} : \mathbf{x}^{(\mathrm{D})} \to (y - \hat{f}_{\mathrm{DSCL}}(\mathbf{x}^{(\mathrm{C})}))$$

- trained on the discrete variables (explanatory variables)

$$\hat{f}_{\mathrm{GLM}} : \mathbf{S}^{(\mathrm{D})} \to \mathbf{R}$$

- dummy or integer coding of discrete variables
- residuals assumed from Gaussian, inverse Gaussian or gamma distribution – the best option is chosen via cross-validation

Model construction

final model

$$\hat{f} : (\mathbf{S}^{(\mathrm{D})}, \mathbf{S}^{(\mathrm{C})}) \to \mathbf{R}$$

- sum of the responses of the two previous models

$$\hat{f}(\mathbf{x}) = \hat{f}^{(k)}_{\mathrm{DSCL}}(\mathbf{x}^{(\mathrm{C})}) + \hat{f}_{\mathrm{GLM}}(\mathbf{x}^{(\mathrm{D})}).$$

evaluation of the final model:

1. identify the nearest cluster $k^\star$
2. compute response of the corresp. $k^\star$-th RBF network $\hat{y}_{\mathrm{DSCL}}$
3. get the value of the GLM model $\hat{y}_{\mathrm{GLM}}$
4. sum these two values $\hat{y} = \hat{y}_{\mathrm{DSCL}} + \hat{y}_{\mathrm{GLM}}$

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Experimental results

Task 1: Data from HCN production

- results from a real application of genetic algorithms: finding the best catalyst for production of HCN
- 11 continuous, 1 discrete and 11 binary variables
- 555 different discrete combinations within 696 datapoints
- training of the model only

Experimental results

Task 2: Benchmark function

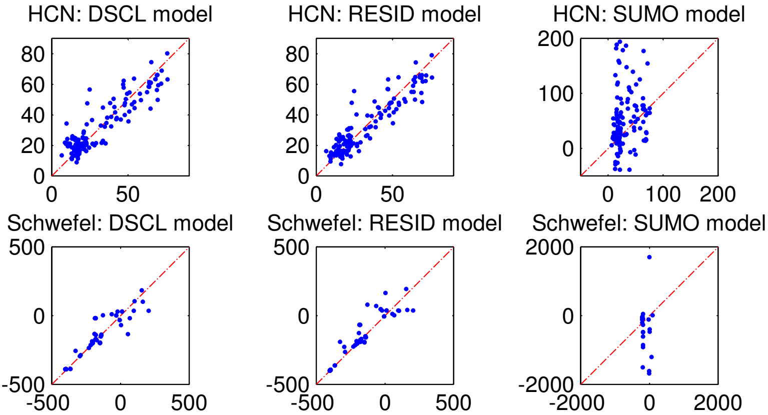
- individuals from the first 10 generations of a run of GA
- modified Schwefel's benchmark function
$$y = \frac{1}{p} \sum_{i=1}^{p} -x_i \sin(\sqrt{|x|})$$
- discrete variables added
$$(x_1^{(\mathrm{D})}, \dots, x_p^{(\mathrm{D})}) \in \{-10, -9, \dots, 10\}$$
- easy to compute for any arbitrary point – possible to test with genetic algorithm

Experimental results

Table: Surrogate-models' regression results on HCN and Schwefel dataset, average results from 50 trainings. RMSE on the testing and training set.

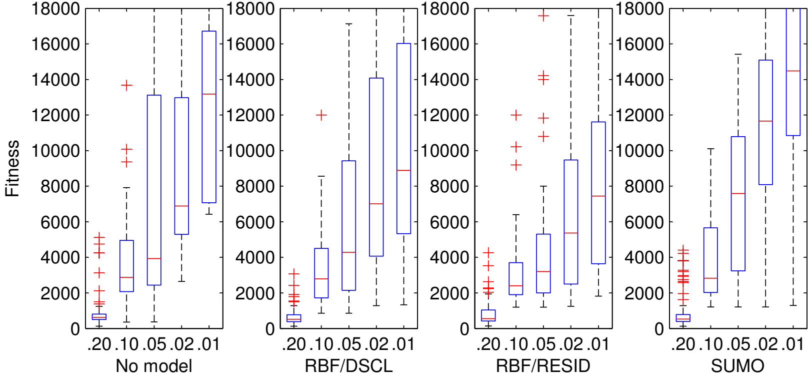
dataset	model	RMSE (test set)	RMSE (train set)
HCN	DSCL	8.2918 ± 0.4373	7.6337
	RESID	$\mathbf{7.6212} \pm \mathbf{0.3187}$	6.6131
	SUMO	115.196 ± 34.1387	**0.5711**
Schwefel	DSCL	62.712 ± 3.4248	83.553
	RESID	$\mathbf{55.605} \pm \mathbf{5.4867}$	73.468
	SUMO	$64576 \pm 1.9e{+}05$	**33.964**

Model fitting



Scatter plots of the DSCL, RESID and SUMO's RBF models on testing data

Benchmark fitness: genetic optimization



The numbers of original evaluations needed to reach 1.2-, 1.1-, 1.05-, 1.02- and 1.01-multiple of minimum, measured on 100 GA runs

Conclusion

Contributions of the work

- detailed description of a surrogate model for genetic optimization
- surrogate model with RBF networks and GLMs, for both continuous and discrete values

Experimental results

- model exhibits significantly lower testing error than competing RBF networks from SUMO toolbox
- utilizing the model on the benchmark fitness saved up to 35 per cent of empirical function evaluations

Conclusion

Thank you for your attention.

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