# Data-Driven Evolutionary Optimization of Complex Systems: Big vs Small Data

**Yaochu Jin**

Head, Nature Inspired Computing and Engineering (NICE)

Department of Computer Science, University of Surrey, United Kingdom

yaochu.jin@surrey.ac.uk

# Outline

UNIVERSITY OF SURREY

- Complexity in evolutionary optimization of real-world problems
- Data driven evolutionary optimization
  - Offline (Big) data driven evolutionary optimization
  - Online small data driven evolutionary optimization
- Concluding remarks

# Strengths and Weaknesses of EAs for Optimization

UNIVERSITY OF SURREY

- No need for analytical objective functions and no requirement for derivative information
- Less vulnerable to local optimums
- Less vulnerable to uncertainty (relative quality is more important)
- Well suited for multi-objective optimization
- No theoretical guarantee for global optimum
- Population based search -- computationally intensive

# Complexities in Real-World Optimization

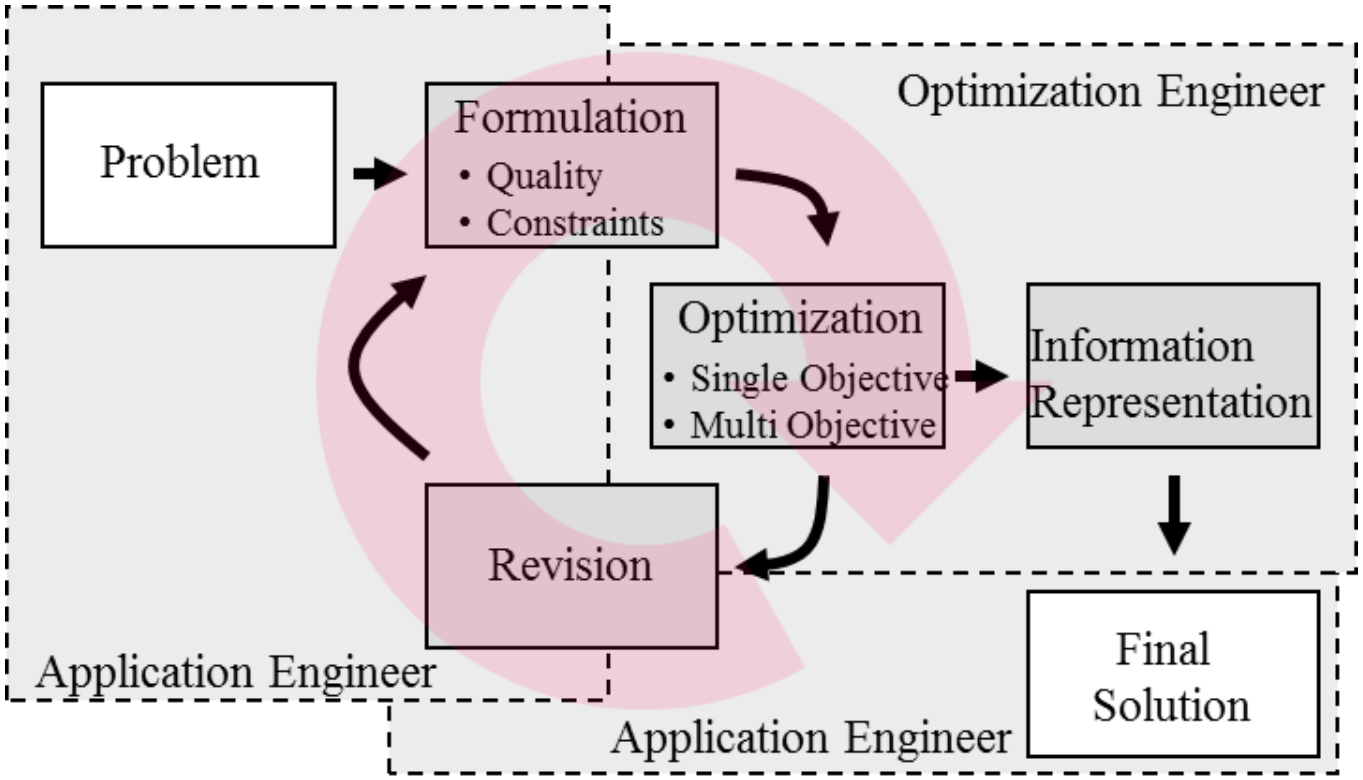
UNIVERSITY OF SURREY

- Complexity in problem formulation and solution representation
- Complexity in scale
  - Large number of decision variables
  - Large number of objectives
- Complexity in handling uncertainty
- Complexity in quality evaluation

UNIVERSITY OF SURREY

# Complexity in Problem Formulation and Solution Representation

# Complexity in Problem Formulation

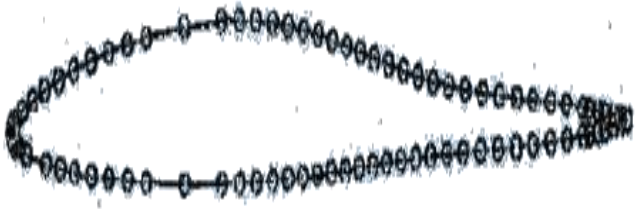


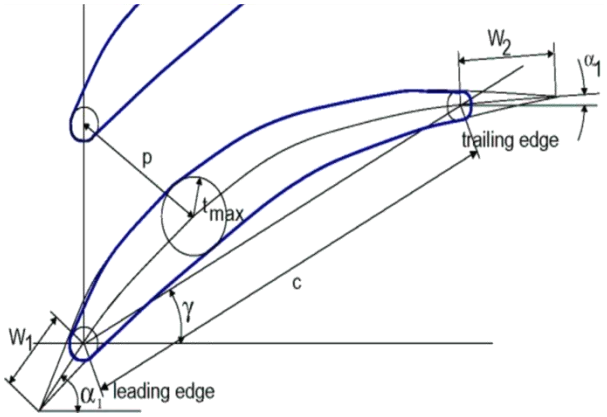

- The formulation of the objective function is an iterative process
- Representation is critical : multiple sub-systems, optimization-control coupling
- Different objectives/ constraints / decision variables may have to be considered / weighted differently at different stages
- Different resources are available at different stages

# Complexity in Shape Representation

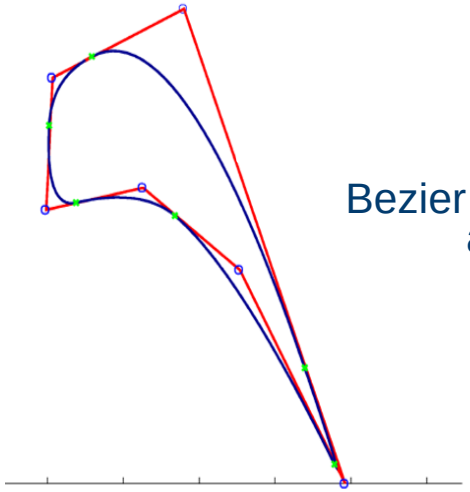
Expert Knowledge

Direct representation

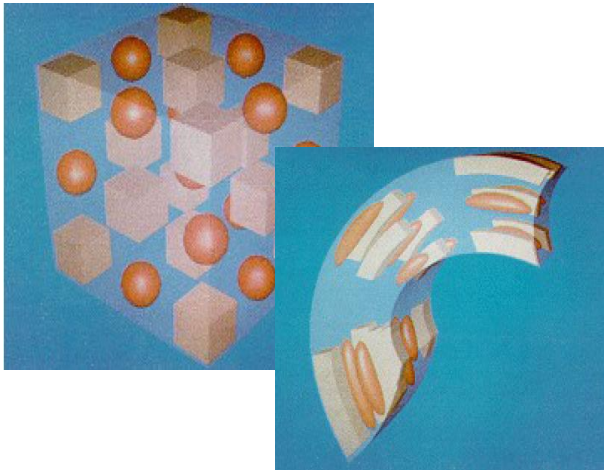




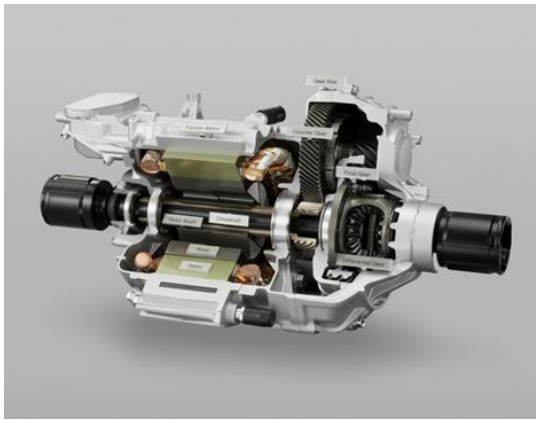

Free Form Deformation(FFD)

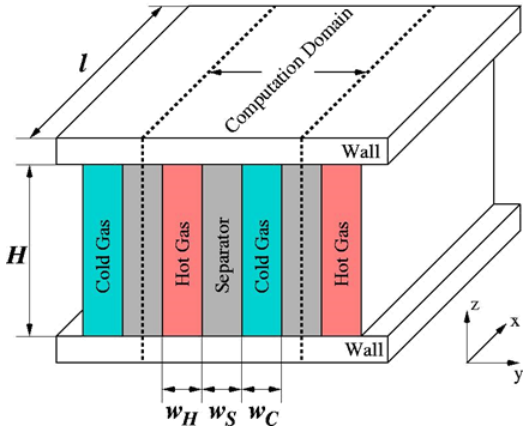


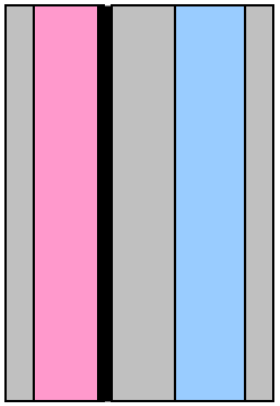
Bezier Curves, B-Splines and NURBS

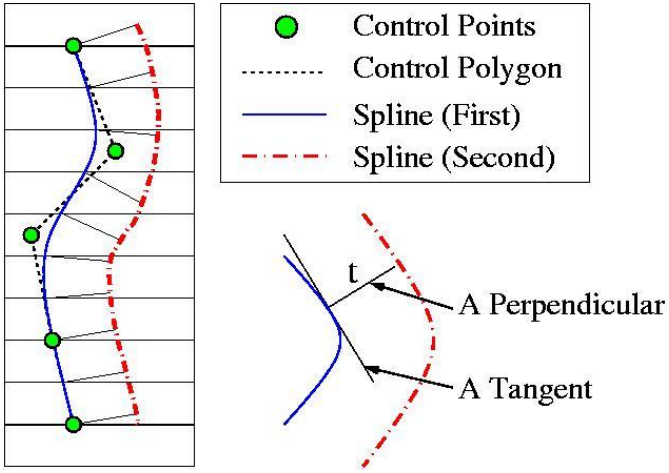


# Shape Representations in Micro Heat Exchanger

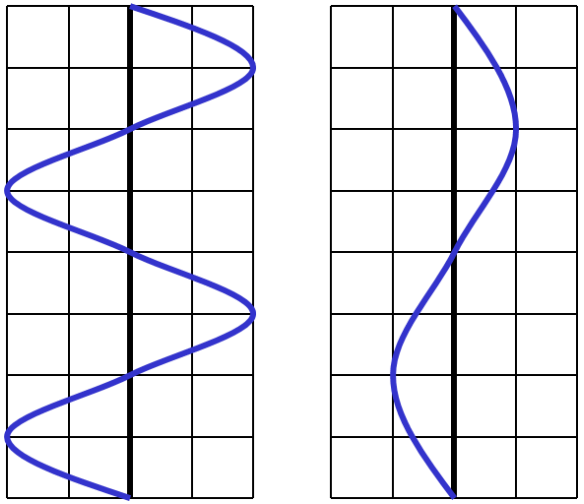




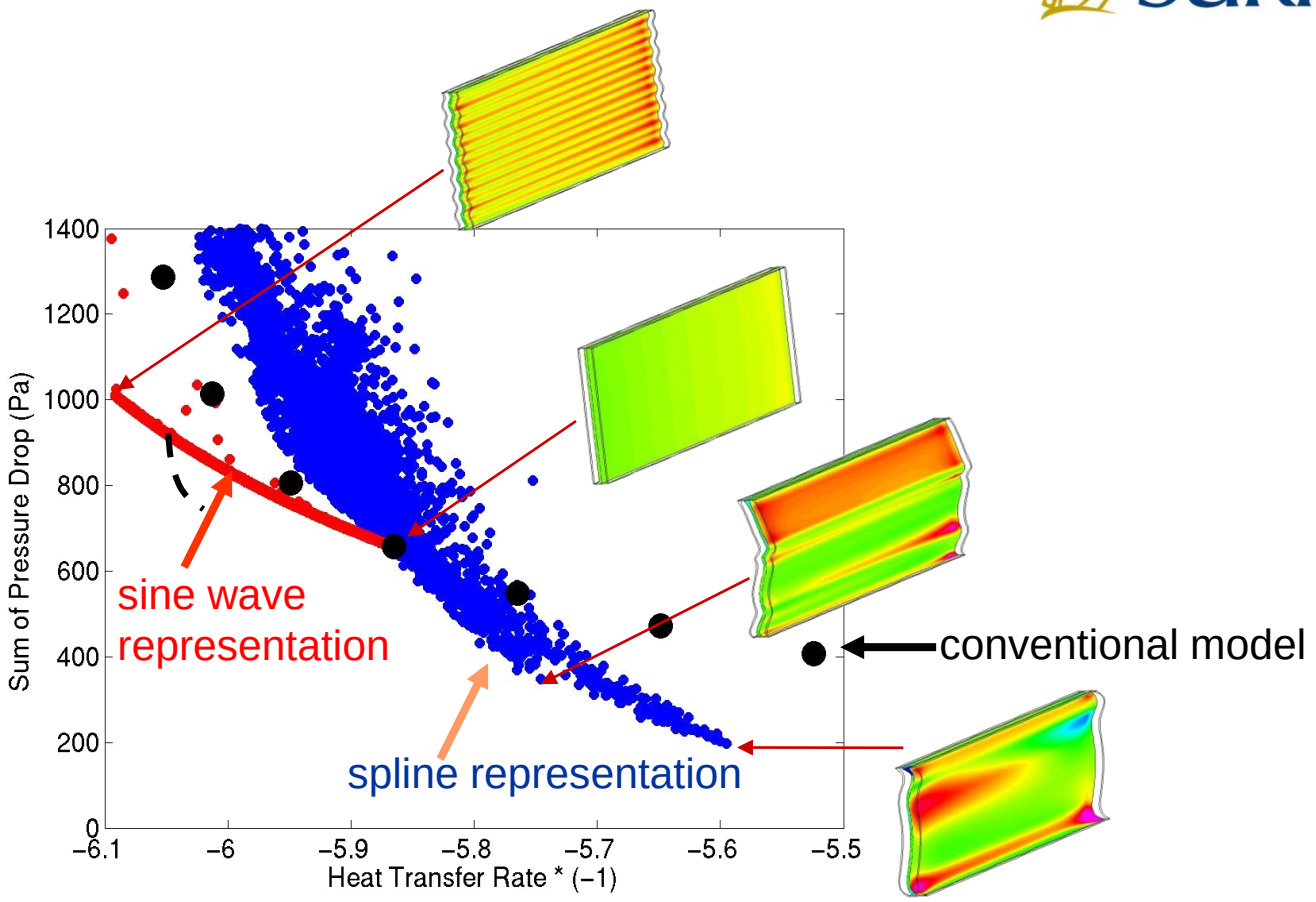




A Spline representation



A frequency-amplitude representation

# Micro Heat Exchanger Optimization - Results




- Maximize the heat transfer rate (thermodynamic)
- Minimize the sum of pressure drop with a penalty (aerodynamic)

UNIVERSITY OF SURREY

# Complexity in Scale: Large Decision and Objective Space

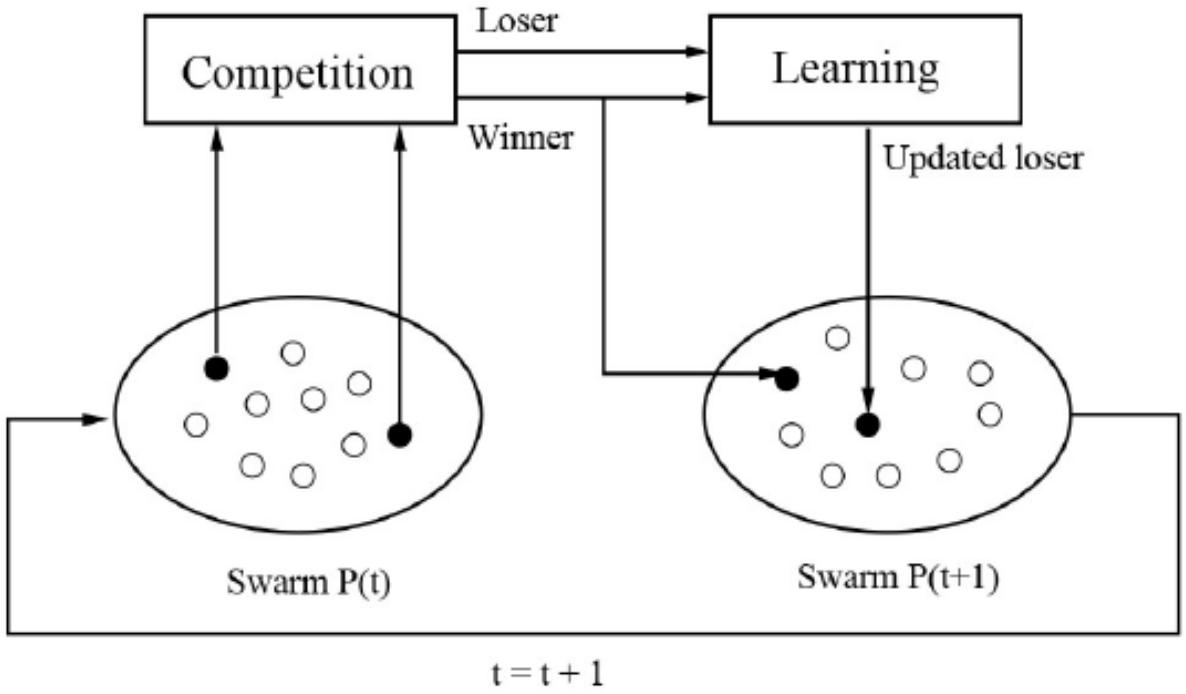
# Swarm Intelligence for Large-Scale Optimization

UNIVERSITY OF SURREY

- Large-scale evolutionary optimization
  - Divide and conquer by random grouping
  - Detection of correlation between decision variables
  - **A competitive swarm optimizer (CSO)**
  - **A social-learning based particle swarm optimizer (SL-PSO)**

R. Cheng and **Y. Jin**. A competitive swarm optimizer for large-scale optimization. *IEEE Transactions on Cybernetics*, 45(2):191-205, 2015
R. Cheng and **Y. Jin**. A social learning particle swarm optimization algorithm for scalable optimization. *Information Sciences*, 291:43-60, 2015

# Competitive Swarm Optimization（CSO）

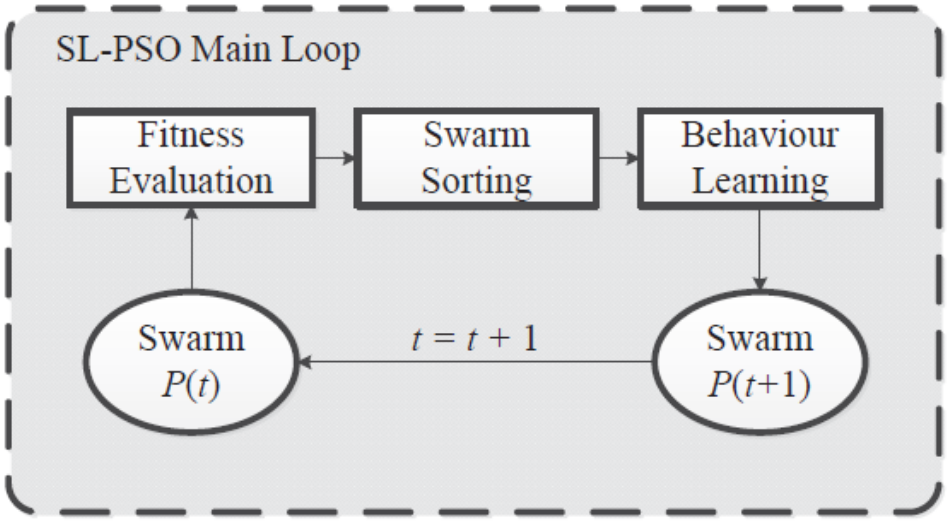


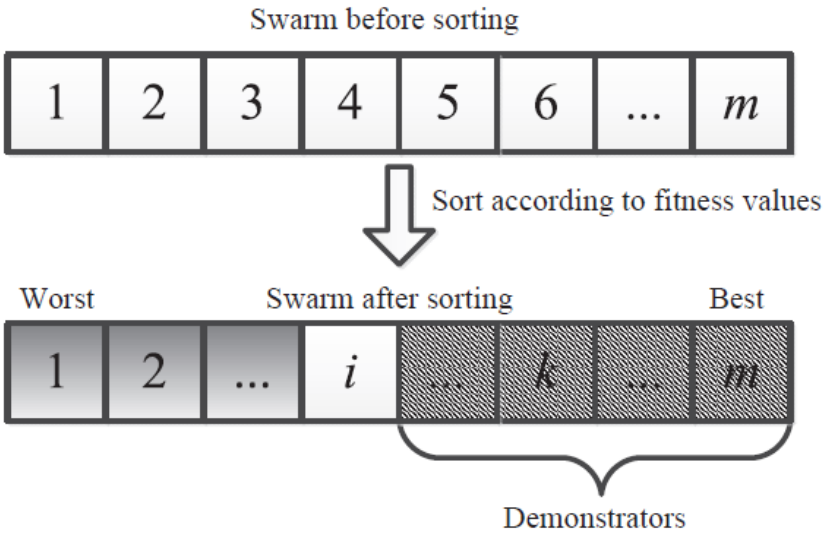

- Randomly pick two solutions
- Compare their fitness. The winner is directly passed to the next generation while the loser will be updated as follows:

$$V_{l,k}(t+1) = R_1(k,t)V_{l,k}(t) + R_2(k,t)(X_{w,k}(t) - X_{l,k}(t)) + \varphi R_3(k,t)\left(\bar{X}_k(t) - X_{l,k}(t)\right)$$

- Neither global nor personal best is used

# A Social Learning PSO (SL-PSO)




$$X_{i,j}(t+1) = \begin{cases} X_{i,j}(t) + \Delta X_{i,j}(t+1), \text{ if } p_i(t) \le P_i^L \\ X_{i,j}(t), \text{ otherwise} \end{cases} \qquad 0 \le p_i(t) \le P_i^L \le 1$$

$$\Delta X_{i,j}(t+1) = r_1(t) \cdot \Delta X_{i,j}(t) + r_2(t) \cdot I_{i,j}(t) + r_3(t) \cdot \epsilon \cdot C_{i,j}(t),$$

$$\begin{cases} I_{i,j}(t) = X_{k,j}(t) - X_{i,j}(t), \\ C_{i,j}(t) = \bar{X}_j(t) - X_{i,j}(t). \end{cases}$$

# Large Number of Objectives – Many-Objective Optimization

- Computational challenges
  - Calculation of performance some indicators becomes intractable
- Performance degradation
  - Loss of selection pressure in Pareto-based approaches
- Solution assessment becomes tricky
  - The performance become very sensitive and also easily biased
  - Solution sets are no loner comparable
  - Diversity becomes trickier to measure
- Can we still be able to find a “representative” subset of the Pareto front?

B. Li, J. Li, K. Tang, and X. Yao. Many-objective evolutionary algorithms: A survey. *ACM Computing Surveys*, 48:13–35, 2015
H. Ishibuchi, N. Tsukamoto, and Y. Nojima. Evolutionary manyobjective optimization: A short review. In: *Proceedings of IEEE Congress on Evolutionary Computation*, pages 2419–2426. IEEE, 2008
H. Wang, Y. Jin and X. Yao. Diversity assessment in many-objective optimization. *IEEE Transactions on Cyber*netics, 2016 (accepted)

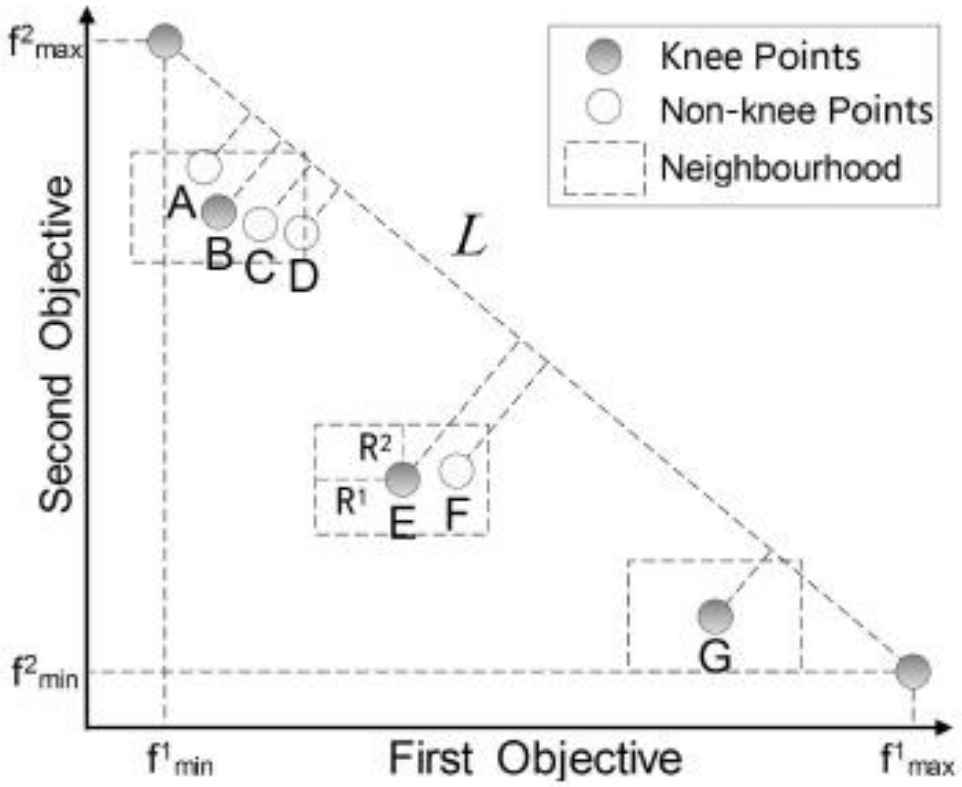
# Evolutionary Many-Objective Optimization

UNIVERSITY OF SURREY

EAs for solving MaOPs may largely be divided into the following categories:

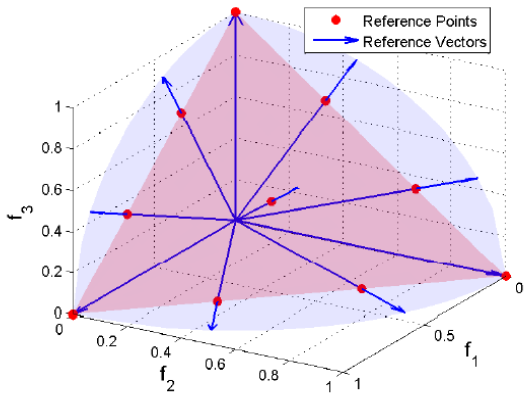
- **Preference based**, including decomposition approaches
- **Convergence acceleration**, mainly by modifying the dominance relationship or by **including additional criteria**
- Performance indicator based

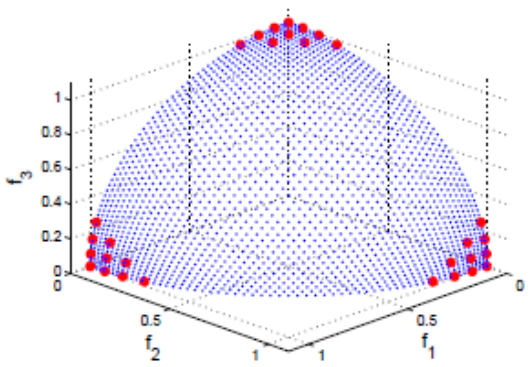
# Use of "Knee-Points" to Accelerate Convergence

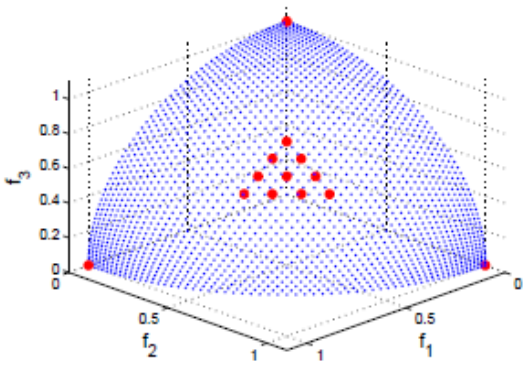



X. Zhang, Y. Tian, and Y. Jin, A Knee Point Driven Evolutionary Algorithm for Many-Objective Optimization. *IEEE Transactions on Evolutionary Computation*, 19(6):761-776, 2015

# Specification of Preferences



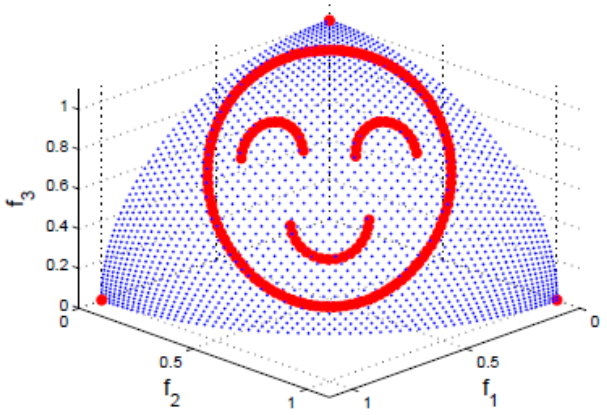




Angle-penalized distance (APD):

$$d^j = (1 + P(\theta^j)) \cdot ||\bar{f}^j||,$$

$$P(\theta^j) = k \cdot (\frac{t}{t_{max}})^\alpha \cdot \frac{\theta^j}{\gamma_v},$$




R. Cheng, Y. Jin, M. Olhofer and B. Sendhoff. A reference vector guided evolutionary algorithm for many-objective optimization. *IEEE Transactions on Evolutionary Computation*, 2016 (Accepted)

# Efficient Non-Dominated Sorting

UNIVERSITY OF SURREY

- Non-dominated sorting becomes extremely time-consuming in case of
  - A large population size
  - A large number of objectives

- Computationally efficient non-dominated sorting
  - **ENS**: An efficient non-dominated sorting algorithm for 2 or 3 objectives with a large population size
  - **A-ENS**: An approximate non-dominated sorting for many objectives
  - **T-ENS**: An accurate tree-based non-dominated sorting for large-scale many-objective optimization

X. Zhang, Y. Tian, R. Cheng, and **Y. Jin**. An efficient approach to non-dominated sorting for evolutionary multi-objective \ optimization. *IEEE Transactions on Evolutionary Computation*, 19(2):201-213, 2015
X. Zhang, Y. Tian, **Y. Jin**. Approximate non-dominated sorting for evolutionary many-objective optimization. *Information Sciences*, 2016 (accepted)
X. Zhang, Y. Tian, R. Cheng, **and Y. Jin**. A decision variable clustering-based evolutionary algorithm for large-scale many-objective optimization. 2016 (Submitted)

**Code for the ENS variants available!**

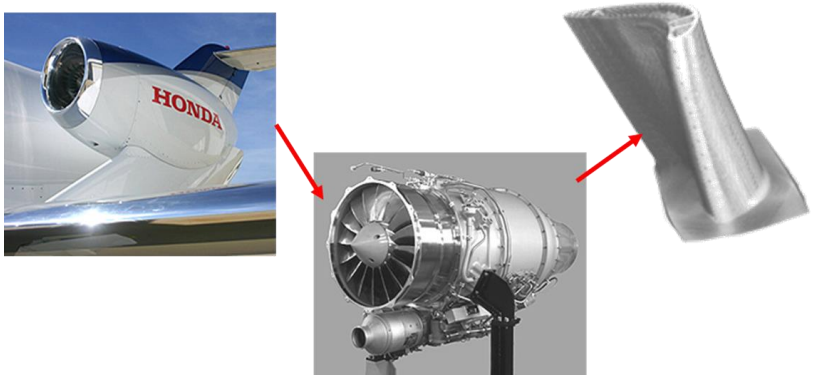
UNIVERSITY OF SURREY

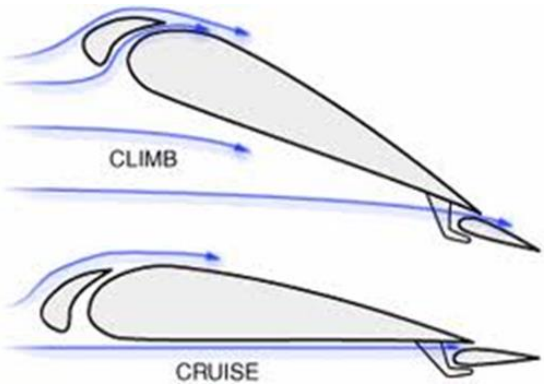
# Complexity in Quality Evaluation

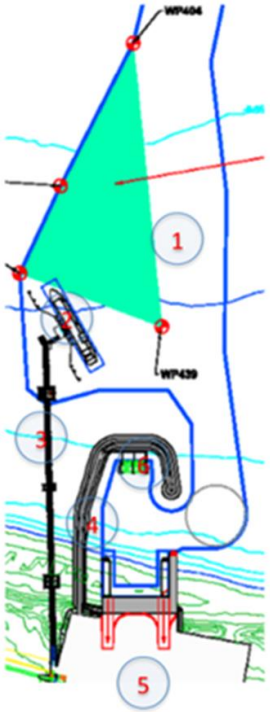
# Complexity in Quality Evaluation

UNIVERSITY OF SURREY

- An analytic fitness function is not available
  - Very time-consuming numerical simulations
  - Expensive experiments
  - History production data only





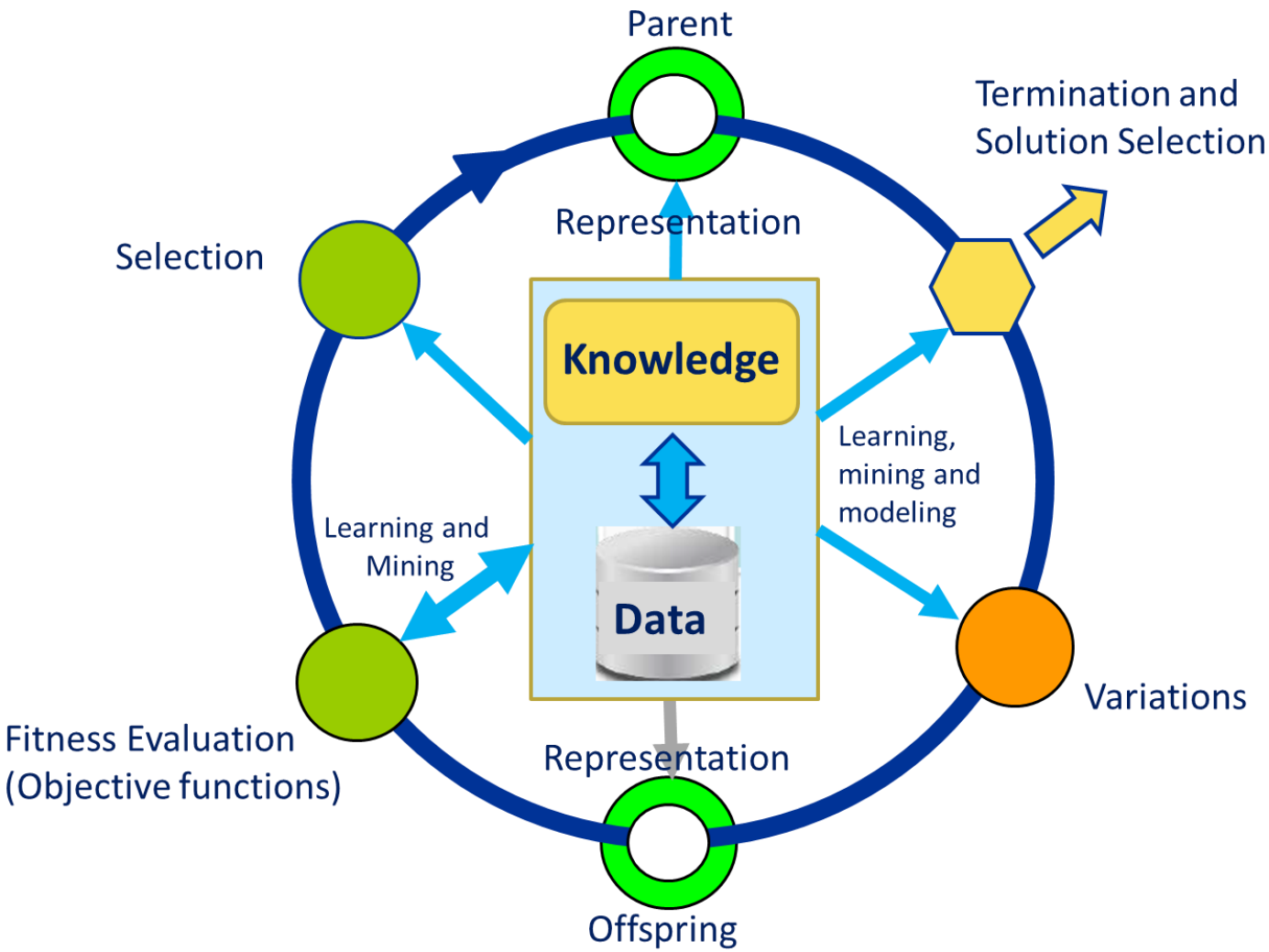



UNIVERSITY OF SURREY

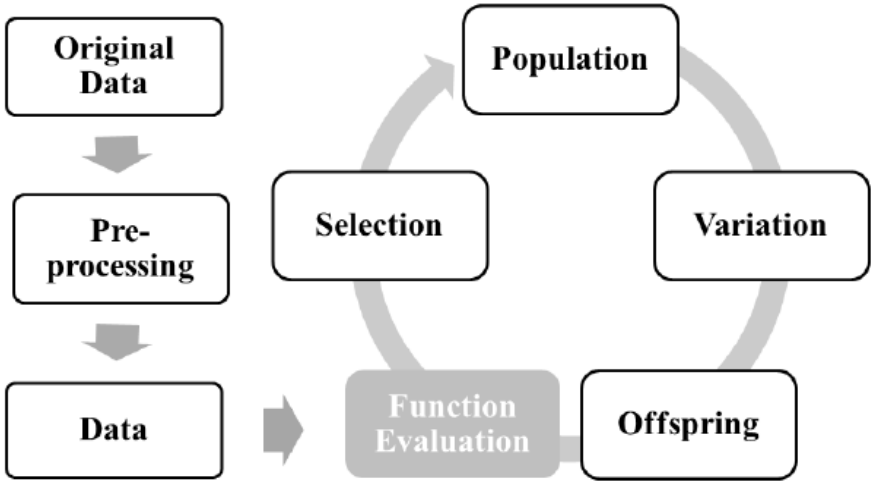
# Data Driven Evolutionary Optimization

# Data Driven Evolutionary Optimization

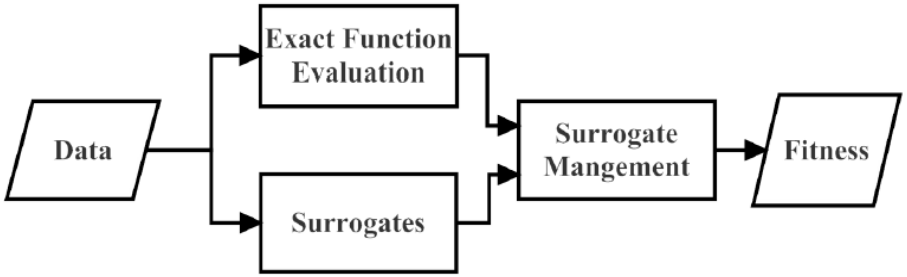
UNIVERSITY OF SURREY



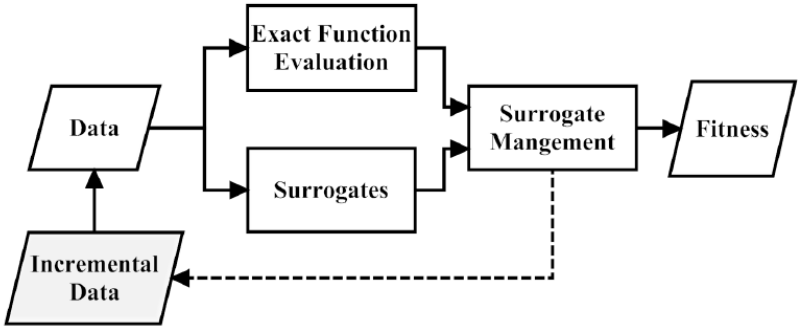
# Data Driven Optimization – Offline and Online




Data-driven evolutionary optimization




Offline data-driven optimization




Online data-driven optimization

H. Wang, Y. Jin and J. O. Jansen. Data-driven surrogate-assisted multi-objective evolutionary optimization of a trauma system. *IEEE Transactions on Evolutionary Computation*, 2016 (accepted)

UNIVERSITY OF SURREY

# Offline (Big) Data Driven Evolutionary Optimization

# Data Driven Evolutionary Trauma System Design

UNIVERSITY OF SURREY

## Scottish Trauma system design

**Major trauma centre (MTC)**

- A specialist hospital responsible for providing a regional or national service for patients with major trauma.

**Trauma unit (TU)**

- A trauma unit is a hospital which manages less severely injured patients.

**Local emergency hospital (LEH)**

- A local emergency hospital is a hospital which only deals with minor injuries.

H. Wang, Y. Jin and J. O. Jansen. Data-driven surrogate-assisted multi-objective evolutionary optimization of a trauma system. *IEEE Transactions on Evolutionary Computation*, 2016 (accepted)

# Data Driven Evolutionary Trauma System Design

UNIVERSITY OF SURREY

**Objective 1**: Minimize total travel time

**Objective 2**: Minimize the exceptions number (the cases "triaged-to-MTC" diverted to a TU)

**Constraint 1**: Number of helicopter transfers

**Constraint 2**: MTC case volume

**Constraint 3**: TU proximity to avoid two close TUs

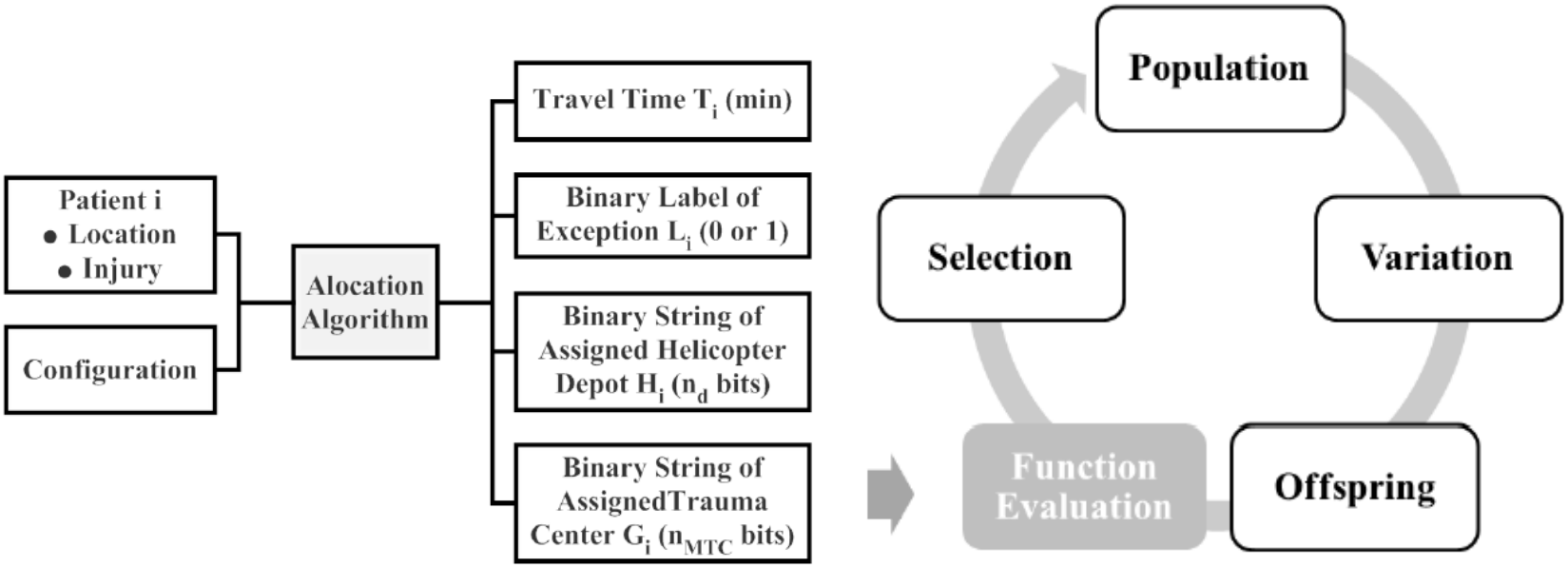
**Main research question is**: how to reduce computational time given the large amount of data (the amount of data could be much larger)?

- The EA is able to find the Pareto optimal solutions
- The computation time can be reduced as much as possible

# Data Driven Evolutionary Trauma System Design

UNIVERSITY OF SURREY

- **40,000** incident records (location, injury, patient)
- 18 trauma centers in Scotland

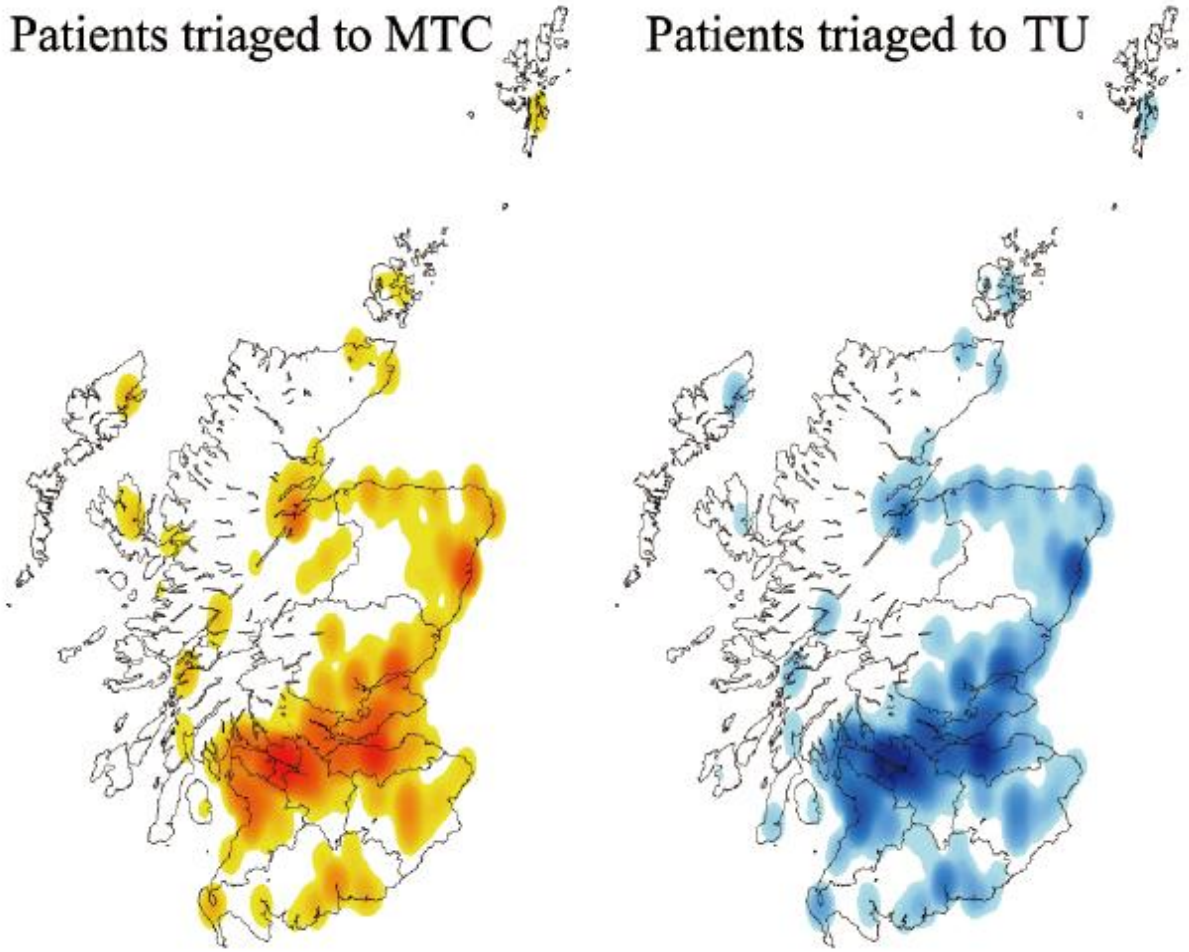



- **Fitness evaluations is highly time-consuming when the number of records is huge**

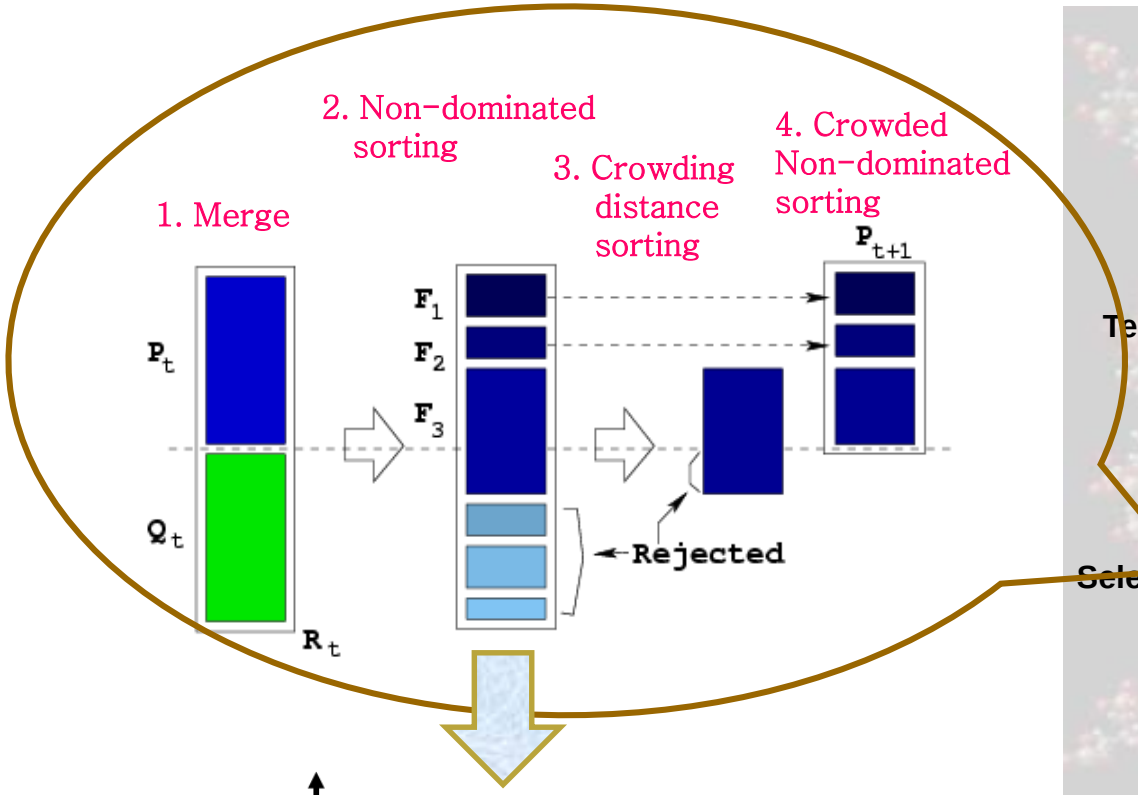
# Data Driven Evolutionary Trauma System Design

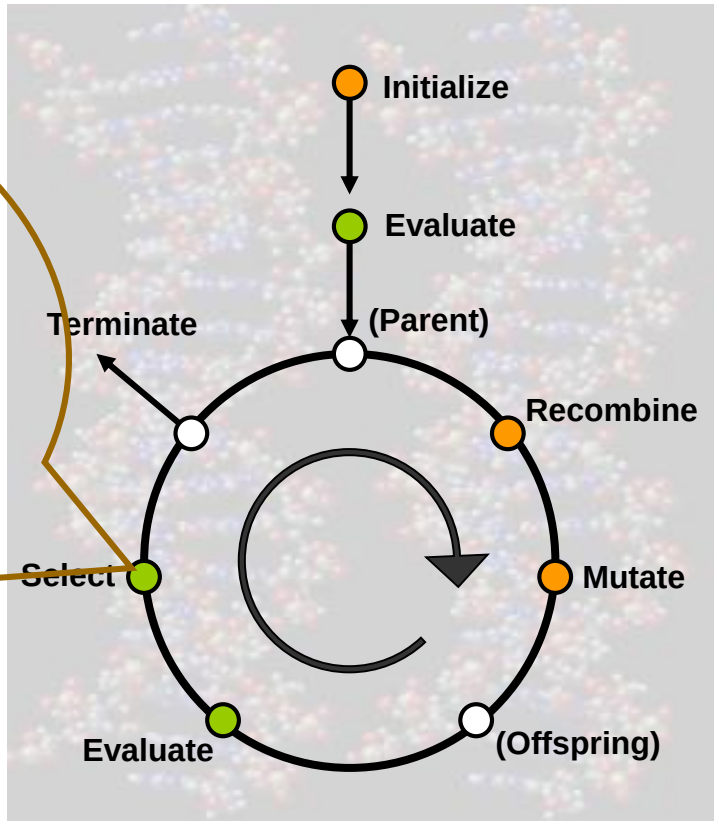
UNIVERSITY OF SURREY

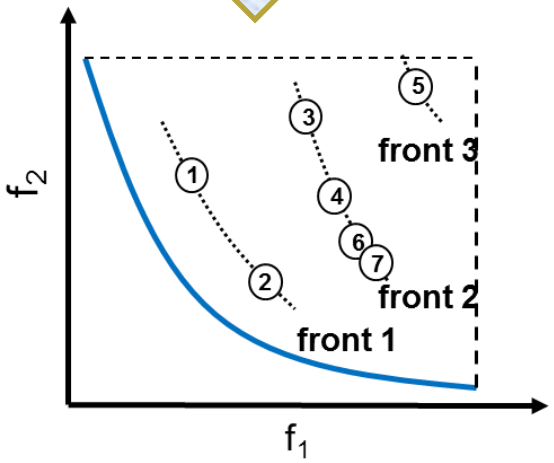
## Distribution of the patient records



# Elitist Non-dominated Sorting GA (NSGA-II)



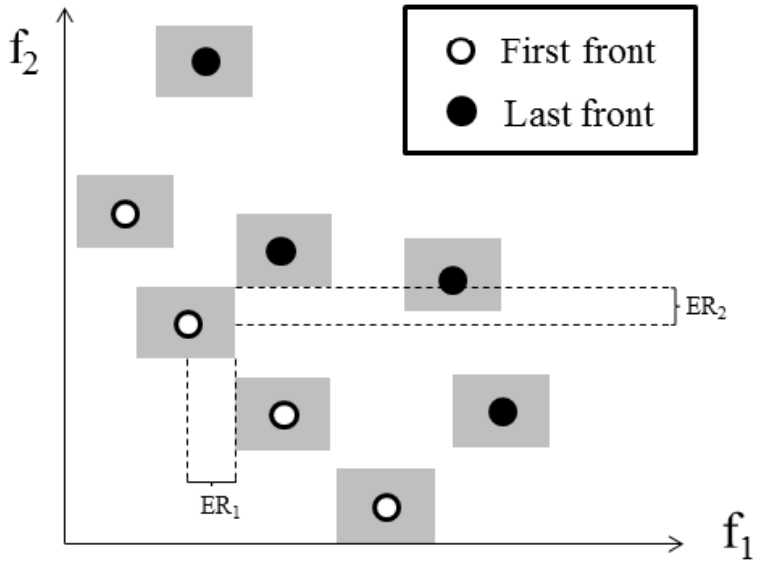

Non-dominated sorting

# Data Driven Evolutionary Trauma System Design

UNIVERSITY OF SURREY

Solution

- Group the data into a number of clusters and use the cluster centers to evaluate the objective and constraint functions
- How to make sure the accuracy is good enough?




First and last front of individuals to be selected

Estimated error for a given number of clusters:

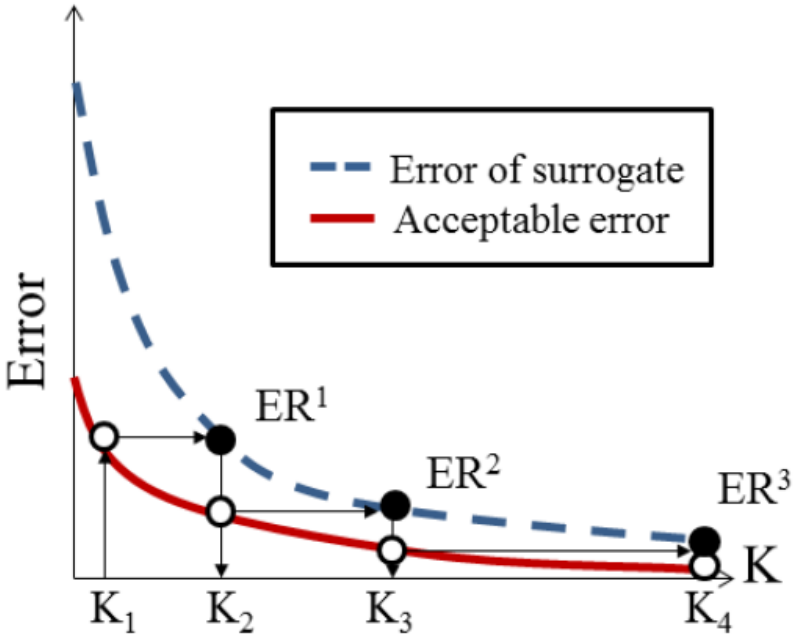
$$ER = \frac{1}{\beta_1 + \beta_2 K},$$

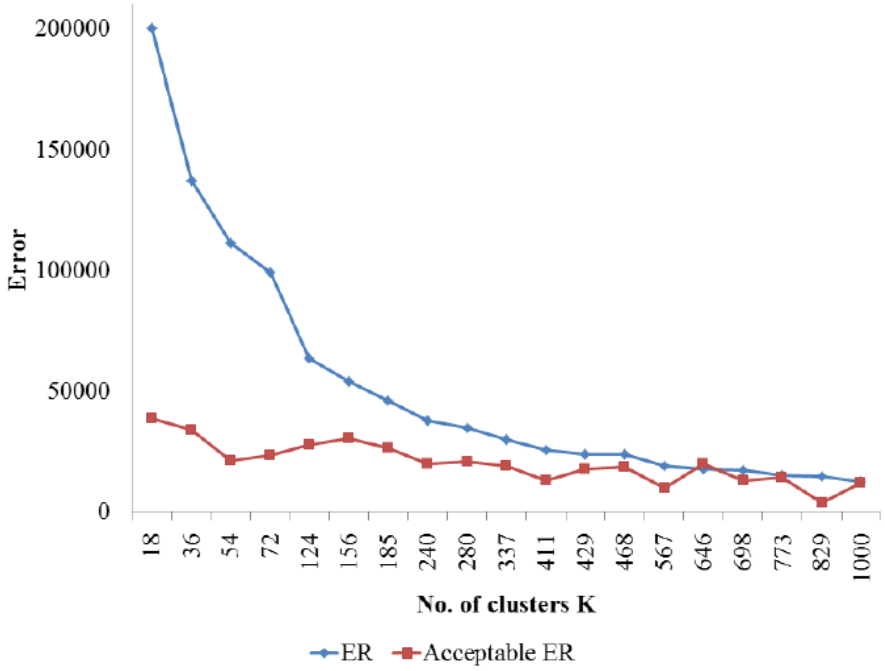
- The maximum error should not change the individuals to be selected

# Data Driven Evolutionary Trauma System Design

UNIVERSITY OF SURREY

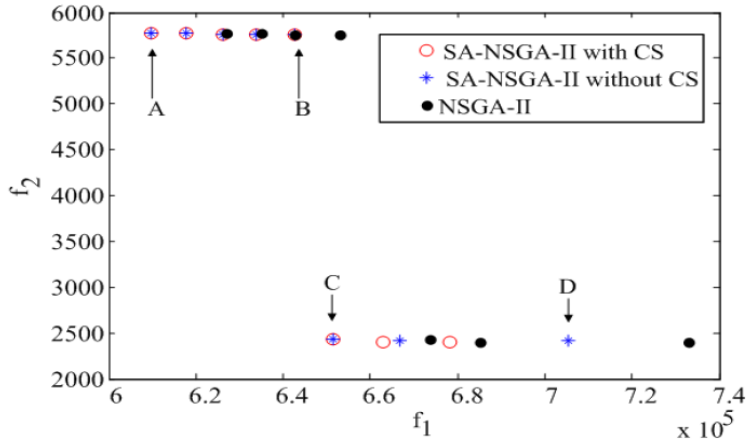
- Adaptation of K

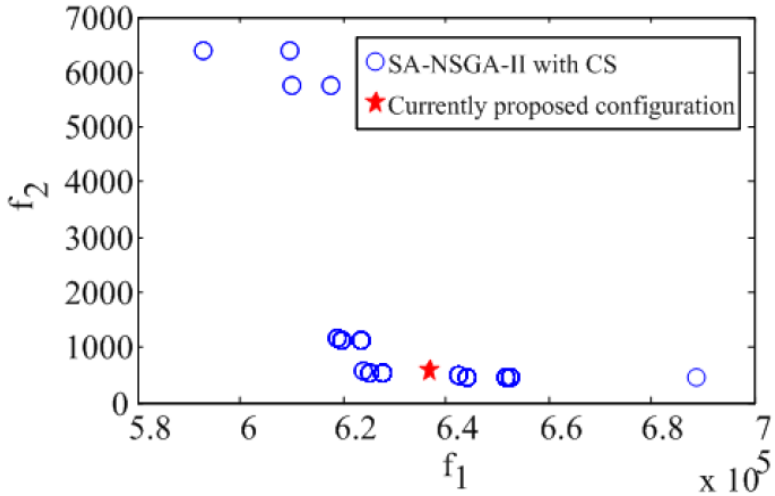


# Data Driven Evolutionary Trauma System Design

UNIVERSITY OF SURREY



▲ MTC

● TU

✚ LEH

| | IGD | Time (s) |
|---|---|---|
| SA-NSGA-II with CS | 2.47e-02±1.96e-02 | 6.54e+03±3.57e+03 |
| SA-NSGA-II without CS | 2.51e-02±2.79e-02 | 10.31e+03±5.00e+03 |
| NSGA-II | 0.00e+00±0.00e+00 | 8.14e+04±5.36e+02 |

# Discussions

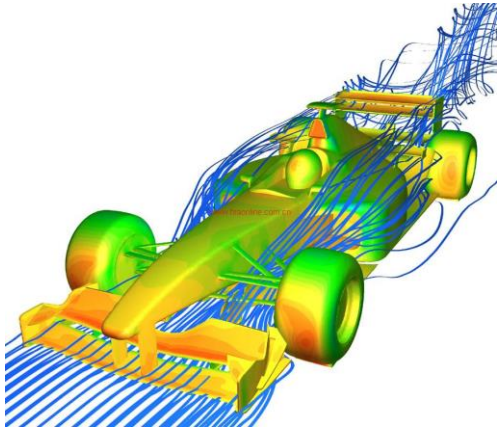
UNIVERSITY OF SURREY

- Online big data driven evolutionary optimization, e.g., stream data
- Efficient learning of big data
- Noisy and / or heterogeneous data

# Online (Small) Data Driven Evolutionary Optimization

# Small Data – Collecting Data is Expensive

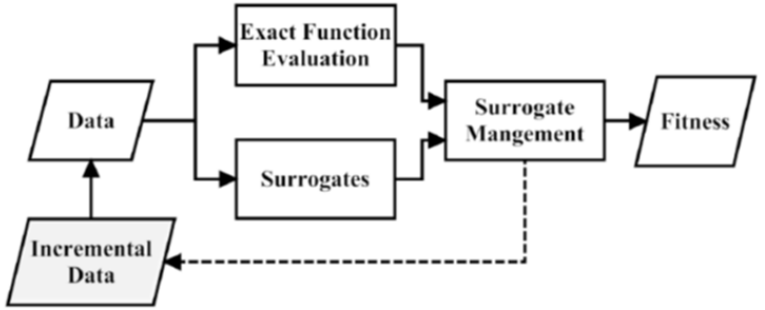
- In many cases, collecting data is very expensive
  - Highly time-consuming numerical simulation
  - Expensive physical experiments
  - Real-industrial processes only

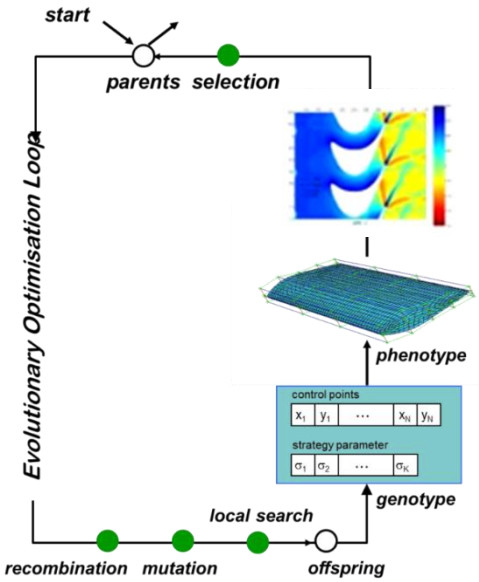


# Surrogate-Assisted Evolutionary Optimization

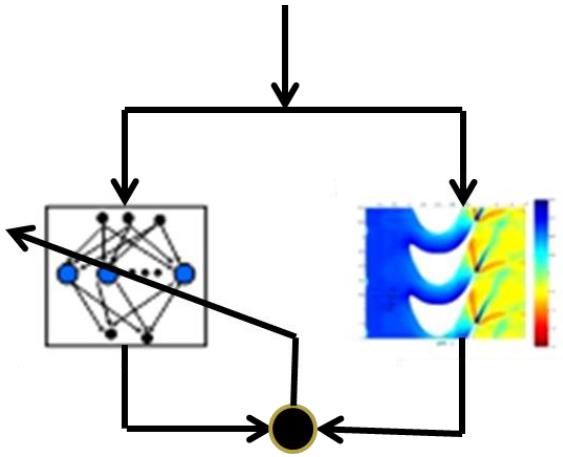
UNIVERSITY OF SURREY

- Use a meta-model /surrogate to replace the expensive fitness evaluations, e.g., CFD simulations
  - Choose a surrogate
  - Collect data
  - Train the surrogate
  - Replace the CFD



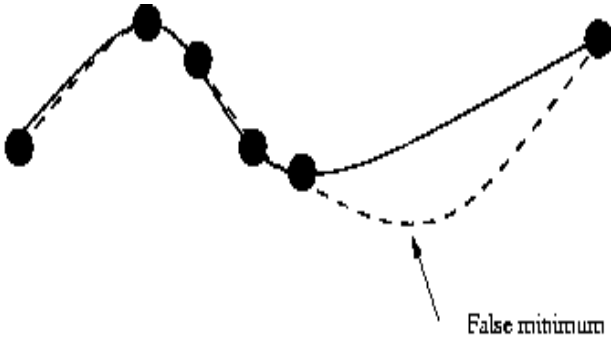

Online data-driven optimization



CFD simulations / Experiments

# Model Management

- Use surrogates only: Risk of converging to a false optimum




- Surrogate management / evolution control
  - population-based
  - generation-based
  - individual-based
  - local search
  - Combination of the above

Y. Jin. A comprehensive survey of fitness approximation in evolutionary computation. *Soft Computing*, 9(1), 3-12, 2005
Y. Jin. Surrogate-assisted evolutionary computation: Recent advances and future challenges. *Swarm and Evolutionary Computation*, 1(2):61-70, 2011

# Model Management – Main Questions

Which individuals are to be re-evaluated using the real-fitness function?

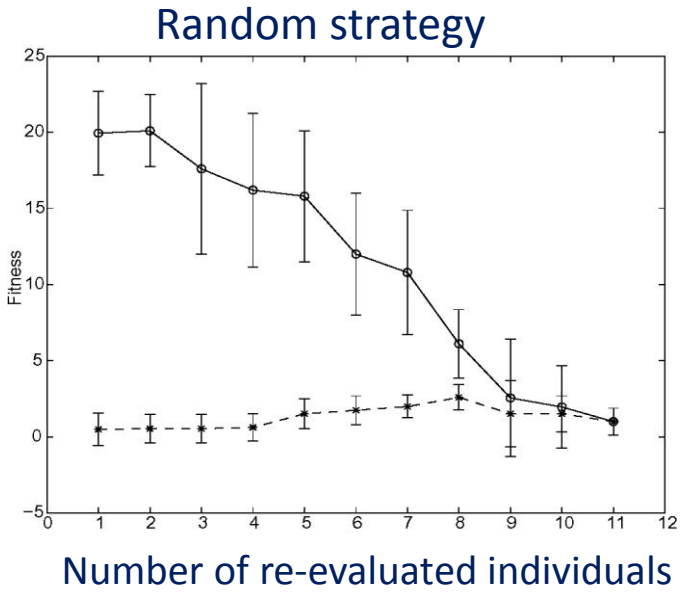
- Solutions that are of potentially good performance
- Solutions whose estimated fitness have large amount of uncertainty
  - Less explored
  - Effective for model improvement

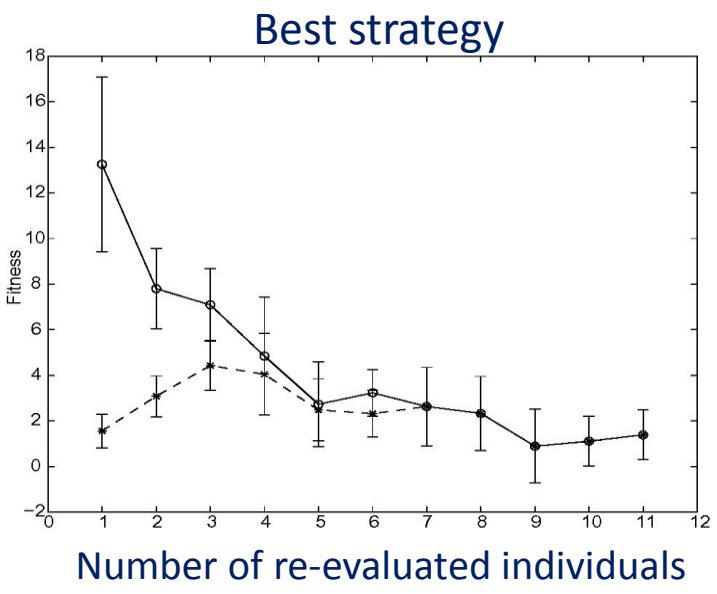
- How to measure uncertainty?

- How to measure model quality? (Jin et al 2003, Huesken et al 2005)

M. Huesken, Y. Jin and B. Sendhoff. Structure optimization of neural networks for evolutionary design optimization. *Soft Computing*, 9(1), 21-28, 2005
Y. Jin, M. Huesken and B. Sendhoff. Quality measures for approximate models in evolutionary computation. In: *Proceedings of the GECCO Workshop on "Learning, Adaptation and Approximation in Evolutionary Computation*", pp.170-174, Chicago, 2003

# Model Management – Promising Ones




- 12-D Ackley function
- (3,12)-ES
- average over 10 runs

- The best strategy is more efficient than the random strategy
- In the best strategy, about half of the individual should be controlled to guarantee correct convergence

Y. Jin, M. Olhofer and B. Sendhoff. A framework for evolutionary optimization with approximate fitness functions. *IEEE Transactions on Evolutionary Computation*, 6(5): 481-494 (2002)

# Model Management – Promising and Uncertain Ones

Given a stochastic model (Gaussian process),

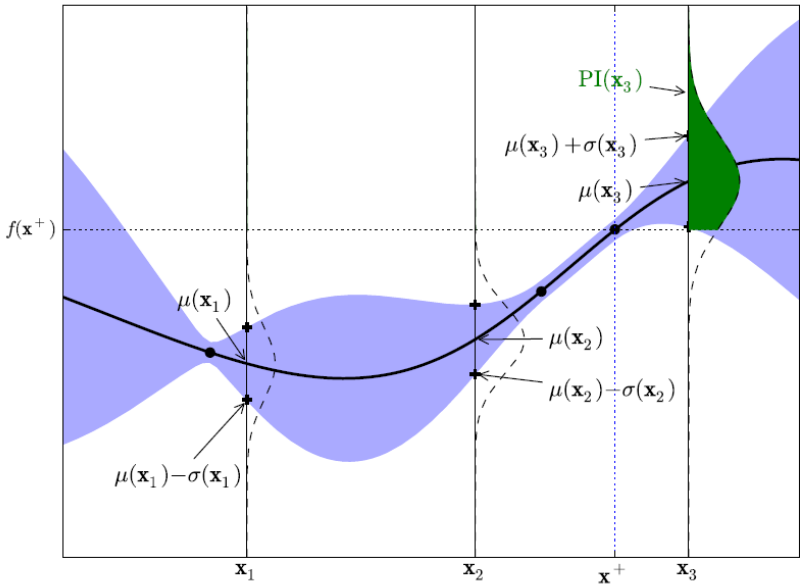
- Mean fitness value:

$$f = \mu(x);$$

- Lower confidence bound (LCB)

$$f = \mu(x) - \alpha\sigma(x) \; (\alpha > 0)$$

- Expected improvement (EI)




(Taken from Brochu et al, 2010)

$$\mathrm{EI}(\mathbf{x}) = \begin{cases} (\mu(\mathbf{x}) - f(\mathbf{x}^+))\Phi(Z) + \sigma(\mathbf{x})\phi(Z) & \text{if } \sigma(\mathbf{x}) > 0 \\ 0 & \text{if } \sigma(\mathbf{x}) = 0 \end{cases} \qquad Z = \frac{\mu(\mathbf{x}) - f(\mathbf{x}^+)}{\sigma(\mathbf{x})}$$

- Probability of Improvement (PI)

$\Phi(\cdot)$ is the normal cumulative distribution function.

$$\mathrm{PI}(\mathbf{x}) = P(f(\mathbf{x}) \geq f(\mathbf{x}^+)) = \Phi\left(\frac{\mu(\mathbf{x}) - f(\mathbf{x}^+)}{\sigma(\mathbf{x})}\right)$$


M. Emmerich, K.C. Giannakoglou, B. Naujoks, Single- and multiobjective evolutionary optimization assisted by Gaussian random field metamodels. *IEEE Transactions on Evolutionary Computation*, 10 (4) : 421–439 (2006)

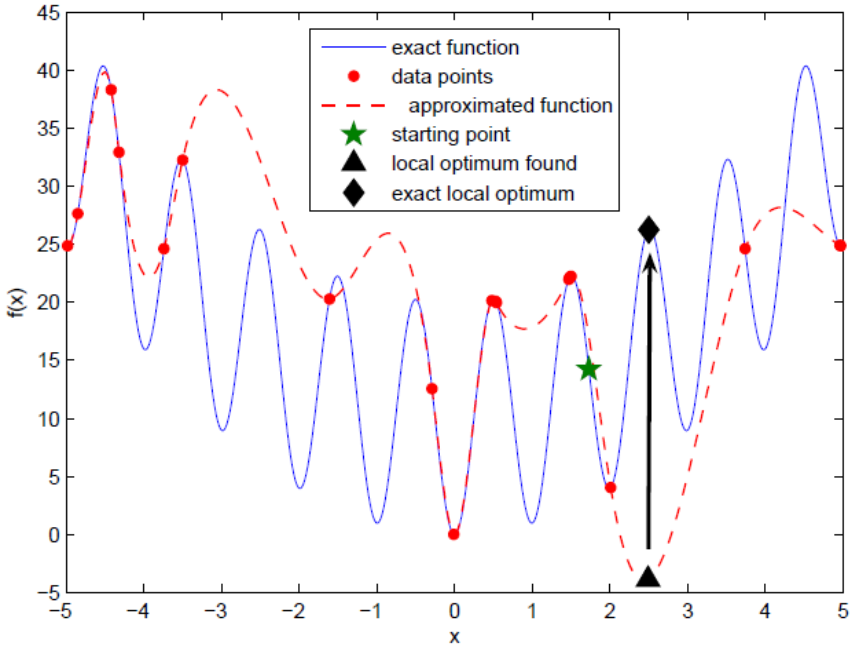
Eric Brochu, Vlad M. Cora and Nando de Freitas. A tutorial on Bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning, 2010. https://arxiv.org/pdf/1012.2599

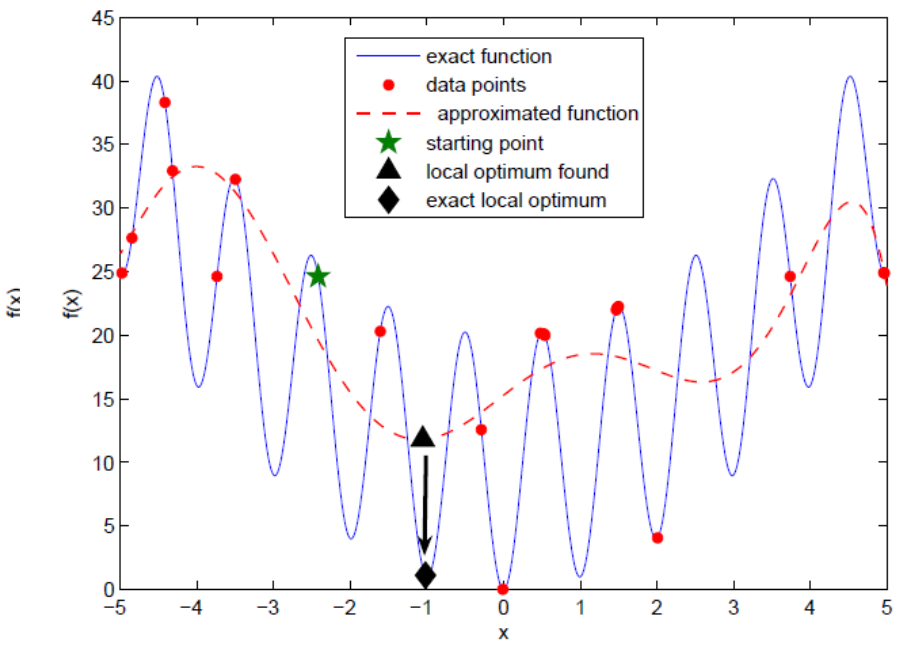
# Model Management in Multi-Objective Optimization

- Each objective is considered separately (similar to single objective optimization)
- Multiple objectives are converted to a scalar objective function and then use the model management criteria for single objective optimization
  - Random weights
  - Uniformly distributed weights
- Use a scalar performance indicator, e.g., hypervolume

D. Horn, T. Wagner, D. Biermann, C. Weihs, and B. Bischl. Model-Based Multi-Objective Optimization: Taxonomy, Multi-Point Proposal, Toolbox and Benchmark. In: *Evolutionary Multi-Criterion Optimization*, LNCS 9018, pages 64–78.

# Potential Benefit of a Global Model



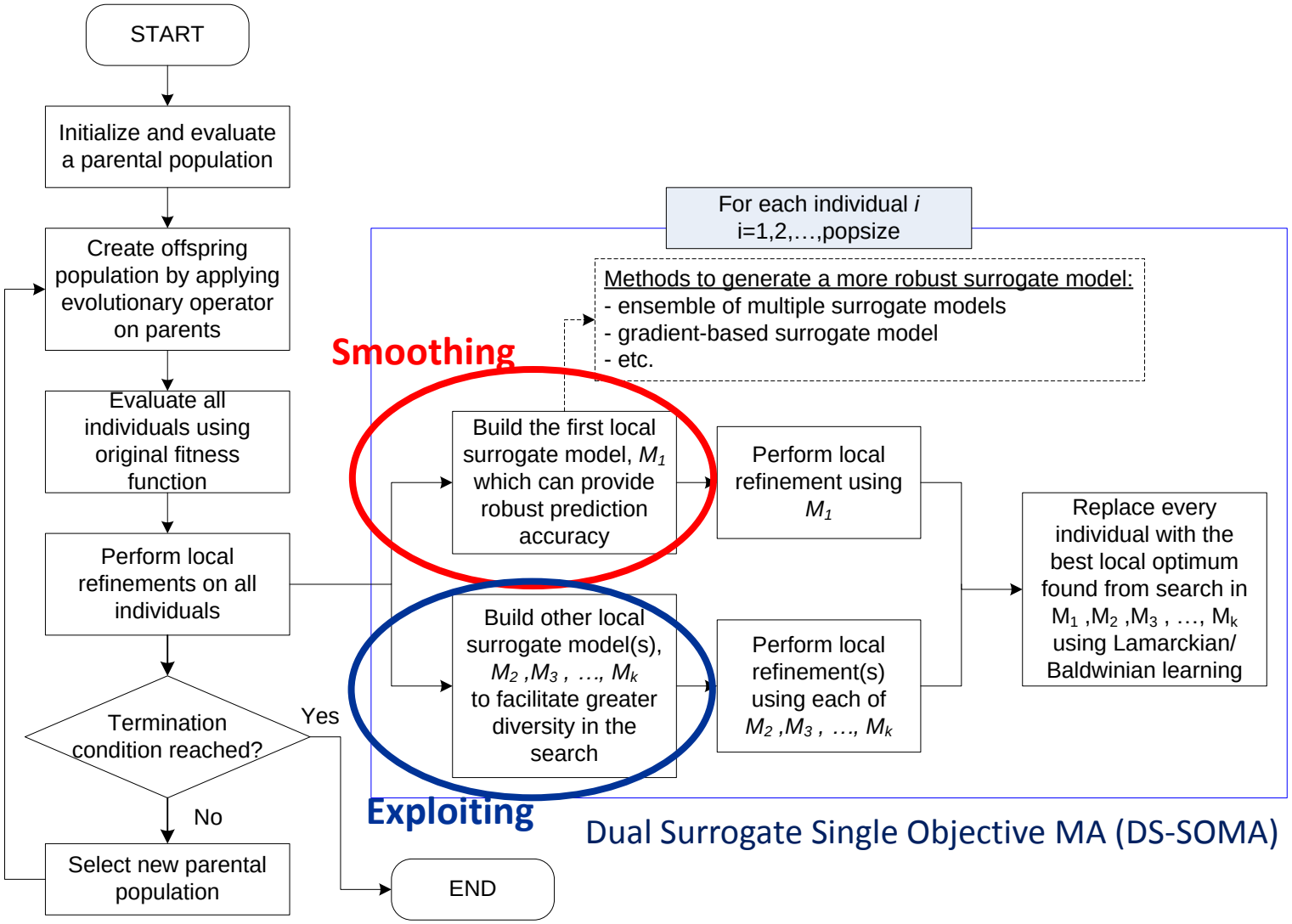




A global model might help smoothen the fitness landscape

D. Lim, Y. Jin, Y.-S. Ong, and B. Sendhoff. Generalizing surrogate-assisted evolutionary computation. *IEEE Transactions on Evolutionary Computation*, 14(3):329 - 355, 2010

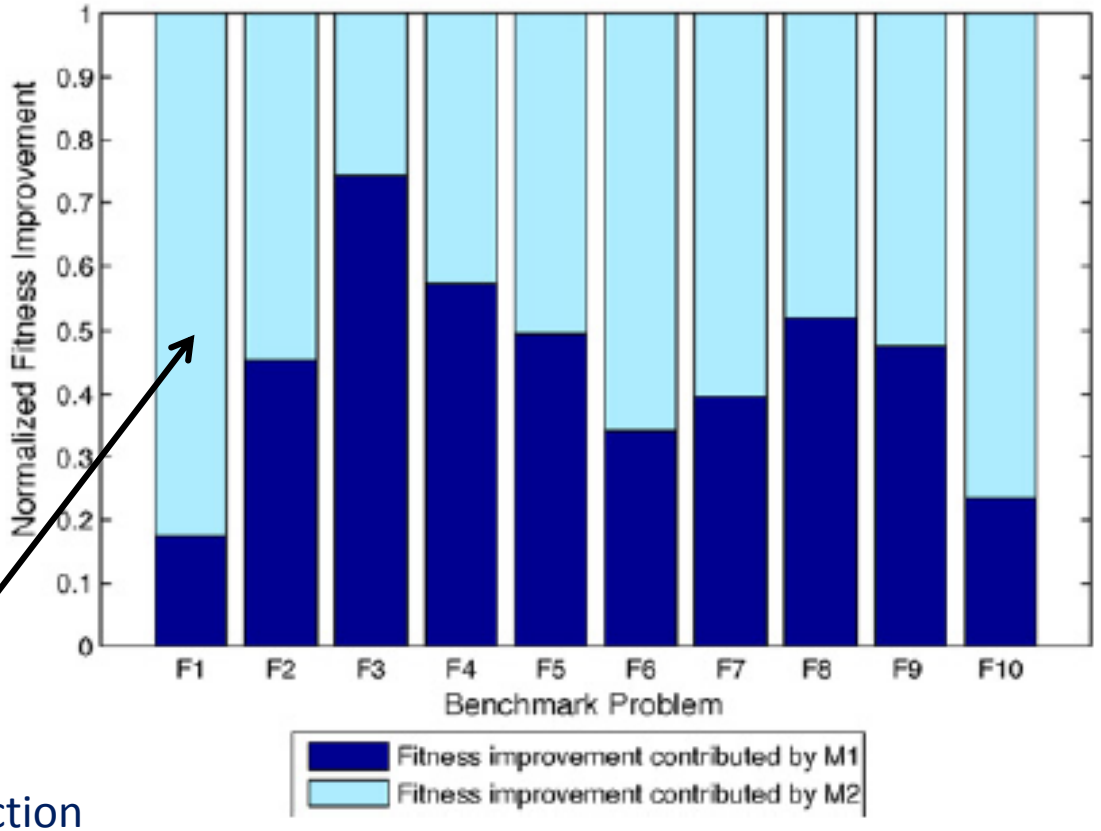
C. Sun, Y. Jin, J. Zeng and Y. Yu. A two-layer surrogate-assisted particle swarm optimization algorithm. *Soft Computing*, 19(6):1461-1475, 2015

# Dual Surrogates in Memetic Algorithms



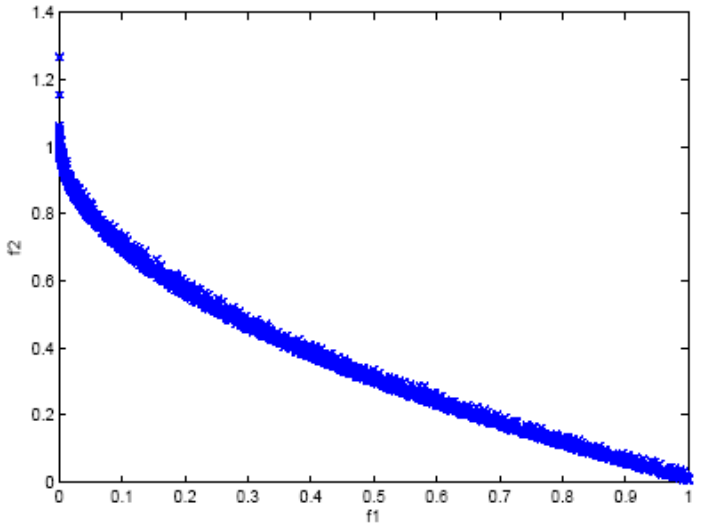

Dual Surrogate Single Objective MA (DS-SOMA)

# Results: Single Objective

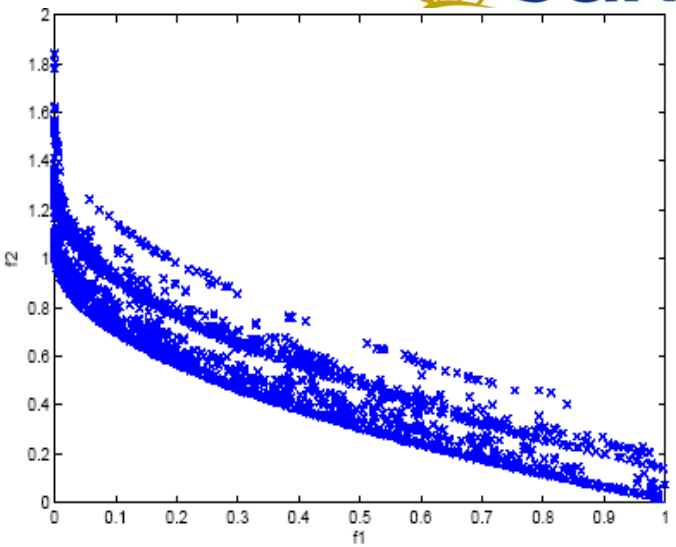



M1 (PR) contributes most on the Ackley function

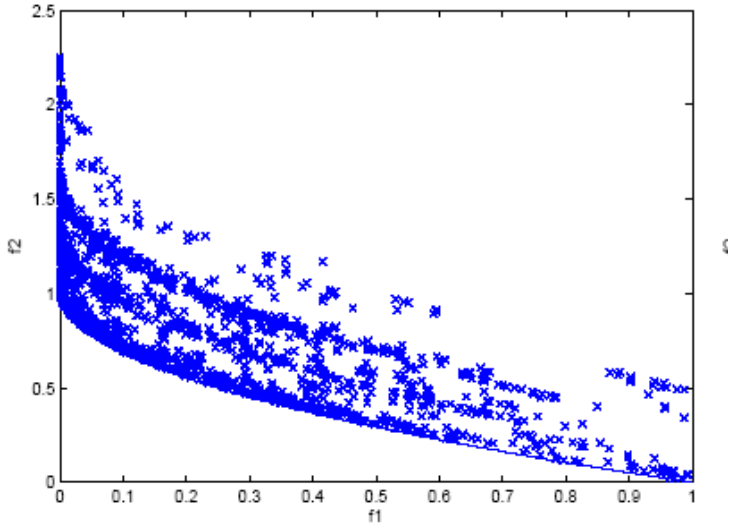
# Results: Multi-Objective



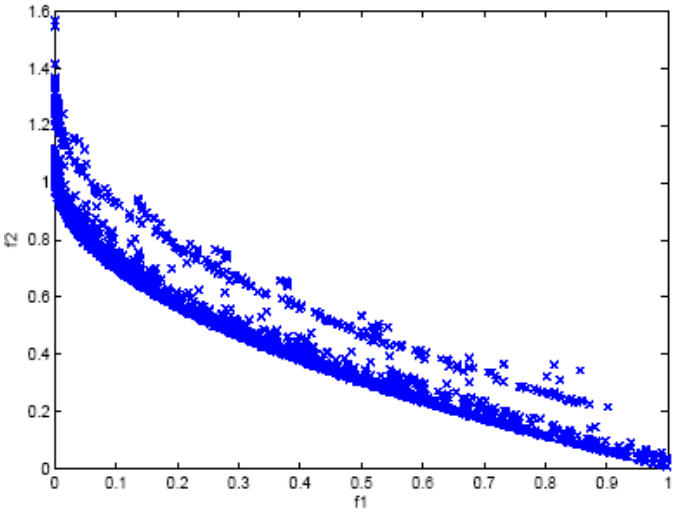

DS-MOMA




SS-MOMA- PR+RBF+GP




SS-MOMA-PR



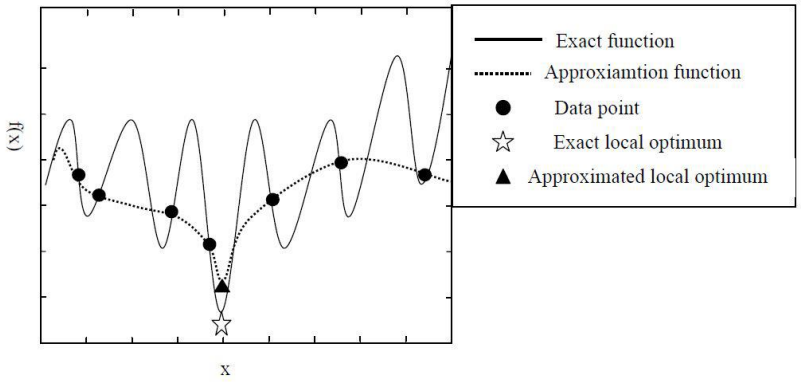

SS-MOMA-Perfect

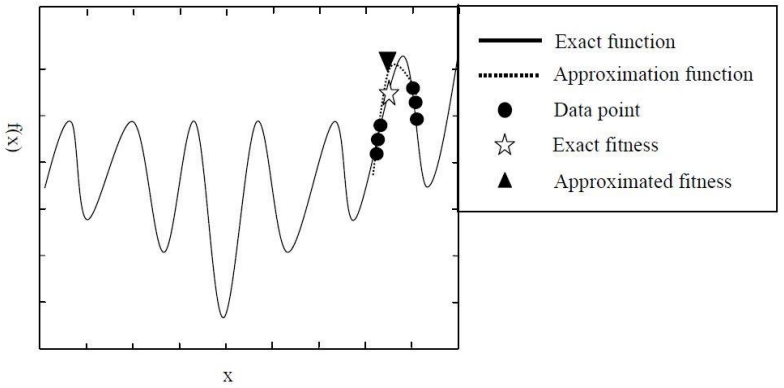
All results from 20 runs

# Global and Local Surrogate Models

## Two-layer (global and local) surrogate-assisted PSO

1: Construct a global surrogate model;
2: Approximate a fitness value for each individual in the swarm using the global surrogate model;
3: **for** each particle $i$ in the swarm **do**
4: Find its neighbors in the local database;
5: **if** there are enough samples to construct a local surrogate **then**
6: Construct a local surrogate model;
7: Approximate the fitness of particle $i$ using the local surrogate model;
8: $\tilde{f}(\mathbf{x}_i) = \min\{\tilde{f}_g(\mathbf{x}_i), \tilde{f}_l(\mathbf{x}_i)\}$
9: **else**
10: $\tilde{f}(\mathbf{x}_i) = \tilde{f}_g(\mathbf{x}_i)$
11: **end if**
12: **end for**



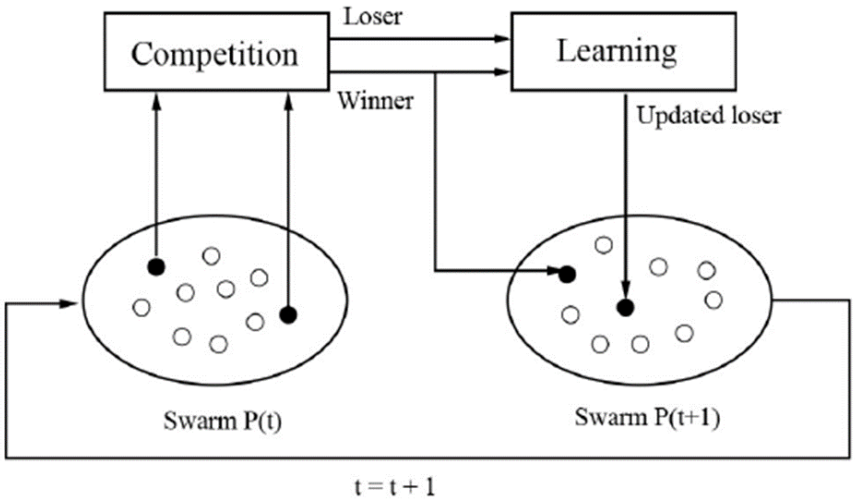

C. Sun, Y. Jin, J. Zeng and Y. Yu. A two-layer surrogate-assisted particle swarm optimization algorithm. *Soft Computing*, 19(6):1461-1475, 2015

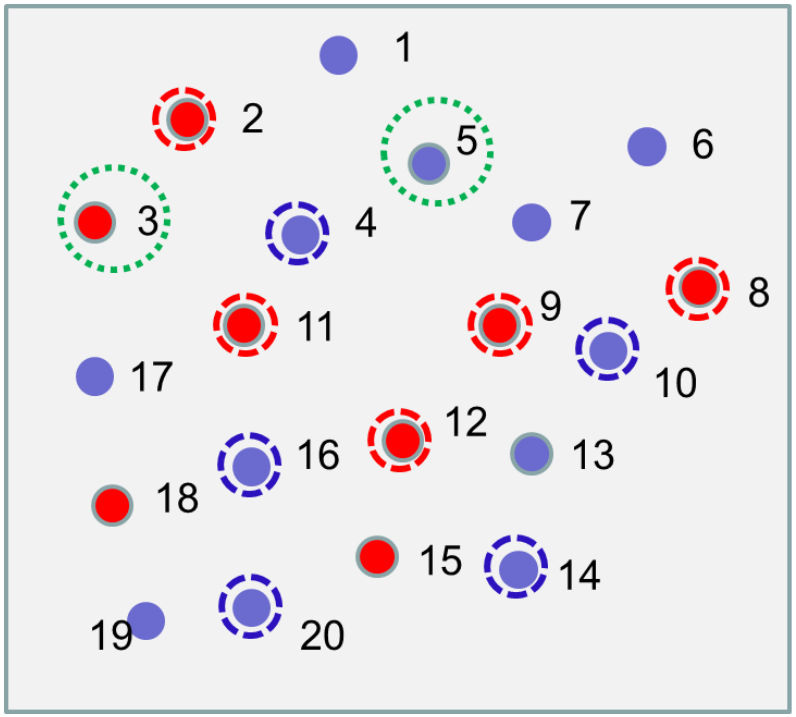
# Surrogate-Assisted Large-Scale Evolutionary Optimization?

UNIVERSITY OF SURREY

- Dimension mostly limited up to 10 in GP-assisted EAs, mostly up to 30
  - ➢ Curse of dimensionality
  - ➢ Dramatic increase in computational cost for training surrogates, e.g., Gaussian processes – **it can take hours to build a GP model** ☹

# Fitness Estimation Assisted CSO for Large-Scale Optimization




- Fitness estimation in competitive swarm optimization for dimensions up to 500
  - ➢ Fitness estimated based on positional relationships

Particles whose fitness is estimated (*ES*)

Particles whose fitness is calculated (*EV*)

Loser particles whose fitness is estimated (*ES*)

Winner particle whose fitness is calculated (*EV*)

C. Sun, J. Ding, J. Zeng and Y. Jin. Fitness approximation assisted competitive swarm optimizer for large scale expensive optimization problems. *Memetic Computing*, 2016 (accepted)

# Concluding Remarks

UNIVERSITY OF SURREY

- Evolutionary optimization of complex systems is promising yet challenging
- Data-driven evolutionary optimization becomes increasing important
- Surrogate-assisted evolutionary optimization will not only be essential for evolutionary optimization of complex systems but also provides a platform for integrating evolution and learning techniques
  - Which to re-evaluate (sample)
    - Active learning
  - Small data
    - Semi-supervised learning
    - Transfer learning
  - big data
    - Deep learning

# 2016 IEEE Symposium Series on Computational Intelligence

**December 6-9, 2016, Athens, Greece**

http://ssci2016.cs.surrey.ac.uk/

**Submission deadline: August 15 2016**

IEEE Computational Intelligence Society

IEEE

# IEEE Transactions on Cognitive and Developmental Systems

*(formerly IEEE Transactions on Autonomous Mental Development)*

**Editor-in-Chief: Yaochu Jin**

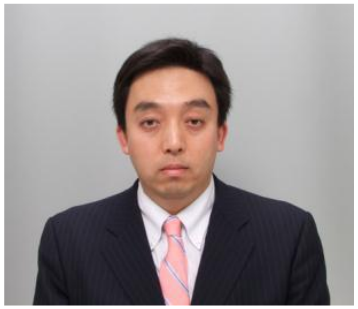
In January 2016 the IEEE Transactions on Autonomous Mental Development (TAMD) changes its name to IEEE Transactions on Cognitive and Developmental Systems (TCDS). This title change aims to widen the scope and audience of the journal to reach the wider community of cognitive systems and cognitive robotics, whilst also keeping an important focus on developmental systems modelling.

***It welcomes contributions from multiple disciplines related to cognition and development, including:***

- cognitive systems
- cognitive robotics
- developmental and epigenetic robotics
- autonomous and evolutionary robotics
- social robotics
- models of cognition and behavior
- multi-agent and artificial life systems
- computational neuroscience
- developmental psychology
- models of neural development

UNIVERSITY OF SURREY

# *Thank you for your attention!*



EPSRC
Engineering and Physical Sciences Research Council

Tekes
Finnish Funding Agency for Innovation