

# Evolutionary Practical Optimization

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## Outline of Tutorial

- ▶ Optimization fundamentals
- ▶ Scope of *optimization* in practice
- ▶ Classical *point-by-point* approaches
- ▶ Advantages of evolutionary *population-based* approaches
- ▶ Scope of evolutionary approaches in different problem solving tasks
  - ▶ Having one algorithm for various practical optimizations is difficult
- ▶ Final words

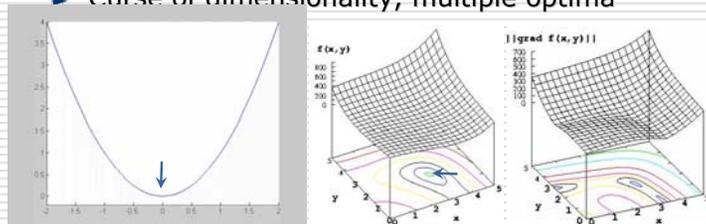


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## Fundamentals of Optimization

- ▶ A generic name for minimization and maximization of a function  $f(\mathbf{x})$
- ▶ Everyone knows:  $df/dx=0$  or  $\nabla f(x)=0$
- ▶ Curse of dimensionality, multiple optima

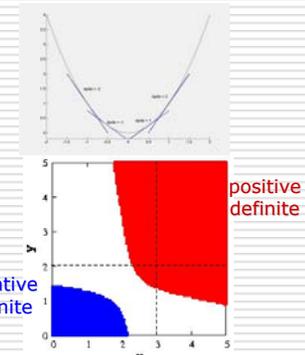


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## Fundamentals (cont.)

- ▶ Concept relates to mathematics
  - ▶ Second and higher-order derivatives
  - $d^2f/dx^2 > 0$ , minimum
  - $d^2f/dx^2 < 0$ , maximum
- if  $\nabla^2 f$  is positive definite at  $x^*$ , it is a minimum
- ▶ **Convex: One optimum**



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## Constrained Optimization Basics

- Decision variables:  $\mathbf{x} = (x_1, x_2, \dots, x_n)$
- Constraints restrict some solutions to be feasible

Min.  $f(\mathbf{x})$   
 s.t.  $g_j(\mathbf{x}) \geq 0 \quad j = 1, 2, \dots, J$   
 $h_k(\mathbf{x}) = 0 \quad k = 1, 2, \dots, K$   
 $x_i^l \leq x_i \leq x_i^u \quad i = 1, 2, \dots, n$

- Equality and inequality constraints
- Minimum of  $f(\mathbf{x})$  need not be constrained minimum
- Constraints can be non-linear



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## Constrained Optimization Basics (cont.)

- Kuhn-Tucker (K-T) conditions for optimality
  - First-order necessary conditions
  - Convex search space, convex  $f$ :**  
K-T point is minimum

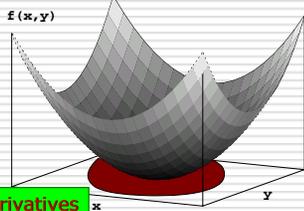
$$\nabla f(\mathbf{x}) - \sum_{j=1}^J u_j \nabla g_j(\mathbf{x}) - \sum_{k=1}^K v_k \nabla h_k(\mathbf{x}) = 0$$

$$g_j(\mathbf{x}) \geq 0 \quad j = 1, 2, \dots, J$$

$$h_k(\mathbf{x}) = 0 \quad k = 1, 2, \dots, K$$

$$u_j g_j(\mathbf{x}) = 0 \quad j = 1, 2, \dots, J$$

$$u_j \geq 0 \quad j = 1, 2, \dots, J$$



Involve Derivatives and solve for roots

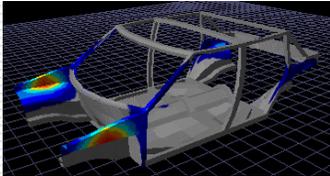


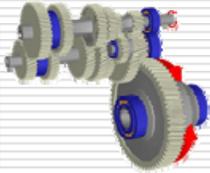
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## Scope of Optimization in Practice

- Optimal design & manufacturing** for desired goals
- Major application in engineering



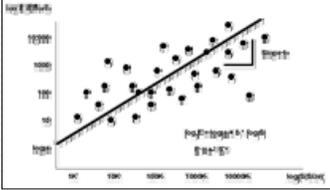


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## Scope of Optimization (cont.)

- Parameter optimization** for optimal performance



- Scientific experiments, computer experiments





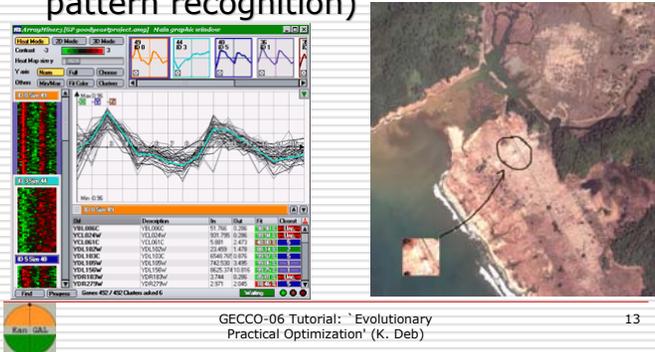

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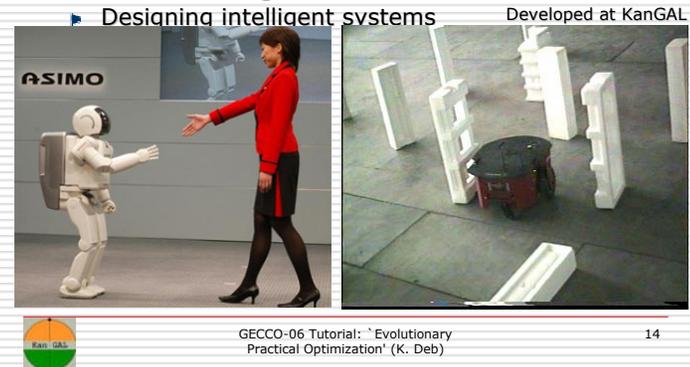
## Scope of Optimization (cont.)

- ▶ **Data mining** (classification, clustering, pattern recognition)



## Scope of Optimization (cont.)

- ▶ **Machine learning**
  - ▶ Designing intelligent systems

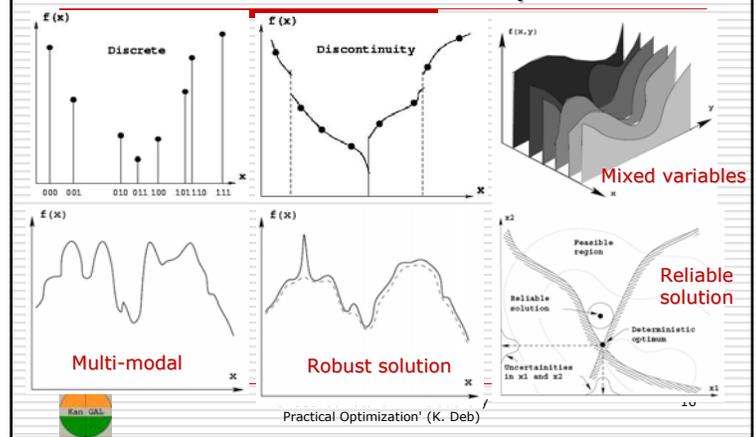


## Properties of Practical Optimization Problems

- ▶ Non-differentiable functions and constraints
- ▶ Discontinuous search space
- ▶ Discrete search space
- ▶ Mixed variables (discrete, continuous, permutation)
- ▶ Large dimension (variables, constraints, objectives)
- ▶ Non-linear constraints
- ▶ Multi-modalities
- ▶ Multi-objectivity
- ▶ Uncertainties in variables
- ▶ Computationally expensive problems
- ▶ Multi-disciplinary optimization

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## Different Problem Complexities



## Classical Optimization Methods and Past

- Exact differentiation & root-finding method
  - Intractable and not sufficient for practical problems
- Numerical algorithms
  - Iterative and **deterministic**
  - Directions based on gradients (mostly)
  - Point-by-point approaches**

*Linear regression:*

$$m = \frac{n\sum(xy) - \sum x \sum y}{n\sum(x^2) - (\sum x)^2}$$

$$b = \frac{\sum y - m\sum x}{n}$$

$y = mx + b$

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## Classical Methods (cont.)

- Direct and gradient based methods**
- Convexity assumption
  - No guarantee otherwise
- Local perspectives**
- Discreteness cause problems
- Non-linear constraints**
- Large-scale application time-consuming
- Serial in nature**

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## Practical Optimization

With a point in each iteration, scope is limited

A need for non-classical, population-based optimization methods exists

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## Evolutionary Optimization: A Motivation from Nature

- Natural evolution + genetics
  - Guided search procedure
  - Offspring are created by duplication, mutation, crossover etc.
  - Good solutions are retained and bad are deleted
  - Information is coded

Random Search

**B  
Y  
E  
L**

Iteration: 1

Directed Search

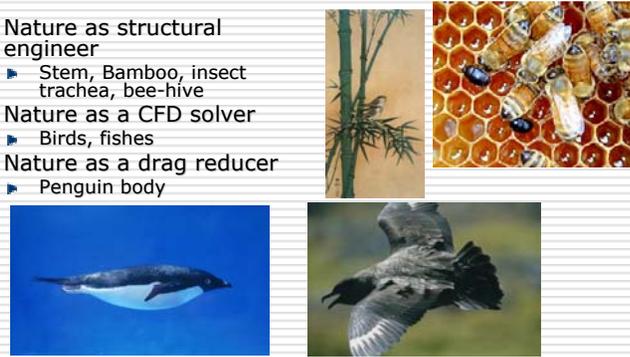
**B  
Y  
E  
L**

Iteration: 1

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## Nature as an Optimizer

- ▶ Nature as structural engineer
  - ▶ Stem, Bamboo, insect trachea, bee-hive
- ▶ Nature as a CFD solver
  - ▶ Birds, fishes
- ▶ Nature as a drag reducer
  - ▶ Penguin body

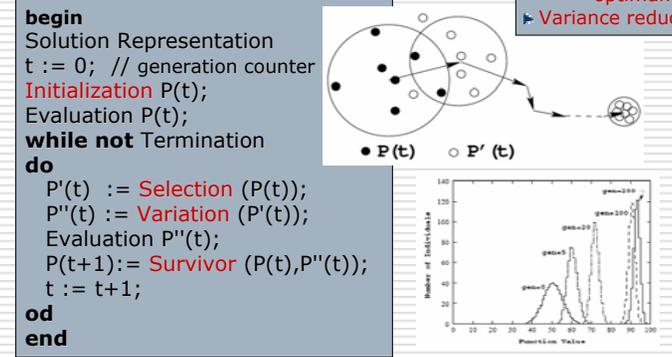


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## Evolutionary Algorithms as Optimizers

```

begin
Solution Representation
t := 0; // generation counter
Initialization P(t);
Evaluation P(t);
while not Termination
do
P'(t) := Selection (P(t));
P''(t) := Variation (P'(t));
Evaluation P''(t);
P(t+1) := Survivor (P(t), P''(t));
t := t+1;
od
end
    
```



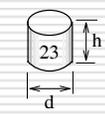
- ▶ Mean approaches optimum
- ▶ Variance reduces

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## Traditional Evolutionary Approach: Binary-Coded Genetic Algorithms

- ▶ Genetic Algorithms (John Holland, 1962)
- ▶ Design of a can for minimum cost having at most V volume
- ▶ **Objective function:** Cost(d,h):  $f(d,h) = \pi dh + 2\pi d^2/4$
- ▶ **Constraint:** Volume (d,h):  $\pi d^2 h/4 \geq V$
- ▶ **Representation** in binary strings
- ▶ **Fitness:** objective value + penalty for constraint

Solution Representation:



(d, h) = (8, 10) cm  
(Chromosome) = 0 1 0 0 0 0 1 0 1 0

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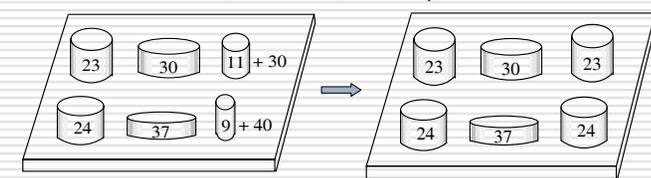
## Binary-Coded Genetic Algorithm: A Hand Simulation

Initialization and Evaluation:

- ▶ Fitness = Cost + Penalty (proportional to constraint violation)

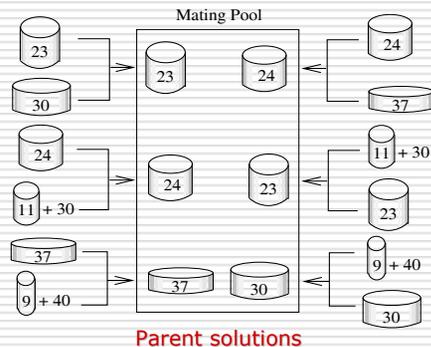
Selection: **Emphasizing better solutions**

Random Initialization (N members)      Population after Selection



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## Tournament Selection Operator

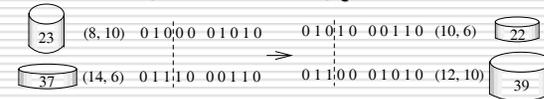


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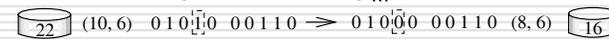
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## Variation Operators: Creating new offspring solutions

- ▶ **Crossover** operator with  $p_c$ :



- ▶ **Mutation** operator with  $p_m$ :

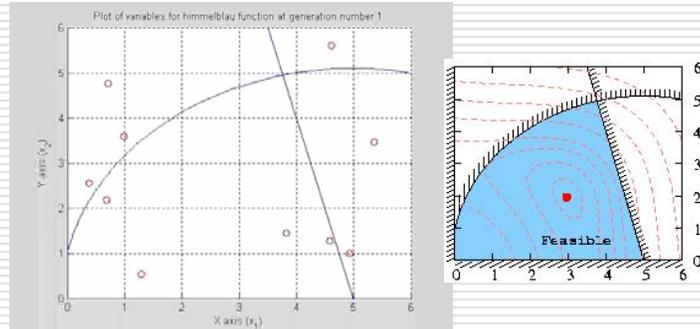


- ▶ Good, partial information propagates leading to optimum
- ▶ Other and modified operators often used

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## Simulation of a GA



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## Differences with Classical Methods

- ▶ **GAs work on a coding of variables**
  - ▶ Mixed variable types can be handled
  - ▶ Permutation, continuous, discrete together
- ▶ **GAs are population-based**
  - ▶ Safety in numbers -> global perspective
  - ▶ *Implicit parallelism*
- ▶ **GA operators are probabilistic**
  - ▶ Less chance of getting stuck
- ▶ **GAs do not use any gradient information**
  - ▶ Black-box search -> wide applicability
- ▶ **Ideal for parallel computation**
  - ▶ Distribute evaluations among processors and more

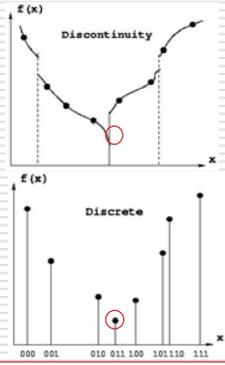
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## Non-smooth Problems

*Handling discrete, discontinuous variables*

- ▶ Non-differentiability, discontinuity, discreteness, non-linearity not a difficulty
- ▶ GAs work with a discrete search space anyway
  - ▶ So, GAs are natural choice for discrete problem solving



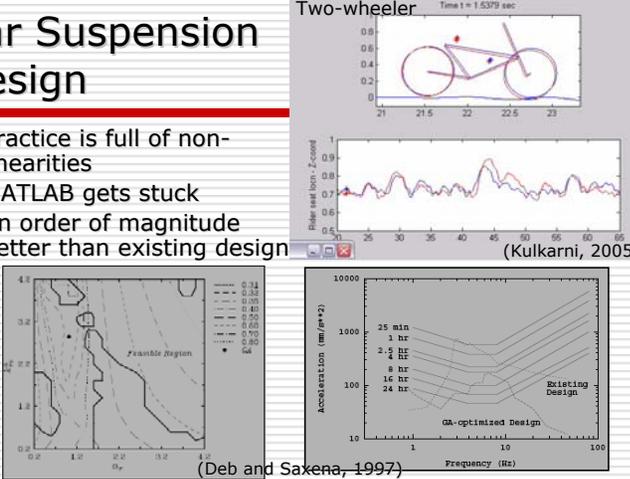


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## Car Suspension Design

- ▶ Practice is full of non-linearities
- ▶ MATLAB gets stuck
- ▶ An order of magnitude better than existing design





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## EAs for Continuous Variables

- ▶ Decision variables are coded directly, instead of using binary strings
- ▶ **Recombination** and **mutation** need structural changes
- ▶ Selection operator remains the same

Recombination

$$\begin{pmatrix} x_1 & x_2 & \dots & x_n \\ y_1 & y_2 & \dots & y_n \end{pmatrix} \Rightarrow ?$$

Mutation

$$(x_1, x_2, \dots, x_n) \Rightarrow ?$$

- ▶ Simple exchanges are not adequate



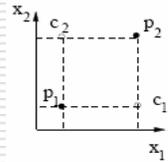
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## Naive Recombination

- ▶ Crossing at boundaries do not constitute adequate search
  - ▶ Least significant digits are taken too seriously

15.345	3.569	→	11.142	3.587
21.142	5.687		25.345	5.669



- ▶ Two Remedies:
  - ▶ Parent values (variable-wise) need to be blended to each other
  - ▶ Vector-wise recombination



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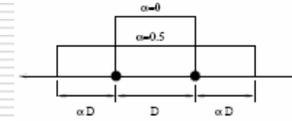
## Variable-wise Blending of Parents

- ▶ Use a probability distribution to create child
- ▶ Different implementations since 1991:
  - ▶ Blend crossover (BLX- $\alpha$ ), 1991
  - ▶ Simulated binary crossover (SBX- $\beta$ ), 1995
  - ▶ Fuzzy recombination (FR-d), 1995
- ▶ Main feature: **Difference between parents used to create children**
  - ▶ Provides self-adaptive property



## Blend Crossover (BLX- $\alpha$ )

- ▶ Uniform probability distribution within a bound controlled by  $\alpha$  (Eshelman and Schaffer, 1991)



- ▶ Diversity in children proportional to that in parents
- ▶ Too wide a search, if parents are distant



## Motivation for the SBX Operator

- ▶ Simulate processing in a binary crossover, say single-point crossover
- ▶ *Gedanken* experiment:
  - ▶ Two parent solutions in real number
  - ▶ Code them in l-bit strings
  - ▶ Use single-point crossover in all (l-1) places and find children strings
  - ▶ In each case map strings back to real numbers as children
  - ▶ Observe the relationship between parents and children
  - ▶ Use this relationship to directly recombine parents to form children



## Properties of Binary Crossover

- ▶ To make crossovers independent of parents, define a **spread factor,  $\beta$**

$$\beta = \left| \frac{c_1 - c_2}{p_1 - p_2} \right|$$

- ▶ Define probability distribution as a function of  $\beta$

- ▶ Two observations:

- ▶ Mean decoded value of parents is same as that of children

- ▶ Child strings crossed at the same place produce the same parent strings

$B_1$	1	0	1	0	1	85	$\Rightarrow$
$B_2$	0	1	1	0	1	51	
$A_2$							68
$B_1$	1	0	1	0	1	83	
$B_2$	0	1	1	0	1	53	
$A_1$							68



## Simulated Binary Crossover (SBX- $\beta$ )

- Probability is large near the parents
- Extent is controlled by  $\beta$
- Diversity in children proportional to that in parents
- Obeys *interval-schema* processing

$$C(\beta) = 0.5(n+1)\beta^n$$

$$E(\beta) = 0.5(n+1)\frac{1}{\beta^{n+2}}$$

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## SBX Procedure

- Step 1: Choose a random number  $u \in [0,1]$ .
- Step 2: Calculate  $\beta_q$ :
 
$$\beta_q = \begin{cases} (2u)^{\frac{1}{n_c+1}}, & \text{if } u \leq 0.5 \\ \left(\frac{1}{2(1-u)}\right)^{\frac{1}{n_c+1}}, & \text{otherwise} \end{cases}$$
- Step 3: Compute two offspring:
 
$$c_1 = 0.5((1 + \beta_q)p_1 + (1 - \beta_q)p_2)$$

$$c_2 = 0.5((1 - \beta_q)p_1 + (1 + \beta_q)p_2)$$

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## Properties of SBX Operator

- If parents are distant, distant offspring are likely
- If parents are close, offspring are close to parents
- Self-adaptive property

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## Variations of SBX

- For bounded and discrete variables

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### Real-Parameter Mutation Operators

- ▶ Idea: Create a neighboring solution
- ▶ Random mutation
- ▶ Normally distributed mutation
- ▶ Non-uniform mutation
- ▶ Extensions to bounded and discrete cases exist

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### Vector-Wise Recombination Operators

- ▶ Variable-wise recombination cannot capture nonlinear interactions
- ▶ Recombine parents as vectors
  - ▶ Parent-centric recombination (PCX)
  - ▶ Unimodal normally-distributed crossover (UNDX)
  - ▶ Simplex crossover (SPX)
- ▶ Difference in parents is used to create offspring solutions
- ▶ DE, PSO, CMA-ES

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### Parent-Centric Recombination

- ▶ SBX (Deb and Agrawal, 1995): variable-wise
- ▶ Vector-wise parent-centric recombination (PCX):  $O(\mu)$  per offspring

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### PCX Operator

- ▶  $\mu$  parents create a offspring
- ▶ Each parent has its turn
- ▶  $e^{(i)}$  orthonormal bases spanning the subspace perpendicular to  $d^{(p)}$
- ▶  $w_c$  and  $w_\eta$  are user-defined parameters, controlling extent of search

$$\vec{y} = \vec{x}_p + w_c |d^{(p)}| + \sum_{i=1, i \neq p}^{\mu} w_\eta \bar{D} e^{(i)}$$

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## Generalized Generation Gap (G3) Model

1. Select the best parent and  $\mu-1$  other parents randomly
  2. Generate  $\lambda$  offspring using a recombination scheme
  3. Choose two parents at random from the population
  4. Form a combination of two parents and  $\lambda$  offspring, choose best two solutions and replace the chosen two parents
- ▶ Parametric studies with  $\lambda$  and  $N$
  - ▶ Desired accuracy in  $F$  is  $10^{-20}$



## Quasi-Newton Method

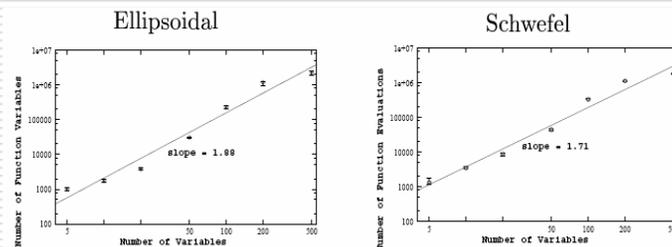
- ▶ Accuracy obtained by G3+PCX is  $10^{-20}$

Func.	FE	Best	Median	Worst
$F_{elp}$	6,000	$8.819(10^{-24})$	$9.718(10^{-24})$	$2.226(10^{-23})$
$F_{sch}$	15,000	$4.118(10^{-12})$	$1.021(10^{-10})$	$7.422(10^{-9})$
$F_{ros}$	15,000	$6.077(10^{-17})$	$4.046(10^{-10})$	3.987
$F_{elp}$	8,000	$5.994(10^{-24})$	$1.038(10^{-23})$	$2.226(10^{-23})$
$F_{sch}$	18,000	$4.118(10^{-12})$	$4.132(10^{-11})$	$7.422(10^{-9})$
$F_{ros}$	26,000	$6.077(10^{-17})$	$4.046(10^{-10})$	3.987

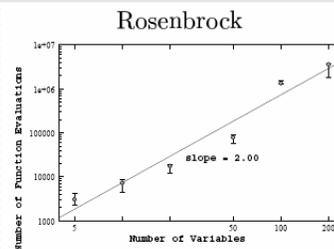


## Scalability Study

- ▶ Accuracy  $10^{-10}$  is set



## Scalability Study (cont.)



- ▶ All polynomial complexity  $O(n^{1.7})$  to  $O(n^2)$  similar to those reported by CMA-ES approach (Hansen and Ostermeier, 2001)



## Differential Evolution (DE)

1. Start with a pool of random solutions
2. Create a child  $v$
3.  $x_k$  and  $v$  are recombined with  $p$

- ▶ Difference of parents in creating a child is important
- ▶ A number of modifications exist

$$- v = x^{(1)} + \lambda(x^{(2)} - x^{(3)})$$

$$- y_i = \begin{cases} v_i, & \text{with a prob. } p \\ x_i^{(k)}, & \text{else} \end{cases}$$

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## DE Results

	$F_{elp}$		
	Best	Median	Worst
DE	9,660	12,033	20,881
G3	5,826	6,800	7,728
<hr/>			
	$F_{sch}$		
	Best	Median	Worst
DE	102,000	119,170	185,590
G3	13,988	15,602	17,188
<hr/>			
	$F_{ros}$		
	Best	Median	Worst
DE	243,800	587,920	942,040
G3	16,508	21,452	25,520

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## Particle Swarm Optimization (PSO)

- ▶ Kennedy and Eberhart, 1995
- ▶ Particles fly through the search space
- ▶ Velocity dynamically adjusted
- ▶  $x_i = x_i + v_i$
- ▶  $v_i = v_i + c_1 \text{rnd}() (p_{i,best} - x_i) + c_2 \text{rnd}() (p_g - x_i)$
- ▶  $p_i$ : best position of  $i$ -th particle
- ▶  $p_g$ : position of best particle so far
  - ▶ 1<sup>st</sup> term: momentum part (history)
  - ▶ 2<sup>nd</sup> term: cognitive part (private thinking)
  - ▶ 3<sup>rd</sup> term: social part (collaboration)

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## PSO Algorithm

1. Initialize a random population
2. For each particle
  - ▶ Evaluate and update  $p_{best}$
3. Identify  $p_g$
4. Compute velocity and position for each particle
5. Loop till termination

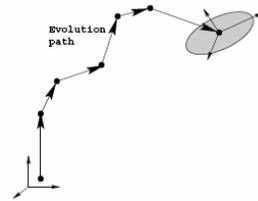
- ▶ Modifications exist
- ▶ Constrained PSO, Hybrid PSO, multi-objective PSO, etc.

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## CMA-ES (Hansen & Ostermeier, 1996)

- ▶ Selecto-mutation ES is run for  $n$  iterations
- ▶ Successful steps are recorded
- ▶ They are analyzed to find uncorrelated basis directions and strengths
- ▶ Required  $O(n^3)$  computations to solve an eigenvalue problem
- ▶ Rotation invariant



## CMA-ES On Three Test Problems

EA	$F_{elp}$			$F_{sch}$		
	Best	Median	Worst	Best	Median	Worst
CMA-ES	8,064	8,472	8,868	15,096	15,672	16,464
DE	9,660	12,033	20,881	102,000	119,170	185,590
G3+PCX	5,826	6,800	7,728	13,988	15,602	17,188
				Accuracy $1 \times 10^{-20}$		
CMA-ES	29,208	33,048	41,076			
DE	243,800	587,920	942,040			
G3+PCX	16,508	21,452	25,520			

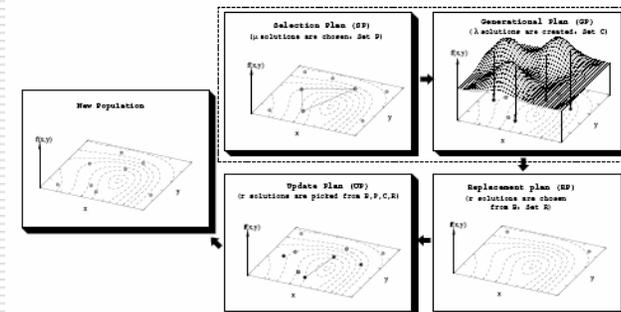


## Population-Based Optimization Algorithm-Generator

- ▶ Four functionally different Plans
  - ▶ **Selection plan (SP)**: choose  $\mu$  solutions from  $B$  to create  $P$
  - ▶ **Generation plan (GP)**: create  $\lambda$  solutions ( $C$ ) using  $P$
  - ▶ **Replacement plan (RP)**: choose  $r$  solutions ( $R$ ) from  $B$
  - ▶ **Update plan (UP)**: update  $B$  by replacing  $R$  ( $r$  solutions) from  $(P, C, R)$



## A Sketch of an Iteration



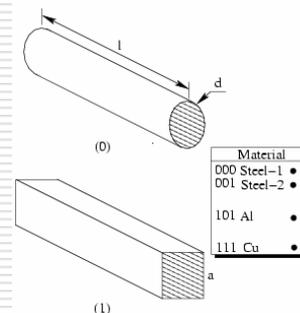
## Designing an Optimization Procedure

1. Choose SP, GP, RP and UP
  2. Perform a parametric study on a set of test problems
    - $N, \mu, \lambda, r$
- ▶ Most classical and non-classical optimization algorithms explained
  - ▶ Interestingly, PSO, DE, ES, EP can also be explained
  - ▶ Possibility for a **unified** optimization approach



## Mixed-Variable Optimization: Handling mixed type of variables

- ▶ Treat type of cross-sections, materials, etc. as decision variables
- ▶ A mixed representation:
  - (1) 14 23.457 (101)
- ▶ (1): circular or square cross-section
- ▶ 14: diameter/side
- ▶ 23.457: length
- ▶ (101): material
- ▶ Permutation + real + cont.
- ▶ **Complete optimization**
- ▶ Deb and Goel, ASME-JMD, 1997



## Constraint Handling: Handling non-linear constraints

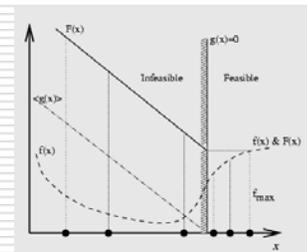
- ▶ Inequality constraints ( $g_j(x) \geq 0$ ) penalized for violation:
 
$$F(x) = f(x) + \sum_{j=1}^J R_j \langle g_j(x) \rangle^2$$
  - ▶  $\langle a \rangle = a$  if  $a$  is -ve, 0 otherwise
- ▶ Performance sensitive to penalty parameters

R	≤ 50%	Infeasible	Best	Median	Worst
$10^0$	12	13	2.41324	7.62465	483.50177
$10^1$	12	0	3.14206	4.33457	7.45453
$10^3$	1	0	3.38227	5.97060	10.65891
$10^6$	0	0	3.72929	5.87715	9.42353



## A Penalty-Parameter-less Population-based Approach

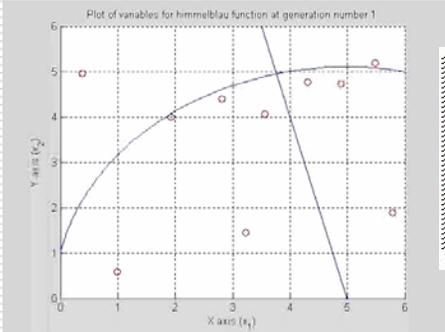
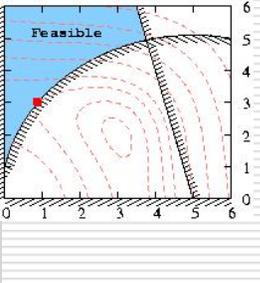
- ▶ Modify tournament sel.:
  - ▶ A feasible is better than an infeasible
  - ▶ For two feasibles, choose the one with better  $f$
  - ▶ For two infeasibles, choose the one with smaller constraint violation ( $\sum_j \langle g_j(x) \rangle$ )
  - ▶ (Deb, 2000)



$$F(x) = \begin{cases} f(x), & \text{if } g_j(x) \geq 0, \forall j \in J \\ f_{\max} + \sum_{j=1}^J \langle g_j(x) \rangle, & \text{otherwise} \end{cases}$$



## A Computer Simulation

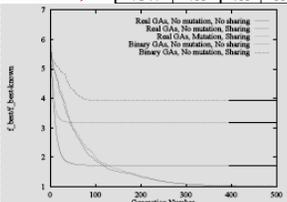


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## Welded-Beam Design Problem

Method	Mutation	sharing	ε						
			< 1%	< 2%	< 5%	< 10%	< 20%	< 50%	> 50%
Maximum generations = 500									
IS-B	No	No	0	0	0	0	0	0	50
TS-B	No	Yes	0	0	0	0	0	0	50
TS-R	No	No	0	0	1	4	8	16	34
TS-R	No	Yes	28	36	44	48	50	50	0
Maximum generations = 4,000									
TS-R	No	Yes	28	37	44	48	50	50	0
TS-R	Yes	Yes	50	50	50	50	50	50	0



Case	Best	Median	Worst
1	4.939027	7.183082	12.084255
2	3.820984	8.899963	14.298933
3	2.442714	3.834121	7.444246
4	2.381191	2.392892	2.645833
5	2.381187	2.392025	2.645833
6	2.381447	2.382634	2.383554



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## Large-Scale Optimization: Handling large number of variables

- ▶ Large n, large pop-size, large computation
- ▶ Knowledge-augmented EAs
  - ▶ Representation
  - ▶ Operators
- ▶ EA's flexibility shows promise
- ▶ A case study involving millions of variables (Deb and Reddy, 2001)

Casting Scheduling



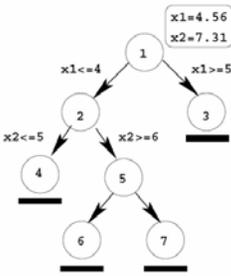


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## Casting Scheduling Problem (cont.)

- ▶ Maximum metal utilization:
 
$$\frac{1}{H} \sum_{i=1}^H \frac{100 \sum_{k=1}^K w_k x_{ki}}{W_i}$$
- ▶ Constraints:
  - Demand satisfaction:  $\sum_{i=1}^H x_{ki} = r_k$  for  $k = 1, \dots, K$
  - Capacity constraint:  $\sum_{k=1}^K w_k x_{ki} \leq W_i$  for  $i = 1, \dots, H$



- ▶ An **integer linear program (ILP)**
- ▶ Branch-and-bound – exponential algorithm



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## Performance of LINGO

- Works up to  $n=500$  on a Pentium IV (7)

LINGO MILP Solver												
Heat No.	Order Number										Utilization/ Cruc. Size	Efficiency (%)
	1	2	3	4	5	6	7	8	9	10		
1	0	1	1	0	0	0	2	1	0	0	623/650	95.85
2	2	0	0	0	1	0	0	0	2	0	615/650	94.62
3	1	0	0	1	3	1	0	0	0	0	611/650	94.00
4	2	0	0	0	1	0	0	1	0	0	645/650	99.23
5	0	0	0	1	0	2	0	0	1	6	612/650	94.15
6	1	1	0	0	2	1	0	0	0	0	591/650	90.92
7	0	0	2	2	1	0	0	0	2	0	585/650	90.00
8	0	3	0	0	0	1	0	0	1	0	611/650	94.00
9	0	2	3	0	1	0	0	0	0	0	650/650	100.00
10	1	0	0	5	0	0	0	0	1	0	635/650	97.69
	7	7	6	9	9	5	2	2	7	6	Average	95.05



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## Off-The-Shelf GA Results

Number of Variables	Binary-coded GAs			Real-coded GAs		
	Population Size	Efficiency	Function Eval.	Population Size	Efficiency	Function Eval.
100	100	96.15	13,600	100	95.94	23,740
200	300	95.01	1,42,200	200	92.81	1,21,760
300	1,000	90.11	14,12,400	700	95.14	5,84,220

- Exponential function evaluations
- Random initialization, standard crossover and mutations are not enough
- Need a **customized EA**



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## No Free Lunch (NFL) Theorem

- No one gives other a **free lunch**
- In the context of *optimization*
  - Wolpert and McCardy (1997)
    - Algorithms A1 and A2
    - All possible problems **F**
    - Performances P1 and P2 using A1 and A2 for a fixed number of evaluations
    - P1 = P2**
- NFL breaks down for a narrow class of problems or algorithms
- Research effort: Find the best algorithm for a class of problems
  - Unimodal, multi-modal, quadratic etc.



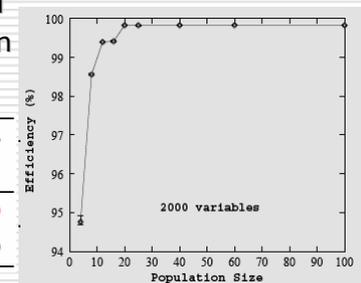
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## A Customized GA: Optimal Population Size

- $N=2000$  variables with max. gen. =  $1000/N$
- A critical population size is needed

N:	4	8	12	16
# Heats:	211	204	201	201
N:	20	25	40	100
# Heats:	200	200	200	200



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## Scale-Up Results

Best-Updates vs Number of Variables (Slope=0.944)

Clock Time (sec) vs Number of Variables (Slope=1.281)

- ▶ Knowledge-augmented GA has sub-quadratic complexity and up to **one million** variables (Deb and Pal, 2003)
- ▶ **Never before such a large problem was solved using EAs**

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## Multi-Modal Optimization: *Handling multiple optimal solutions*

- ▶ To solve problems with multiple local/global optimum
- ▶ Classical methods can find only one optimum at a time
- ▶ EAs can, in principle, find multiple optima simultaneously

Efficiency vs x

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## Niching Concept

Multiple niches (human and animal) coexist in nature

- ▶ By sharing resources (land, food, etc.)
- ▶ How to mimmick the concept in EAs?
- ▶ Reduce selection pressure for crowded solutions
- ▶ Use a **sharing function** based on two-armed bandit problem

$Sh(d)$  vs  $d$

Efficiency vs x

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## Two-Armed Bandit Problem

- ▶ If we know which arm pays more, all population members crowd there
  - ▶ Same as converging to one optima
- ▶ Introduce sharing payoff strategy
- ▶ All player share payoff with others interested in playing the same arm
- ▶ Steady-state distribution: Players in both arms

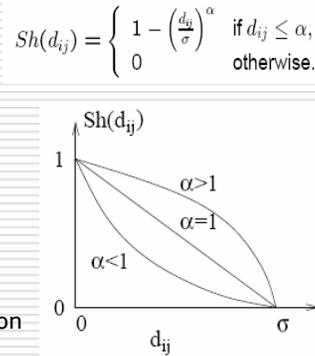
left arm right arm

$f_L/m_L = f_R/m_R$

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## Sharing Function

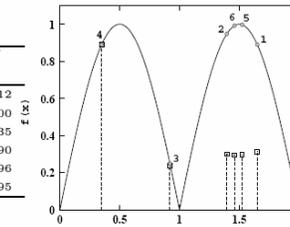
- ▶ Goldberg and Richardson (1997)
- ▶  $d$  is a distance measure between two solns.
  - ▶ Phenotypic distance:  $d(x_i, x_j)$ ,  $x$ : variable
  - ▶ Genotypic distance:  $d(s_i, s_j)$ ,  $s$ : string
- ▶ Calculate niche count,  $nc_i = \sum_j Sh(d_{ij})$
- ▶ Shared fitness:  $f'_i = f_i / nc_i$
- ▶ Use proportionate selection operator



## An Example: Phenotypic Sharing

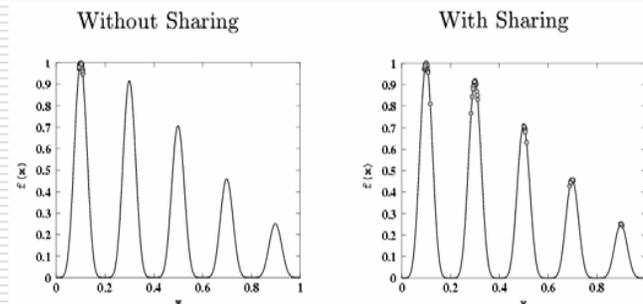
- Maximize  $f(x) = |\sin(\pi x)|$ ,  $x \in [0, 2]$
- $nc_i = \sum_{j=1}^N Sh(d_{ij})$

Sol. $i$	String	$x^{(i)}$	$f_i$	$nc_i$	$f'_i$
1	110100	1.651	0.890	2.856	0.312
2	101100	1.397	0.948	3.160	0.300
3	011101	0.921	0.246	1.048	0.235
4	001011	0.349	0.890	1.000	0.890
5	110000	1.524	0.997	3.364	0.296
6	101110	1.460	0.992	3.364	0.295

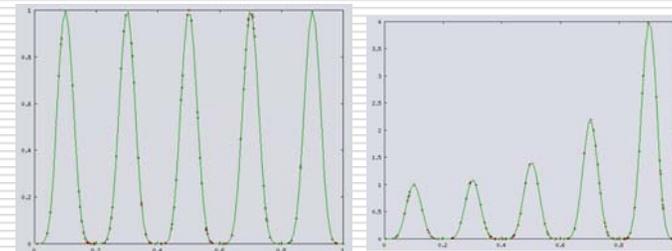


## Simulation Results

- ▶ Inclusion of niche-formation strategy

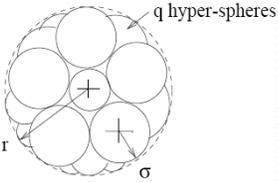


## Simulation on Two Problems



## Phenotypic $\sigma_{share}$

- Assume number of optima:  $q$
- 1-D space:  $\sigma_{share} = (x_{max} - x_{min}) / 2q$
- $p$ -D space:
  - $r$ : Euclidean length of radius of entire  $p$ -D hyper-sphere
  - Volume:  $V = cr^p$
  - Divide volume into  $q$  parts
  - $\sigma_{share}$  is the radius of each part
  - $V = cr^p = q c \sigma_{share}^p$  yields  $\sigma_{share} = r/q^{1/p}$



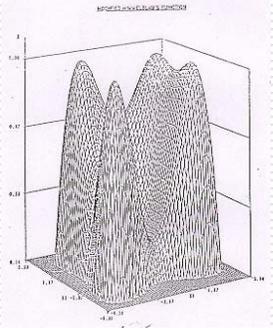
q hyper-spheres

$\sigma_{share} = r/q^{1/p}$

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## More Simulation Results

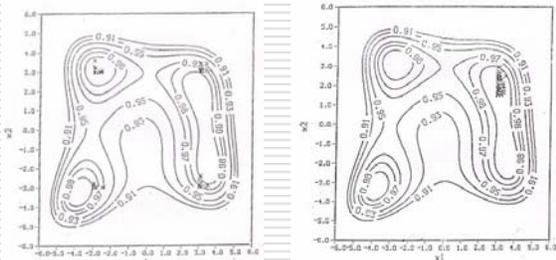
- A two-dimensional function
- Four optima
- Interested in finding all four optima



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## More Simulation Results (cont.)

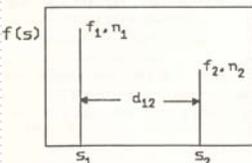
- With and without sharing (phenotypic)



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## Genotypic Sharing

- $d$ =Hamming distance (# of bit differences)
- $q$  niches:  $\frac{1}{2^l} \prod_{i=0}^{l-1} \binom{l}{i} = \frac{1}{q}$
- Approximate:  $\sigma = \frac{1}{2}(l + z^* \sqrt{l})$
- $z^*$  found from cum. Normal distribution chart for  $1/q$
- Restriction on gen. sharing:
  - Need a minimum distance between optima ( $\gamma = f_1/f_2$ )

$$d \geq \left(1 - \frac{1}{\gamma}\right) \sigma$$


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## Other Niching Approaches

- ▶ Clearing approach
- ▶ Clustering approach
- ▶ Crowding approach
- ▶ Pre-selection approach
- ▶ Restrictive tournament selection approach
- ▶ All require at least one tunable parameter



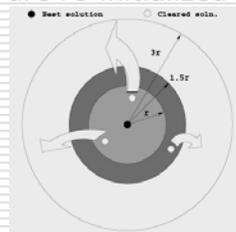
## Clearing Strategy

- ▶ Clear bad near good solutions
  - ▶ Sort population according to fitness
  - ▶ Keep the best and assign zero fitness to all others within  $d$  from best
  - ▶ Keep the next best and assign zero fitness to others within  $d$  from next best
  - ▶ Continue
  - ▶ Perform a selection with assigned fitness
- ▶ Petrowski (1996)



## Modified Clearing Strategy

- ▶ Most members are wasted
- ▶ A better approach
  - All zero-fitness solutions are re-initialized outside  $1.5r$  of best
  - Performs better
- Singh and Deb (2006)



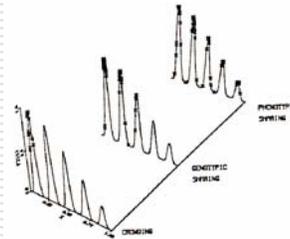
## Clustering Approach

- ▶ Based on phenotypic space, a clustering is performed
  - ▶ With a predefined  $d$
  - ▶ With a predefined number of clusters
  - ▶ Niching within each cluster
  - ▶ Mating restriction can also be performed
- ▶ Parameter sensitive
- ▶ Yin and Gernay (1993)



## Crowding Approach

- ▶ De Jong (1975)
  - ▶ Child solution replaces the most similar solution from a subpopulation
  - ▶ Subpopulation size
- ▶ Mahfoud (1993)
- ▶ Maintains diversity
- ▶ Not as good as sharing (Deb and Goldberg, 1989)



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## Comparison on a Scalable Problem



- ▶ Optima are placed randomly
- ▶ Gaussian shape
- ▶ A8 (Mod. Clearing) performs the best
  - ▶ A1: Clearing
  - ▶ A2: Clustering
  - ▶ A4: Crowding

No. of Peaks		A1	A2	A4	A8
20	SR	15.78	19.0	19.28	<b>20.0</b>
	SD	4.18	1.44	1.20	<b>0.0</b>
	TT	112.6	23.39	120.4	2156.7
30	SR	25.0	27.38	28.58	<b>30.0</b>
	SD	3.02	2.82	1.56	<b>0.0</b>
	TT	155.0	36.72	144.8	2526.8
40	SR	35.14	36.24	38.12	<b>40.0</b>
	SD	4.50	2.80	2.23	<b>0.0</b>
	TT	121.6	120.7	125.0	2967.9
50	SR	44.86	42.2	47.6	<b>50.0</b>
	SD	2.53	4.40	2.43	<b>0.0</b>
	TT	321.8	222.8	335.6	3326.0
	SD	64.14	60.92	138.9	2142.7



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## Optimization with Meta-Models:

*Handling computationally expensive problems*

- ▶ Evaluation of most real-world problems is computationally expensive
- ▶ Optimization algorithm run into days
- ▶ To save time, use **approximate models** of objective function and constraints
- ▶ Different techniques
  - ▶ A fixed model
  - ▶ Updating the model with iteration



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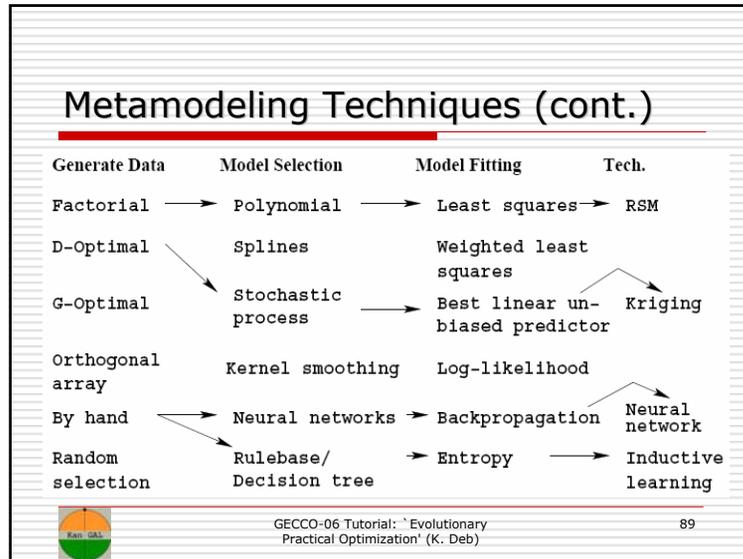
## Metamodeling Techniques

- ▶ Three tasks
  - ▶ Generate data using an experimental design method or a computer
  - ▶ Choose a model to represent data
  - ▶ Fit the model to the data
- ▶ Some common techniques
  - ▶ Response surface methodology (RSM)
  - ▶ Neural networks
  - ▶ Kriging
  - ▶ Inductive learning



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### Response Surface Method (RSM)

- ▶ Box and Wilson (1951)
- ▶ Model: Error is independent of x
  - $y(\mathbf{x}) = g(\mathbf{x}) + \epsilon, \epsilon = N(0, \sigma),$
  - $\hat{y}(\mathbf{x}) = g(\mathbf{x})$
- ▶ Assume  $g(\mathbf{x})$ , usually parametric linear or quadratic

$$\hat{y} = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \sum_{j=1}^k \beta_{ij} x_i x_j$$

- ▶  $\beta_i$  determine data from observed data
- ▶ Optimize to minimize error: Find mean  $\beta_i$
- ▶ Variance of  $\beta_i$  determine predictive capability

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### RSM Tips

- ▶ Popular and most widely used
- ▶ Best suited in applications with random error
- ▶ However, limited handling on non-linearity
- ▶ Usually applied for  $k < 10$
- ▶ Sequential RSM with move limits and trust region approach is better

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### Artificial Neural Networks (ANN)

- ▶ Mimicking natural neural processing
- ▶ Input: Variables (n)
- ▶ Output: Objective and constraint functions
- ▶ Sigmoidal activation function for hidden and output neurons

$$y = \frac{1}{1 + \exp(-(\sum_i w_i x_i + \beta)/T)}$$

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## ANN (cont.)

- ▶ Obtain relationship among input-output
- ▶ Optimal connection and its weights for minimum error

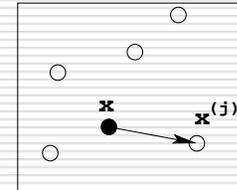
$$E = \|\mathbf{y}_p - \hat{\mathbf{y}}_p\|$$

- ▶ A non-linear regression method
- ▶ Suitable for large (104) parameters
- ▶ Best suited for deterministic problems (no random error)
- ▶ Computationally expensive procedure



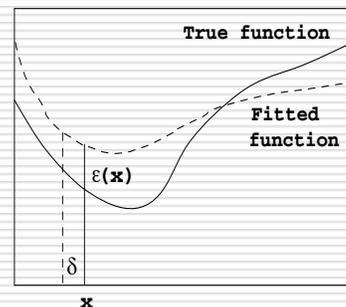
## Kriging Procedure

- ▶ D. G. Krige (a geologist): Statistical analysis of mining data
  - ▶ Predict a value at a point from a given set of observations
- $$f(\mathbf{x}) = \sum_{i=1}^M \lambda_i y(\mathbf{x}^{(i)})$$
- ▶  $\lambda_i$  depends on distance of  $\mathbf{x}$  from observed points
  - ▶ Flexible, but complex
  - ▶ Suited for  $k < 50$ , deterministic problems



## Fundamentals of Kriging

- ▶  $F(\mathbf{x})$  is true function
- ▶  $f(\mathbf{x})$  is fitted function
- ▶  $\varepsilon(\mathbf{x}) = F(\mathbf{x}) - f(\mathbf{x})$
- ▶ If error at  $\mathbf{x}$  is large, it is reasonable to believe that
  - ▶ Error at  $\mathbf{x} + \delta$  is also large



## Fundamentals of Kriging (cont.)

- Say,  $M$  data points:  $(\mathbf{x}^{(j)}, y_j)$ ,  $j = 1, 2, \dots, M$
- Assume model:  $Y(\mathbf{x}) = \sum_{k=1}^K \beta_k \mathbf{f}_k(\mathbf{x}) + Z(\mathbf{x})$
- $\mathbf{f}_k(\mathbf{x})$  assumed **global model**, can be taken as **constant**, polynomial or others
- $Z(\mathbf{x})$  is a **local variation** and stochastic:
  - $E(Z(\mathbf{x})) = 0$
  - $Cov(Z(\mathbf{w}), Z(\mathbf{x})) = \sigma_Z^2 R(\mathbf{w}, \mathbf{x})$
  - $\sigma_Z^2$  is the process variance
  - $R(\mathbf{w}, \mathbf{x})$  is spatial correlation function (SCF)
  - $R(\mathbf{w}, \mathbf{x}) = \prod_{j=1}^n R_j(\mathbf{w}_j, \mathbf{x}_j)$
  - SCF ( $R_j$ ) is function of distance between  $\mathbf{w}_i$  and  $\mathbf{x}_i$



## Commonly Used SCFs

Exponential:  
 $\exp(-\theta_j | \mathbf{w}_j - \mathbf{x}_j |^\alpha) \quad 0 < \alpha \leq 2$

Gaussian:  
 $\exp(-\theta_j | \mathbf{w}_j - \mathbf{x}_j |^2)$

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## Kriging Procedure

**Step 1:** Normalize  $\mathbf{x}^{(j)}$  and  $y^{(j)}$  and set  $\mathbf{Y} = [y^{(j)}]$

**Step 2:** Maximize log-likelihood function:

$$\max_{\boldsymbol{\theta}} -\frac{1}{2} [M \log \sigma_Z^2 + \log R(\boldsymbol{\theta})]$$

and obtain  $\boldsymbol{\theta}^*$

- $R(\boldsymbol{\theta})$  is a matrix:  $\prod_{j=1}^n R_j(\mathbf{w}_j, \mathbf{x}_j; \theta_j)$
- MLE of  $\sigma_Z^2$ :  $\sigma_Z^2 = \frac{1}{M} (\mathbf{Y} - \mathbf{I}\hat{\boldsymbol{\beta}}(\boldsymbol{\theta}))^T R(\boldsymbol{\theta})^{-1} (\mathbf{Y} - \mathbf{I}\hat{\boldsymbol{\beta}}(\boldsymbol{\theta}))$
- MLE of  $\hat{\boldsymbol{\beta}}$ :  $\hat{\boldsymbol{\beta}}(\boldsymbol{\theta}) = (\mathbf{I}^T R(\boldsymbol{\theta})^{-1} \mathbf{I})^{-1} \mathbf{I}^T R(\boldsymbol{\theta})^{-1} \mathbf{Y}$

**Step 3:** Compute  $\hat{\boldsymbol{\beta}}^* = \hat{\boldsymbol{\beta}}(\boldsymbol{\theta}^*)$ ,  $R(\boldsymbol{\theta}^*)$ , and  $\sigma_Z^{2*}$

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## Kriging Procedure (cont.)

**Step 4:** Compute fitted function at any point  $\mathbf{x}$ :

$$\hat{y}(\mathbf{x}) = \hat{\boldsymbol{\beta}}^* + \mathbf{r}^T(\mathbf{x}) R(\boldsymbol{\theta}^*)^{-1} (\mathbf{Y} - \mathbf{I}\hat{\boldsymbol{\beta}}^*)$$

where  $\mathbf{r}(\mathbf{x}) = [R(\mathbf{x}, \mathbf{x}^{(i)})] \quad i = 1, 2, \dots, M$

**Step 5:** The corresponding MSE (error):

$$MSE(\mathbf{x}) = \sigma_Z^{2*} \left[ 1 - \left( \mathbf{1} \quad \mathbf{r}^T(\mathbf{x}) \right) \begin{pmatrix} 0 & \mathbf{I}^T \\ \mathbf{I} & R(\boldsymbol{\theta}^*) \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ \mathbf{r}(\mathbf{x}) \end{pmatrix} \right]$$

- If  $\mathbf{x}$  is closer to an observed point, the MLE will be small

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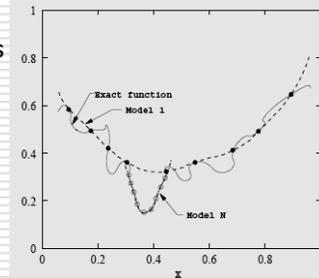
## Model Verification

- ▶ Leave-one-out-cross-validation scheme
- ▶ Leave out one observation (say  $\mathbf{x}^{(j)}$  and  $y^{(j)}$ )
- ▶ Find the kriging model with  $(M-1)$  points and find  $\hat{y}^{(j)}$
- ▶ Compute the error  $s^j = \sqrt{MSE(\mathbf{x}^{(j)})}$
- ▶ If the normalized error  $(y^{(j)} - \hat{y}^{(j)})/s^j$  is within  $[-3, 3]$ , the model is acceptable

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## Successive Modeling Procedure

- ▶ Nain and Deb (2003)
- ▶ Successive approximations to the problem
- ▶ Initial coarse approximate model defined over the whole range of decision variables with small database
- ▶ Gradual finer approximate models localized in the search space

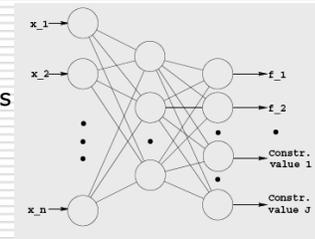


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## ANN Model

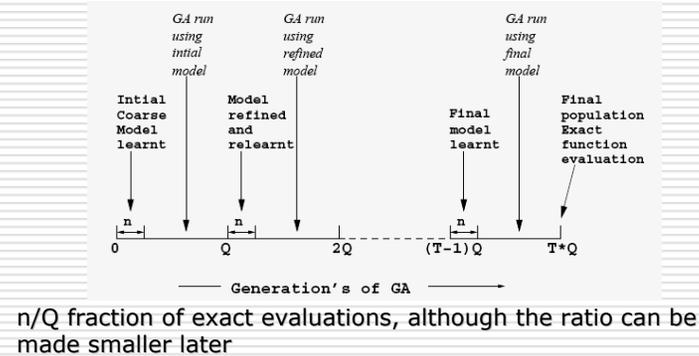
- ▶ A feed-forward neural network
- ▶ Input: Decision variables (size  $n$ )
- ▶ Output: Objective functions and constraint violations (size  $M+J$ )
- ▶ One hidden layer with  $H$  neurons
- ▶ Sigmoidal activation for hidden and output neurons



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## Generation-wise Sketch of Proposed Approach



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## Flip Side: Parameters Involved

- ▶ Frequency of ANN modeling
- ▶ Number of training points (can reduce with iteration)
- ▶ Learning rate in training
- ▶ Final RMS error in ANN training
- ▶ Learning models (incremental or batch)
- ▶ ANN architecture (connectivity and hidden layers)

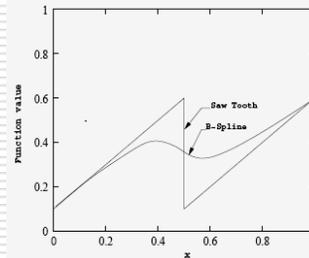


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## A Case Study from Curve-Fitting

- ▶ Two-objective problem:
  - ▶ Minimize error from the curve
  - ▶ Minimize the maximize curvature
- ▶ 41 control points forming a B-spline curve (39 varied)



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## Formulation of the Problem

- ▶ A B-spline curve  $S$  having 41 control points in  $[0,1]$
- ▶ Numerical computation of the integral with 400 intermediate points:

$$f_1(S) = \int_{x=0}^{x=1} |f_{\text{saw-tooth}} - S| dx$$

- ▶ Differentials are computed exactly

$$f_2(S) = \max_{x=0}^{x=1} \frac{\frac{d^2 S}{dx^2}}{\left[1 + \left(\frac{dS}{dx}\right)^2\right]^{3/2}}$$

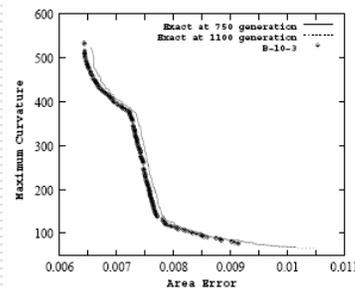


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## Savings in Function Evaluations

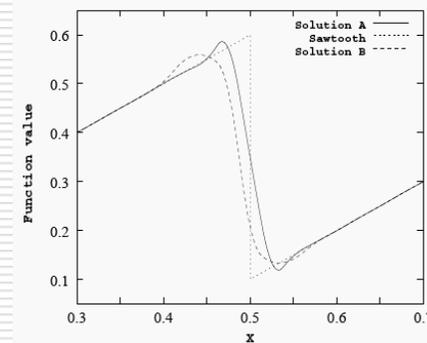
- ▶ B-10-3 finds a front in (750x200) evaluations similar to NSGA-II in (1100x200) evaluations
- ▶ A saving of 32% evaluations



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## Extreme Trade-off Solutions



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### Multi-Objective Optimization: *Handling multiple conflicting objectives*

- ▶ We often face them

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### Classical Approach: *Weighted-Sum Method*

- ▶ Construct a weighted sum of objectives and optimize

$$F(x) = \sum_{i=1}^M w_i f_i(x)$$

- ▶ User supplies weight vector  $w$
- ▶ Non-convexity a problem

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### Classical Approach: *$\epsilon$ -Constraint Method*

- ▶ Constrain all but one objective
- ▶ Need to know relevant  $\epsilon$  vectors
- ▶ Non-uniformity in Pareto-optimal solutions
- ▶ Any Pareto-optimal solutions can be found with this approach

Minimize  $f_\mu(x)$ ,  
subject to  $f_m(x) \leq \epsilon_m, m \neq \mu$

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### Evolutionary Multi-Objective Optimization (EMO)

- Step 1 : Find a set of Pareto-optimal solutions
- Step 2 : Choose one from the set (Deb, 2001)

- Ideal for an EA

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## Elitist Non-dominated Sorting Genetic Algorithm (NSGA-II)

- ▶ NSGA-II can extract Pareto-optimal frontier
- ▶ Also find a well-distributed set of solutions
- ▶ **iSIGHT and modeFrontier adopted NSGA-II**

Fast-Breaking Paper in Engineering by ISI Web of Science (Feb'04)

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## NSGA-II Procedure

Elites are preserved  
Non-dominated solutions are emphasized

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## NSGA-II (cont.)

Diversity is maintained

Overall Complexity  $O(N \log^{M-1} N)$

Improve diversity by

- k-mean clustering
- Euclidean distance measure
- Other techniques

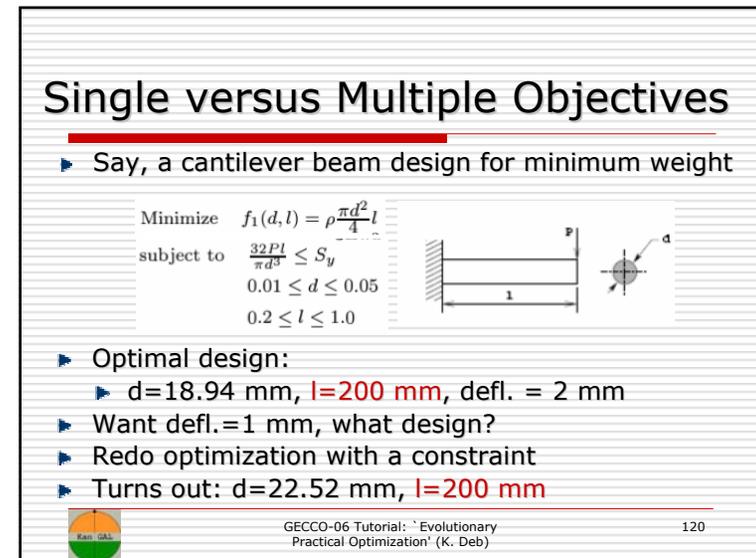
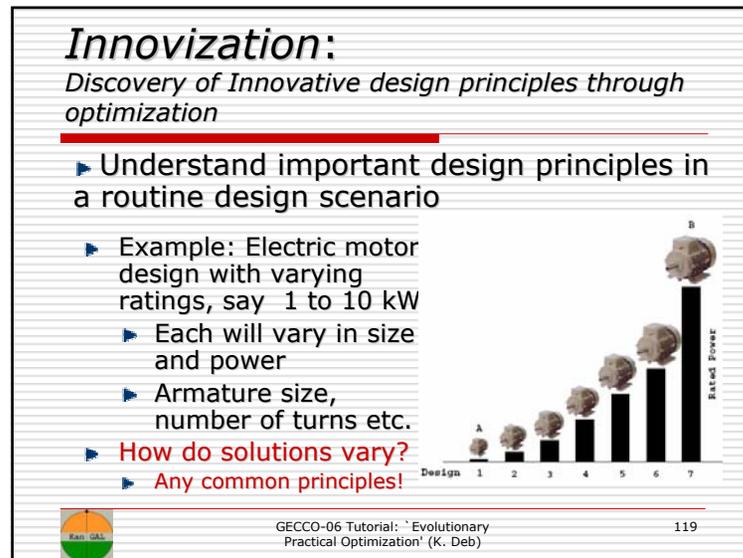
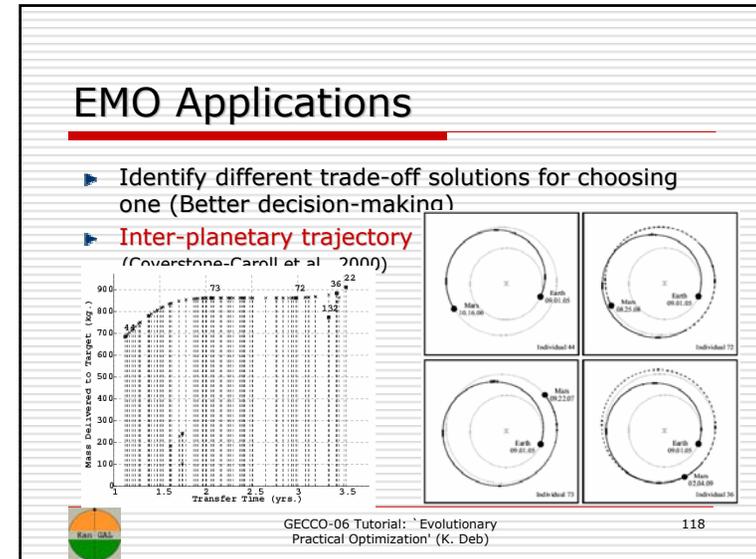
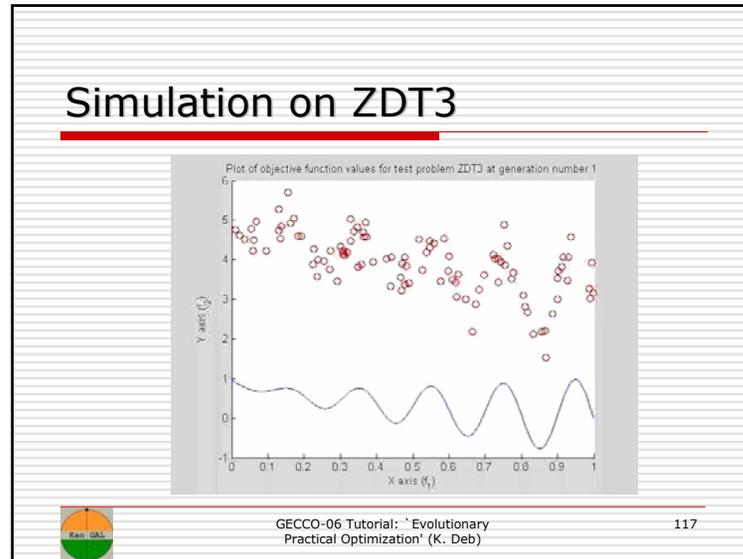
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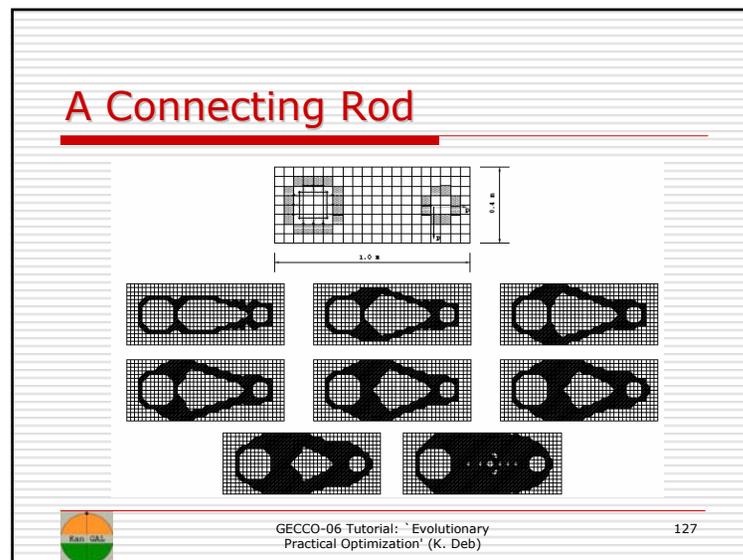
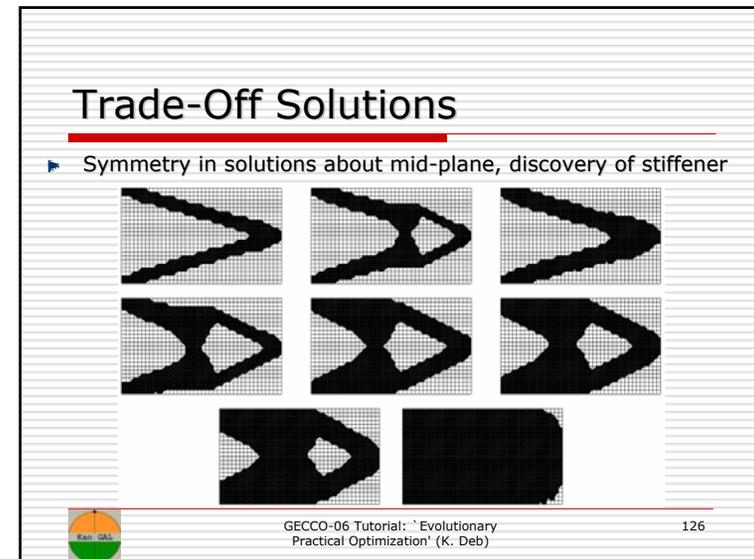
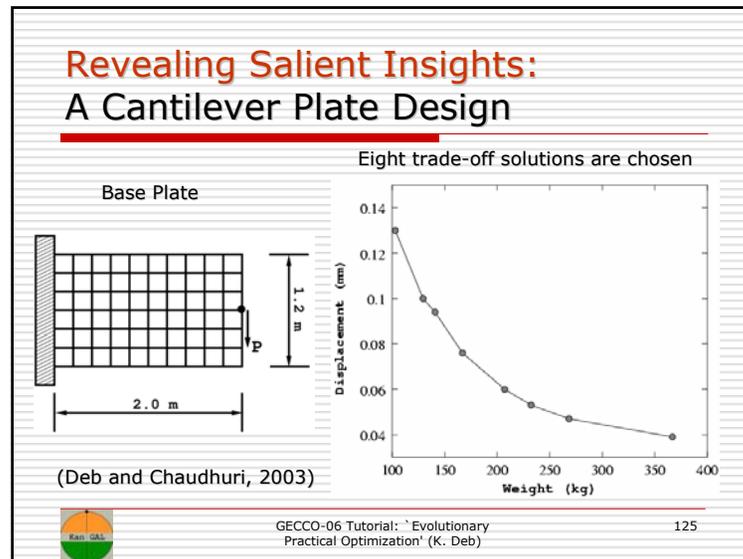
## Simulation on ZDT1

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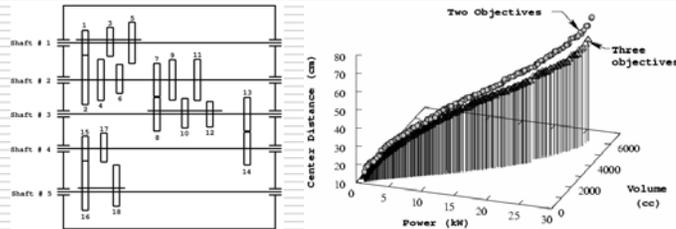




- ### Innovized Principles
- Mid-line symmetry
  - Straight arms to reach load is minimum-weight strategy
  - Two ways to increase stiffness
    - Thickening of arms
    - Use of a stiffener
    - Additional stiffening by a combination
  - Chamfering of corners helpful
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## Gear-box Design

- ▶ A multi-spindle gear-box design (Deb and Jain, 2003)
- ▶ 28 variables (integer, discrete, real-valued)
- ▶ 101 non-linear constraints
- ▶ Important insights obtained (larger module for more power)

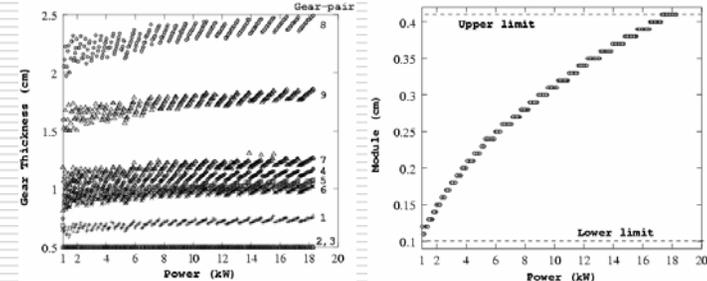


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## Innovized Principles

- ▶ Module varies proportional to square-root of power
- ▶ Keep other 27 variables more or less the same



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## Mechanical Spring Design

- ▶ Minimize material volume
- ▶ Minimize developed stress
- ▶ Three variables: (d, D, N): discrete, real, integer
- ▶ Eight non-linear constraints
  - ▶ Solid length restriction
  - ▶ Maximum allowable deflection ( $P/k \leq 6\text{in}$ )
  - ▶ Dynamic deflection ( $(P_m - P)/k \geq 1.25\text{in}$ )
  - ▶ Volume and stress limitations

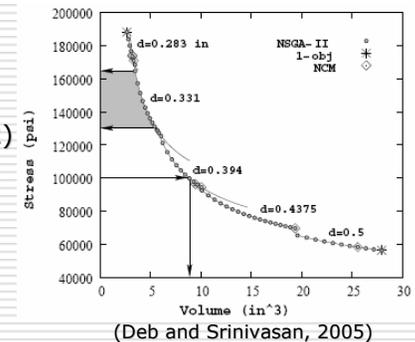


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## Innovized Principles

- ▶ Pareto-optimal front have niches with d
- ▶ Only 5 (out of 42) values of d (large ones) are optimal
- ▶ A blue-print for optimal design



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## Epoxy Polymerization

- ▶ Three ingredients added hourly
- ▶ 54 ODEs solved for a 7-hour simulation
- ▶ Maximize chain length (Mn)
- ▶ Minimize polydispersity index (PDI)
- ▶ Total 3x7 or 21 variables
- ▶ (Deb et al., 2004)

A non-convex frontier

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## Epoxy Polymerization (cont.)

- ▶ Some patterns emerge among obtained solutions
- ▶ Chemical significance unveiled

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## Innovized Principles: An Optimal Operating Chart

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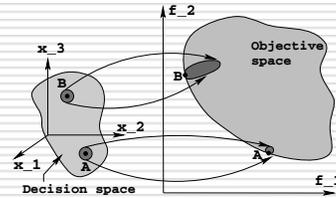
## Robust Optimization: Handling uncertainties in variables

- ▶ Parameters are **uncertain** and **sensitive** to implementation
  - ▶ Tolerances in manufacturing
  - ▶ Material properties are uncertain
  - ▶ Loading is uncertain
- ▶ Who wants a sensitive optimum solution?
- ▶ Single-objective robust EAs (Branke and others)

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## Multi-Objective Robust Solutions

- ▶ Solutions are averaged in  $\delta$ -neighborhood
- ▶ Not all Pareto-optimal points may be robust
- ▶ A is robust, but B is not
- ▶ Decision-makers will be interested in knowing robust part of the front



## Multi-Objective Robust Solutions of Type I and II

- ▶ Similar to single-objective robust solution of type I

$$\begin{aligned} & \text{Minimize } (f_1^{\text{eff}}(\mathbf{x}), f_2^{\text{eff}}(\mathbf{x}), \dots, f_M^{\text{eff}}(\mathbf{x})), \\ & \text{subject to } \mathbf{x} \in S, \end{aligned}$$

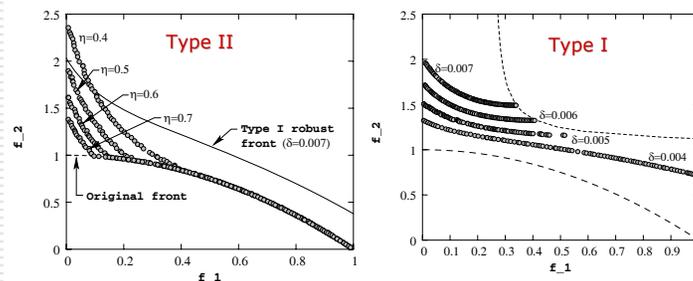
- ▶ Type II

$$\begin{aligned} & \text{Minimize } \mathbf{f}(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_M(\mathbf{x})), \\ & \text{subject to } \frac{\|\mathbf{f}^p(\mathbf{x}) - \mathbf{f}(\mathbf{x})\|}{\|\mathbf{f}(\mathbf{x})\|} \leq \eta, \\ & \mathbf{x} \in S. \end{aligned}$$



## Robust Frontier for Two Objectives

- ▶ Identify robust region
- ▶ Allows a control on desired robustness



## Robustness with Constraints

- ▶ Constraints will make boundary solutions infeasible
- ▶ Simply declare a solution infeasible, if any of H neighboring points is infeasible
- ▶ Use constraint tournament selection in NSGA-II



## Test Problem 1

Constrained effective front is different

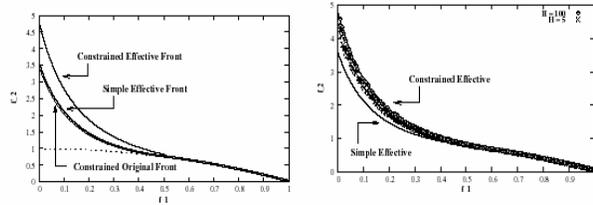


Fig. 1. Theoretical simple and constrained effective fronts on test problem 1.

Fig. 2. Constrained effective fronts showing the effect of number of points H on test problem 1.



## Effect of H

Larger H, more shift

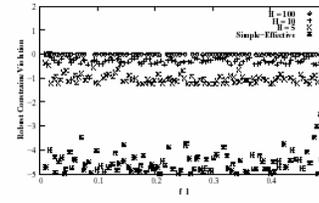


Fig. 3. Robust constraint violation for the points obtained on test problem 1 with different values of H.

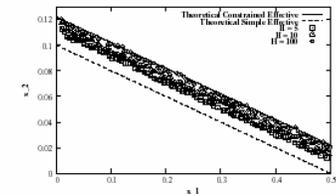


Fig. 4.  $x_1$  vs  $x_2$  relationship for different values of H on test problem 1.



## Faster Computation for Robustness

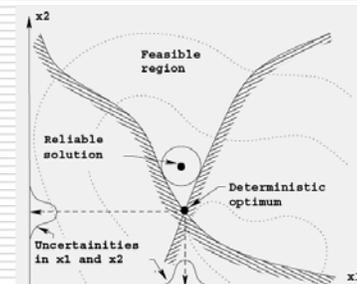
- ▶ Use of an archive to store already computed solutions
- ▶ Later, select solutions from the archive within  $\delta$ -neighborhood
- ▶ If H points not found, create a solution
- ▶ Although reported quicker single-objective runs, multi-objective runs are not quicker
- ▶ A diverse set is needed, requiring archive to be large



## Reliability-Based Optimization:

*Making designs safe against failures*

- ▶ Deterministic optimum is not usually reliable
- ▶ Reliable solution is an interior point
- ▶ Chance constraints with a given reliability



Minimize  $\mu_f + k\sigma_f$   
 Subject to  $Pr(g_i(x) \geq 0) \geq \beta_j$   
 $\beta_j$  is user-supplied



### Nested Optimization: Check if a solution is reliable

▶ PMA approach

Minimize  $G_j(\mathbf{U})$ ,  
Subject to  $\|\mathbf{U}\| = \beta_j^r$ ,

$G_j(\mathbf{U}^*) \geq 0.$

▶ RIA approach

Minimize  $\|\mathbf{U}\|$ ,  
Subject to  $G_j(\mathbf{U}) = 0.$

$\|\mathbf{U}\| \geq \beta_j^r.$

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### Proposed Faster Procedure

- ▶ Single-loop method
- ▶ Faster computation of  $\mathbf{U}^*$ 
  - ▶ PMA: MPP as computed
  - ▶ RIA: Apply Newton's search to find MPP

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### Finding Global Reliable Solution: Single-objective reliable solution

- ▶ Multiple deterministic optima
- ▶ Reliable solution for local is better
- ▶ Classical methods starts from deterministic global optimum
- ▶ GAs solve the overall problem and are better

PMA approach is used

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### Multiple Reliability Solutions: Get a better insight

RIA approach is used

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## Multi-Objective Reliable Frontier

- ▶ Instead of finding deterministic Pareto-optimal front, find **reliable front**
- ▶ Chance constraints
- ▶ Objectives as they are
- ▶ PMA approach is used

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## Multi-Objective Reliability-Based Optimization

- ▶ Reliable fronts show rate of movement
- ▶ What remains unchanged and what

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## Interactive Optimizers

- ▶ Needs to involve a decision-maker (DM)
- ▶ No concrete study yet
- ▶ A few difficulties:
  - ▶ The act of a DM makes it a single-obj. problem
  - ▶ But, obj. is not known precisely and changes with iteration
  - ▶ EMO finds many solutions, but only one is desired
- ▶ **EMO**: Find potentially good solutions – robust, knee-like, etc.
- ▶ **Classical**: Concentrate in an area based DM's preference

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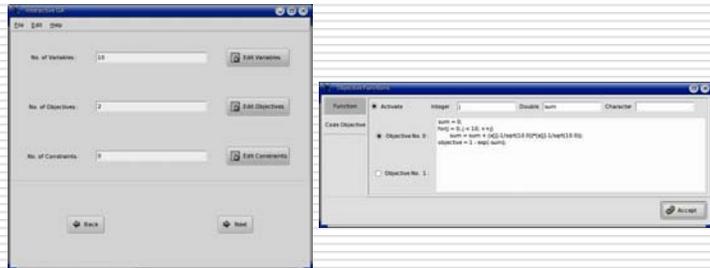
## I-EMO Being Developed at KanGAL

- ▶ GUI-based interactive EMO
  - ▶ Start with a front obtained with NSGA-II
  - ▶ Verify solutions with local searches & classical point-by-point approaches
  - ▶ Help choose a particular solution
    - ▶ Knee solutions
    - ▶ Robust solutions
    - ▶ Partial front
    - ▶  $L_p$  and other utility-based metrics
- ▶ An iterative procedure

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## I-EMO Snap-shots

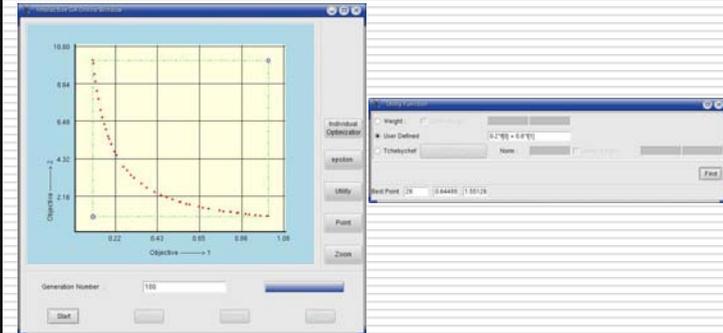
► On a Linux platform



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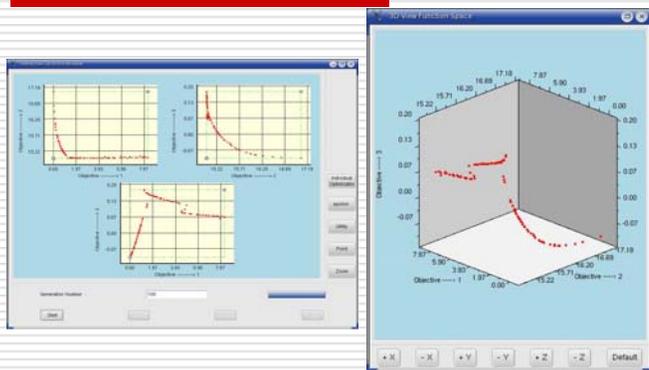
## I-EMO (cont.)



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## I-EMO (cont.)

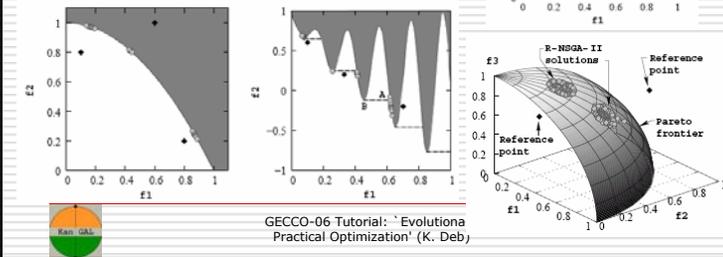


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## Making Decisions: Reference Point Based EMO

- Ranking based on closeness to each reference point
- Clearing within each niche with  $\epsilon$



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## Finding Knee Solutions

Branke et al. (2004) for more details

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## Goal Programming: *Not to find Optimum*

- ▶ Target function values are specified
- ▶ Convert them to objectives and perform domination check with them

Type	Goal	Objective function
$\leq$	$f_j(x) \leq t_j$	Minimize $(f_j(x) - t_j)$
$\geq$	$f_j(x) \geq t_j$	Minimize $(t_j - f_j(x))$
$=$	$f_j(x) = t_j$	Minimize $ f_j(x) - t_j $
Range	$f_j(x) \in [t_j^l, t_j^u]$	Minimize $\max((t_j^l - f_j(x)), (f_j(x) - t_j^u))$

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## Omni-Optimizer: *Motivation from Computation*

- ▶ Multiple is a generic case, single is specific
- ▶ Single objective as a degenerate case multi-objective case
- ▶ One algorithm for single and multi-objective problem solving (Deb and Tiwari, 2005)
- ▶ Accommodating NFL theorem
  - ▶ Single-objective, uni-optimum problems
  - ▶ Single-objective, multi-optima problems
  - ▶ Multi-objective, uni-optimal front problems
  - ▶ Multi-objective, multi-optimal front problems

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## Single-Objective, Uni-Optimum

- ▶ Dominance reduced to simple ' $<$ '
- ▶ Epsilon-dominance to  $f^a < f^b - \epsilon$ 
  - ▶ Allows multiple solutions within  $\epsilon$  to exist
- ▶ Elite-preservation is similar to CHC and  $(\mu + \lambda)$ -ES

Function	$f(x)$	$n$	Range	$N$	Target $f^*$	Func. Eval.		
						Best	Median	Worst
Rastrigin	$\sum_{i=1}^n x_i^2 + 10(1 - \cos(2\pi x_i))$	10	$[-10, 10]$	40	0.01	8,120	15,520	53,480
Rastrigin	$\sum_{i=1}^n x_i^2 + 10(1 - \cos(2\pi x_i))$	20	$[-10, 10]$	40	0.01	24,520	41,760	106,440
Schwefel	$418.9829n - \sum_{i=1}^n x_i \sin \sqrt{ x_i }$	10	$[-500, 500]$	16	0.01	6,304	11,360	24,704
Schwefel	$418.9829n - \sum_{i=1}^n x_i \sin \sqrt{ x_i }$	20	$[-500, 500]$	16	0.01	26,128	36,272	82,096

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## Shinn et al.

12 problems

Definition of benchmark function	Variable bound	Optimum value
$f_1 = \sum_{i=1}^{D-1}  \sin(x_i) + \sin(\frac{2\pi i}{D}) $	[3, 13]	1.21598D (max)
$f_2 = -\sum_{i=1}^{D-1} \sin(x_i + x_{i+1}) + \sin(\frac{2\pi x_{D+1}}{D})$	[3, 13]	$\approx 2D$ (max)
$f_3 = \sum_{i=1}^D  x_i + 0.5 ^2$	[-100, 100]	0 (min)
$f_4 = \sum_{i=1}^{D-1}  x_i^2 - 10 \cos(2\pi x_i) + 10 $	[-5.12, 5.12]	0 (min)
$f_5 = \sum_{i=1}^{D-1}  x_i^2 $	[-5.12, 5.12]	0 (min)
$f_6 = \sum_{i=1}^{D-1}  x_i \sin(10\pi x_i) $	[-1.0, 2.0]	1.85D (max)
$f_7 = \sum_{i=1}^D \frac{\sin(10\pi x_i)}{10\pi x_i}$	[-0.5, 0.5]	0 (min)
$f_8 = 20 + e - 20e^{-0.2\sqrt{\frac{1}{D} \sum_{i=1}^D x_i^2}} - e^{\sum_{i=1}^D \frac{\cos(2\pi x_i)}{\sqrt{x_i}}}$	[-30, 30]	0 (min)
$f_9 = 418.9829D - \sum_{i=1}^D x_i \sin(\sqrt{ x_i })$	[-500, 500]	0 (min)
$f_{10} = \sum_{i=1}^{D-1}  100(x_{i+1} - x_i)^2 + (x_i - 1)^2 $	[-5.12, 5.12]	0 (min)
$f_{11} = 6D + \sum_{i=1}^D  x_i $	[-5.12, 5.12]	0 (min)
$f_{12} = \frac{1}{200} \sum_{i=1}^D x_i^2 - \prod_{i=1}^D \cos(\frac{x_i}{\sqrt{x_i}}) + 1$	[-600, 600]	0 (min)

Dimension Function	60	70	80	90	100	Shinn et al. D = 100
$f_1$	$1.36 \times 10^{-3}$	$2.14 \times 10^{-3}$	$3.00 \times 10^{-3}$	$3.95 \times 10^{-3}$	$5.05 \times 10^{-3}$	$1.20 \times 10^{02}$
$f_2$	$3.32 \times 10^{-1}$	$3.50 \times 10^{-1}$	$3.59 \times 10^{-1}$	$3.72 \times 10^{-1}$	$3.88 \times 10^{-1}$	$1.53 \times 10^{02}$
$f_3$	$7.00 \times 10^{-2}$	$1.61 \times 10^{-1}$	$2.96 \times 10^{-1}$	$5.29 \times 10^{-1}$	$8.91 \times 10^{-1}$	$6.21 \times 10^{02}$
$f_4$	$3.75 \times 10^{-1}$	$5.00 \times 10^{-1}$	$6.40 \times 10^{-1}$	$7.85 \times 10^{-1}$	$9.37 \times 10^{-1}$	$2.13 \times 10^{02}$
$f_5$	$2.09 \times 10^{-4}$	$3.67 \times 10^{-4}$	$6.72 \times 10^{-4}$	$1.08 \times 10^{-3}$	$1.90 \times 10^{-3}$	$1.60 \times 10^{00}$
$f_6$	$1.74 \times 10^{-1}$	$2.17 \times 10^{-1}$	$2.68 \times 10^{-1}$	$3.05 \times 10^{-1}$	$3.41 \times 10^{-1}$	$1.31 \times 10^{02}$
$f_7$	$1.20 \times 10^{-3}$	$1.50 \times 10^{-3}$	$1.81 \times 10^{-3}$	$2.14 \times 10^{-3}$	$2.40 \times 10^{-3}$	$6.50 \times 10^{-1}$
$f_8$	$1.46 \times 10^{-2}$	$1.94 \times 10^{-2}$	$2.29 \times 10^{-2}$	$2.52 \times 10^{-2}$	$2.64 \times 10^{-2}$	$3.69 \times 10^{00}$
$f_9$	$9.62 \times 10^0$	$1.16 \times 10^1$	$1.37 \times 10^1$	$1.48 \times 10^1$	$1.63 \times 10^1$	$8.01 \times 10^{03}$
$f_{10}$	$3.70 \times 10^0$	$4.22 \times 10^0$	$4.68 \times 10^0$	$5.09 \times 10^0$	$5.57 \times 10^0$	$2.08 \times 10^{03}$
$f_{11}$	$0.00 \times 10^0$	$0.00 \times 10^0$	$1.26 \times 10^{-4}$	$1.26 \times 10^{-4}$	$1.26 \times 10^{-4}$	$4.39 \times 10^{01}$
$f_{12}$	$1.37 \times 10^{-2}$	$1.42 \times 10^{-2}$	$1.34 \times 10^{-2}$	$1.28 \times 10^{-2}$	$1.29 \times 10^{-2}$	$3.29 \times 10^{01}$

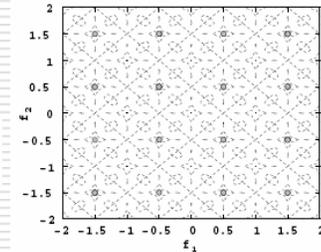
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## Single-Objective, Multi-Optima

- ▶ Variable-space niching help find multiple solutions
- ▶ Weierstrass function
  - ▶ 16 minima with  $f=0$

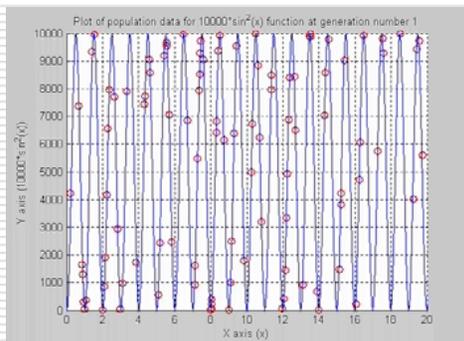
$$f(x) = \sum_{i=1}^D \left[ \sum_{k=0}^{k_{max}} [a^k \cos(2\pi b^k x_i)] \right], \quad x_i \in [-2, 2]$$



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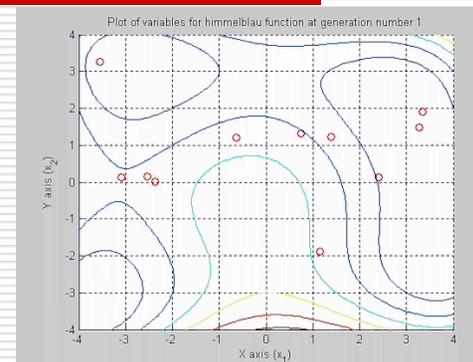
## $10^4 \sin^2(x)$ : 20 Minima



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## Himmelblau's Function: 4 Minima



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### Multi-Objective, Uni-Pareto front

- Constrained and unconstrained test problems

Fig. 7. Efficient points for ZDT1. Fig. 8. Efficient points for ZDT6.

Fig. 9. Efficient points for OSY. Fig. 10. Efficient points for CTP4.

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### More Results

- Comparable performance to existing EMO methods

Test Problem	MOEA	Convergence measure		Sparsity		Hyper-volume	
		Avg.	SD	Avg.	SD	Avg.	SD
ZDT1	NSGA-II	0.00054898	6.62e-05	0.858	0.0202	0.8701	3.85e-04
	C-NSGA-II	0.00061178	7.86e-05	0.994	0.0043	0.8713	2.25e-04
	PESA	0.00053481	12.62e-05	0.754	0.0331	0.8680	6.76e-04
	SPEA2	0.00100589	12.06e-05	0.999	0.0014	0.8708	1.86e-04
	e-MOEA	0.00039545	1.22e-05	0.991	0.0050	0.8702	1.86e-04
	OMNI	0.01089320	9.14e-04	0.922	0.0200	0.8546	9.28e-04
ZDT4	OMNI*	0.00536259	4.32e-04	0.911	0.0251	0.8626	6.54e-04
	OMNP	0.00416721	3.80e-04	0.960	0.0151	0.8649	6.00e-04
	NSGA-II	0.00639002	0.0043	0.958	0.0328	0.8613	0.00610
	C-NSGA-II	0.00618386	0.0744	0.998	0.0029	0.8558	0.00301
	PESA	0.00730242	0.0047	0.798	0.0352	0.8566	0.00710
	SPEA2	0.00769278	0.0043	0.989	0.0132	0.8609	0.00536
ZDT6	e-MOEA	0.00259063	0.0006	0.987	0.0076	0.8509	0.01537
	OMNI	1.69495000	1.0766	0.765	0.0708	0.4819	0.71756
	OMNI*	0.01105010	0.0097	0.899	0.0389	0.8483	0.01779
	OMNP	0.00545542	0.0025	0.958	0.0184	0.8566	0.01522
	NSGA-II	0.07896111	0.0067	0.815	0.0157	0.3959	0.00894
	C-NSGA-II	0.07940667	0.0110	0.995	0.0029	0.3990	0.01154
ZDT6	PESA	0.06415652	0.0073	0.748	0.0345	0.4145	0.00990
	SPEA2	0.00573584	0.0009	0.908	0.0029	0.4968	0.00117
	e-MOEA	0.06792800	0.0118	0.996	0.0023	0.4112	0.01573
	OMNI	0.05342110	0.0055	0.863	0.0228	0.4176	0.00645
	OMNI*	0.02528650	0.0024	0.872	0.0288	0.4511	0.00291
	OMNP	0.021418	0.0023	0.956	0.0143	0.4559	0.00275

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### Multi-Objective, Multi-Optima

$$\text{Minimize } f_1(x) = \sum_{i=1}^n \sin(\pi x_i),$$

$$\text{Minimize } f_2(x) = \sum_{i=1}^n \cos(\pi x_i),$$

$$0 \leq x_i \leq 6, \quad i = 1, 2, \dots, n.$$

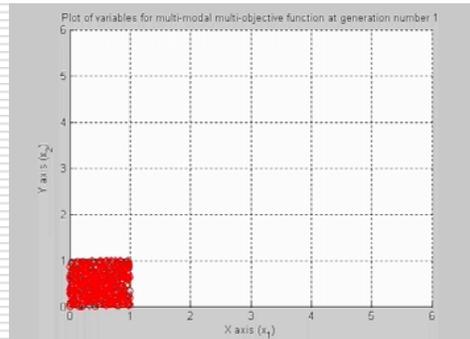
- Nine regions leading to the same Pareto-optimal front
- Multiple solutions cause a single Pareto-optimal point

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### Nine Optimal Regions

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## Nine Optimal Fronts



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## Conclusions

- ▶ Most application activities require optimization routinely
- ▶ Classical methods provide foundation
  - ▶ If applicable, good accuracy is achievable
- ▶ Evolutionary methods enable applicability to near-optimality
  - ▶ Try when classical methods fail
  - ▶ Parallel search ability
- ▶ A good optimization task through EAs and local search



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## How are EAs Unique?

- ▶ Broader applicability
  - ▶ Mixed variables, non-linearity, non...
  - ▶ Constraint handling
- ▶ Easy to use for distributed computing
- ▶ Beyond optimization
  - ▶ Learn your problem better
  - ▶ What makes a solution optimum, robust, or reliable?



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## Practical Optimization

### Final words

- ▶ Seems impossible to have one algorithm for many practical problems
- ▶ Needs a customized optimization
  - ▶ Calls for collaborations
- ▶ An application requires
  - ▶ Domain-specific knowledge
  - ▶ Thorough knowledge in optimization basics
  - ▶ Good knowledge in optimization algorithms
  - ▶ Good computing background
- ▶ Have successful show-cases, have a practice choose one



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## What we have not discussed?

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- ▶ Combinatorial optimization
  - ▶ Non-linearity, large dimension
- ▶ Problem Formulation aspects
  - ▶ Objectives, constraints, etc.
- ▶ Very large computational overhead
  - ▶ One evaluation takes a day or more
- ▶ Parallel EAs
- ▶ Termination criteria



## Thank You for Your Attention

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