Simulated Annealing

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In this lesson we'll learn the theory behind using simulated annealing as an optimization and search technique. We'll then use simulated annealing to search for a solution to the famous Travelling Salesman Problem in R.

Additional packages needed

To run the code you may need additional packages.

- If necessary install the followings packages.

```
install.packages("ggplot2");
install.packages("stats");
```

```
require(ggplot2)

## Loading required package: ggplot2

require(stats)
```

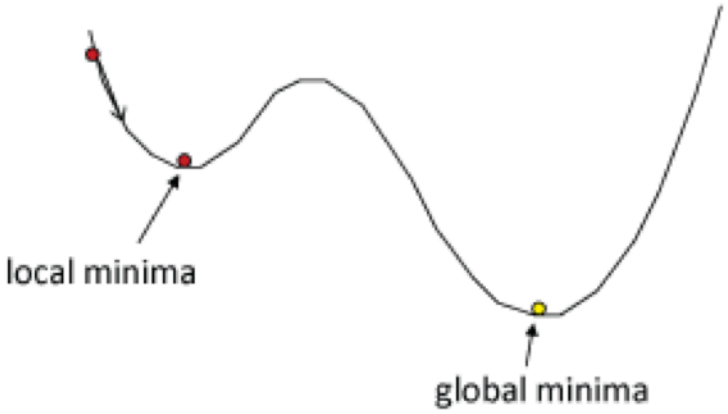
Data

We will be using the R stats library mapping of distances between European cities to generate out data.

Simulated Annealing

A Simulated Annealing (SA) is a probabilistic search heuristic that mimics the process of cooling in thermodynamic systems. This heuristic is often used to generate useful solutions to optimization and search problems. The method is an adaptation of the Metropolis–Hastings algorithm, a Monte Carlo method to generate sample states of a thermodynamic system, invented by M.N. Rosenbluth and published in a paper by N. Metropolis et al. in 1953.

Basically simulated annealing perturbs the current solution and then checks to see whether the new solution is good or not. If its an improvement it will accept it and if the new solution is worse it may accept it with a probability inversely proportional to how much worse the new solution changes the current one. Compared to pure gradient descent the main difference is that SA allows "uphill" steps. Simulated annealing also differs from gradient descent in that a move is selected at random.



Gradient Descent

Metropolis–Hastings algorithm

Metropolis algorithm (symmetric proposal distribution) Let f(x) be a function that is proportional to the desired probability distribution P(x)

This algorithm proceeds by randomly attempting to move about the sample space, sometimes accepting the moves and sometimes remaining in place.

Perturb (randomly) the current state to a new state. ΔE is the difference in energy between current and new state.
If $\Delta E < 0$ (new state is lower), accept new state as current state If $\Delta E > 0$ accept new state with probability inversely proportional to the increase in system energy. Traditionally the change in Gibbs free energy is used for thermodynamic free energy systems.

This can be run for a fixed number of iterations or if the overall system energy can measured then it can be run until the overall system energy settles.

Simulated Annealing Pseudocode

Simulated Annealing uses the Metropolis–Hastings algorithm with a temperature parameter T that effects the acceptance probability of an "uphill" transition. At higher"temperatures" accpeting "uphill" transitions is more probable. The algorithm starts initially with T set to a high value , and then it is decreased at each step following some annealing schedule—which is often specified by the user, but must end with $T = 0$. At $T = 0$ there is no chance of accpeting "uphill" transitions and so it becomes gradient descent.

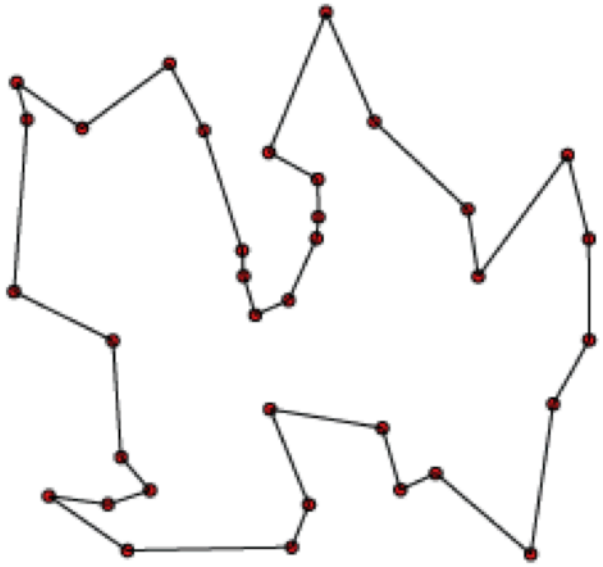
At a fixed temperature T:
Perturb (randomly) the current state to a new state. ΔE is the difference in energy between current and new state.

If $\Delta E < 0$ (new state is lower), accept new state as current state If $\Delta E > 0$ accept new state with probability inversely proportional to the increase in system energy as a function of T.

Eventually the systems evolves into thermal equilibrium at temperature T ; then the formula mentioned before holds When equilibrium is reached, temperature T can be lowered and the process can be repeated.

Travelling Salesman Problem

The travelling salesman problem (TSP) asks the following question: Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city? It is an NP-hard problem in combinatorial optimization, important in operations research and theoretical computer science.



Travelling Salesman Problem

Simulated Annealing to solve the Travelling Salesman Problem in R

Simulated Annealing to solve the Travelling Salesman Problem in R

```
CityDistMatx <- as.matrix(eurodist)
CityDistMatx
```

```
##                 Athens Barcelona Brussels Calais Cherbourg Cologne
## Athens               0      3313     2963   3175      3339    2762
## Barcelona         3313         0     1318   1326      1294    1498
## Brussels          2963      1318        0    204       583     206
```

```
## Calais             3175      1326      204      0       460     409
## Cherbourg          3339      1294      583    460         0     785
## Cologne            2762      1498      206    409       785       0
## Copenhagen         3276      2218      966   1136      1545     760
## Geneva             2610       803      677    747       853    1662
## Gibraltar          4485      1172     2256   2224      2047    2436
## Hamburg            2977      2018      597    714      1115     460
## Hook of Holland    3030      1490      172    330       731     269
## Lisbon             4532      1305     2084   2052      1827    2290
## Lyons              2753       645      690    739       789     714
## Madrid             3949       636     1558   1550      1347    1764
## Marseilles         2865       521     1011   1059      1101    1035
## Milan              2282      1014      925   1077      1209     911
## Munich             2179      1365      747    977      1160     583
## Paris              3000      1033      285    280       340     465
## Rome                817      1460     1511   1662      1794    1497
## Stockholm          3927      2868     1616   1786      2196    1403
## Vienna             1991      1802     1175   1381      1588     937
##                 Copenhagen Geneva Gibraltar Hamburg Hook of Holland
Lisbon
## Athens               3276   2610      4485    2977            3030
4532
## Barcelona            2218    803      1172    2018            1490
1305
## Brussels              966    677      2256     597             172
2084
## Calais               1136    747      2224     714             330
2052
## Cherbourg            1545    853      2047    1115             731
1827
## Cologne               760   1662      2436     460             269
2290
## Copenhagen              0   1418      3196     460             269
2971
## Geneva               1418      0      1975    1118             895
1936
## Gibraltar            3196   1975         0    2897            2428
676
## Hamburg               460   1118      2897       0             550
2671
## Hook of Holland       269    895      2428     550               0
2280
## Lisbon               2971   1936       676    2671            2280
0
## Lyons                1458    158      1817    1159             863
1178
## Madrid               2498   1439       698    2198            1730
668
## Marseilles           1778    425      1693    1479            1183
1762
```

```
## Milan                1537    328      2185    1238            1098
2250
## Munich               1104    591      2565     805             851
2507
## Paris                1176    513      1971     877             457
1799
## Rome                 2050    995      2631    1751            1683
2700
## Stockholm             650   2068      3886     949            1500
3231
## Vienna               1455   1019      2974    1155            1205
2937
##                 Lyons Madrid Marseilles Milan Munich Paris Rome
Stockholm
## Athens           2753   3949       2865  2282   2179  3000  817
3927
## Barcelona         645    636        521  1014   1365  1033 1460
2868
## Brussels          690   1558       1011   925    747   285 1511
1616
## Calais            739   1550       1059  1077    977   280 1662
1786
## Cherbourg         789   1347       1101  1209   1160   340 1794
2196
## Cologne           714   1764       1035   911    583   465 1497
1403
## Copenhagen       1458   2498       1778  1537   1104  1176 2050
650
## Geneva            158   1439        425   328    591   513  995
2068
## Gibraltar        1817    698       1693  2185   2565  1971 2631
3886
## Hamburg          1159   2198       1479  1238    805   877 1751
949
## Hook of Holland   863   1730       1183  1098    851   457 1683
1500
## Lisbon           1178    668       1762  2250   2507  1799 2700
3231
## Lyons               0   1281        320   328    724   471 1048
2108
## Madrid           1281      0       1157  1724   2010  1273 2097
3188
## Marseilles        320   1157          0   618   1109   792 1011
2428
## Milan             328   1724        618     0    331   856  586
2187
## Munich            724   2010       1109   331      0   821  946
1754
## Paris             471   1273        792   856    821     0 1476
1827
```

```
## Rome              1048   2097       1011   586    946  1476    0
2707
## Stockholm         2108   3188       2428  2187   1754  1827 2707
0
## Vienna            1157   2409       1363   898    428  1249 1209
2105
##                 Vienna
## Athens            1991
## Barcelona         1802
## Brussels          1175
## Calais            1381
## Cherbourg         1588
## Cologne            937
## Copenhagen        1455
## Geneva            1019
## Gibraltar         2974
## Hamburg           1155
## Hook of Holland   1205
## Lisbon            2937
## Lyons             1157
## Madrid            2409
## Marseilles        1363
## Milan              898
## Munich             428
## Paris             1249
## Rome              1209
## Stockholm         2105
## Vienna               0
```

```r
# Distance function
distance <- function(sq)
  {  # Target function
  sq2 <- embed(sq, 2)
  return(as.numeric(sum(CityDistMatx[cbind(sq2[,2],sq2[,1])])))
}

# Generate new candidates
GenSeq <- function(sq) {  # Generate new candidate sequence
  idx <- seq(2, NROW(CityDistMatx)-1, by=1)
  ChangePoints <- sample(idx, size=2, replace=FALSE)
  tmp <- sq[ChangePoints[1]]
  sq[ChangePoints[1]] <- sq[ChangePoints[2]]
  sq[ChangePoints[2]] <- tmp
  return(as.numeric(sq))
}

cities<-labels(eurodist)
cities
```

```
##  [1] "Athens"          "Barcelona"       "Brussels"
##  [4] "Calais"          "Cherbourg"       "Cologne"
##  [7] "Copenhagen"      "Geneva"          "Gibraltar"
## [10] "Hamburg"         "Hook of Holland" "Lisbon"
## [13] "Lyons"           "Madrid"          "Marseilles"
## [16] "Milan"           "Munich"          "Paris"
## [19] "Rome"            "Stockholm"       "Vienna"
```

```
initial.tour <- c(1,2:NROW(CityDistMatx),1)
# Initial sequence
initial.tour
```

```
##  [1]  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21
1
```

```
initial.d<-distance(initial.tour)
initial.d
```

```
## [1] 29625
```

```
for(i in 1:length(initial.tour))
{
  print(cities[initial.tour[i]])
}
```

```
## [1] "Athens"
## [1] "Barcelona"
## [1] "Brussels"
## [1] "Calais"
## [1] "Cherbourg"
## [1] "Cologne"
## [1] "Copenhagen"
## [1] "Geneva"
## [1] "Gibraltar"
## [1] "Hamburg"
## [1] "Hook of Holland"
## [1] "Lisbon"
## [1] "Lyons"
## [1] "Madrid"
## [1] "Marseilles"
## [1] "Milan"
## [1] "Munich"
## [1] "Paris"
## [1] "Rome"
## [1] "Stockholm"
## [1] "Vienna"
## [1] "Athens"
```

```
set.seed(333) # chosen to get a good soln relatively quickly

#  box-constrained optimization and simulated annealing
```

```r
# method = "SANN" performs simulated annealing
# Method "SANN" is by default a variant of simulated annealing given in
Belisle (1992)
res <- optim(initial.tour, distance, GenSeq, method = "SANN",
             control = list(maxit = 30000, temp = 2000, trace = TRUE,
                            REPORT = 500))

## sann objective function values
## initial       value 29625.000000
## iter     5000 value 13044.000000
## iter    10000 value 13044.000000
## iter    15000 value 12907.000000
## iter    20000 value 12907.000000
## iter    25000 value 12907.000000
## iter    29999 value 12907.000000
## final         value 12907.000000
## sann stopped after 29999 iterations

res  # Near optimum distance around 12842

## $par
##  [1]  1 19 16 15  2 14  9 12 13  8 18  5  4  3 11  7 20 10  6 17 21
1
##
## $value
## [1] 12907
##
## $counts
## function gradient
##    30000       NA
##
## $convergence
## [1] 0
##
## $message
## NULL

final.tour<-res$par
final.tour

##  [1]  1 19 16 15  2 14  9 12 13  8 18  5  4  3 11  7 20 10  6 17 21
1

final.d<-distance(final.tour)
final.d

## [1] 12907

initial.d

## [1] 29625
```

```
final.d/initial.d
```

```
## [1] 0.4356793
```

```
cities.xy <- cmdscale(eurodist)
cities.xy
```

```
##                          [,1]        [,2]
## Athens           2290.274680  1798.80293
## Barcelona        -825.382790   546.81148
## Brussels           59.183341  -367.08135
## Calais            -82.845973  -429.91466
## Cherbourg        -352.499435  -290.90843
## Cologne           293.689633  -405.31194
## Copenhagen        681.931545 -1108.64478
## Geneva             -9.423364   240.40600
## Gibraltar       -2048.449113   642.45854
## Hamburg           561.108970  -773.36929
## Hook of Holland   164.921799  -549.36704
## Lisbon          -1935.040811    49.12514
## Lyons            -226.423236   187.08779
## Madrid          -1423.353697   305.87513
## Marseilles       -299.498710   388.80726
## Milan             260.878046   416.67381
## Munich            587.675679    81.18224
## Paris            -156.836257  -211.13911
## Rome              709.413282  1109.36665
## Stockholm         839.445911 -1836.79055
## Vienna            911.230500   205.93020
```

```
for(i in 1:length(final.tour))
{
  print(cities[final.tour[i]])
}
```

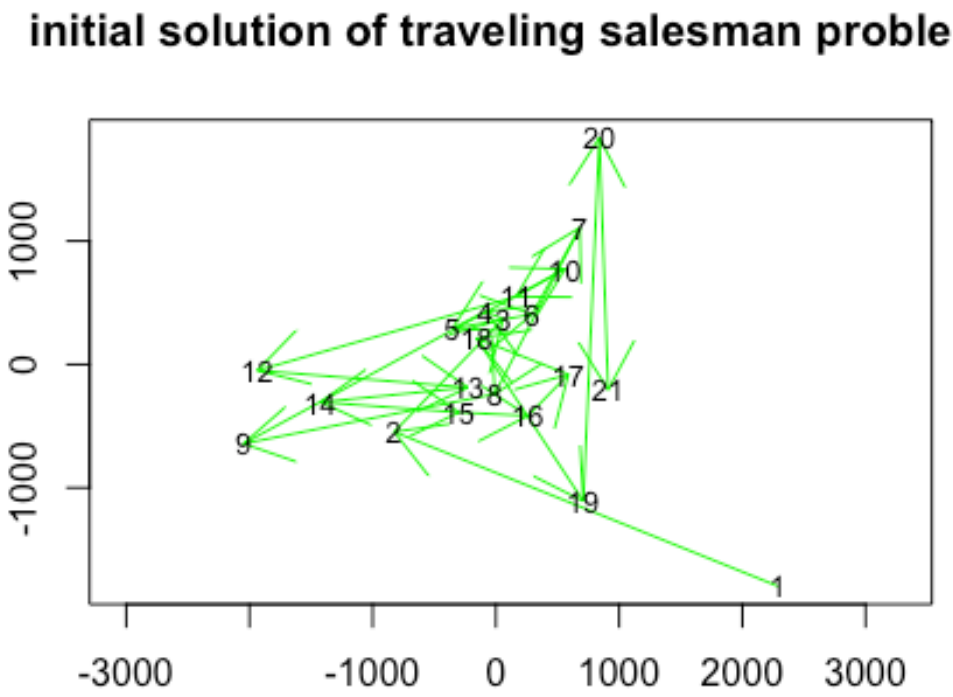
```
## [1] "Athens"
## [1] "Rome"
## [1] "Milan"
## [1] "Marseilles"
## [1] "Barcelona"
## [1] "Madrid"
## [1] "Gibraltar"
## [1] "Lisbon"
## [1] "Lyons"
## [1] "Geneva"
## [1] "Paris"
## [1] "Cherbourg"
## [1] "Calais"
## [1] "Brussels"
## [1] "Hook of Holland"
## [1] "Copenhagen"
```

```
## [1] "Stockholm"
## [1] "Hamburg"
## [1] "Cologne"
## [1] "Munich"
## [1] "Vienna"
## [1] "Athens"

rx <- range(x <- cities.xy[,1])
ry <- range(y <- -cities.xy[,2])
rx

## [1] -2048.449  2290.275

ry

## [1] -1798.803  1836.791

x

##          Athens       Barcelona        Brussels          Calais
##     2290.274680     -825.382790       59.183341      -82.845973
##       Cherbourg         Cologne      Copenhagen          Geneva
##     -352.499435      293.689633      681.931545       -9.423364
##       Gibraltar         Hamburg Hook of Holland          Lisbon
##    -2048.449113      561.108970      164.921799    -1935.040811
##           Lyons          Madrid      Marseilles           Milan
##     -226.423236    -1423.353697     -299.498710      260.878046
##           Munich           Paris            Rome       Stockholm
##      587.675679     -156.836257      709.413282      839.445911
##           Vienna
##      911.230500

y

##          Athens       Barcelona        Brussels          Calais
##     -1798.80293      -546.81148       367.08135       429.91466
##       Cherbourg         Cologne      Copenhagen          Geneva
##       290.90843       405.31194      1108.64478      -240.40600
##       Gibraltar         Hamburg Hook of Holland          Lisbon
##      -642.45854       773.36929       549.36704       -49.12514
##           Lyons          Madrid      Marseilles           Milan
##      -187.08779      -305.87513      -388.80726      -416.67381
##           Munich           Paris            Rome       Stockholm
##       -81.18224       211.13911     -1109.36665      1836.79055
##           Vienna
##      -205.93020

initial.tour

##  [1]  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21
1
```

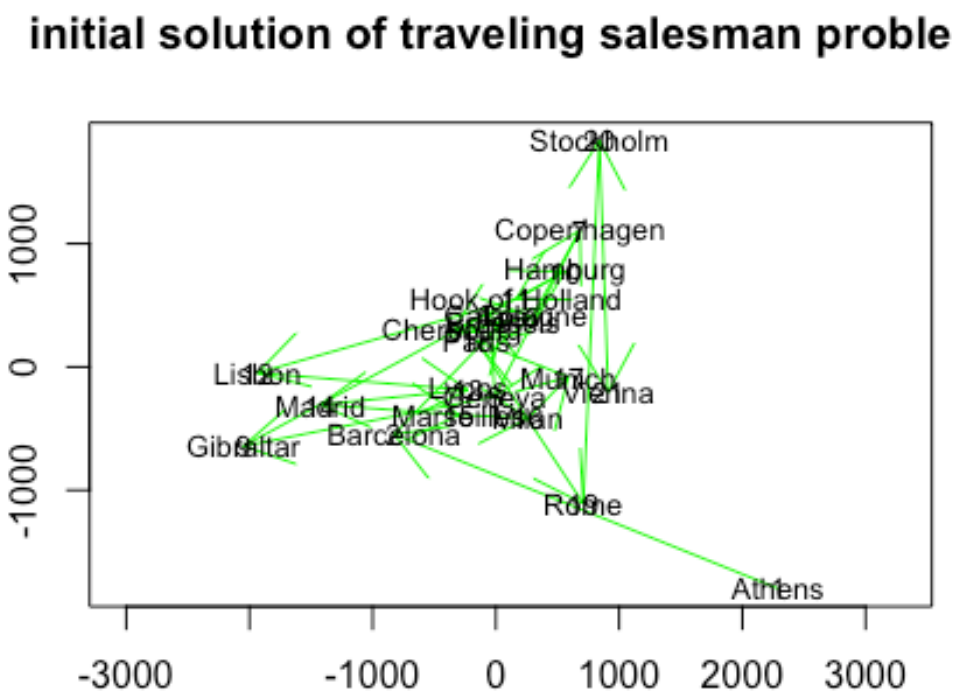
```
## remove last element to draw arrows from point to point
s <-head(initial.tour, -1)
s
```

```
##  [1]  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21
```

```
plot(x, y, type="n", asp=1, xlab="", ylab="", main="initial solution of
traveling salesman problem")
arrows(x[s], y[s], x[s+1], y[s+1], col="green")
text(x, y, labels(cities), cex=0.8)
```




```
plot(x, y, type="n", asp=1, xlab="", ylab="", main="initial solution of
traveling salesman problem")
arrows(x[s], y[s], x[s+1], y[s+1], col="green")
text(x, y, labels(cities), cex=0.8)
text(x, y, labels(eurodist), cex=0.8)
```




```
final.tour
```

```
##  [1]  1 19 16 15  2 14  9 12 13  8 18  5  4  3 11  7 20 10  6 17 21
1
```

```
## draw lines from point to point
s <-head(final.tour, -1)
s
```

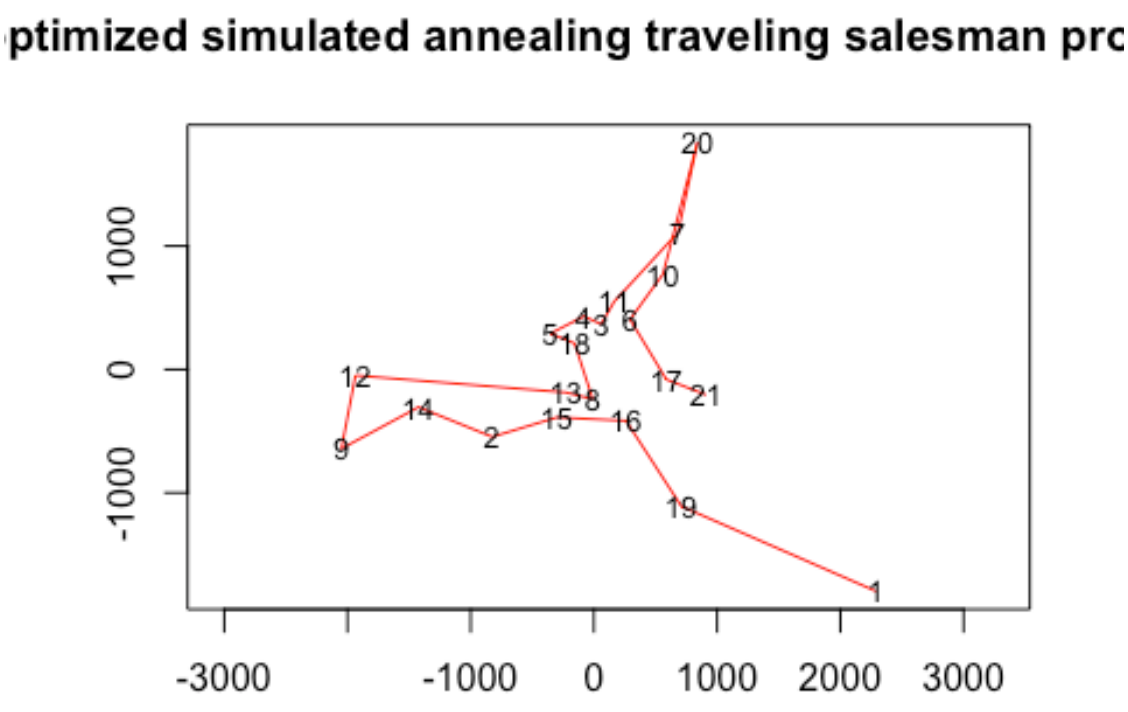
```
##  [1]  1 19 16 15  2 14  9 12 13  8 18  5  4  3 11  7 20 10  6 17 21
```

```
df = data.frame(x[s],y[s])
df
```

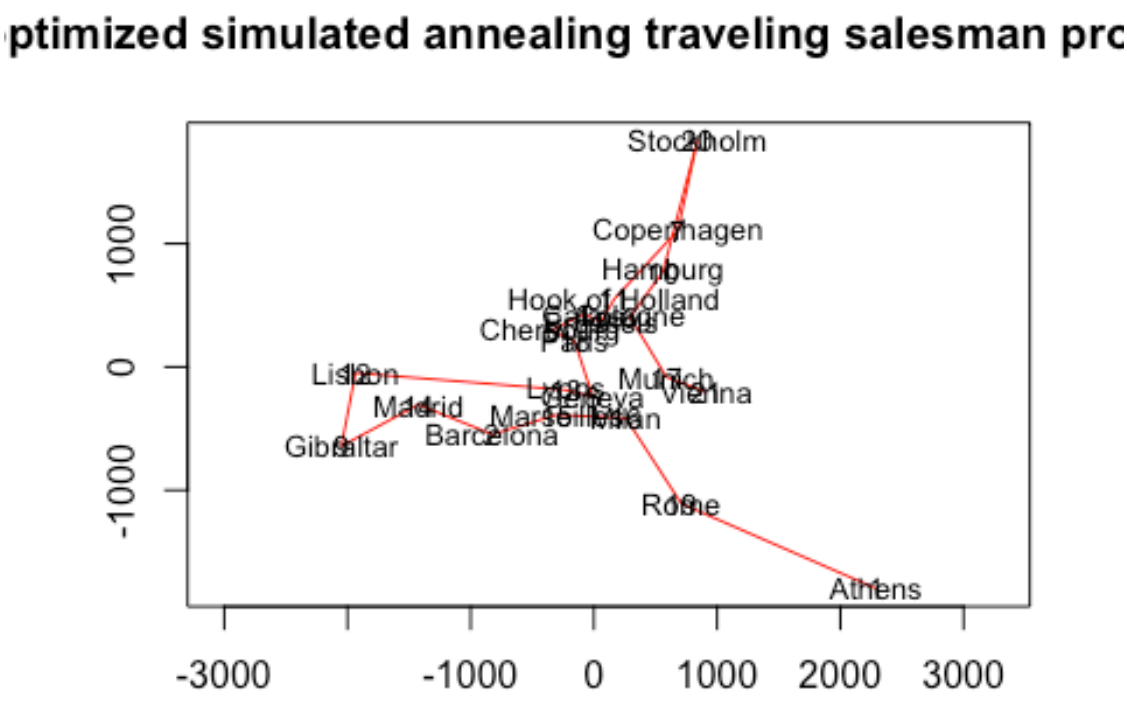
```
##                          x.s.        y.s.
## Athens           2290.274680 -1798.80293
## Rome              709.413282 -1109.36665
## Milan             260.878046  -416.67381
## Marseilles       -299.498710  -388.80726
## Barcelona        -825.382790  -546.81148
## Madrid          -1423.353697  -305.87513
## Gibraltar       -2048.449113  -642.45854
## Lisbon          -1935.040811   -49.12514
## Lyons            -226.423236  -187.08779
```

```
## Geneva              -9.423364  -240.40600
## Paris             -156.836257   211.13911
## Cherbourg         -352.499435   290.90843
## Calais             -82.845973   429.91466
## Brussels            59.183341   367.08135
## Hook of Holland    164.921799   549.36704
## Copenhagen         681.931545  1108.64478
## Stockholm          839.445911  1836.79055
## Hamburg            561.108970   773.36929
## Cologne            293.689633   405.31194
## Munich             587.675679   -81.18224
## Vienna             911.230500  -205.93020
```

```
plot(x, y, type="n", asp=1, xlab="", ylab="", main="optimized simulated
annealing traveling salesman problem")
lines(df$x, df$y, col="red")
text(x, y, labels(cities), cex=0.8)
```




```
plot(x, y, type="n", asp=1, xlab="", ylab="", main="optimized simulated
annealing traveling salesman problem")
lines(df$x, df$y, col="red")
text(x, y, labels(cities), cex=0.8)
text(x, y, labels(eurodist), cex=0.8)
```



Resources

- The Traveling Salesman with Simulated Annealing, R, and Shiny
- Simulated Annealing Feature Selection

```
```