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# Global Optimization of Self Avoiding Random Walks using Simulated Annealing Method.

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***Abstract***

***In this paper we have reported the application of self avoiding random walk (SARW) and evaluation of the simulated annealing (SA) optimization method in solving the Feyman problem which is an application of self ad voiding random walks. From the results of simulation, graphs of the shortest path among N randomly positioned cities for N=5, 10, 20, 25, 30, 35, 40, 45, 60, 65, 70, 200, 500, and 1000 were sketched. We have equally studied the variation of root mean square value of the displacement $\langle d_N \rangle$, the mean square value of the end to end distance $d^2_N$, (persistence distance) and we have compared the result with other theoretical results.***

**Key words:** Fey man problem; self avoiding, random walks; simulated annealing; Global optimization.

## 1.0 Introduction

Self-avoiding random walk is a path from one point to another, which never intersects itself. Such paths are usually considered to occur on lattices. The most familiar form of self-avoiding walk is obtained by enumerating all self-avoiding walks of length N. Such a walk is described by a function [1].

The history of SARW began in the mid 1940s and was first papered by Orr in 1947 [2]. In 1954, Hamersley proved that the N-step SARW grow like $\mu^N$ where N is the connective constant.

The main characteristic of SARW is the infinite memory of the walk, resulting from excluded volume constraint. This property raises question whether an initial bias persists along the entire walk, and affect the distribution of the end point. This problem was first considered by Grass Berger in 1982 [3] who investigated the dependence of the persistence length on the number of steps of two-dimensional SARW. The persistence length of a SARW ($d_N$) is defined as the average displacement of the end point of an n-step walk along the direction of the first step. He showed that $\langle d_N \rangle \approx n^{\upsilon}$ diverges $\upsilon$=0.063. Base on exact enumeration and monte Carlo (MC) data, the divergence is logarithmic in n [3]. E. Eisenberg and A.baram 2003 [3] showed that persistence length of 2-dimensional SARW do not diverge neither as a power law nor logarithmically but rather converge to a constant. They investigated the persistency problem by analyzing the decay rate of the angular correlation function $C_{1j(n)} = \frac{\sum_{k=1}^{Cn} \cos\left(\theta_1, j(k)\right)}{C_n}$

between the direction of the first step and the j[th] step of an n-step SARW on a square lattice. Thus $C_{1j(n)}$ described the average x component of the j[th]-step of the walk, and the persistence length is given by the summation over j of the angular correlations that is $< x_n >=< d_n >= \sum_{j=1}^{n} C_1, j(n).$

$(\theta_1, j(k))$ is the angle between the directions of the first step and the j[th] step of the walk.

The generator of SARW statistics or distribution function $G_{N(r)}$, which represent the number of N-stepped SARW configurations with end -to-end distance r, is not Gaussian as in the case of random walk (for random walk $G_N(r) = \exp(-r^2/N)$ [4]. From the distribution function $G_{N(r)}$, one obtain the asymptotic behavior of various movements The statistics of SARW, are determined by the connectivity constant $\mu$ which is non-universal and depend on the lattice types, and the universal exponents like the radius of revolution exponent ν which depends on the lattice dimension d. The growth of the (total) number $G_N = \left(\sum_r G_N(r)\right)$ of walks with steps size N is determined by the connective constant $\mu = \left(\frac{G_N}{G_{N-1}}, N \to \infty\right)$ and the radius of revolution $R_N$ of the SARW grows with N as $N^{\nu}$. Extensive numerical studies gives $\mu = \mu_o$ =2.638, 4.151 and 4.684 for square, triangular and simple cubic lattices respectively [5]. Theoretical studies gives the value of $\nu=\nu_0^s$ =3/4, 0592±0.003 and ½ for d=2, 3 and 4 respectively (the subscript $^o$ stand for a pure lattice) [5].

E. Eisenberg and A Baram (2003) [3] showed that the persistent length for all temperature range (Low and high) is $< d_N^2 >= \frac{\sum r^2 G_{NM}(r)\exp\left(\frac{-MJ}{kT}\right)}{\sum_r G_{NM}(r)\exp\left(\frac{-MJ}{kT}\right)}$ and that at high temperatures, $< d_N^2 >\approx N^{2\nu}$.

The study of SARW encompasses a broad range of areas of Mathematics, Biology, Chemistry and Physics. In our paper we have studied an example of SARW: The Fey man Problem due to its academic significances and its real World applications. The Fey man in our context is a person with a dubious character. The Fey man problem is generally define as the task of finding the cheapest way of connecting N cities in a closed tour where a cost is associated with each link between the cities. The proverbial Fey man visits N cities with positions $(x_1,y_1)$, returning finally to his or her city of origin. Each city is visited once. This problem can be considered as a constraint or unconstraint optimization problem, which in general is non-linear and potentially nonconvex. A reliable solution to the Fey man problem is obtained using stochastic optimization methods such as the Simulated Annealing (SA) or genetic algorithm (GA). Even though these methods provide no formal guarantee for global optimization, they are reliable strategies and offer a reasonable computational effect in the optimization of multivariable functions [6].

In our work, we have used the method of Simulated Annealing which is an individual optimization technique. The Fey man problem belongs to class of minimization problems for which the objective function has many local minima (or local maxima). In practical cases, it is enough to chose from these minima, a minimum even if not absolute. The Annealing method manages to achieve this, while limiting its calculations to scale as a small power of N.

## 2.0 Methodology

### 2.1 Problem formulation.

The cities are numbered i=1…N and each has coordinates $(x_i,y_i)$. The objective function in it simplest form, E is taken just as the total length of the journey

$$E = L = \sqrt{(x_i - x_{i+1})^2 + (y_i - y_{i+1})^2}$$

Starting in an initial state $x_0$, we pick up another state from the neighborhood of $x_o$ and we compute the

quantity $\Delta E = E(x) - E(x_o)$. Then if $\Delta E > 0$, It would be accepted according to the Boltzmann factor exp(-$\Delta E/KT$), where T is an external control interpreted as a temperature and E is the cost function of the problem. If $\Delta E \leq 0$, the state is always accepted. This is an iterative stochastic producer [7], and at low temperature, it expected that it will jump between low cost (low energy) configurations. In this case, our function is the unconstrained function.

## 2.2 Simulated Annealing (SA)

Simulated annealing is a stochastic optimization technique inspired by the thermodynamic process of cooling of molten metals to attain the lowest free energy state [6]. Starting with an initial solution and armed with adequate perturbation and evaluation functions, the algorithm performs a stochastic partial search of the state space. In minimization problems, uphill moves are occasionally accepted with a probability controlled by a parameter called annealing temperature, $T_{SA}$ . The probability of acceptance of uphill moves decreases as $T_{SA}$ decreases. At high temperatures, the search is almost greedy. At zero temperature, the search becomes totally greedy that is only good moves are accepted [6]. The core of the algorithm is the metropolis procedure, which simulates the annealing process at a given $T_{SA}$ [Metropolis 1953] [8]. The metropolis criterion is used to accept or reject the uphill moves. Several algorithms have been proposed for SA method. We have used the algorithm proposed by Corana et al (1987) [9] because previous papers have reported it reliability and efficiency in thermodynamic calculations (Henderson et al, [10], Rangaiah, 2001 [11]).

The metropolis algorithm has the function of setting up the initial routes of the Fey man and printing final results. For each value of density it chooses random coordinates x(i), y(i) using the subroutine ran 3, put an entry of each city in the array IPTR(i). The array indicates the order in which the cities will be visited. On the original specified path, the cities are in the order i=1…N so that the sample programme initially takes IPTR (i) = i (it is assume that the Fey man will return to the first city after visiting the last). A call is then made to anneal, which attempts the shortest alternative route, which is recorded in the array.

## 3.0 Results of simulation

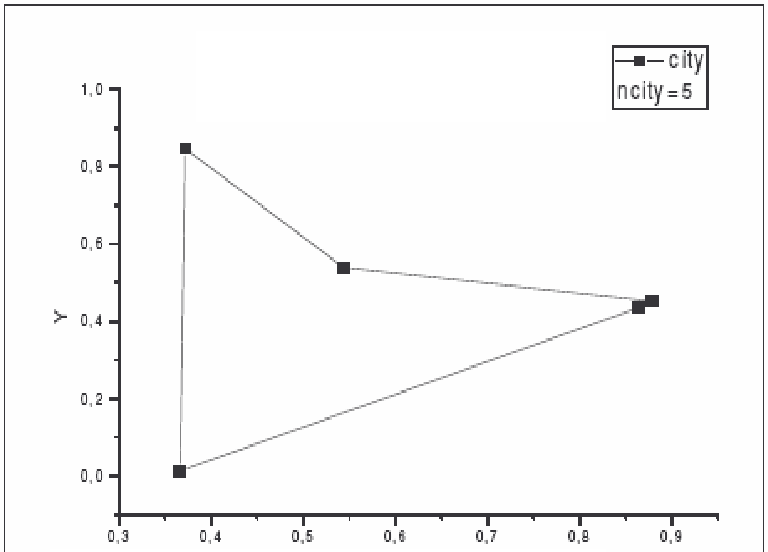



Fig. a

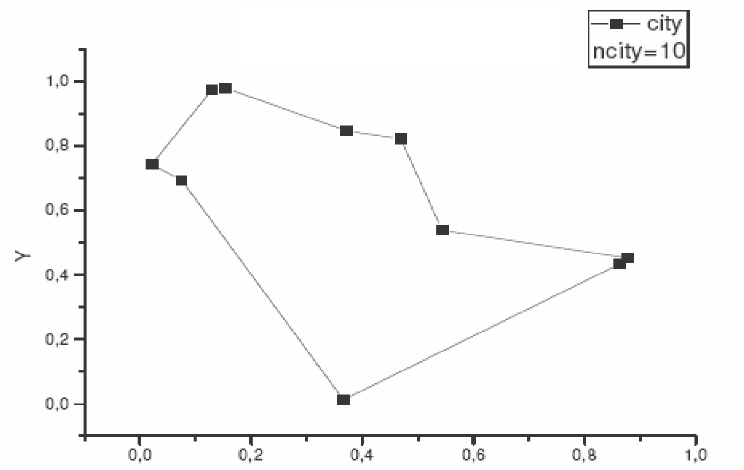
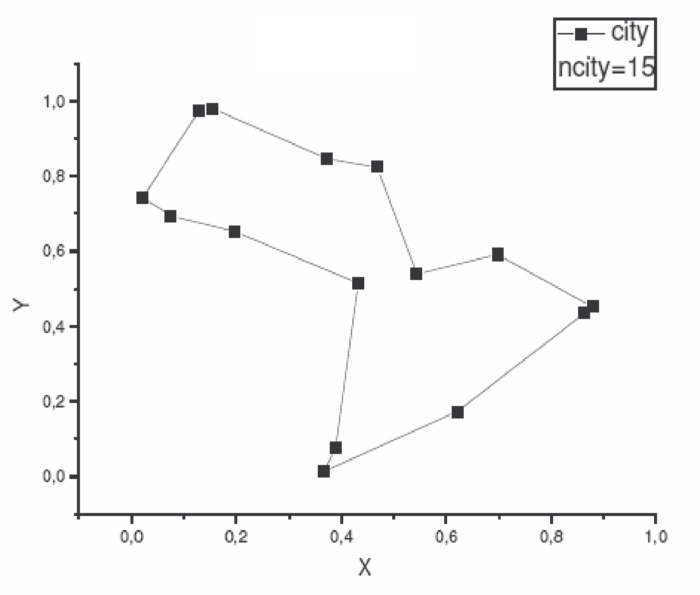



Fig. b



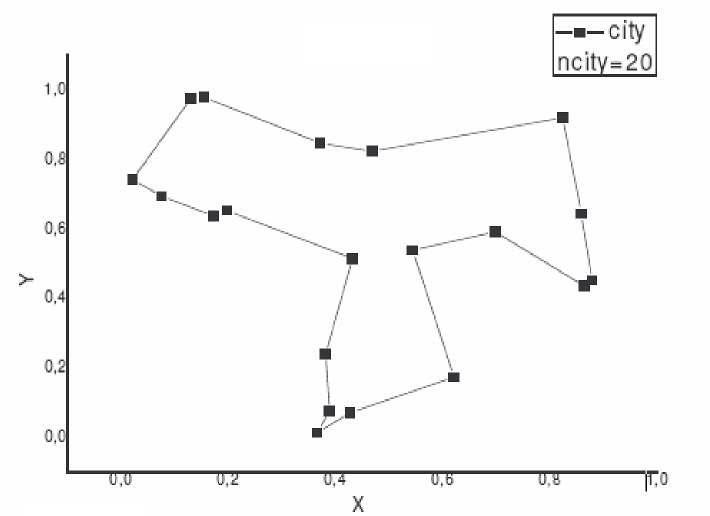
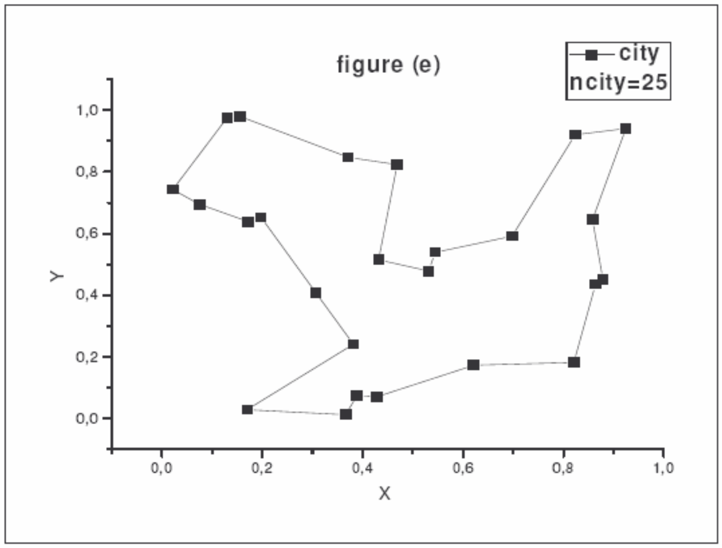


Fig. d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city
ncity=25
1,0
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0,2
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Y
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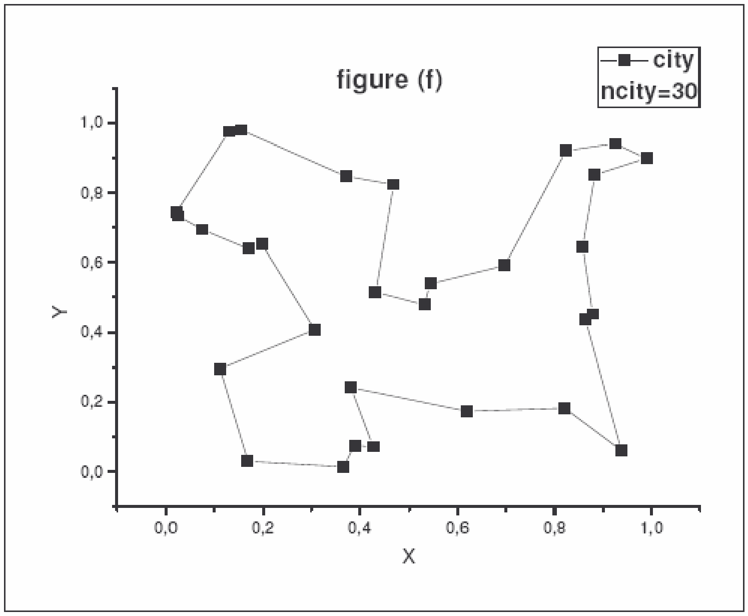
0,2
0,4
0,6
0,8
1,0
X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city
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Y
X

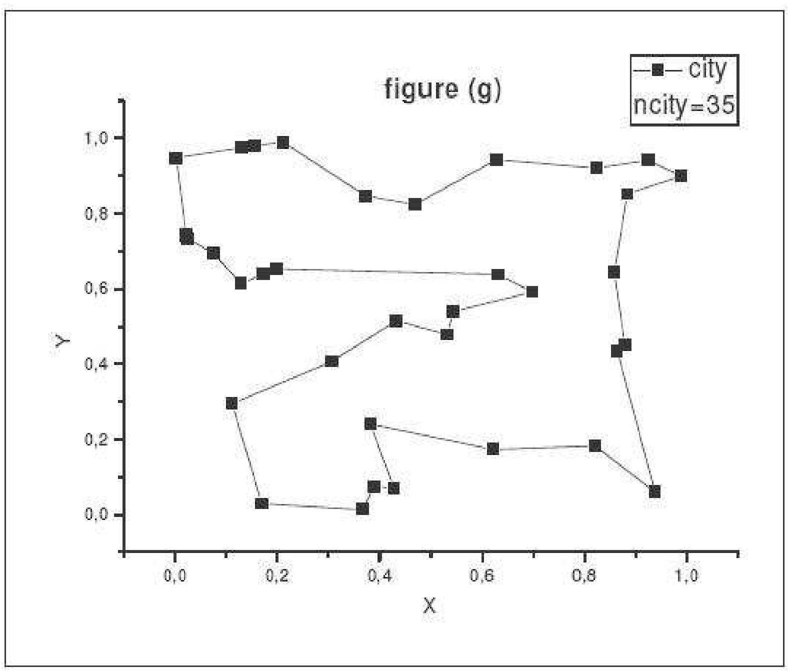
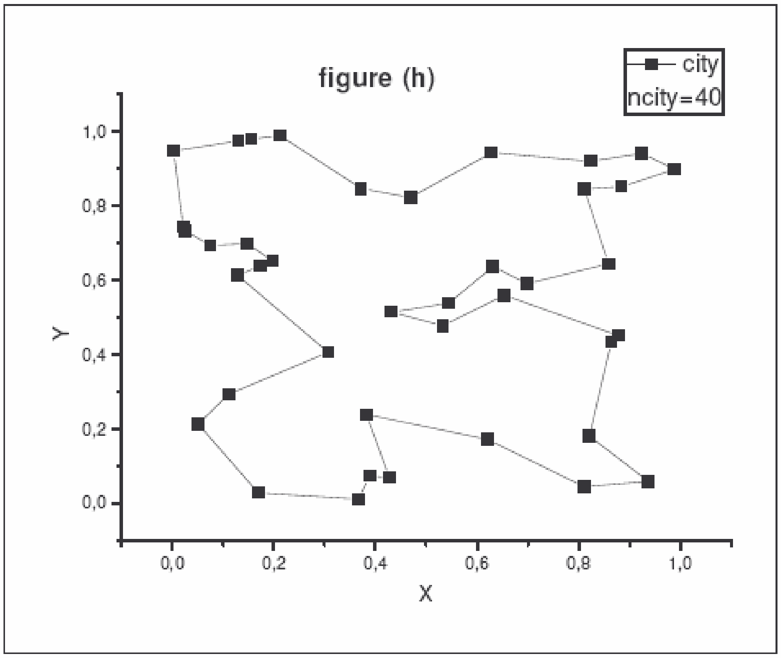


figure (g)
city
ncity=35
Y
X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city
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1,0
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0,2
0,0
Y
0,0
0,2
0,4
0,6
0,8
1,0
X

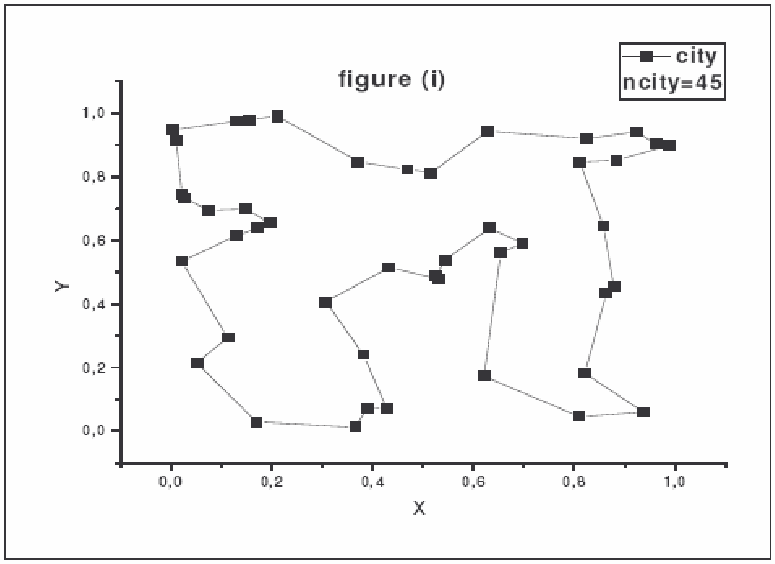
figure (i)
city
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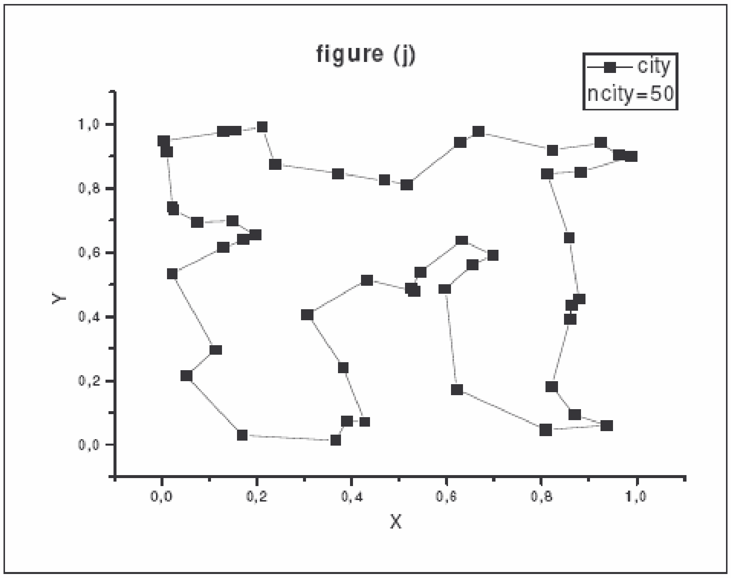
0,0
Y
0,0
0,2
0,4
0,6
0,8
1,0
X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city
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Y
X
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0,4
0,2
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0,0
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0,6
0,8
1,0

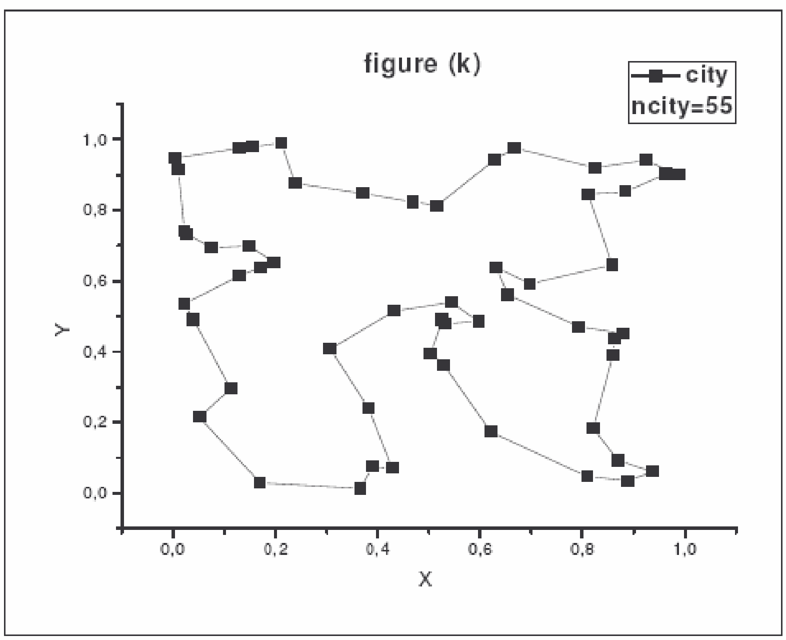
figure (k)
city
ncity=55
Y
X
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0,2
0,0
0,0
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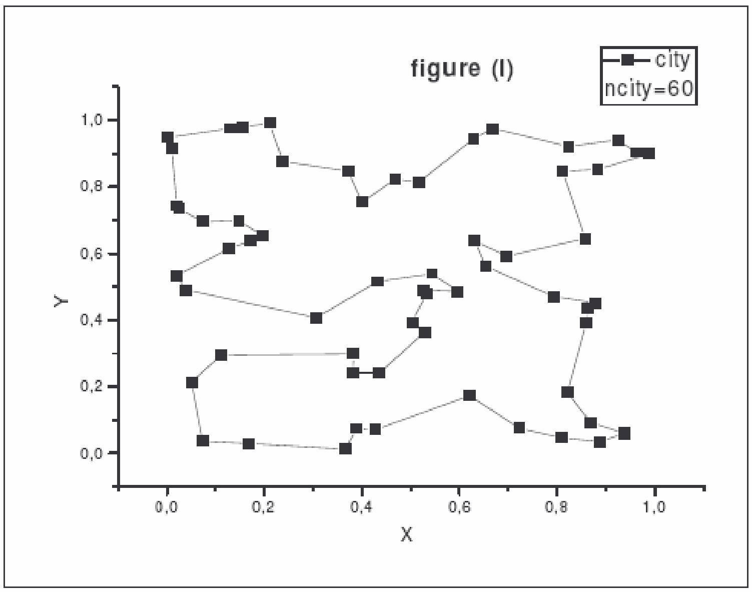
0,6
0,8
1,0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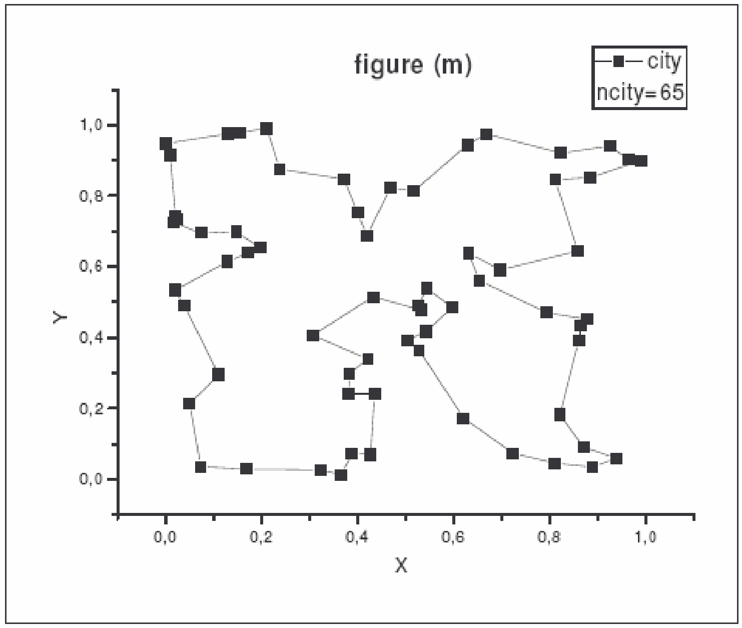
0,4
0,2
0,0
Y
0,0
0,2
0,4
0,6
0,8
1,0
X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city
ncity=65
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Y
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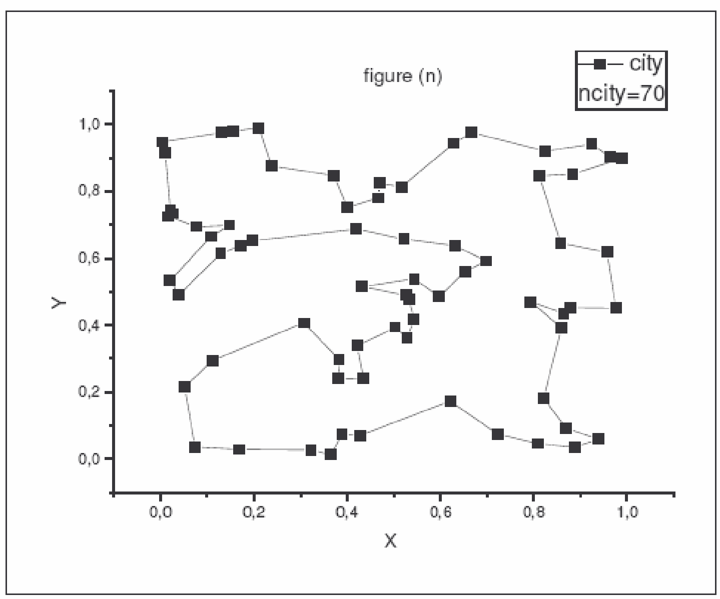
0,2
0,4
0,6
0,8
1,0
X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city
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Y
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0,4
0,6
0,8
1,0
X

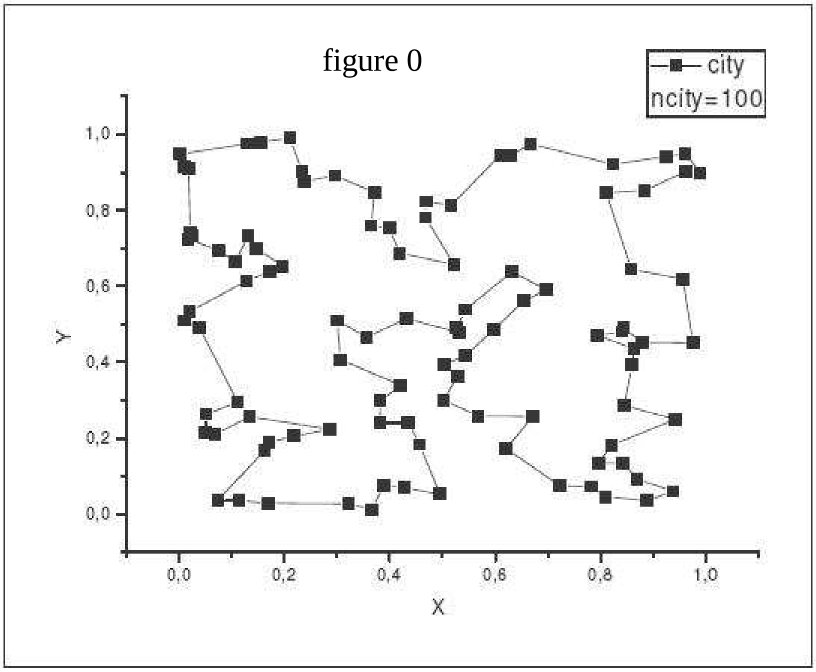
figure 0
city
ncity=100
1,0
0,8
0,6
0,4
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Y
0,0
0,2
0,4
0,6
0,8
1,0
X

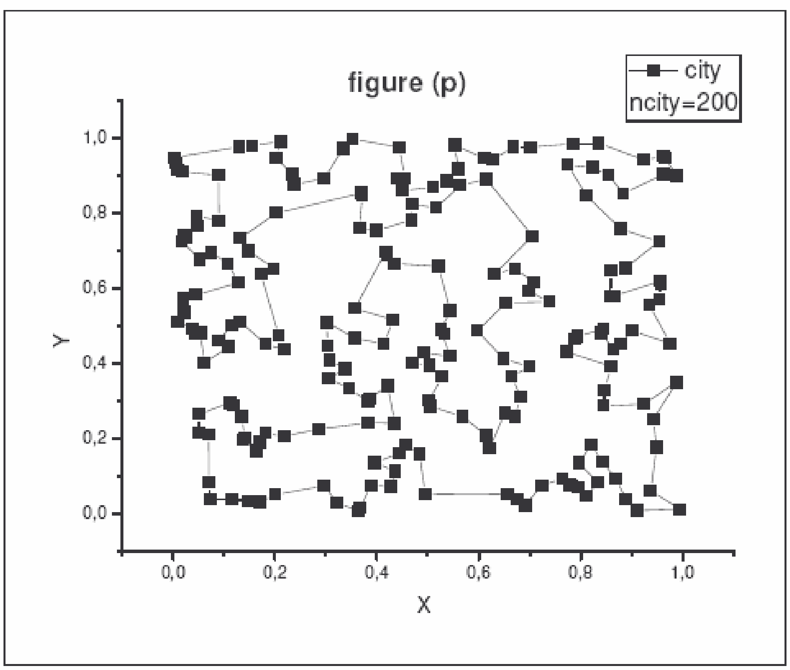
figure (p)
city
ncity=200
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Y
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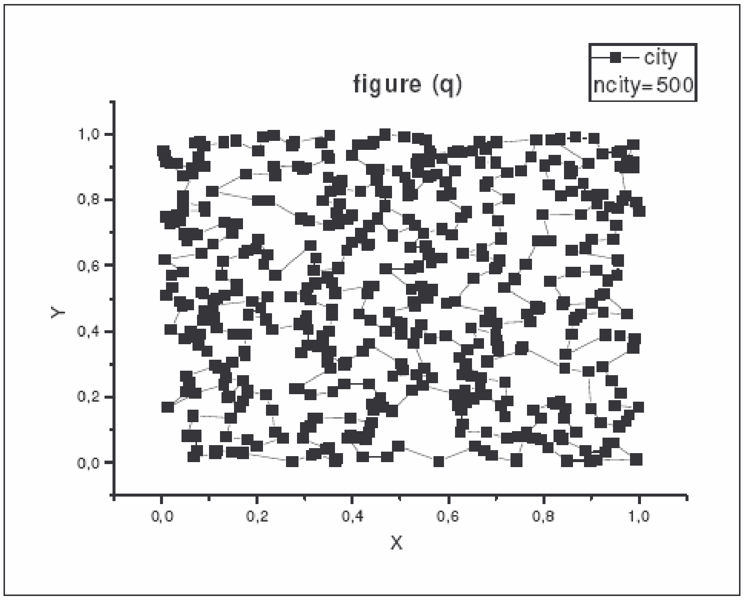
0,2
0,4
0,6
0,8
1,0
X



city
ncity=500
figure (q)
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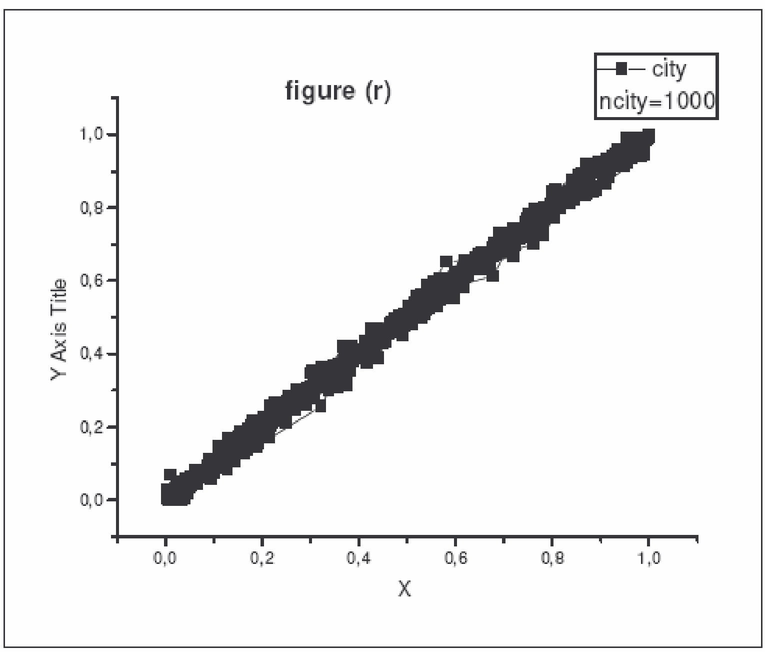
0,6
0,4
0,2
0,0
Y
0,0
0,2
0,4
0,6
0,8
1,0
X

city
ncity=1000
figure (r)
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0,8
0,6
0,4
0,2
0,0
Y Axis Title
0,0
0,2
0,4
0,6
0,8
1,0
X

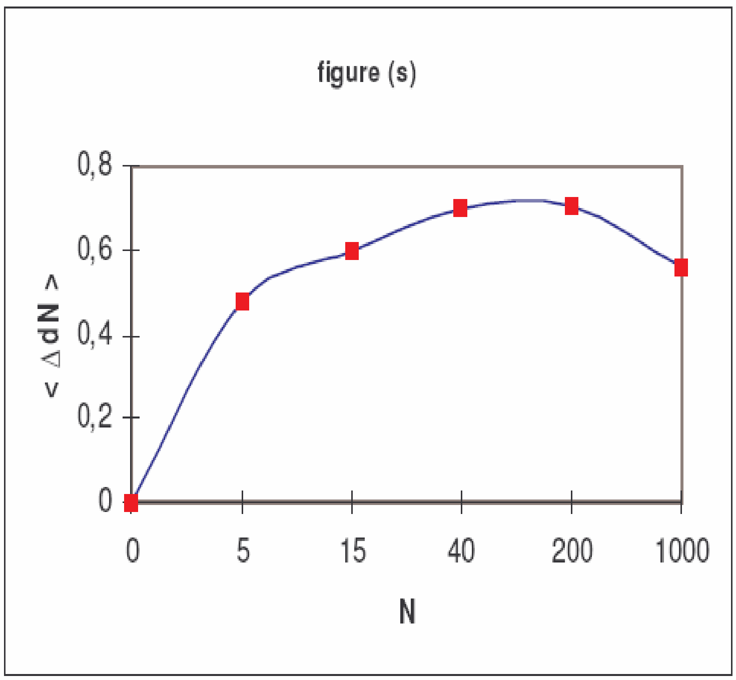
figure (s)
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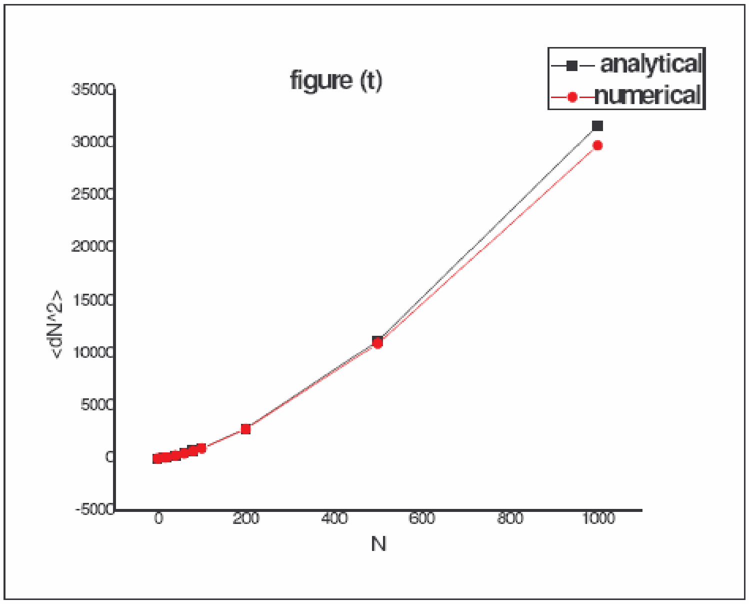
0,4
0,2
0
< Δ d N >
0
5
15
40
200
1000
N




The figures (a)-(r) shows the Fey man problem solved by simulated annealing.

The cities are represented by the black squared dots which are randomly occupied. The shortest path among N randomly positioned cities is shown in each case (that is the optimized path). We have studied the numerical results for N=5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 200, 500 and 1000. These results are shown above on the figures (a)-(r) respectively. For N=1000, the displacement of the Fey man is practically on a straight line. For values of N greater than 1000 (N>1000), no results were obtained. We can say that N=1000 is a critical value.

Figure (s) shows the variation of the root mean square value of the Fey man displacement and figures (t) shows how mean square of the end to end distance varies with the number of cities. A careful look at the figures (t) and (s) indicates that the mean square of the end to end distance is proportional to $N^{2\nu}$ (that is $< d_N^2 >= N^{2\nu}$) and that the variation of mean square distance is proportional to $N^{1/2}$ (that is $\Delta d_N \propto N^{1/2}$) respectively which are in good agreement with other theoretical results [3], [12].

## 4.0 Some applications of the Fey man Problem (FP).

Much of the works on the FP are not motivated by direct application, but rather by the fact that it provides an ideal platform for the study of general methods that can be applied to a wide range of discrete optimization problems. This is not to say, however, that the FP does not find application in many fields. Indeed, the numerous direct applications of the FP bring life to the research area and help to direct future works.

The FP naturally arises as a sub problem in many transportation and logistics applications, for example the problem of arranging school bus routes to pick up the children in a school district. More recent applications involve the scheduling of service calls at cable firms, the delivery of meal to homebound persons, the scheduling of stacker cranes in warehouses, the routing of trucks for parcel post pickup .

Although transportation applications are the most natural setting for the FP, the simplicity of the model has lead to many interesting applications in other areas. A classical example is the scheduling of a machine to drill holes in a secured board or other objects. In this case, the holes to be drilled are the cities and the cost of travel is the time it takes to move the drill head from one hole to the next. The technology for drilling vary from one industry to the other, but whenever the travel time of the drilling device is a significant portion of the overall manufacturing process then, the FP can play a role in reducing cost. Here are some of these applications.

FP's implementation can be used by a semi conductor manufacturer to optimize scan chains in integrated circuits. Scan chains are routes included on a chip for testing purposes and it is useful to minimize their length for both timing and power reason

FP can be used to locate cables to deliver power to electronic devices associated with fibre optics connections to homes

It is used to optimize the sequence of celestial objects to be imaged in an interferometer program. The goal of the study is to minimize the use of fuel in targeting and imaging manoeuvres for the pair of satellites involved in the mission (the cities in the FP are the celestial objects to be images, and the cost of travel is the amount of fuel needed to reposition the two satellites from one image to the next).

It can be used as a tool for designing fibre optical networks. The FP aspect of the problem arises in the routing of sonet rings, which provide communications links through a set of sites organized in a ring. The ring structure provides a backup mechanism in case of a link failure, since traffic can be rerouted in the opposite direction on the ring.

## 5.0 Conclusion

From the numerical study of the FP and its applications, we can conclude that the FP is very important to the society as it is used in daily life activities. We hope that this work shall be one day exploited by some industries as a practical example in our country and also to solve some problem of road construction in urban area so as to minimize transportation cost. We hope that in our future studies, we shall solve the same problem in more than 2 dimensions which is more realistic.

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