Fig. 2 Concentration of Se IV (∇) and total Se (+) as a function of pH. Where pH values were unavailable they have been interpolated from the alkalinity of the samples and its relationship to pH observed in other samples of the same region. These are designated ($\triangle$) Se IV and ($\times$) total Se.

for limestones. The molar selenium/sulphate ratio of 7.5×10^{-6} is also hard to reconcile with marine evaporites in which a ratio similar to that of surface sea water (1.8×10^{-8}) would be expected. The occurrence of the highest values in samples collected before the rivers cross the Llanos precludes the reworking of fluvial or lacustrine sediments as a source. This conclusion is reinforced by data from the Capanaparo and Cinaruco which, as the only left bank rivers whose drainage is entirely within the Llanos, are observed to contain relatively low levels of selenium. Weathering of Upper Cretaceous calcareous black shales would appear to be the most likely explanation of the elevated levels of selenium in this region. Black shales in general are known to contain high levels of selenium[8] probably in a reduced form (0 or $-$II). Data from the Julia Creek[9], Green river, and Bear Paw shales (K. L. Von Damm, personal communication) show pyritic Se/S levels in the range 10^{-3} to 10^{-5}. Unfortunately no other measured tracer in the Orinoco data set is able to quantify the shale weathering signal.

The relationship between oxidation states of selenium and pH in this data set (Fig. 2) imply that, under the conditions prevalent in the drainage, mobilization of reduced Se is proceeding at pH above 7; this is in broad agreement with the work of Howard[10]. The technique used will include any $-$II and 0 oxidation state selenium in with the $+$VI state, but it seems likely that the majority of the fraction, that is the difference between total selenium and selenite, is composed of selenate and not dissolved organic selenium. Support for this argument comes from the relatively low total selenium observed in the black, low pH, organic-rich rivers of the Shield. More significantly though, organic selenium levels are only some 10-15% of the total even in the highly contaminated agricultural drainage waters which feed Kesterson reservoir in California[11]. The occurrence of selenate as the dominant species in the Orinoco samples would also imply that oxidation potentials in the Se VI stability field[10] are reached in natural weathering systems. When this is coupled with shales that contain high levels of carbonates, such that weathering pHs above 7 are achieved, significant mobilization of selenium is observed.

The region of high fluvial selenium concentrations appears to coincide with an area of Venezuela reported to produce vegetation with potentially toxic levels of the element[12,13]. It is well known that shales frequently weather to soils in which the bio-availability of the element is such that seleniferous vegetation is produced[8]. The fact that the dissolved selenium levels in rivers and groundwater appear to reflect this bio-availability suggests that a relatively simple river survey of a region could be a useful precursor in identifying areas prone to such problems.

Total selenium in the Amazon (645 pM), the Chang Jiang

(2,953 and 2,802 pM), and the Hudson (1,081 pM) fall within the range observed for the Orinoco. Selenium IV values were 155 (Amazon), 490 and $<$170 (Chiang Jiang) and $<$170 pM (Hudson). Using the Amazon concentration of 645 pM, the annual riverine flux of total selenium to the oceans is 2.3×10^7 moles. This would imply an oceanic residence time of some 150,000 yr. This value, although some seven times higher than that estimated by Goldberg et al.[14] must be considered somewhat unconstrained as it is based only on river data with no provision made for hydrothermal or volcanic inputs or recycled marine emissions which may be important.

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An analogue approach to the travelling salesman problem using an elastic net method

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The travelling salesman problem[1] is a classical problem in the field of combinatorial optimization, concerned with efficient methods for maximizing or minimizing a function of many independent variables. Given the positions of N cities, which in the simplest case lie in the plane, what is the shortest closed tour in which each city can be visited once? We describe how a parallel analogue algorithm, derived from a formal model[2-3] for the establishment of topographically ordered projections in the brain[4-10], can be applied to the travelling salesman problem[1,11,12]. Using an iterative procedure, a circular closed path is gradually elongated non-uniformly until it eventually passes sufficiently near to all the cities to define a tour. This produces shorter tour lengths than another recent parallel analogue algorithm[13], scales well with the size of the problem, and is naturally extendable to a large class of optimization problems involving topographic mappings between geometrical structures[14].

Although easy to state, the travelling salesman problem (TSP)

Fig. 1 Example of the progress of the elastic net method for 100 cities randomly distributed in the unit square. *a*, The initial path. To break symmetry, this was set up to be a ring of radius 0.1 about the centroid of the cities. A starting configuration with each point on the path placed at a small, randomly chosen distance away from the centroid (see ref. 13) was found to be adequate as long as a large number of iterations at a high value of K were allowed. *b*, *c* and *d*, Paths generated as the value of K was gradually lowered. *e*, The tour of length 7.78 deduced from the final configuration shown in *d*. *f*, The shortest tour so far found by us by any method (simulated annealing[15,16] with eight million trials; see Table 1 for details). This tour had a length of 7.70. The parameter values used for the computations described in this paper which used the elastic net method were: $M = 2.5\ N$, $\alpha = 0.2$, $\beta = 2.0$; the initial value of K was 0.2, and was reduced by 1% every n iterations to a final value in the range 0.01–0.02. In the calculation shown here, K was reduced to 0.01 in 7,000 iterations by

taking $n = 25$. The rate at which K can be reduced is limited by situations such as that shown by the arrow in *c*, where the system must be sufficiently relaxed to prevent the occurrence of crossovers, which would increase the tour length. The function ϕ had the form $\phi(d, K) = \exp(-d^2/2K^2)$. In this case an energy function E can be defined as $E = -\alpha K \sum_i \ln \sum_j \phi(|\mathbf{x}_i - \mathbf{y}_j|, K) + \beta \sum_j |\mathbf{y}_{j+1} - \mathbf{y}_j|^2$. This has the property that $\Delta \mathbf{y}_j = -K\ \partial E/\partial \mathbf{y}_j$, which means that any change in $\mathbf{y}_j$ according to equation (1) results in a reduction in the value of E and, because E is bounded below, local minima of E will eventually be reached. In the limit where K tends to zero, for E to remain bounded the limiting path must pass through all the cities (for every i there must be a j such that $|\mathbf{x}_i - \mathbf{y}_j|$ tends to zero). As M gets large, the second term in the expression for E is then minimized by spacing the M path points equally around the path at a distance D/M apart, where D is the path length. This term then takes the value D^2/M, which is minimized by minimizing the tour length D.
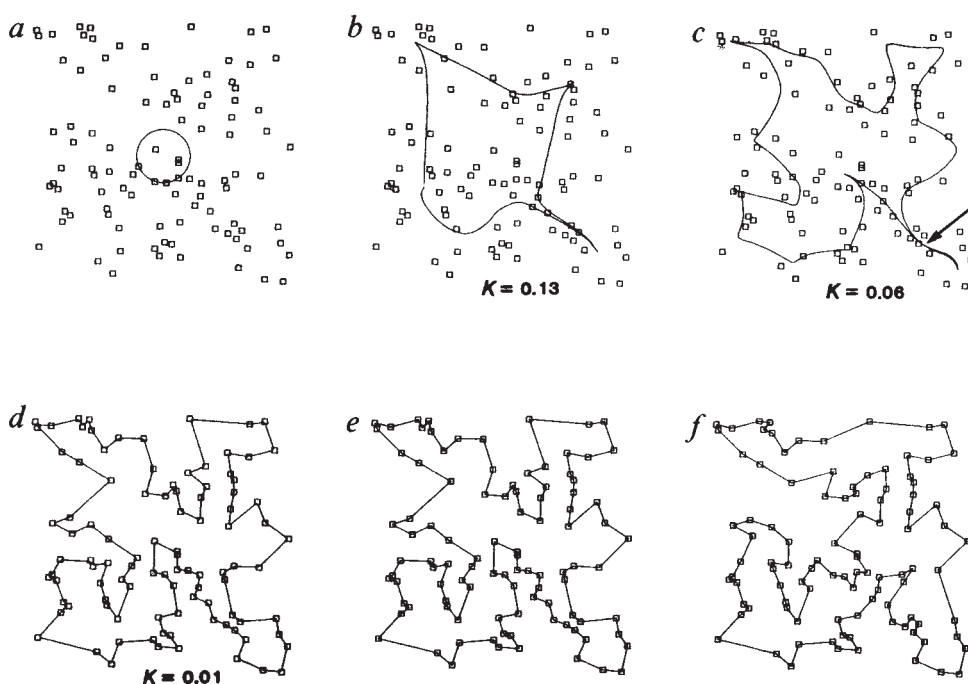
is hard to solve; the number of possible tours increases exponentially with the number of cities. It is representative of the an important class of optimization problems[1,12], called NP-complete[11], which are all interconvertible, but the computing effort needed to solve them increases faster than any power of N. Because perfect solutions are unattainable for problems of any appreciable size, there has been interest in heuristic methods that find near-optimal solutions in a reasonable time[1].

Hopfield and Tank[13] have recently discussed how problems such as the TSP can be represented in the dynamical behaviour of a network of simple model neurons. The activity of the network evolves into a stable configuration which represents a good solution to the problem. This procedure was shown to be equivalent to gradient descent of an energy function which contains the tour length as a major term. For the 30-city problem discussed, the best tour found was only 19% longer than the shortest known tour. A related analogue algorithm (G. Tesauro, personal communication) obtains shorter tours for 30 cities, but does not, in general, produce valid solutions for larger problems.

Our approach is more geometrical. A tour can be viewed as a mapping from a circle to the plane so that each city in the plane is mapped to by some point on the circle. We consider mappings from a circular path of points to the plane in which neighbouring points on the circle are mapped as close as possible on the plane. This is a special case of the general problem of best preserving neighbourhood relationships when mapping between different geometrical spaces. Our algorithm was developed from the tea-trade model[2,3] for the establishment of topographically ordered, neighbour-preserving projections between neural structures with matching geometries[4-10], such as the projection of the vertebrate retina onto the optic tectum[5,6].

The algorithm is a procedure for the successive recalculation of the positions of a number of points in the plane in which the

cities lie. The points describe a closed path which is initially a small circle centred on the centre of the distribution of cities and is gradually elongated non-uniformly to pass eventually near all the cities and thus define a tour around them (Fig. 1). Each point on the path moves under the influence of two types of force. The first moves it towards those cities to which it is nearest; the second pulls it towards its neighbours on the path, acting to minimize the total path length. By this means, each city becomes associated with a particular section of the path. The tightness of the association is determined by how the force contributed from a city depends on distance, and the nature of this dependence changes as the algorithm progresses. Initially all cities have a roughly equal influence on each point on the path. Subsequently, longer distances become less favoured, and each city gradually becomes more specific for the points on the path closest to it. This gradual increase of specificity (informally equivalent to the lowering of the 'temperature' in optimal simulated annealing[15,16]) is controlled by a reduction of the length parameter K. We call this algorithm the elastic net method because of the way in which the initial path is gradually deformed to produce the final tour.

Let the coordinates of the position of a typical city i be denoted by the vector $\mathbf{x}_i$ and those of a typical point j on the path by $\mathbf{y}_j$. Then the rule for the change $\Delta \mathbf{y}_j$ in the coordinates $\mathbf{y}_j$ of point j at each iteration is

$$\Delta \mathbf{y}_j = \alpha \sum_i w_{ij}(\mathbf{x}_i - \mathbf{y}_j) + \beta K(\mathbf{y}_{j+1} - 2\mathbf{y}_j + \mathbf{y}_{j-1}) \tag{1}$$

where the constants α and β determine the relative strengths of the forces from the cities and the forces from its neighbours on the path. The coefficient w_{ij} specifies the influence of city i on path point j, and can be thought of as the strength of the connection between i and j. This is a function of the distance $|\mathbf{x}_i - \mathbf{y}_j|$ between i and j and of the length parameter K. It is

Table 1 Tour lengths obtained from comparative studies on five sets of 50 randomly positioned cities

City set	Elastic net method*	Simulated annealing†	All algorithms‡
1	5.98	5.88	5.84, 3
2	6.03	6.01	5.99, 3
3	5.74 [5.70]	5.65	5.57, 6
4	5.90 [5.86]	5.81	5.70, 4
5	6.49	6.33	6.17, 1

* For each set of cities, the algorithm was run for 1,250 iterations, with $n = 5$. For sets 3 and 4, a slower schedule for reducing the value of K resulted in shorter tours, shown in brackets.

† At each trial, three cuts in the tour were made at random and rearrangements which produced shorter tours were accepted; in the absence of a shorter tour, the rearrangement which lengthened the tour least was accepted with probability $\exp(-\Delta D/T)$[15,16], where ΔD is the increase in tour length and the parameter T corresponds to the parameter K of the elastic net method. T was reduced from 0.5 to 0.003 (5×10^5 steps, $n = 1,000$), which took 30% more computer time than the elastic net method. Each figure is the average of 5 simulations.

‡ Tour optimization was also attempted by systematic trial of all possible three-cut rearrangements and accepting only those rearrangements which shortened the tour, the procedure being repeated from many different randomly generated initial configurations. This strategy has been shown to be efficient in the use of time for this size of problem[29]. Each pair of figures in the final column represents respectively the shortest tour obtained from any of these methods and the number of times this tour was obtained.

normalized so that the total influence of each city is equal.

$$w_{ij} = \phi(|\mathbf{x}_i - \mathbf{y}_j|, K)/\sum_k \phi(|\mathbf{x}_i - \mathbf{y}_k|, K) \qquad (2)$$

where $\phi(d, K)$ is a positive, bounded decreasing function of d that approaches zero for $d > K$.

Taking $\phi(d, K)$ as the gaussian function $\exp(-d^2/2K^2)$, an energy function can be defined which has the property that successive changes in the path calculated according to equation (1) lead to a stable state which represents a local minimum of energy (see Fig. 1 legend). In the limit where K tends to zero and the number of points M on the path tends to infinity, the global minima of the energy function are optimal solutions of the TSP. This suggests that even when these limits are not achieved, good tours will be obtained.

The elastic net method was applied to the distribution of 30 cities used by Hopfield and Tank[13]. It generated the shortest known tour[17] in 1,000 iterations; Hopfield and Tank's shortest tour was 19% longer. A comparison of our algorithm with more conventional algorithms is shown in Fig. 1 and Table 1. The length of the best tour around 100 cities distributed at random in the unit square was 7.78, which is within 1% of the best tour length (7.70) we have found by any method (Fig. 1). When applied to 5 sets of 50 randomly distributed cities, the best tour length was within $3.0 \pm 1.4\%$ (mean $\pm$ s.d.) of the best tour length we have found by any method, and within $1.5 \pm 0.7\%$ of the average length we found by simulated annealing[15,16] in approximately the same amount of computing time (Table 1).

The elastic net method operates by integrating a set of simultaneous first-order difference equations, an essentially parallel operation, and it therefore naturally lends itself to implementation in parallel hardware. Even when implemented on conventional computers, its complexity scales well with the number of cities N. It produces shorter tours than the parallel algorithm of Hopfield and Tank[13] and it is not as sensitive to the choice of parameter values. The main computational cost is in calculating the distances at each iteration and is therefore proportional to the product of the number of iterations required with the number of significant connections (connections with near-zero strength can be ignored). The number of connections is of the order N^2 (given that the number of points on the path is of

order N), but this could be reduced by starting with a small number of path points and gradually interpolating additional points in the path to keep a constant average number of significant connections from each city. The number of connections required by the algorithm of Hopfield and Tank[13] is of the order of N^3, although these are fixed in value. The number of iterations required seems to increase more slowly than a linear function of N, and this number could probably be significantly decreased by optimizing the schedule for decreasing K. Because an energy function can be defined, a more sophisticated approach to minimization[18] might also reduce the computational time required.

Our algorithm is fundamentally geometrical. It can be extended to the more general TSP with cities in any euclidean space, but not to the case where an arbitrary matrix of distances is given. However, it is applicable to a wide range of geometrical optimization problems. For instance, we can alter the dimension and topology of either space (by, for example, replacing the ring by any other graph), and also remove the condition that points in the 'ring' space are to be evenly spaced (by varying the strength of the force between neighbours). The algorithm therefore provides a general method for matching a set of arbitrarily connected points to a second set of points located in a geometrical space of any dimensionality. It may thus be applicable to a variety of matching and representational problems[1,16,19], such as those that arise in early visual processing[20,21].

Our interest in this problem originated in an interest in mechanisms[2,3] for the establishment of ordered neural projections between structures of similar geometry. There are other neural projections which involve topographical mappings between spaces of different dimensionality[22-24], for which several formal models have been proposed[25-28]. The elastic-net approach suggests a new way of looking at these phenomena and we are currently investigating how simple parallel algorithms of the type discussed here could give rise to the projection patterns observed.

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