Metaheuristics and Optimization in R

DS 775

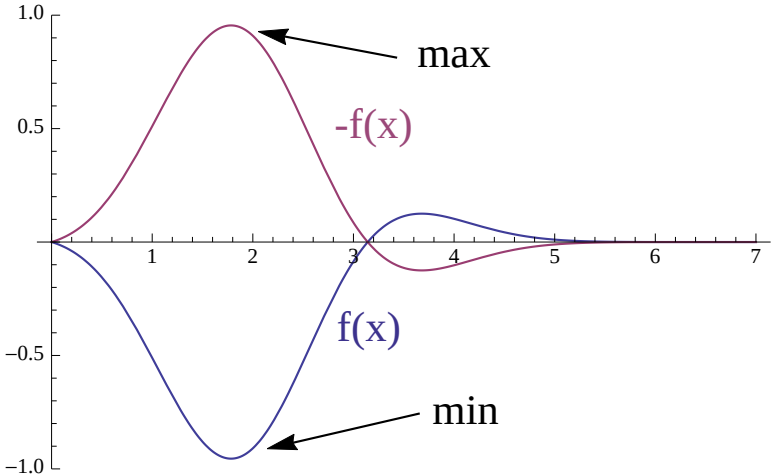
This Unit

- Goal 1: introduce three metaheuristic (optimization) techniques
  - Multistart methods
  - Simulated Annealing
  - Genetic Algorithms
- Goal 2: introduce some optimization tools available in R including
  - optim() in the 'stats' package for local search
  - genetic algorithms in 'GA' and 'gramEvol' packages
  - multiple algorithms in NLopt accessible through 'nloptr'
  - simulated annealing through optim() and GenSA()

Metaheuristics

- problems so complex that we cannot guarantee an optimal solution
  - complex nonlinearities leading to many potentially optimal points
  - combinatorial optimization with too many possible solutions
- Goal: find a good feasible solutions
- algorithms are often iterative

Maximize vs Minimize

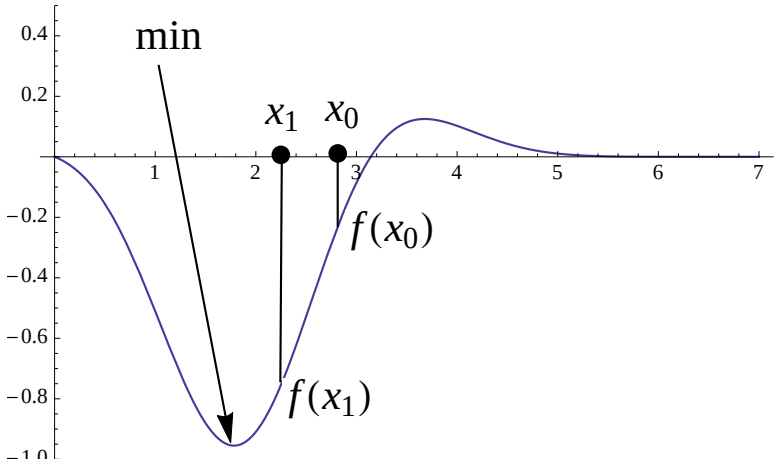


- from now on we'll talk about minimization

Local Search

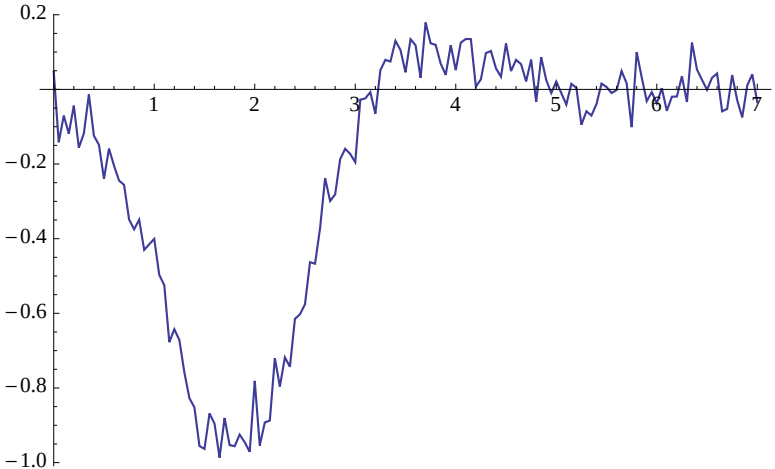
- start with x_0 and evaluate $f(x_0)$
- choose x_1 close to x_0 so that hopefully $f(x_1)$ is smaller
- repeat until close enough to minimum

Local Search - Continuous Variables



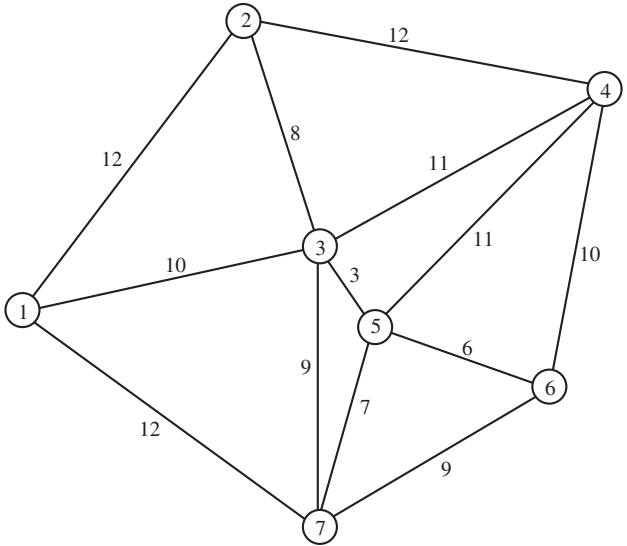
- for smooth functions like this one we can use (approximate) calculus to descend the hill until we reach the bottom

Local Search - Rough Functions



- for rough functions calculus won't help but other search methods like a genetic algorithm or simulated annealing can be used

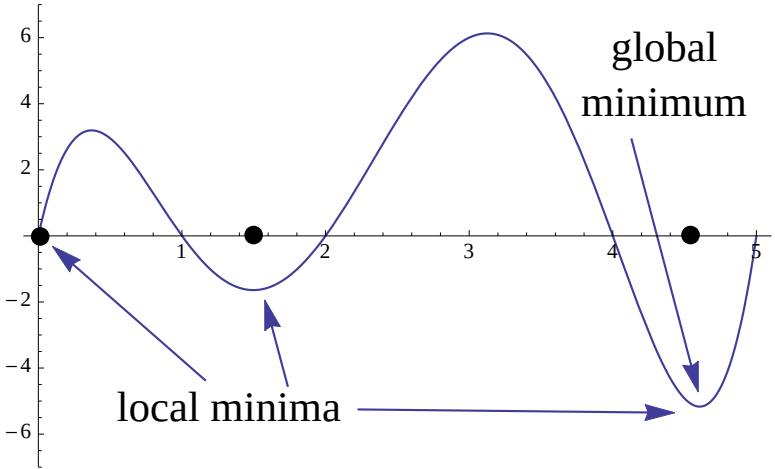
Local Search - Discrete Variables



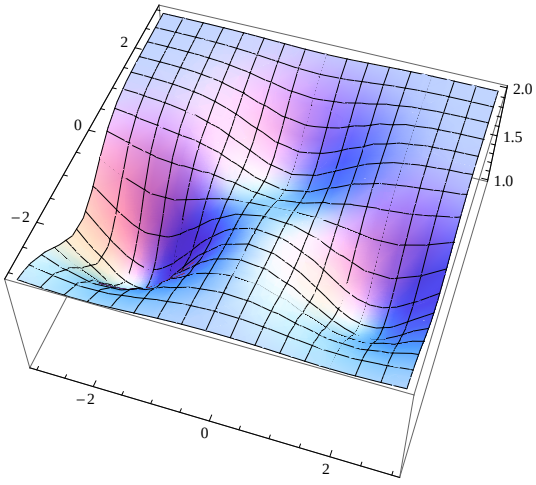
- Let $x_0 = 1\text{-}2\text{-}3\text{-}4\text{-}5\text{-}6\text{-}7\text{-}1$, with cost 69
- Swap cities 2 and 3 to get $x_1 = 1\text{-}3\text{-}2\text{-}4\text{-}5\text{-}6\text{-}7\text{-}1$, with cost 68
- Continue making swaps that improve the cost
- Stop when no improving swaps are possible
- No guarantee that result is best possible tour

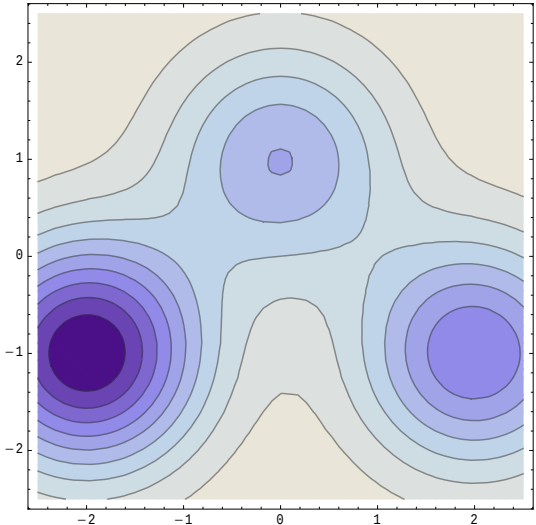
Local or Global Minimum?

Minimize $f(x) = 0.5x^5 - 6x^4 + 24.5x^3 - 39x^2 + 20x$ subject to $0 \leq x \leq 5$.



Local vs Global again





Local Search in R

For a smooth function (differentiable):

```
f <- function(x){
  0.5*x^5 - 6*x^4 + 24.5*x^3 - 39*x^2 + 20*x;
}
# find a local min starting from x = 2
x0 <- 2
optim(x0, f)
```

```
## $par
## [1] 1.497807
##
## $value
## [1] -1.640659
```

optimize() for 1D function in R

```
f <- function(x){
  0.5*x^5 - 6*x^4 + 24.5*x^3 - 39*x^2 + 20*x;
}
optimize(f,c(0,5)) # specify the interval
```

```
## $minimum
## [1] 1.497809
##
## $objective
## [1] -1.640659
```

optimize() is supposed to find *the* minimum of a continuous f on $[a, b]$, but it's really just another local search. It will find other minima if you choose a good interval.

Local search for higher dimensions

```
f3 <- function(x){ # 3 minima 2D function from earlier
  -.5*exp(-.7*( x[1]^2   +(x[2]-1)^2))
  -.7*exp(-.7*((x[1]-2)^2+(x[2]+1)^2))
  -   exp(-.7*((x[1]+2)^2+(x[2]+1)^2));
}
x0 <- c(1,1)
optim(x0,f3)
```

```
## $par
## [1] -1.999999 -1.000000
##
## $value
## [1] -1
```

optim() in package ‘stats’

- optim() is really a gradient based search method
- if the gradient is not supplied, it is approximated numerically
- for a smooth function for which the gradient is not available, it is probably better to use a “derivative-free” method from package ‘nloptr’
  - use newuoa() in ‘nloptr’ for unconstrained optimization
  - use bobyqa() in ‘nloptr’ for box constrained problems
  - use cobyla() for more complex constraints
- for large numbers of variables it really pays to get the gradient if possible, but the derivative-free algorithms can handle 100’s of variables

nloptr package

- provides interface to open-source NLopt
- uniform syntax for many optimization algorithms
- can be a bit tricky to install (not required for homework)
  - some instructions in download packet (but Google is your friend)
  - for Windows get precompiled NLopt binaries and also Rtools
  - for Mac/Linux download NLopt source and compile
  - install.packages('nloptr') in R

newuoa() from nloptr

- local search, derivative-free method for unconstrained optimization
- many more options are possible, see documentation

```
library(nloptr); x0 <- c(1,1);
opts <- list("algorithm"="NLOPT_LN_NEWUOA", "xtol_rel"=1.0e-7);
result <- nloptr(x0=x0,eval_f=f3,opts=opts)
result
```

- output on next slide
- algorithm due to Michael Powell (in “Mathematical Programming”, v. 100, p. 183-214, 2004)

newuoa() output

- happens to find global optimum even though it doesn't start nearby

```
## Minimization using NLopt version 2.4.2
##
## NLopt solver status: 1 ( NLOPT_SUCCESS: Generic success return valu
##
## Number of Iterations....: 47
## Termination conditions:  xtol_rel: 1e-07
## Number of inequality constraints:  0
## Number of equality constraints:    0
## Optimal value of objective function:  -1
## Optimal value of controls: -2 -1
```

bobyqa() from nloptr

- local search, derivative-free method for box constrained optimization
- many more options are possible, see documentation

```
library(nloptr)
opts <- list("algorithm"="NLOPT_LN_BOBYQA", "xtol_rel"=1.0e-7,
             lb=c(-2.5,-2.5),ub =c(2.5,2.5));
result <- nloptr(x0=x0,eval_f=f3,opts=opts)
result
```

- output on next slide
- algorithm due to Michael Powell (in "Mathematical Programming", v. 100, p. 183-214, 2004)

bobyqa() output

- happens to find global optimum even though it doesn't start nearby

```
## Minimization using NLopt version 2.4.2
##
## NLopt solver status: 4 ( NLOPT_XTOL_REACHED: Optimization stopped
## xtol_rel or xtol_abs (above) was reached. )
##
## Number of Iterations....: 44
## Termination conditions:  xtol_rel: 1e-07
## Number of inequality constraints:  0
## Number of equality constraints:    0
## Optimal value of objective function:  -1
## Optimal value of controls: -2 -1
```

Multistart Methods

Naive Multistart

- Choose a random sample of starting points in the feasible domain.
- Start a local search at each one.
- Return the coordinates and function value of the lowest minimum.

Naive Multistart in R

```
bestmin <- 100000;
for (j in 1:10){
  x0 <- as.vector(runif(2,min=-2.5,max=2.5));
  result <- optim(x0,f3,method="L-BFGS-B",lower=c(-2.5,-2.5),upper=c(
  if (result$value<bestmin){ bestmin = result$value; bestx = result$p
}
bestmin
```

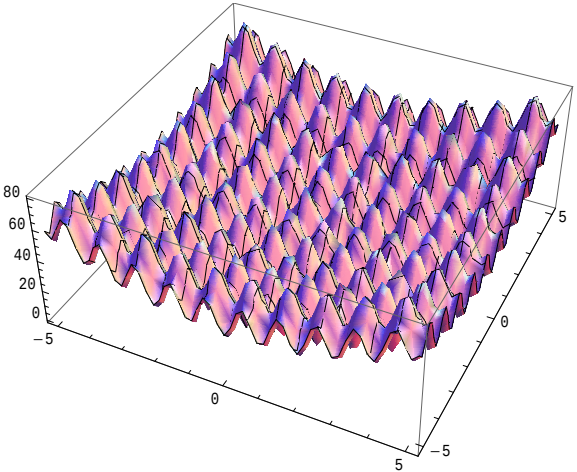
```
## [1] -1
```

```
bestx
```

```
## [1] -2 -1
```

Rastrigin Function

in 2D $f(x, y) = 20 + x^2 + y^2 - 10\cos(2\pi x) - 10\cos(2\pi y), -5.12 \leq x, y \leq 5.12$



Naive Multistart on Rastrigin

```
fr <- function(x){
  20 + x[1]^2 + x[2]^2 - 10*cos(2*pi*x[1]) - 10*cos(2*pi*x[2])
}
bestmin <- 100000; set.seed(126)
for (j in 1:50){
  x0 <- as.vector(runif(2,min=-5.12,max=5.12));
  result <- optim(x0,fr,method="L-BFGS-B",lower=c(-5.12,-5.12),upper=
  if (result$value<bestmin){ bestmin = result$value; bestx = result$p
}
bestmin
bestx
```

- output on next slide

Naive Multistart on Rastrigin - output

```
round(bestmin)
```

```
## [1] 1
```

```
round(bestx,4)
```

```
## [1] 0.000 0.995
```

MLSL

- MLSL = Multi-Level Single Linkage algorithm for global optimization (Kan and Timmer, "Stochastic global optimization methods", Mathematical Programming, vol.39, p. 27-78, 1987)
- "clustering" method to avoid repeated detection of the same minimum
  - randomly pick a small set of potential local search starting points
  - evaluate f at these points
  - start a local search at a point if it is one of the lowest starting points and is not too close to a previous local search starting point
  - repeat three above steps until satisfied with result
- available in R package 'nloptr' (uses an approximate gradient local search)

MLSL applied to Rastigrin Function

```
require(nloptr); x0<-c(5,5);
result <- mlsl(x0,fr,lower=c(-5.12,-5.12),upper=c(5.12,5.12),nl.info=
```

```
## NLopt solver status: 5 ( NLOPT_MAXEVAL_REACHED: Optimization stopp
## because maxeval (above) was reached. )
##
## Number of Iterations....: 1001
## Termination conditions:  xtol_rel: 1e-06 maxeval: 1000   ftol_rel:
## Number of inequality constraints:  0
## Number of equality constraints:    0
## Current value of objective function:  0
## Current value of controls: 3.529593e-13 -3.529593e-13
```

Genetic Algorithms

- objective function not smooth or very complicated
- finding "good enough" solutions in combinatorial optimization problems
- basic idea
  1. start with population of potential solutions (chromosomes)
  2. fittest individuals selected for breeding (selection)
  3. offspring formed by crossover and mutation
  4. offspring placed in new population and repeat
  5. if satisfied stop, else goto step 2.

Binary Encoding

- variables are represented as string of bits
  - chromosome A: 100100101
  - chromosome B: 011010110
- Knapsack Problem
  - have a number of items of given value and size
  - knapsack with given capacity
  - select items to maximize value in knapsack
  - encoding: each bit represents whether an item is the knapsack or not

Permutation Encoding

- each chromosome is a permutation of the numbers $1, 2, ..., n$
- useful for ordering problems
- Traveling Salesman Problem
  - salesman visits all cities while minimizing cost (or distance)
  - chromosome represents order of visiting cities

Value Encoding

- each chromosome is string of some values such as reals, integers, characters
- real chromosomes can be used for complex optimization problems such as Rastrigin
- in the homework is an integer chromosome problem where integers represent assignment of cities to numbered congressional districts

Genetic Algorithms in R

- the 'GA' package is very good and can deal with binary, permutation, and real encoding
- the 'gramEvol' package has a useful genetic algorithm for integer encoded problems
- both can be installed easily using `install.packages('name of package')`

GA for Knapsack Problem in R

```
value = c(4,6,5,3,6,3,7,8,9,10);
size = c(3,2,5,3,2,4,3,2,4,2); capacity = 15;
totalValue = function(xb){
  sum(value*xb)*(sum(size*xb)<=capacity)
}
require(GA)
result = ga("binary",fitness=totalValue,nBits=10) # approx *max*
result@fitnessValue # total value of best knapsack
result@solution # binary vector showing which items to include
sum(size*result@solution) # capacity used
```

- output on next slide
- run this a few times, you won't always get the same solution!

Knapsack output

```
## [1] 46
```

```
##      x1 x2 x3 x4 x5 x6 x7 x8 x9 x10
## [1,]  0  1  0  0  1  0  1  1  1   1
```

```
## [1] 15
```

GA for a TSP Problem in R

We'll use GA to approximate a solution to the sample TSP problem with 7 cities from an earlier slide. Here is the cost matrix with a large cost for infeasible connections:

```
M = 100000;
costMatrix = as.matrix(rbind(
                    c( 0,12,10, M, M, M,12),
                    c(12, 0, 8,12, M, M, M),
                    c(10, 8, 0,11, 3, M, 9),
                    c( M,12,11, 0,11,10, M),
                    c( M, M, 3,11, 0, 6, 7),
                    c( M, M, M,10, 6, 0, 9),
                    c(12, M, 9, M, 7, 9, 0)));
numcities = 7;
```

GA for TSP

Here is the fitness function:

```
# given a tour, calculate the total cost
tourCost <- function(tour, costMatrix) {
  tour <- c(tour, tour[1])
  route <- embed(tour, 2)[, 2:1]
  sum(costMatrix[route])
}
# inverse of the total distance is the fitness
tspFitness <- function(tour, ...) 1/tourCost(tour, ...)
```

GA for TSP

Run the GA:

```
result <- ga(type = "permutation", fitness = tspFitness, costMatrix=c
             max = numcities, popSize = 10, maxiter = 500, run = 100,
             , monitor = NULL)
soln <- as.vector(result@solution[1,]) # use first soln
tourCost(soln,costMatrix)
tour <- c(soln,result@solution[1]);
tour # approx best tour
```

- for a large problem increase popSize and maxiter
- run=100 means the algorithm will terminate if there are 100 iterations without improvement
- pmutation = 0.2 is the probability of a mutation, default is 0.1
- output on next slide

GA for TSP

```
## [1] "tour cost: "
```

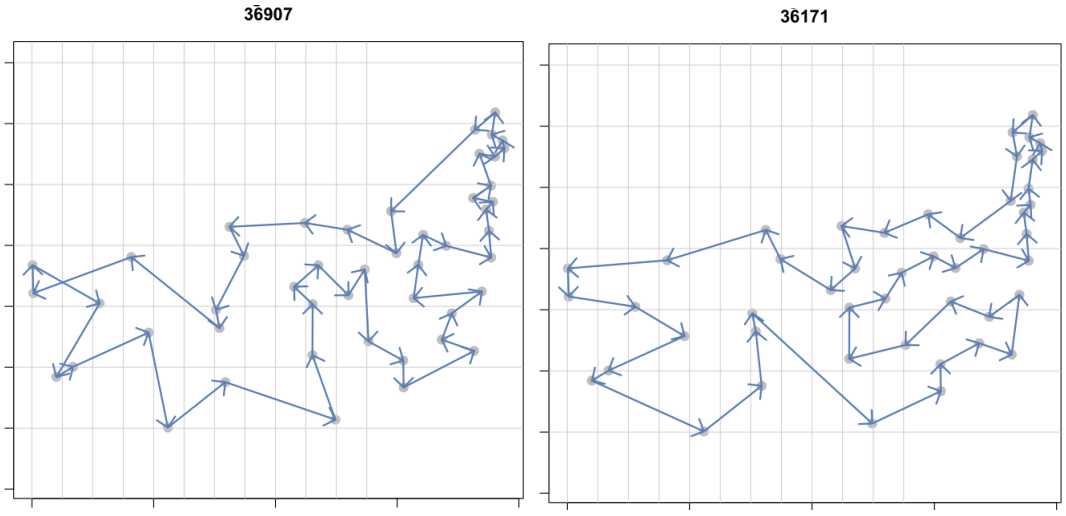
```
## [1] 63
```

```
## [1] "approx best tour"
```

```
## [1] 4 6 7 5 3 1 2 4
```

- usually finds a tour equivalent to tour in textbook (p. 624)

GA for a larger TSP in R



GA for the Rastrigin Problem

```
Rastrigin <- function(x) {
            -(sum(x^2 - 10 * cos(2 * pi  * x)) + 10 * length(x))
        }
dimension = 10;
lower = rep(-5.12,dimension);
upper = rep(5.12,dimension);
result = ga(type="real-valued",fitness=Rastrigin,min=lower,max=upper,
round(result@solution,5)
result@fitnessValue
```

- results on next slide

GA Rastrigin Results

- real-valued GA explores large solution space well, but converges slowly near optimum

```
##             x1       x2     x3       x4       x5       x6      x7     x
## [1,] -0.00619 0.00506 0.0036 0.00033 0.00053 -0.00273 0.00482 7e-04
##            x10
## [1,] -0.00053

## [1] -0.0227812
```

GA plus local search

- add optim=TRUE to ga() call to use optim() to do local search using each chromosome as an initial value to determine fitness

```
result = ga(type="real-valued",fitness=Rastrigin,
            min=lower,max=upper,maxiter=1000,optim=TRUE)
```

```
##       x1 x2 x3 x4 x5 x6 x7 x8 x9 x10
## [1,]  0  0  0  0  0  0  0  0  0   0
```

```
## [1] 0
```

Simulated Annealing

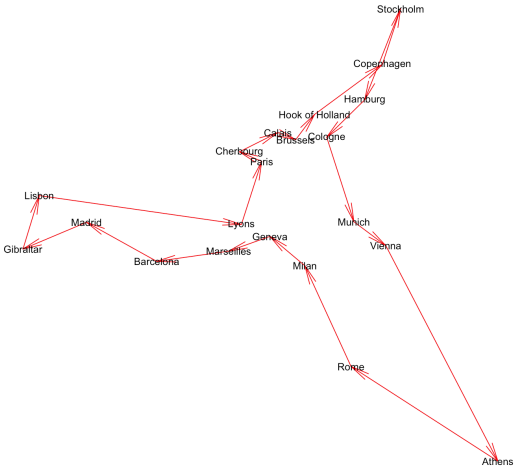
- objective function not smooth or very complicated
- finding "good enough" solutions in combinatorial optimization problems
- basic idea for minimizing
  1. start with initial guess x_o with fitness $f(x_n)$
  2. randomly choose a nearby point x_n with fitness $f(x_n)$
  3. if $f(x_n) < f(x_o)$ then $x_o = x_n$ and goto step 2 if not converged
  4. if $f(x_n) \geq f(x_o)$ then $x_o = x_n$ with probability P otherwise don't change x_o, goto step 2 if not converged
- probability P of accepting worse solution decreases over time as simulation "cools"

Simulated Annealing in R

- simulated annealing is an option in optim() in package 'stats'
- 'GenSA' package (check out the example of 30 dimensional Rastrigrin in documentation - hard problem!)

SA for TSP Problem in R

- see saTSP.R in download packet for the code



SA for the Rastrigin Problem

```
Rastrigin <- function(x) {
            (sum(x^2 - 10 * cos(2 * pi  * x)) + 10 * length(x))
        }
dimension = 10;
lower = rep(-5.12,dimension); upper = rep(5.12,dimension);
x0 = runif(dimension,-5.12,5.12)
require(GenSA)
result = GenSA(x0,Rastrigin,lower=lower,upper=upper,
               control=list(max.call=5000))
result$value
result$par
```

- output on next slide

SA for Rastrigin output

```
## Loading required package: GenSA

## [1] "approximate minimum value"

## [1] 0.995

## [1] "occurs at"

##  [1] 0.000 0.000 0.000 0.995 0.000 0.000 0.000 0.000 0.000 0.000
```