Derivative-based Optimization

(chapter 6)

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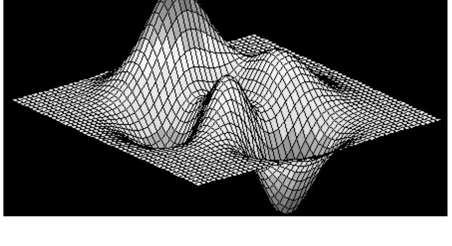
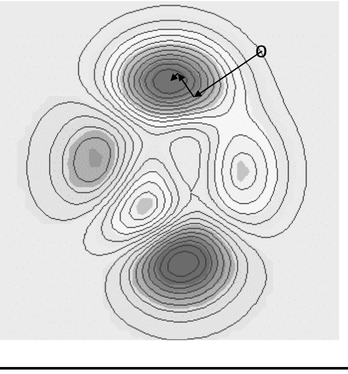
- used for neural network learning
- used for multidimensional input spaces

Steepest Descent

Determine search direction according to an objective function's derivative information

- find locally steepest direction
- find best point on line
- repeat

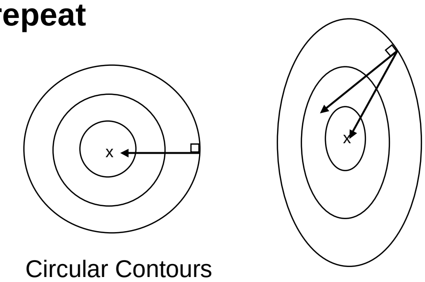




Newton’s method

Determine search direction according to an objective function’s second derivative

- **find Newton direction**
- **find best point on line**
- **repeat**



Steepest descent
Newton’s method
both

Circular Contours

Elliptical Contours

Peaks Function

Issues with Derivative-based Optimization

- **Assumes there is an objective function**
- **Only finds local minima/maxima**
- **Newton only works when close to minima/maxima**
- **Calculating derivatives could be difficult**

Example: Find the max. of the “peaks” function

z = f(x, y) = 3*(1-x)^2*exp(-(x^2) - (y+1)^2) - 10*(x/5 - x^3 - y^5)*exp(-x^2-y^2) -1/3*exp(-(x+1)^2 - y^2).

Peaks Derivative

Derivatives of the “peaks” function

- dz/dx = -6*(1-x)*exp(-x^2-(y+1)^2) - 6*(1-x)^2*x*exp(-x^2-(y+1)^2) - 10*(1/5-3*x^2)*exp(-x^2-y^2) + 20*(1/5*x-x^3-y^5)*x*exp(-x^2-y^2) - 1/3*(-2*x-2)*exp(-(x+1)^2-y^2)
- dz/dy = 3*(1-x)^2*(-2*y-2)*exp(-x^2-(y+1)^2) + 50*y^4*exp(-x^2-y^2) + 20*(1/5*x-x^3-y^5)*y*exp(-x^2-y^2) + 2/3*y*exp(-(x+1)^2-y^2)
- d(dz/dx)/dx = 36*x*exp(-x^2-(y+1)^2) - 18*x^2*exp(-x^2-(y+1)^2) - 24*x^3*exp(-x^2-(y+1)^2) + 12*x^4*exp(-x^2-(y+1)^2) + 72*x*exp(-x^2-y^2) - 148*x^3*exp(-x^2-y^2) - 20*y^5*exp(-x^2-y^2) + 40*x^5*exp(-x^2-y^2) + 40*x^2*exp(-x^2-y^2)*y^5 - 2/3*exp(-(x+1)^2-y^2) - 4/3*exp(-(x+1)^2-y^2)*x^2 -8/3*exp(-(x+1)^2-y^2)*x
- d(dz/dy)/dy = -6*(1-x)^2*exp(-x^2-(y+1)^2) + 3*(1-x)^2*(-2*y-2)^2*exp(-x^2-(y+1)^2) + 200*y^3*exp(-x^2-y^2)-200*y^5*exp(-x^2-y^2) + 20*(1/5*x-x^3-y^5)*exp(-x^2-y^2) - 40*(1/5*x-x^3-y^5)*y^2*exp(-x^2-y^2) + 2/3*exp(-(x+1)^2-y^2)-4/3*y^2*exp(-(x+1)^2-y^2)

5

Derivative-Free Optimization

(chapter 7)

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6

Soft Computing: Derivative-Free Optimization

Derivative-Free Optimization

Genetic algorithms (GAs)

Simulated annealing (SA)

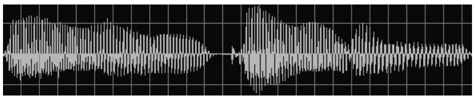
7

Soft Computing: Derivative-Free Optimization

Genetic Algorithms

Motivation

- **Look at what evolution brings us?**
  - Vision
  - Hearing
  - Smell
  - Taste
  - Touch
  - Learning and reasoning
- **Can we emulate the evolutionary process with today's fast computers?**



8

Genetic Algorithms

Terminology:

- **Population - a set of possible solutions to a problem**
- **Fitness function - how to evaluate the quality of a member of the population**
- **Encoding schemes - a binary representation for a member of the population**
- **Selection - how to determine which members of the population will survive to the next generation**
- **Crossover - combining two members of the population**
- **Mutation - changing a single member of the population**
- **Elitism - allowing the best members to pass to the next generation**

9

Genetic Algorithms

Binary encoding

Chromosome

(11, 6, 9) ⇒ 1011 0110 1001

Gene

Crossover

1 0 0 | 1 1 1 1 0 ⇒ 1 0 0 | 1 0 0 1 0
1 0 1 | 1 0 0 1 0 ⇒ 1 0 1 | 1 1 1 1 0

Crossover point

Mutation

1 0 0 1 1 1 1 0 ⇒ 1 0 0 1 1 0 1 0

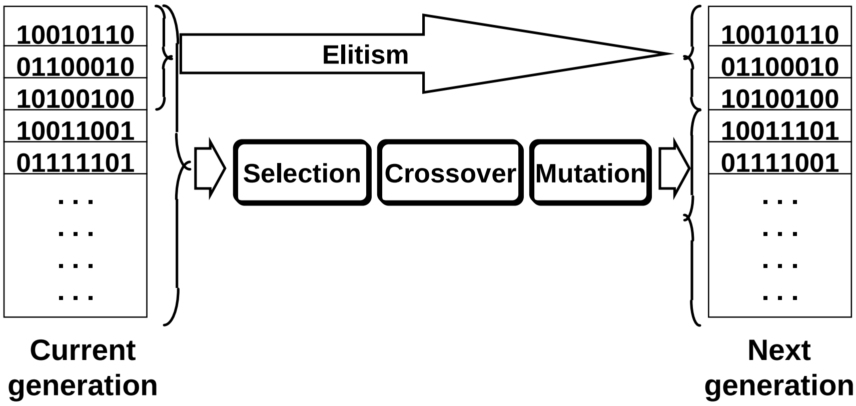
Mutation bit

10

Soft Computing: Derivative-Free Optimization

Genetic Algorithms

Flowchart



11

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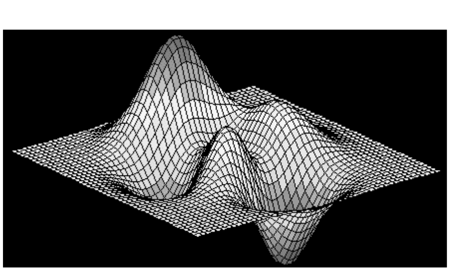
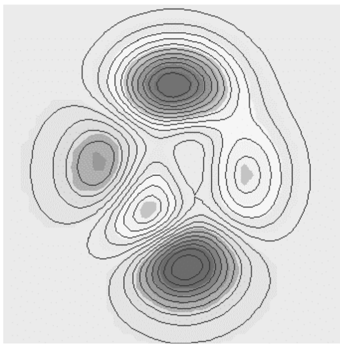
Genetic Algorithms

Plotting the function





12

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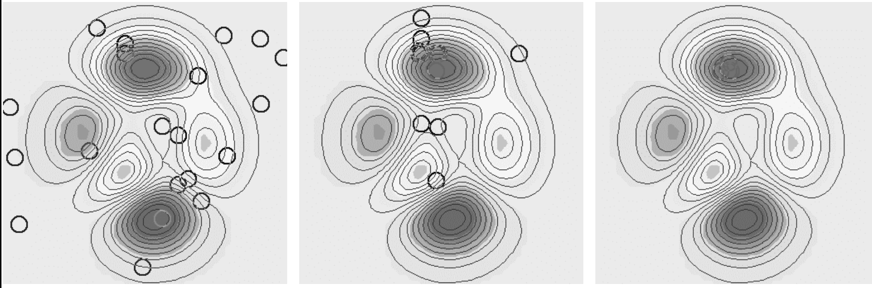
Genetic Algorithms

GA process:



Initial population 5th generation 10th generation

13

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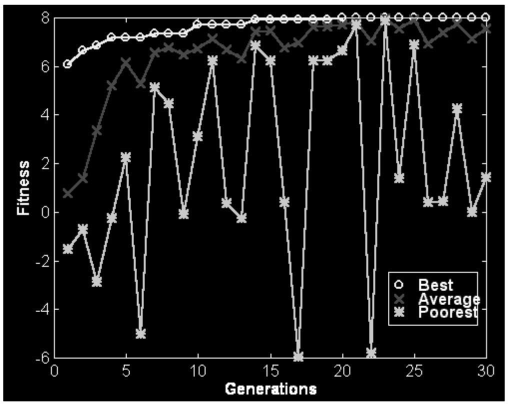
Genetic Algorithms

Performance profile



14

Example

Let us consider the equation:

a+2b+3c+4d=30,

where a,b,c,d are positive integers

given the constraints 1 =< a,b,c,d =< 30

GA systems allow for a solution to be reached quicker since "better" solutions have a better chance of surviving and procreating, as opposed to random search

15

Soft Computing: Derivative-Free Optimization

Example

First we will choose 5 random initial solution sets

Chrom	(a,b,c,d)	bit representation
1	(1,28,15,3)	(00001 11100 01111 00011)
2	(14,9,2,4)	(01110 01001 00010 00100)
3	(13,5,7,3)	(01101 00101 00111 00011)
4	(23,8,16,19)	(10111 01000 10000 10011)
5	(9,13,5,2)	(01001 01101 00101 00010)

16

Soft Computing: Derivative-Free Optimization

Example

fitness function

a+2b+3c+4d - 30

Chromosome	Fitness Value
1	|114-30|=84
2	|54-30|=24
3	|58-30|=28
4	|163-30|=133
5	|58-30|=28

17

Soft Computing: Derivative-Free Optimization

Example

more desirable fitness values are more likely to be chosen as parents

Chromosome	Likelihood
1	(1/84)/0.135266 = 8.80%
2	(1/24)/0.135266 = 30.8%
3	(1/28)/0.135266 = 26.4%
4	(1/133)/0.135266 = 5.56%
5	(1/28)/0.135266 = 26.4%

18

Example

Crossover

Father	Mother	Offspring
(13 | 5,7,3)	(1 | 28,15,3)	(13,28,15,3)
(9,13 | 5,2)	(14,9 | 2,4)	(9,13,2,4)
(13,5,7 | 3)	(9,13,5 | 2)	(13,5,7,2)
(14 | 9,2,4)	(9 | 13,5,2)	(14,13,5,2)
(13,5 | 7, 3)	(9,13 | 5, 2)	(13,5,5,2)

19

Example

Mutation

Before-Mutation	After Mutation
(1,28,15,3)	(1,29,15,3)
(14,9,2,4)	(14,25,2,4)

(00001 11100 01111 00011) (00001 11101 01111 00011)
(01110 01001 00010 00100) (01110 11001 00010 00100)

20

Example

Now we can calculate the fitness values for the new generation of offspring.

Offspring	Fitness Value
(13,28,15,3)	|126-30|=96
(9,13,2,4)	|57-30|=27
(13,5,7,2)	|57-30|=22
(14,13,5,2)	|63-30|=33
(13,5,5,2)	|46-30|=16

21

Last GA Slide

22

Break up into groups of 3 or 4
Design a GA to determine the maximum of the peaks function in the range –2 < x < 3, -2 < y < 3

1) Design a binary chromosome that can represent the possible solutions accurate to two digits after the decimal point. Give an example of an (x, y) pair represented by the chromosome.
2) How do you decode your chromosome to evaluate the peaks function?
3) How do you determine the probability of selection?
4) What values do you use for population size, generations, elitism, crossover rate, mutation rate? Why did you pick these values?

23

Soft Computing: Derivative-Free Optimization

2) How do you decode your chromosome to evaluate the peaks function?

```
function num = bit2num(bit, range)
%
%  bit2num([1 1 0 1], [0, 15])
%  bit2num([0 1 1 0 0 0 1], [0, 127])
%  Roger Jang, 12-24-94

integer = polyval(bit, 2);
num = integer*((range(2)-range(1))/(2^length(bit)-1))
    + range(1);
```

24

3) How do you determine the probability of selection?

```
% rescaling the fitness
fitness = fitness - min(fitness);  % keep it positive
total = sum(fitness);
if total == 0,
    fprintf(' Warning: converge to a single point\n');
    fitness = ones(popu_s, 1)/popu_s; % sum is 1
else
    fitness = fitness/sum(fitness);       % sum is 1
end
cum_prob = cumsum(fitness);
```

25

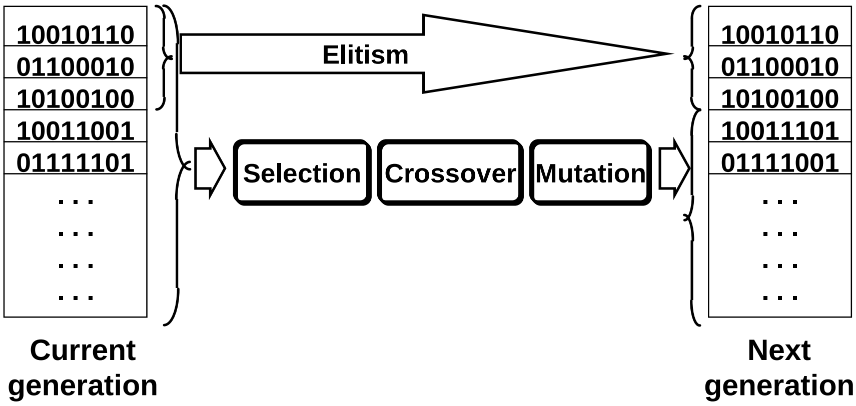
GA Summary

26

Soft Computing: Derivative-Free Optimization

Genetic Algorithms

Flowchart



27

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GA Issues

1) How to design the chromosome

   Chrom (a,b,c,d) (00001 11100 01111 00011)

2) How to create fitness function

   numerical ranking for best of population

3) How to set parameters

   population, generations, crossover, mutation

GA's are good for Optimization

28

Soft Computing: Derivative-Free Optimization

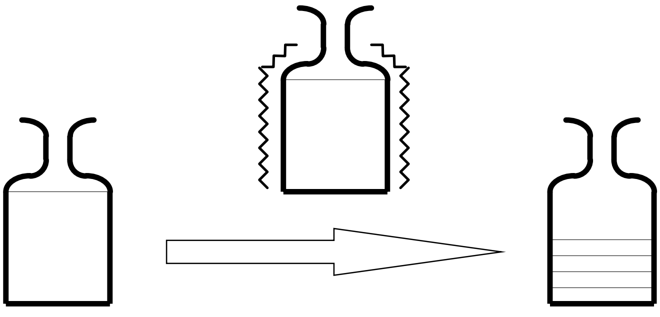
Last GA Slide

29

Soft Computing: Derivative-Free Optimization

Simulated Annealing

Analogy



College is where your thoughts anneal
- entertainment weekly magazine

30

Soft Computing: Derivative-Free Optimization

Simulated Annealing

Terminology:

- Objective function E(x): function to be optimized
- Move set: set of next points to explore
- Generating function: to select next point
- Acceptance function h(ΔE, T): to determine if the selected point should be accept or not. Usually h(ΔE, T) = 1/(1+exp(ΔE/(cT)).
- Annealing (cooling) schedule: schedule for reducing the temperature T

31

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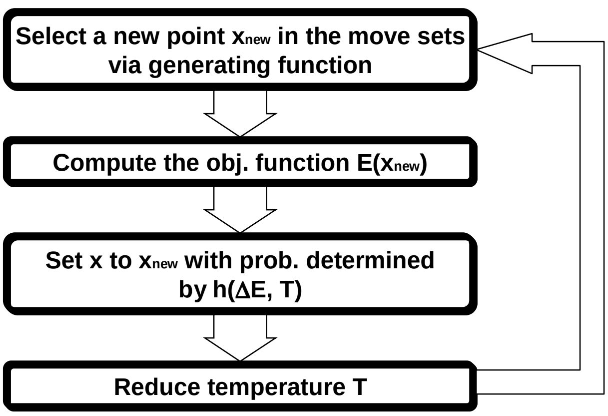
Simulated Annealing

Flowchart



32

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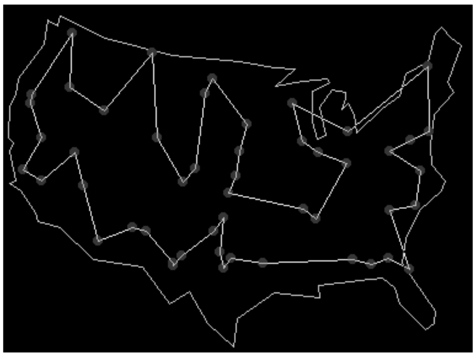
Simulated Annealing

Example: Travel Salesperson Problem (TSP)

How to transverse n cities once and only once with a minimal total distance?



33

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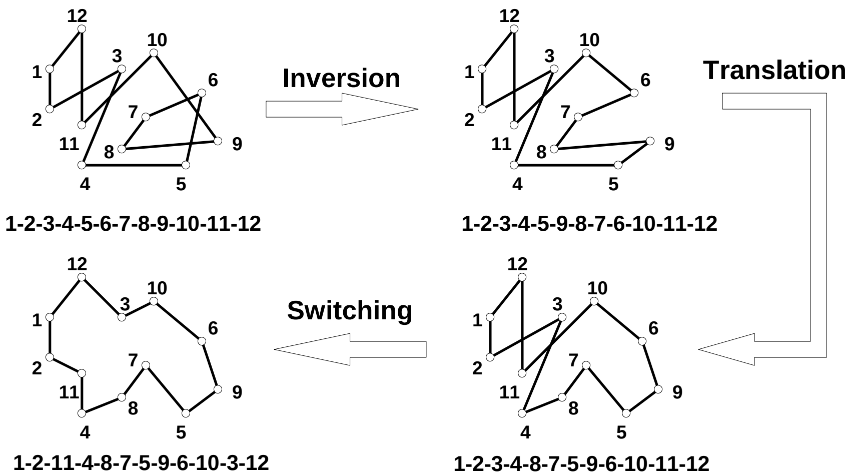
Simulated Annealing

Move sets for TSP



34

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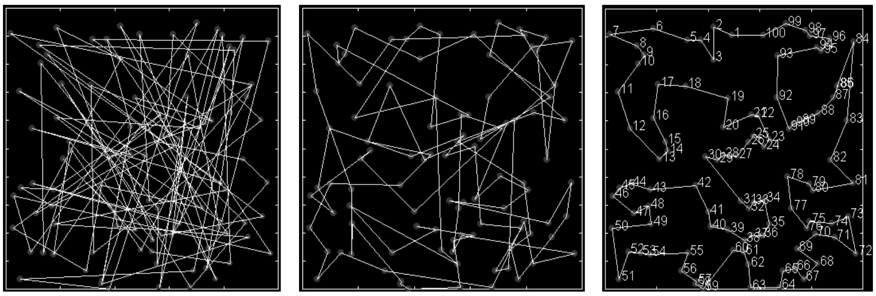
Simulated Annealing

A 100-city TSP using SA



Initial random path   During SA process   Final path

35

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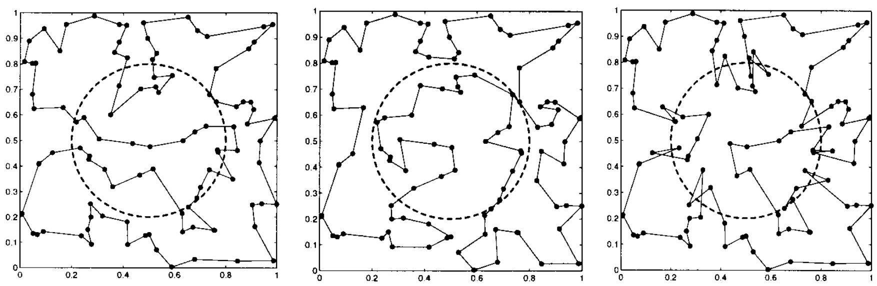
Simulated Annealing

100-city TSP with penalties when crossing the circle



Penalty = 0   Penalty = 0.5   Penalty = -0.3

36