submitted for publication in *Evolutionary Computation* (1997)

Optimization of Road Networks Using Evolutionary Strategies

F. Schweitzer, W. Ebeling, H. Rosé, O. Weiss

Institute of Physics, Humboldt University
Unter den Linden 6, 10099 Berlin, Germany

e-mail: frank@summa.physik.hu-berlin.de

Abstract

A road network usually has to fulfill two requirements: (i) it should as far as possible provide direct connections between nodes, to avoid large detours, (ii) the costs for road construction and maintainance, which are assumed proportional to the total length of the roads, should be low. The optimal solution is a compromise between these contradicting demands, which in our model can be weighted by a parameter.

The road optimization problem belongs to the class of frustrated optimization problems. In this paper, a special class of evolutionary strategies, such as the Boltzmann and Darwin and mixed strategies, are applied to find differently optimized solutions (graphs of varying density) for the road network in dependence on the degree of frustration. We show, that the optimization process occurs on two different time scales. In the asymptotic limit, a fixed relation between the mean connection distance (detour) and the total length (costs) of the network exists, which defines a range of possible compromises.

Further, we investigate the density of states, which describes the number of solutions with a certain fitness value in the stationary regime. We find that the network problem belongs to a class of optimization problems, where more effort in optimization certainly yields better solutions. An analytical approximation for the relation between effort and improvement is derived.

Key words: network, evolutionary strategy, frustrated problem, compromise

1 Introduction

The optimization of networks which connect a given set of nodes is of common interest in many different areas, among them electrical engineering, telecommunication, or road construction and trade-logistics. The problem turned out to be a challenge both for practical applications and theoretical investigations [2, 19, 20, 36]. As one example, we consider here a road network, however the optimization method as well as the results can be generalized for similar network problems.

Usually, the optimization of a road network has to consider different requirements, e.g. (i) to minimize the total costs of constructing and maintaining the roads, which should be proportional to the total length of the roads between the different points of interest (nodes), (ii) to minimize the effort (detour) to reach any given node from any other node, which should be proportional to the length of the roads along the shortest existing connection between the two nodes. Both demands could not be completely satisfied at the same time, since a minimized detour means a direct connection between all nodes and therefore, a maximum total length of the road network, and minimal costs for the network mean the shortest possible total length for the roads.

This perspective of course neglects all problems which usually occur with the use of roads, such as traffic density, flow capacity, etc. Here, we mainly focus on the optimized establishment of links, thus the definition of "costs" takes into account only the length of the road, and not the width or the equipment, and "detour" takes into account only the travelling distance, not the travelling time or the travelling velocity.

Considering only the first demand mentioned, the solution of the optimization process is given by a road network where every node is connected to the network by just one (the possible shortest) link, which leads to the *minimal link system*, also known as *minimal spanning tree*. Contrary, considering only the second demand, the solution is simply given by a network where every node is connected to every other node by a direct link, which leads to the *direct link system* (cf. also Fig. 1). Compared to these two idealized limiting cases, the road network in most real applications is a compromise between these requirements.

Optimization problems like this are known as *frustrated problems* in statistical physics or multi-objective problems in optimization theory. Problems of this kind are characterized by a tremendous number of nearly evenly matched solutions which have to be found in a very rugged landscape of the related optimization function. For the Pareto optimization, the In general, first Pareto-optimal solutions are obtained

Dependent on how the Pareto-optimal solutions are obtained, we can distinguish between different approaches to incorporate preference information about the different objectives of the optimization process: (i)

In order to find some of these matched solutions, evolutionary algorithms are applied [15, 17, 18, 24, 28, 32]. These algorithms deal with stochastic search strategies in an ensemble of searchers which adapt certain features from natural evolution.

We use a special class of evolutionary strategies, namely the Boltzmann and the Darwin strategy, as well as a mix of both of them, which have been successfully applied to a number of complex optimization problems [3, 7, 9, 11, 12]. In this paper, the major focus is on the applications of these strategies to the optimization of road networks, however, in order to elucidate the simulation procedure, we need to comprise some theoretical facts about these strategies.

In Sect. 2, we introduce the evolutionary strategies and the simulation method used in this paper. In Sect. 3, we propose an optimization function for the evaluation of the road network, which consists of two parts, representing the mean detour (averaged local demand) and the total lenght of the road network (global demand). A parameter λ can weight between these two contributions. By means of computer simulations, we investigate the evolution of the network and the related fitness function during the optimization process, and present different optimized solutions for the road network in dependence on λ. In Sect. 4, we discuss the asymptotic limit of the Boltzmann optimization process. For the road network, we find a fixed relation between detour and costs. Further, we investigate the density of states, resulting from the stationary distribution of the Boltzmann strategy, which can be considered as a heuristic measure of the number and the quality of not yet found optimized solution. We derive a relation between the possibility of further improvement of the solutions and the effort (computer time) needed.

2 Evolutionary Optimization Strategies

2.1 Boltzmann Strategy

An optimization process can be described as a special search for minima of a related potential in the configuration space. Evolutionary optimization strategies are based on the idea of an ensemble of searchers which move through the configuration space, searching for minima. Let us consider a numbered set of states $i = 1, ..., s$ in the configuration space, each of them characterized by a scalar U_i (the potential energy). Further, we assume a total number N of searchers participating. Then, $N_i(t)$ is the actual number of searchers occupying the state i at time t. The occupation number should be an integer, but in the limit case $N \to \infty$ discussed first, the occupation fraction $N_i(t)/N$ may be replaced by a probability of occupation at time t denoted by $p_i(t)$.

The search strategy has to ensure that the occupation probability for the minima of the potential will increase during the search. However, since due to the frustration of the problem a large quantity of suitable minima exist, the search strategy should also avoid a total locking of the searchers in the minima found so far in order to guarantee further search. The so called Boltzmann strategy is a *thermodynamic strategy* used during evolution to find the minima of certain thermodynamic functions. This strategy is based on three elements:

(i) due to motion along gradients the steepest local ascent of the entropy or the steepest local descent of a potential is reached

(ii) due to thermal fluctuations the locking in local minima of the potential is avoided

(iii) due to a continous decrease of the temperature the search becomes more precise in the course of time

We note that different optimization routines like the Metropolis algorithm [22] or the *simulated annealing* approach [21, 26, 35] are based on these elements.

The analogy between equilibrium statistical mechanics and the Metropolis algorithm was first discussed in [?]

A dynamics which finds the minimum among a discrete set of scalar values, e.g. energy values U_i with $i = 1, \ldots, s$ is given by

$$\frac{dp_i(t)}{dt} = \sum_{i \neq j} \left[A_{ij}\, p_j(t) - A_{ji}\, p_i(t) \right] \tag{1}$$

where A_{ij} denotes the transition rate for the searcher to move from state j to state i. In accordance to the description above, it is defined as follows:

$$A_{ij} = A^0_{ij} * \begin{cases} 1 & \text{if } U_i < U_j \\ \exp\left(-(U_i - U_j)/T(t)\right) & \text{if } U_i \geq U_j \end{cases} \tag{2}$$

This means that transitions $j \to i$ towards a lower value $U_i < U_j$ are always accepted, but transitions which lead to a deterioration, $U_i > U_j$, are accepted only with a rate related to the difference in the potential, scaled by the temperature. Thus, due to the motion along the gradients the steepest local descent of the potential will be reached; however, due to thermal fluctuations locking in those local minima will be avoided.

The prefactor A^0_{ij} is symmetric ($A^0_{ij} = A^0_{ji}$), it defines a set of possible states i which can be reached by the searcher from state j. The simplest definition might be

$$A^0_{ij} = \begin{cases} 1 & \text{if} \quad i \text{ is adjacent to } j \\ 0 & \text{if} \quad i \text{ is not adjacent to } j \end{cases} \tag{3}$$

The term *adjacent* means here that state i results only from a single elementary mutation of state j, in other words, a change between the different states can only occur in small steps. Another, but more complicated case is given by $A^0_{ij} = g(d_{ij})$, where g is a monotonously decreasing function of the minimal number of elementary mutations to reach state j from state i and vice versa.

The temperature T, which appears in eq. (2) allows to adjust the transition rates for the deterioration case. For $T \to \infty$, all movements of the searchers are equally accepted, whereas for $T \to 0$ only improvements in the search are accepted. The latter case is equivalent to the gradient method in optimization theory. In the Boltzmann strategy, similar to simulated annealing, the temperature $T(t)$ decreases during the search by a certain rule, e.g. by a power law. This decrease leads to the consequence that first the larger basins of the potential minima are explored ("coarse grained search") and later on a "fine grained" search occurs within these minimum regions.

For constant temperatures the stationary solution of eq. (1)

$$p^0_i = \lim_{t \to \infty} p_i(t) \tag{4}$$

is known to be the canonical or Boltzmann distribution (which gives the strategy its name)

$$p^0_i \sim \exp\left(-U_i/T\right) \tag{5}$$

The Boltzmann process asymptotically finds the minimum in a given set of scalars U_i, since the minimum of the potential has the highest probability. One can further show [14], that during the search process the function

$$K(t) = \sum_i p_i(t) \log \frac{p_i(t)}{p_i^0} = \frac{F(t) - F_0}{T} \tag{6}$$

is monotonically decreasing. Here $F(t)$ has the meaning of a *free energy* of the system with the equilibrium value F_0.

2.2 Darwin Stragegy and Mixed Strategy

In biological evolution, some new elements occured in the optimization process, namely

(i) self-reproduction of species with a fitness above the average fitness

(ii) mutation processes due to error reproduction

(iii) increase of the precision of self-reproduction in the course of evolution

We adapt these elements for our search strategy, which is then called Darwin strategy because it includes some biological elements known from population dynamics [7, 12, 13]. Biological strategies are different from the above thermodynamic strategies in that here the searchers do not remain constant, but can be changed with respect to fundamental processes, such as *reproduction* and *selection*.

Let us consider again the population of N searchers, which are now distributed in different subpopulations $x_i = N_i/N$; $(i = 1, ..., N)$, each characterized by a replication rate E_i which might be proportional to the fitness. Then, the average replication rate $\langle E \rangle$ is given by

$$\langle E \rangle = \frac{1}{N} \sum_{i=1}^{N} E_i \, x_i(t) \;\; ; \;\; N = \sum_{i=1}^{N} x_i(t) \tag{7}$$

According to the Eigen – Fischer dynamics, the evolution of the subpopulations is given by the equation:

$$\frac{dx_i}{dt} = (E_i - \langle E \rangle)\, x_i + \sum_{j \neq i} [A_{ij}^D \, x_j - A_{ji}^D \, x_i] \tag{8}$$

Here the transition rates A_{ij}^D are assumed to be symmetric, since there are no directed mutations. The effect of an increasing precision in self-reproduction can be considered again by a temperature dependence of the transition rates, where a decreasing temperature leads to a smaller probability of mutation. For $A_{ij}^D \to 0$, this evolutionary dynamics is known to approach asymptotically a final state where the average fitness $\langle E \rangle$ is equal to the maximal fitness, which means that only the (one) subpopulation with the best fitness value will survive. For finite mutation rates, $A_{ij}^D > 0$, the target of the search is the eigenvector of eq. (8) corresponding to the highest eigenvalue, which for small mutations rates is close to the maximal value E_{max}.

To compare both strategies [3, 7, 11] we note that the Boltzmann strategy is able to detect the appropiate potential minima even in an unknown, rugged optimization landscape as long as the potential barriers between local minima are not too high, which forces the locking in side minima. On the other hand, the Darwin strategy is able to cross high barriers by tunneling if the next minimum is close enough.

In order to combine the advantages of both stragegies, a *mixed Boltzmann–Darwin strategy* has been introduced [7, 11]. Here, the asymmmetric transition rates (eq. 2) are adopted which favor the transition towards the minimum. On the other hand, the fitness E_i of the subspecies i is chosen to be the negative of the potential U_i indicating that the subspecies which has found the better minimum in the potential landscape, also has the higher reprodution rate.

Here, we introduce a new, more general formulation for the mixed strategy which covers different limit cases:

$$\frac{dx_i}{dt} = \sum_{j \neq i} \Big[\kappa\, \boldsymbol{g}(U_j - U_i)\, x_j\, x_i + A_{ij}\, x_j - A_{ji}\, x_i \Big] \tag{9}$$

with the transition matrices A_{ij} obtained from eq. (2). The function $\boldsymbol{g}(x)$ can be any linear or nonlinear monotonously non-decreasing function. For the applications discussed here, we use two limiting cases for the choice of $\boldsymbol{g}(x)$, namely:

$$\begin{array}{lll} \text{(i)} \quad \boldsymbol{g}(U_j - U_i) = U_j - U_i & & \text{difference selection} \\ \text{(ii)} \quad \boldsymbol{g}(U_j - U_i) = \boldsymbol{\Theta}(U_j - U_i) = & \left\{ \begin{array}{ll} 1 & \text{if} \quad U_j > U_i \\ 0 & \text{if} \quad U_j > U_i \end{array} \right. & \text{tournament selection} \end{array} \tag{10}$$

The function $\boldsymbol{g}(U_j - U_i)$ allows to describe different selection processes. The *tournament selection* (cf. also [4, 5, 17]) means a “hard” or k.o. selection, where the better one wins regardless of the value of the advantage. Compared to this, the *difference selection*, which also occurs in the Eigen–Fischer model, weights this advantage, and therefore is a “weak” selection. For $\mathbf{g}(U_j - U_i) = U_j - U_i$, eq. (9) can be transformed into

$$\frac{dx_i}{dt} = \kappa(\langle U \rangle - U_i)\, x_i + \sum_{j \neq i} [A_{ij}\, x_j - A_{ji}\, x_i] \tag{11}$$

We note, that in eq. (11), as well as in eq. (9), a global coupling between the different subpopulations exists [33].

From the general equation (9), we can obtain different limit cases of evolutionary strategies, which are appropriate to solve the optimization problem of minimizing U_i. By changing the parameters κ and T in the range $0 \leq \kappa \leq 1$, $0 < T \leq \infty$, eq. (9) yields:

$$\begin{array}{ll} \kappa = 0, \quad T > 0 & \text{Boltzmann strategy (eq. 1)} \\ \kappa = 1, \quad T \to \infty, \quad \boldsymbol{g}(U_j - U_i) = U_j - U_i & \text{Eigen-Fischer strategy (eq. 8)} \\ \kappa = 1, \quad T \to \infty, \quad \boldsymbol{g}(U_j - U_i) = \boldsymbol{\Theta}(U_j - U_i) & \text{tournament stragegy} \end{array} \tag{12}$$

2.3 Master Equation Approach to Searching

So far we considered the case $N \to \infty$ where the discrete numbers of searchers occupying state i, $N_i(t)$, might be replaced by probabilities $p_i(t)$ or population densities $x_i(t)$. During the simulations, however, one always deals with a finite number of searchers, hence, the search process may be reformulated now in terms of a stochastic approach. Let us introduce the discrete distribution of searchers

$$\mathbf{N}(t) = N_1(t), N_2(t), ..., N_s(t)\ ; \quad N = \sum_{i=1}^{s} N_i(t) = const. \tag{13}$$

The probability to find a particular distribution $\mathbf{N}$ at time t should be described by $P(\mathbf{N},t) = P(N_1, N_2, ..., N_s, t)$. The change of this probability distribution in the course of time can be described by a *master equation* which considers all possible processes leading to the change of the particular distribution $\mathbf{N}$:

$$\frac{\partial P(\mathbf{N},t)}{\partial t} = \sum_{\mathbf{N'}\neq\mathbf{N}} \{w(\mathbf{N}|\mathbf{N'})P(\mathbf{N'},t) - w(\mathbf{N'}|\mathbf{N})P(\mathbf{N},t)\} \tag{14}$$

The terms $w(\mathbf{N'}|\mathbf{N})$ are the transition probabilities per time unit to change the distribution $\mathbf{N}$ into distributions $\mathbf{N'}$. For the strategies introduced above, we have now two different sets of transition probabilities.

The transition probability for *mutation* processes reads

$$w_M(N_1, ..., N_i + 1, N_j - 1, ..., N_s|N_1, ..., N_i, N_j, ..., N_s) = A_{ij}\ N_j \tag{15}$$

which means that the probability for a searcher occupying state j to move to state i is proportional to the number of searchers in state j and the transition rates for the Boltzmann process, eq. (2). With respect to computer simulations, eq. 15, is consistent with the rules:

(i) select one among the N searchers (say searcher j)

(ii) choose a possible mutation A_{ij}

(iii) decide according to eq. 2 whether the mutation is accepted or not

For strategies including Darwinian elements, we have to consider in addition the transition probability for *selection* processes, which reads:

$$w_S(N_1, ..., N_i + \omega_{ij}, N_j - \omega_{ij}, ..., N_s|N_1, ..., N_i, N_j, ..., N_s) = \kappa\, \|\boldsymbol{g}(U_j - U_i)\|\, N_i N_j/N \tag{16}$$

with

$$\omega_{ij} = \begin{cases} 1 & \text{if } U_i < U_j \\ -1 & \text{if } U_i > U_j \end{cases}$$

Eq. (16) means that the probability for the searchers in state j to compete with searchers of state i depends on the occupation number (or size of the subpopulation) and the fitness, which is related to the potential of the occupied state. For the selection function, $g(x)$ two possibilities have been introduced in eq. (10). For the computer simulations discussed below, we prefer the tournament selection (k.o. selection) which in most cases is more effective than the difference selection. It is consistent with the rules:

(i) select a pair of searchers (say i and j) out of the $N\,(N-1)/2$ possibilities

(ii) compare the potentials U_i and U_j

(iii) transform the searcher with the higher value of U to the class of searchers with the lower U (which is related to the better fitness)

During the stochastic simulation of the search, the transition probabilities for all possible changes of the distribution $\mathbf{N}$ are calculated for every time step. The probability that a particular transition occurs during the next time step, is given by $w(\mathbf{N'}|\mathbf{N})/\sum_{\mathbf{N'}} w(\mathbf{N'}|\mathbf{N})$. The actual transition is chosen randomly, with respect to the different weights of the possible transition.

It can be proved that the stochastic approach based on the transition probabilities, eqs. (15), (16), in the average and for large numbers of N results in the equation for the mixed Boltzmann–Darwin strategy, eq. (9) and therefore has the same search properties.

3 Evaluation and Optimization of Road Networks

3.1 The Evaluation Function

In order to apply evolutinary strategies to the optimization of road networks, we first have to define a potential function (or a *fitness function*) which evaluates a given network.

Let us consider a set of nodes $p_1 ... p_N$ which shall be connected by straight lines representing the roads. The configuration space is defined by the number of all possible graphs g to connect the nodes, and is of the order $2^{N(N-1)/2}$. Each graph should be evaluated due to the following potential function:

$$U(g, \lambda) = (1 - \lambda) D(g) + \lambda C(g) \quad ; 0 \leq \lambda \leq 1 \tag{17}$$

Here, $D(g)$ represents the mean detour to reach different nodes on the existing network, whereas $C(g)$ represents the total costs for construction and maintainace of the network, which should be proportional to the total length of the links.

In order to minimize the potential $U(g)$, both terms should be minimized. The demand for a minimized detour between two points represents a *local constraint* to the network. Hence, a minimized mean detour between *every* two nodes is considered as an averaged local constraint, whereas the demand of a minimized total length of the network means a *global constraint*. For the considered example of a road network, the local constraints represent the interest of the users who don't like detours, and the global constraints are given by the interests of the government which has to pay for the road construction and therefore tries to minimize it.

The parameter λ is introduced to weight between the two contradicting demands. The case $\lambda \to 0$ leads to a potential function, which only minimizes the detour regardless of the costs of the network, and finally results in the *direct link system* (Fig. 1a). In this case, any two nodes are connected by the shortest possible link (equal to the length of the metric distance), the total length of the network, however, reaches a maximum.

In the opposite case, $\lambda \to 1$, only the costs of the network will be minimized, which finally leads to the *minimal link system* (Fig. 1b). This implies a very long connection between arbitrary nodes, which includes large detours, since the connection on the existing network exceeds the metric distance by far. Moreover, a minimal link system might be susceptible to breakdown, because every node has only one connection to the net. We note, that in the node system considered here, the minimal link system will be different from the known Steiner tree (Fig. 1c), since we assume that any link between nodes should be a straight line and no additional sub-nodes should be constructed to connect given nodes. To give an estimate about the difference, we note that the ratio of the length of the Steiner tree and the length of the minimal spanning tree is always $\geq \sqrt{3}/2$ [16, 39].

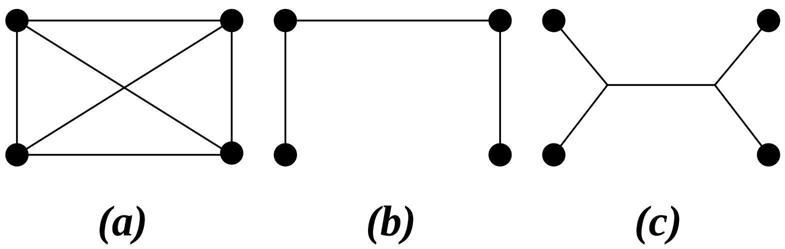

Figure 1: (a) direct link system, (b) minimal link system, (c) Steiner tree for a set of 4 nodes

For practical applications, both limiting cases, $\lambda = \{0, 1\}$, could be sufficient under certain circumstances. A minimal link system is appropriate e.g. if the connection distance can be passed with a very high speed. Then the time to reach a given node does not count, and a detour on the network could be easily accepted. On the other hand, a direct link system will be appropriate if the costs of establishing a network do not count compared to the traveling time which should be as short as possible. For road networks, however, λ should be different from 0 or 1, then it can be a measure for the *degree of frustration* of the problem, or a measure for accepting compromises.

In this paper, the direct link system will be used as a *reference state*, indicated by the symbol $\star$. The direct link system has the advantage, that the values both for the detour and the costs of the road network are known. The total length of the network is simply given by all direct (metric) distances, $l_{i,j}$, between the nodes and gets its maximum value $L^\star$:

$$L^\star = \frac{1}{2} \sum_{i,j=1}^{N} \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} = \frac{1}{2} \sum_{i,j=1}^{N} l_{i,j} \tag{18}$$

x_i, y_i are the coordinates of node i in a two-dimensional plane. For values of $0 \leq \lambda \leq 1$, the mean detour $D(g)$ is defined as follows:

$$D(g) = \frac{1}{2} \sum_{i,j=1}^{N} h_{i,j} - l_{i,j} \quad ; \quad D(g^\star) = 0 \tag{19}$$

where $h_{i,j}$ is the length of the *shortest route* which connects nodes i and j *on the existing graph.* Obviously, for a graph representing the direct link system, $h_{i,j} = l_{i,j}$, yields, hence the detour $D(g^\star)$ is zero.

The expression $D(g)$ can be normalized by the total length of the direct link system, which is a known constant for a given set of nodes,

$$d(g) = \frac{D(g)}{L^\star} = \frac{1}{2}\sum_{i,j=1}^{N} \frac{h_{i,j} - l_{i,j}}{L^\star} \tag{20}$$

Another possibility, proposed in [31, p. 82], reads

$$d(g) = \frac{1}{2}\sum_{i,j=1}^{N} \frac{h_{i,j} - l_{i,j}}{l_{i,j}} \tag{21}$$

Here, the detours related to shorter distances, are weighted higher than those for larger distances, which seems to be more reasonable for practical cases. In this paper, we restrict ourselves to eq. (20).

In order to specify the term representing the costs, we assume the costs simply proportional to the total length of the graph

$$C(g) = \frac{1}{2}\sum_{i,j=1}^{N} \vartheta_{ij} l_{i,j} \tag{22}$$

Here, ϑ_{ij} expresses the connectivity of the nodes: $\vartheta_{ij} = 1$, if there is a *direct* connection between nodes i and j, and $\vartheta_{ij} = 0$ else. After a normalization of $C(g)$ similar to eq. (20),

$$c(g) = \frac{C(g)}{L^\star} = \frac{1}{2}\sum_{i,j=1}^{N} \frac{\vartheta_{ij} l_{i,j}}{L^\star} \tag{23}$$

the potential function describing the road network reads finally:

$$u(g,\lambda) = \frac{U(g)}{2L^\star} = \frac{1}{2L^\star}\sum_{i,j=1}^{N} (1-\lambda)\,(h_{i,j} - l_{i,j}) + \lambda\,\vartheta_{ij} l_{ij} \tag{24}$$

For the reference state (direct link system), the values are $d(g^\star) = d_{min} = 0$ for the mean detour, $c(g^\star) = c_{max} = 1$ for the costs, and $u(g^\star) = \lambda$ for the potential. Based on eq. (24), a hypothetic network will be optimized with respect to the mean detour and the total length of the network.

3.2 Results of Computer Simulations

We have carried out our computer simulations of the evolutionary optimization of a road network for a system of 39 nodes. The coordinates of the nodes are listed in Table 1.

The initial state for the simulations is given by the graph presented in Fig. 2 for $t = 0$. Here, a very dense connection between the nodes exists. There is no need to start the simulations exactly with a direct link system, because for $\lambda \neq 0$ this is is not an optimized state of the problem. Basically, the simulations could start with an arbitrary graph. During every time step of the simulation, the graph is first mutated by adding, removing or exchanging one link between nodes, and then evaluated due to eq. (24).

Table 1: Coordinates of the nodes in the (x,y) plane, used for the simulations.

node	x	y
1	0.121667	0.388333
2	0.131667	0.291667
3	0.203333	0.438333
4	0.218333	0.233333
5	0.231667	0.078333
6	0.231667	0.331667
7	0.256667	0.163333
8	0.305000	0.370000
9	0.310000	0.463333
10	0.321667	0.086667
11	0.336667	0.253333
12	0.361667	0.160000
13	0.396667	0.478333
14	0.398333	0.325000
15	0.440000	0.260000
16	0.448333	0.063333
17	0.480000	0.145000
18	0.488333	0.415000
19	0.493333	0.503333
20	0.508333	0.171667

node	x	y
21	0.518333	0.340000
22	0.556667	0.246667
23	0.598333	0.415000
24	0.598333	0.536667
25	0.601667	0.121667
26	0.638333	0.160000
27	0.645000	0.463333
28	0.648333	0.320000
29	0.661667	0.190000
30	0.695000	0.550000
31	0.718333	0.120000
32	0.718333	0.356667
33	0.731667	0.485000
34	0.760000	0.393333
35	0.788333	0.293333
36	0.811667	0.221667
37	0.826667	0.463333
38	0.833333	0.360000
39	0.863333	0.273333

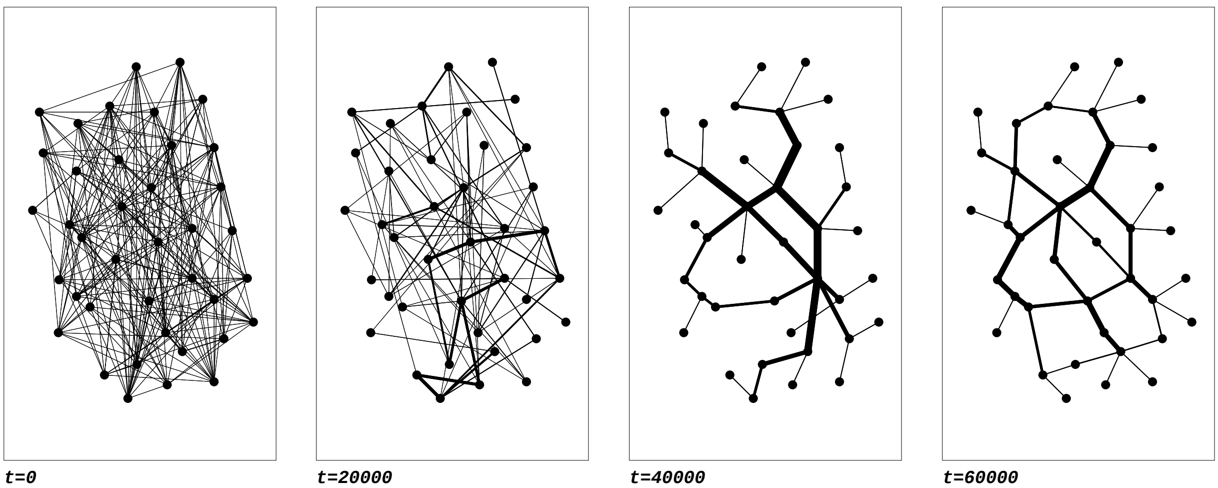

Figure 2: Optimization of a network of 39 nodes ($\lambda = 0.975$) The graph is shown after different time steps.

Fig. 2 shows a time series displaying different stages of the optimization process for $\lambda = 0.975$. The decrease of the temperature is due to $T(t+1) = T_0/(1+at)$, where $T_0 = 0.01$ is the initial temperature, and $a = 0.002$ is the cooling rate. The thickness of the lines indicates how much a given road is used for the shortest possible connection of any node to any other.

When we start the simulations with a dense graph, the optimization process occurs in two stages: During the first stage the network is strictly thinned out, whereas during the second and much longer stage the links between the different nodes are balanced with respect to the costs and the mean detour. How long the second stage takes compared to the first one, depends of course on the value of λ: For $\lambda \to 0$ the thin-out of the network does not play an important role for the optimization, therefore the first stage should be rather short.

The two stages of the optimization process are, for the given initial situation, a rather typical scenario, because for a dense graph the removal of links results in a larger "gain", whereas the exchange of links does not affect the value of the optimization function considerably. On the other hand, if already a thinned-out network exists, the strict removal of links eventually leads again to increasing values in the optimization function, which are rarely accepted, but the exchange of links may still result in improvements for the graph.

These two stages are investigated in more detail in Fig. 3. As we see in Fig. 3(a), the re-arrangements in the network during the first stage are characterized by rather large fluctuations in the evaluation function, but do not affect the mean detour considerably. The second stage starts with a steep decrease in the potential function, which is related to a remarkable increase of the mean detour. This increase is reduced only during a long period of time, indicating the painstaking process of balancing the contradictory requirements, costs and detour, to optimize the network.

Fig. 3(b) displays the ratio between costs and mean detour during the optimization process. With respect to the time, the curve starts in the lower right corner and ends in the lower left corner. Again, the first stage (which is related to the right part of the curve), is characterized by a steep decrease in the costs function and a moderate change in the detour function. The transition into the second stage is indicated by a large increase in the detour, and the crossover is marked by the maximum region of the curve. During the second stage, a slow decrease of both detour and costs occurs which eventually results in the quasistationary state of a balanced network.

With respect to practical applications, it is very remarkable that during the last stage a considerable decrease in the detour occurs, whereas the costs remain nearly constant. That means that the global constraints (e.g. the costs payed by the "government") are already satisfied, but regarding the local constraints (e.g. the interests of the users) further improvements can be achieved if the optimization proceeds long enough. As mentioned above, this should be rather typical for the final stage of the simulations, since the removal of links (which mostly affect the costs) is rarely accepted, but the exchange of links (which mostly affect the detour) still results in better solutions. In Sect. 4, we give an analytical approximation, whether more effort in the optimization may finally yield still better solutions for the graph, and estimate the computer time needed for additional improvements.

The optimized final state of course depends on the parameter λ which influences the density of the graph. Fig. 4 presents results for the optimized network for different values of λ. In agreement with the discussion in Sect. 3.1., for small λ we find networks, where most of the nodes are connected to all neighboring nodes, and for large λ networks which are close to the minimal link system.

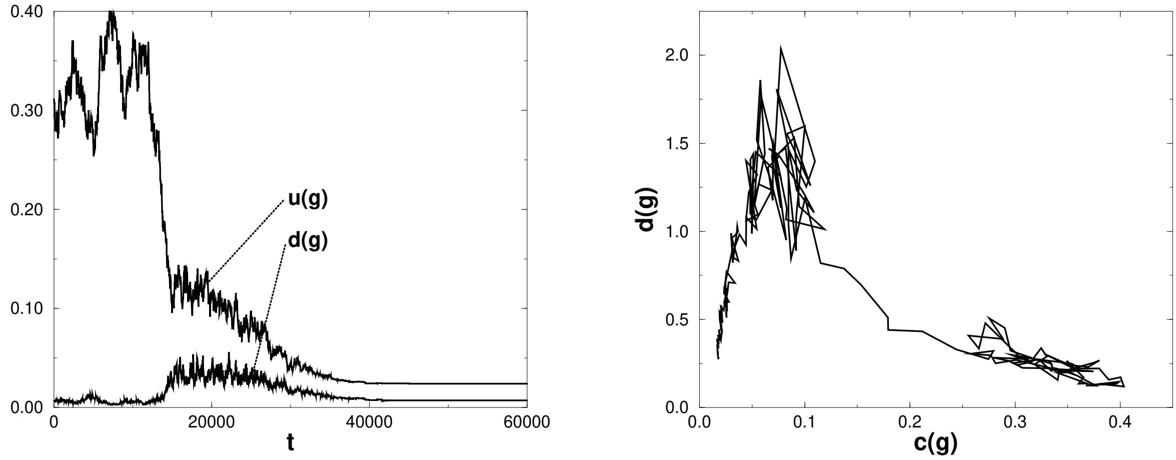

Figure 3: (a) Time dependence of the potential $u(g)$ and the mean detour $d(g)$, (b) mean detour $d(g)$ versus costs $c(g)$ during the optimization of the network. The data points are picked from a single run every 200 time steps. ($\lambda = 0.975$).

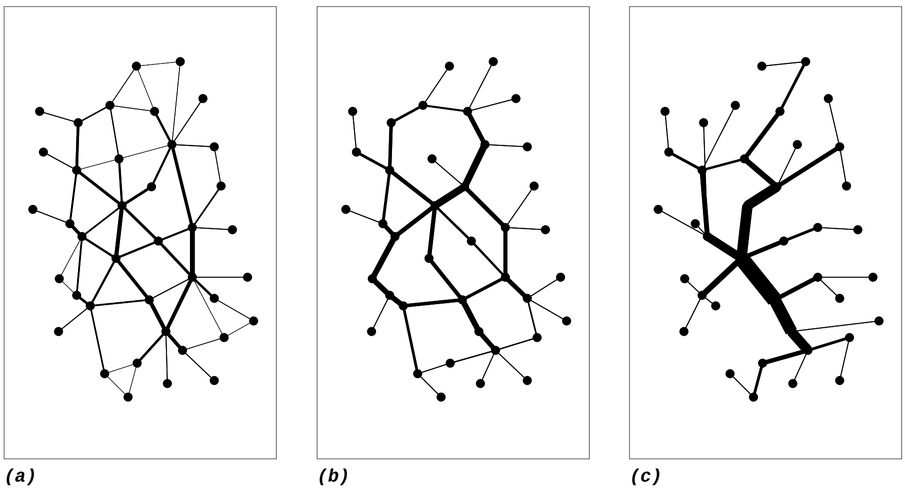

Figure 4: Optimized networks after t=60.000 simulation steps for different values of the parameter λ: (a)$\lambda = 0.900$, (b)$\lambda = 0.975$, (c)$\lambda = 0.990$

Finally, we would like to compare the results of the Boltzmann strategy and the mixed strategy which also includes Darwinian elements. As shown in the simulations in the previous section, the Boltzmann strategy finds suitable results in the asymptotic limit (about 60.000 simulation steps). However, the mixed Boltzmann-Darwin strategy already finds optimal graphs in a much shorter simulation time, as shown in Fig. 5 for 10.000 simulation steps (obtained for the same number of searchers in both simulations).

The optimization function relaxes very fast compared to the Boltzmann curve. With respect to the networks obtained after 10.000 time steps, we find already balanced graphs with the mixed optimization strategy, whereas the graphs obtained from the Boltzmann strategy still display failures in optimization. For larger values of the parameter λ, which means for networks closer to the minimal link system, this advantage becomes even more

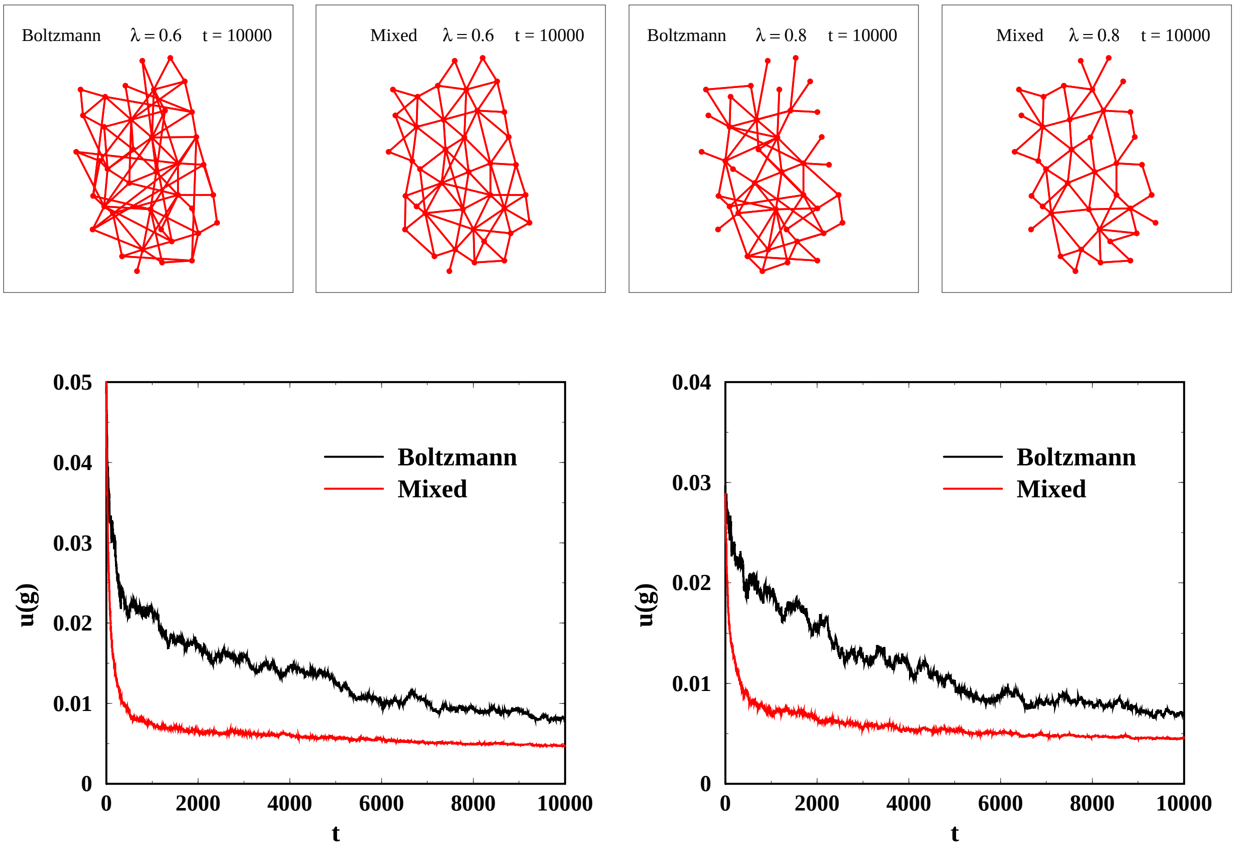

Figure 5: Comparison of Boltzmann and mixed strategies for network optimization. (left) $\lambda = 0.6$, (right) $\lambda = 0.8$. The networks presented are obtained after 10.000 simulation steps, the related potential is displayed below. The ensemble consists of 16 searchers for both strategies. For the selection process, a tournament selection is used, with a probability of 0.3 per searcher and time step.

remarkable, as shown for the comparison of $\lambda = 0.6$ and $\lambda = 0.8$ in Fig. 5.

Aussagen "uber Konvergenzgeschwindigkeit -¿ Eb., Asselmeyer ??

4 Asymptotic Results on the Optimization Landscape

4.1 Optimization Values in the Asymptotic Limit

In order to characterize the optimization landscape of road networks in more detail, we finally investigate some asymptotic features, obtained from the Boltzmann strategy. First, the depencence of the optimized state on the parameter λ is discussed. Whereas Fig. 4 shows some realizations of the network obtained for different λ, in Fig. 6 the potential values for the optimized network, u^{opt}, obtained asymptotically are plotted versus the parameter λ. As the plot shows, the potential minimum in the asymptotic regime can be well approximated by a 4th order power function of λ:

$$u^{opt}(\lambda) = \lambda \{0.2155 - 0.4949\,\lambda + 0.6380\,\lambda^2 - 0.3395\,\lambda^3\} \tag{25}$$

This allows a prediction of the asympotic value of $u(g)$, and can be used as an estimate whether a simulation has already reached the asymptotic stage. On the other hand, this relation can also be used to test different functions for the decrease of the temperature, $T(t)$, which finally have to yield the known asymptotic value.

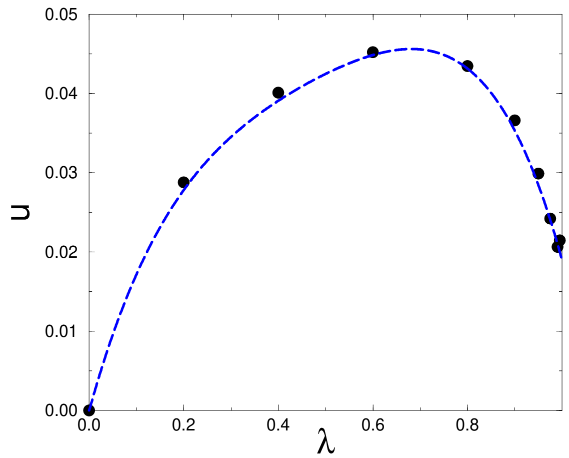

Figure 6: Dependence of the asymptotic potential minimum on the parameter λ. Dots mark the results of the simulations, averaged over 50 runs; the dashed line is given by eq. (25)

For the optimized network, eq. (25) does not completely determine the best possible cost and the best affordable detour. From eq. (17), eq. (25), a linear relation between the asymptotic values of $d(g)$ and $c(g)$ results:

$$d^{opt}(c^{opt}) = \frac{u^{opt}(\lambda)}{1-\lambda} - \frac{\lambda}{1-\lambda}\,c^{opt} \tag{26}$$

Eq. (26) characterizes the *range of compromises*, which can be found asymptotically for a fixed value of λ. For $\lambda < 1$, c^{opt} has to be larger than the costs for the minimal link system, c_{min}, which defines the lower boundary for $c(g)$, and less than $c(g^\star) = c_{max} = 1$, which is the upper boundary, obtained for the direct link system. For a medium range of $0 \leq \lambda \leq 1$ and an appropriate large number of nodes, there should be many sets of c^{opt}, d^{opt}, which fulfill eq. (26), as also indicated by Fig. 7.

This means that an optimized road network for a given λ allows different realizations regarding costs and mean detours. Within the range of possible compromises defined by eq. (26), we obtain different graphs to connect the nodes. Here, those sets of c^{opt}, d^{opt} which are related to lower costs, lead to graphs with dominating trunk routes (such as in Fig. 4(c)), whereas sets related to smaller mean detours, lead to graphs with ring routes. This interesting feature will be investigated by subsequent computer simulations.

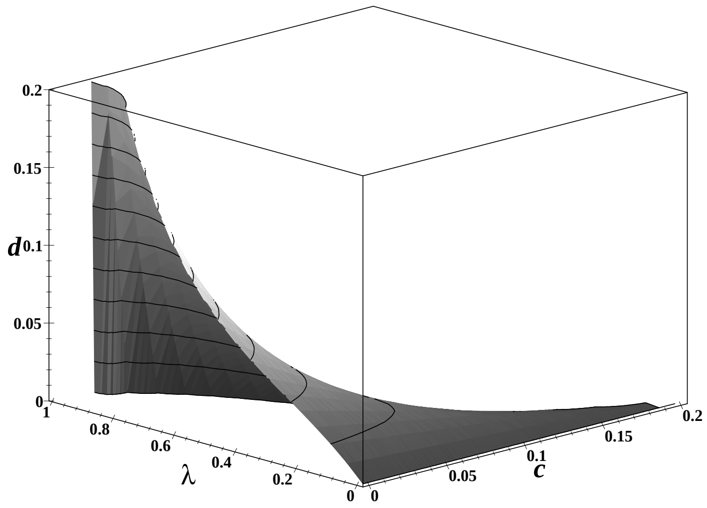

Figure 7: Range of compromises (eq. 26) between detour, d^{opt}, and costs, c^{opt}, for the optimized network, dependent on λ.

4.2 Density of States in the Asymptotic Limit

From the Boltzmann distribution reached in the asymptotic limit, $p_i^0 \sim \exp(-U_i/T)$, eq. (5), we obtain the probability $P^0(U)$ to find a certain value of U in the intervall dU:

$$P^0(U)\, dU = n(U)\, \exp(-U/T)\, dU \tag{27}$$

The function $n(U)$ is called the degeneracy function or *density of states*. It contains important information about the structure of the opimization landscape [29], because it tells us how sparsely states of a given quality are distributed. The density of states, however, measures only the number and the order of possible solutions, but not the geometry and topology of the search space itself.

Usually, the best available optimization states are found in the tail of the distribution $n(U)$, corresponding to a very small density of state. Thus, in the limit $n(U) \to 0$, the best possible potential value of a given problem can be estimated. Formally, the density of states may be found from the equilibrium solution:

$$n(U) = P^0(U)\, \exp(U/T) \tag{28}$$

After determining the equilibrium probability distribution $P^0(U)$ for the optimization of the road network by means of a Boltzmann strategy, we find the density of states, eq. (28), presented in Fig. 8.

We want to note that the density of states provides useful information for optimization problems which can be characterized by a monotonous function $n(U)$, with $n(U) \to 0$ both in the limit of $U \to 0$ and $U \to U_{max}$. This does not include problems which deal with a singular solution, such as the "needle-in-a-haystack" problem.

From the density of states, information about the *effort* of optimization for a given problem can be derived. Optimization problems characterized by a very steep decay in $n(U)$ for the good values of U, in general do not need too much effort in simulations, since the

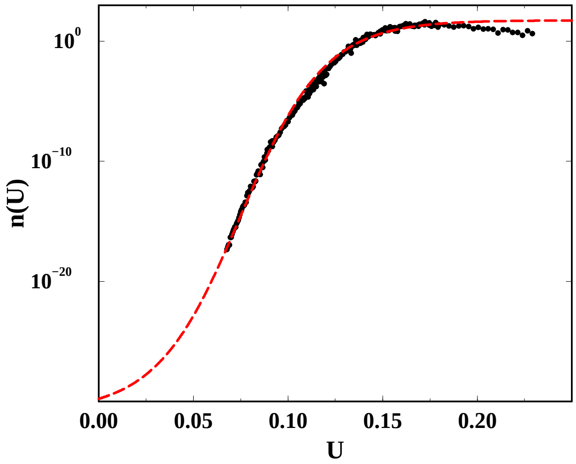

Figure 8: Density of states $n(U)$ in the asymptotic limit (t=100.000 time steps). The probability distribution $P^0(U)$ was obtained from a simulation of 1.000 graphs, carried out for different temperatures: T=0.001, 0.002, 0.005, 0.1 (λ=0.950). Dots mark the results of the simulations, the dashed line results from eq. (29).

number of good solutions is very limited. Once a good solution is found, one can almost be sure that more effort does not necessarily result in better optimization values.

Most interesting, however, are optimization problems which display long tails in the density of state $n(U)$ in the limit $U \to 0$. Here, the number of better solutions is figuratively "non-exhaustable", which means that more effort in optimization always has a good chance to yield better solutions. As Fig. 7 indicates, the network problem discussed here, belongs to this class of problems. For the considered network with $\lambda = 0.950$, we find that the frequency of the better solutions can be estimated by

$$\begin{gathered} n(U) = c_0 \exp\{c_1 \tanh[c_2(U - c_3)]\} \\ c_0 = 2.8306 \times 10^{-15}\ ; c_1 = 37.4982\ ; c_2 = 22.6000\ ; c_3 = 0.0750 \end{gathered} \tag{29}$$

which, in the limit $U \to 0$, can be approximated by

$$n(U) \sim \exp\{-b + aU\} \quad \text{with} \;\; a = c_1 c_2\ ;\ b = c_1 c_2 c_3 \tag{30}$$

The non-Gaussian distribution of $n(U)$ is a notable difference to other optimization problems, which yield either a Gaussian distribution for $n(U)$ [29], or display an very steep decay, such as the LABS–problem [6]. Compared to these cases, the frustrated network problem is characterized by a rather weak decay in $n(U)$. The best values we have obtained so far, namely $U \approx 0.07$, are not yet in the region of saturation, which indicates a good chance to find better solutions (e.g. $U \approx 0.03 - 0.05$) in the long run.

Let us estimate the effort needed to improve a given solution U_0 by the amount ΔU, in order to obtain $U_0 - \Delta U$. Assuming the time to find the better solution proportional to the reciprocal density of states,

$$\frac{\tau}{\tau_0} \simeq \frac{n(U_0)}{n(U_0 - \Delta U)} \tag{31}$$

we obtain with eq. (30) for the network problem

$$\frac{\tau}{\tau_0} \simeq \exp\{a\Delta U\} \qquad (32)$$

This gives a useful estimate for the computer time (or effort, respectively) needed to improve a given optimal solution by a certain amount, which depends on only one characteristic parameter, a.

5 Conclusions

The optimization of road networks has to consider both the connection distance (detour) between different nodes and the total length (costs) of the network. Since both requirements cannot be completely satisfied at the same time, the optimization problem belongs to the class of frustrated problems, where numerous evenly matched solutions exist. In this paper, we have applied evolutionary strategies to the optimization of road networks which include both thermodynamic and biological elements (mixed strategies of simulated annealing, ensemble search, mutation, selection and recombination).

As the computer simulations have shown, these strategies provide a suitable tool for finding optimized solutions. The consideration of biological elements in the strategies allows to reduce the number of time steps in the simulation and enhance the performance of the optimization, compared to Boltzmann–like strategies.

In order to evaluate the road network, we have introduced a potential function, which consists of two parts, related to the mean detour to reach any given node (averaged local constraint), and to the costs proportional to the length of the network (global constraint). A parameter λ, which is a measure of the frustration of the problem, can weight between these two parts.

We want to note again, that this optimization function does not consider the requirements which result from a use of the network, such as traffic density or flow capacity. The simulation results, displaying the graphs for the optimized road networks, however indicate the strength of the possible use of the different links, obtained from a connection between any two nodes.

Further, the evaluation function does not consider any requirements related to the use of the area covered by the road network. In cities or urban areas, the optimization of road networks usually has to take into account, that many subareas are occupied or preserved, and therefore cannot be devided by an "optimized" road. Thus, for applications of the model to cities, the evaluation function should include a third term expressing the optimization of sub-areas as well. This should be discussed in a forthcoming paper. So far, our model may be applied to road networks which link different cities at certain distances. In this range, the terms of a minimal and a direct link system and the compromise between these limit cases make sense for geographic applications.

We want to summarize some results obtained from the simulation of the road network, which can be generalized to other types of networks obeying the same evaluation function:

(i) Starting with a direct link system, the optimization of networks occurs on two different time scales: (a) thin-out of the network (short time scale), (b) balancing of detour compared to costs (long time scale). Both time scales can be well separated in the curves, displaying the potential, the mean detour and the costs.

(ii) In the asymptotic limit, the potential (fitness) of the optimized network can be described by a power function in terms of the parameter λ. This relation defines a range of possible compromises between the mean connection distance (detour) and the total lenght (costs) for the optimized network.

(iii) The density of states measures how sparsely the best available optimized solutions can be reached, and therefore allows an estimation, whether more effort in the optimization process will yield better results. For the network optimization, we found a weak, non-Gaussian distribution in the range of the best potential values, indicating a good chance for finding better solutions in the long run.

(iv) The existence of long tails of the density of states distribution in the range of better potential values corresponds to the fact, that during the final stage of the simulation global constraints are already satisfied, but further improvements can be made to match the local constraints. Hence, the search for more comfort in the solutions is worthwhile.

(v) From the density of states, which can be approximated by a simple exponential function, an estimate of the effort can be derived, needed to improve an optimized solution by a certain value. For the network problem, this effort is characterized by only one parameter.

Finally, we want to note that the network problem discussed in this paper, is a very graphic example for elucidating frustrated optimization problems; it therefore may serve as a toy model for testing different approaches.

Acknowledgment

This work has been supported by the Deutsche Forschungsgemeinschaft via SFB 230 “Natural Constructions” (Stuttgart, Germany).

References

[1] ANDRESEN, B., HOFFMANN, K.H., MOSEGAARD, K., NULTON, J., PEDERSEN, J. M., SALAMON, P. (1988): On lumped models for thermodynamic properties of simulated annealing problems, J. Phys. (France) **49**, 1485.

[2] APPLEBY, S. (1995): Estimating the cost of a telecommunications network using the fractal structure of the human population distribution, IEEE Proc.-Communic. **142**, 172-178.

[3] ASSELMEYER, T., EBELING, W. (1997): Mixing of Thermodynamic and Biological Strategies in Optimization, in: F. Schweitzer (ed.): *Self-Organization of Complex Structures: From Individual to Collective Dynamics*, London: Gordon and Breach, pp. 153-163.

[4] BÄCK, T. (1994): Selective Pressure in Evolutionary Algorithms: A Characterization of Selection Mechanisms, in: R.K. Belew, L.B. Booker (eds.): Proc. 1st IEEE Conf. on Evolutionary Computation, Piscataway, NJ: IEEE Press, pp. 57-62.

[5] BÄCK, T. (1995): Generalized Convergence Models for Tournament- and (5 ,l)-Selection, in: L. Eshelman (ed.): Proc. 6th Intern. Conf. on Genetic Algorithms, San Francisco: Morgan Kaufmann, pp. 2-8.

[6] BERNASCONI, J. (1987): Low autocorrelation binary sequences: statistical mechanics and configuration space analysis, J. Physique **48**, 559.

[7] BOSENIUK, T., EBELING, W., ENGEL, A. (1987): Boltzmann and Darwin Strategies in Complex Optimization, Physics Letters **125**, 307-310.

[8] CARRAWAY, R.L., MORIN, T.L., MOSKOWITZ, H. (1990): Generalized Dynamic Programming for Multicriteria Optimization, Europ. J. Operational Res. **44**, 95-104.

[9] EBELING, W. (1990): Applications of Evolutionary Stragegies, Syst. Anal. Model. Simul. **7**, 3–16.

[10] EBELING, W. (1994): Self–Organization, Valuation and Optimization, in: R.K. Mishra, D. Maaß, E. Zwierlein (eds): *On Self–Organization*, Springer Series in Synergetics, vol. 61, Berlin: Springer, pp. 185-196.

[11] EBELING, W., ENGEL, A. (1986): Models of Evolutionary Systems and Their Application to Optimization Problems, Syst. Anal. Model. Simul. **3**, 377-385.

[12] EBELING, W., ROSÉ, H., SCHUCHHARDT, J. (1994): Evolutionary Strategies for Solving Frustrated Problems, in: R.K. Belew, L.B. Booker (eds.): Proc. 1st IEEE Conf. on Evolutionary Computation, Piscataway, NJ: IEEE Press, pp. 79-81.

[13] FEISTEL, R., EBELING, W. (1982): Models of Darwin Proceses and Evolutionary Principles, BioSystems **15**, 291.

[14] FEISTEL, R.; EBELING, W. (1989): *Evolution of Complex Systems*, Dordrecht: Kluwer.

[15] FOGEL, D.B. (1995): *Evolutionary Computation – Towards a new Philosophy of Machine Intelligence*, Piscataway, NJ: IEEE Press.

[16] GILBERT, E.N.; POLLACK, H.O. (1968): Steiner Minimal Trees, SIAM J. App. Math. **16**, 1-29.

[17] GOLDBERG, D.E. (1989): *Genetic Algorithms in Search, Optimization and Machine Learning*, Reading: Addison-Wesley.

[18] HOLLAND, J.H. (1975): *Adaptation in Natural and Artificial Sytstems*, Ann Arbor: University of Michigan Press.

[19] HOPFIELD, J.J.; TANK, D.W. (1985): Computing RC-Networks, Biol. Cybernetics **52**, 141.

[20] Johnson, D.S.; Lenstra, J.K.; Rinooy Kan, A.H.G. (1978): The Complexity of the Network Design Problem, Networks **8**, 279–285.

[21] Kirkpatrick, S.; Gelatt, C.D.; Vecchi, M.P. (1983): Optimization by Simulated Annealing, Science **220**, 671.

[22] Metropolis, N.; Rosenbluth, A.; Rosenbluth, M.; Teller, A.; Teller, E. (1953): J. Chem. Phys. **21**, 1087.

[23] Misra, K.B. (1991): Multicriteria Redundancy Optimization Using an Efficient Search Procedure, Int. J. Systems Sci. **22**, 2171-2183.

[24] Mühlenbein, H. (1989): Parallel genetic algorithm, population dynamics and combinatorial optimization, in: H. Schaffer (ed.): Proc. 3rd Int. Conf. on Genetic Algorithms, San Francisco: Morgan Kaufmann, pp. 416-421.

[25] Mühlenbein, H.; Schlierkamp–Voosen, D. (1994): The science of breeding and its application to the breeder genetic alogorithm, Evolutionary Computation **1**, 335-360.

[26] Nulton, J.D.; Salamon, P. (1988): Statistical Mechanics of Combinatorial Optimization, Phys. Rev. **A 37**, 1351.

[27] Osyczka, A., Kundu, S. (1995): A New Method to Solve Generalized Multicriteria Optimization Problems Using the Simple Genetic Algorithm, Structural Optimization **10**, 94-99.

[28] Rechenberg, I. (1994): *Evolutionsstrategie '94*, Stuttgart: Frommann-Holzboog.

[29] Rosé, H., Ebeling, W.; Asselmeyer, T. (1996): The Density of States – A Measure of the Difficulty of Optimization Problems, in: H.-M. Voigt, W. Ebeling, H.-P. Schwefel, I. Rechenberg (eds): *Parallel Problem Solving from Nature – PPSN IV*, Berlin: Springer, pp. 208-217.

[30] Salamon, P., Nulton, J., Robinson, J., Pedersen, J. M., Ruppeiner, G., Liao, L. (1988): Simulated annealing with constant thermodynamic speed, Comput. Phys. Comm. **49**, 423.

[31] Schaur, E. (1991): *Non-Planned Settlements: Characteristic Features - Path Systems, Surface Subdivision*, IL 39, Universtität Stuttgart.

[32] Schwefel, H.-P. (1981): *Numerical Optimization of Computer Models*, New York: Wiley.

[33] Schweitzer, F. (1997): Active Brownian Particles: Artificial Agents in Physics, in: L. Schimansky-Geier, T. Pöschel (eds.): *Lectures on Stochastic Dynamics*, Berlin: Springer, pp. 339-352.

[34] Schweitzer, F., Ebeling, W., Rosé, H., Weiss, O. (1996): Network Optimization Using Evolutionary Strategies, in: H.-M. Voigt, W. Ebeling, H.-P. Schwefel, I. Rechenberg (eds): *Parallel Problem Solving from Nature – PPSN IV*, Berlin: Springer, pp. 940-949.

[35] SIBIANI, P.; PEDERSEN, K.M.; HOFFMANN, K.H.; SALAMON, P. (1990): Monte Carlo Dynamics of Optimization: A Scaling Description, Phys. Rev. **A 42**, 7080.

[36] STEIGLITZ, K.; WEINER, P.; KLEITMAN, D.J. (1969): The Design of Minimum-cost Servivable Networks, IEEE Trans. Circuit Theory **CT-16/4**, 455–460.

[37] STEUER, R.E. (1989): *Multiple Criteria Optimization: Theory, Computation, and Application*, Malabar, FL: Robert E. Krieger Publ..

[38] WHITE, D.J. (1982): The Set of Efficient Solutions for Multiple Objective Shortest Path Problems, Computers and Operations Research **9/2**, 101-107.

[39] WINTER, P.: (1987): Steiner Problems in Networks: A Survey, Networks **17**, 129-167.

[40] YU, P. L. (1985): *Multiple-Criteria Decison Making*, New York: Plenum Press.