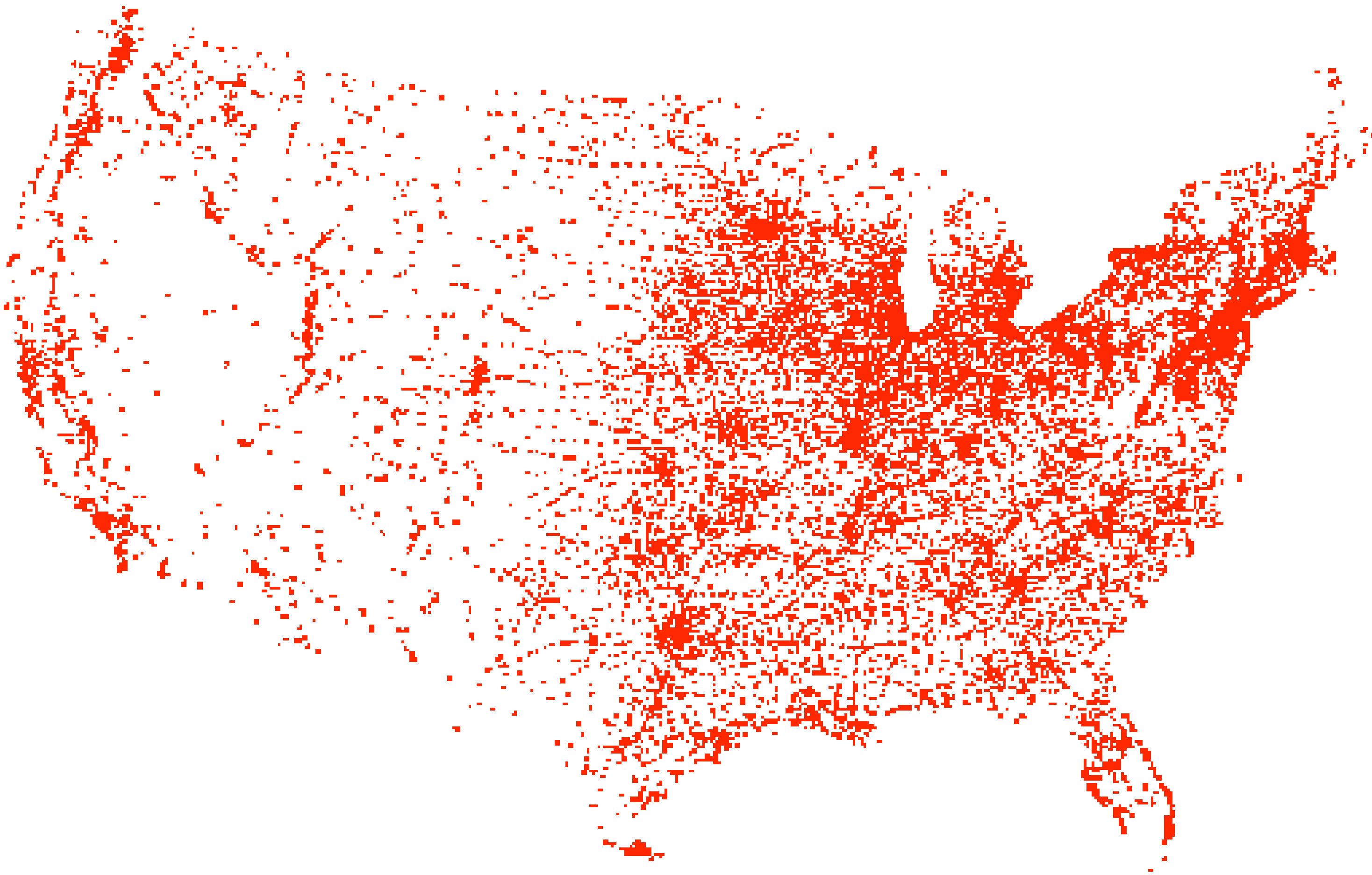
1. Monte Carlo in Statistical Physics
2. Monte Carlo for optimization and simulation of evolution
3. Dynamic Monte Carlo for simulations of (bio)chemical reactions

Simulated Annealing

1. Stat at high T_0
2. Make Monte Carlo.
   Save $\mathbf{s}_{\mathbf{min}}$ with the lowest energy $E(\mathbf{s}_{\mathbf{min}})$.
3. <u>*Slightly*</u> decrease T.
   $T_m = T_{m-1} - \Delta T$ OR $T_m = \alpha T_{m-1}$
4. Goto step 2

Kirkpatrick, S., Gerlatt, C. D. Jr., and Vecchi, M.P., Optimization by Simulated Annealing, Science 220, 671-680, 1983.

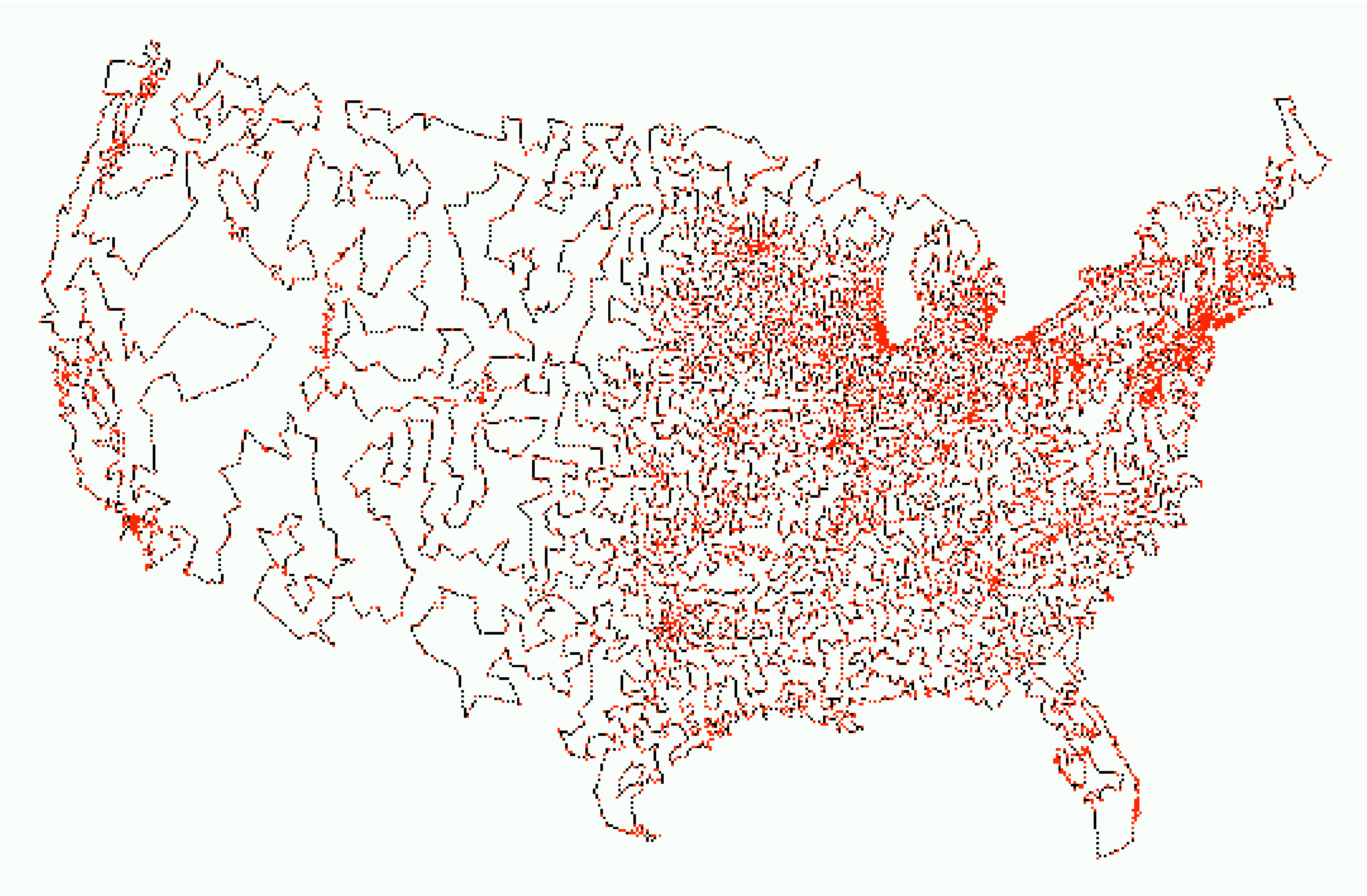
Traveling Salesman Problem



Find shortest route through all the cities and towns.

Courtesy of the TSP research group at Georgia Tech. Used with permission.

Traveling Salesman Problem



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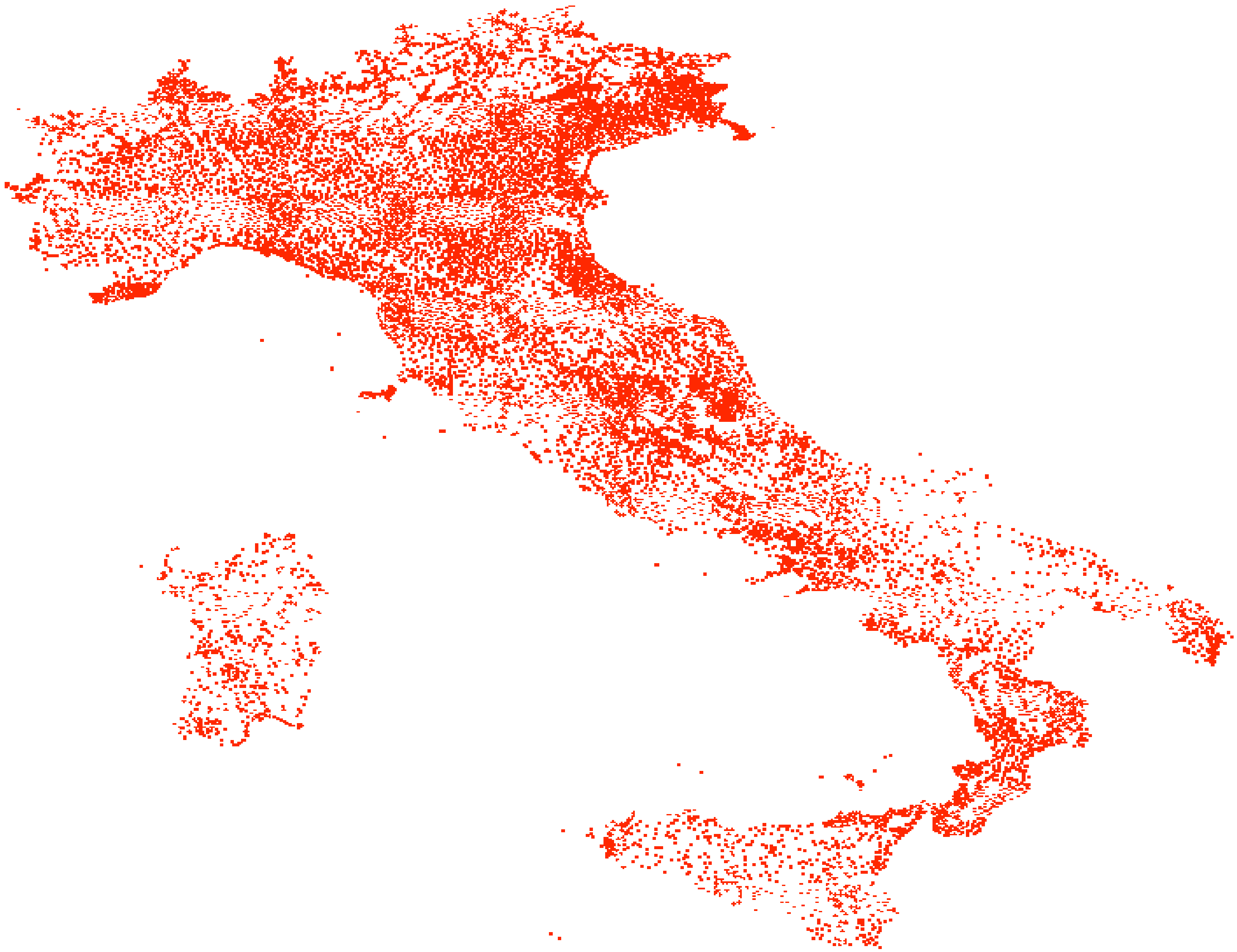
Traveling Salesman Problem



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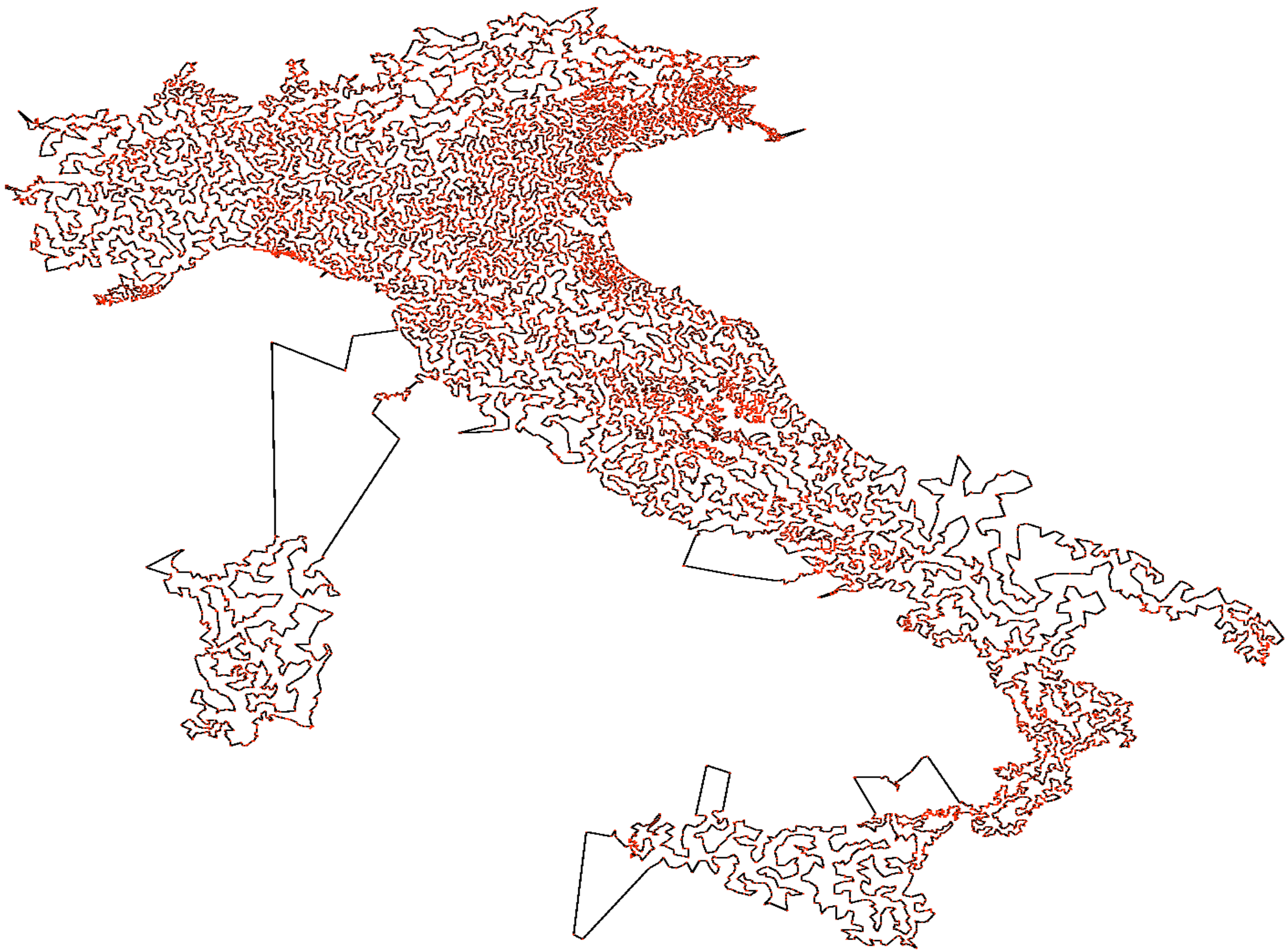
Traveling Salesman Problem



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TSP demo

http://www.math.ruu.nl/people/beukers/anneal/anneal.html

Evolution and genetic algorithm (also MC)

1. Start with **N** random organisms
   $[\mathbf{s}_1,\mathbf{s}_2,\mathbf{s}_3,\mathbf{s}_4,\mathbf{s}_5]$
2. Make mutations [flip some spins in $\mathbf{s}_k$]
3. Compute fitness of all organisms
   $F(\mathbf{s}_k)=-E(\mathbf{s}_k)$
4. Generate offsprings:
   More fit leave more offsprings.
5. Reduce population to size **N**

5. Goto step 2.

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Population of solutions

-1, 1, 1, 1,-1,-1, 1

1, 1,-1, 1,-1,-1,-1

1,-1,-1,-1, 1,-1, 1

-1,-1, 1,-1, 1, 1,-1

-1,-1,-1,-1,-1,-1, 1

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Mutations

-1, 1, 1, 1,-1,-1, 1		-1, 1, 1, 1, 1,-1, 1
1, 1,-1, 1,-1,-1,-1		1, 1,-1, 1,-1, 1,-1
1,-1,-1,-1, 1,-1, 1	→	1, 1,-1,-1, 1,-1, 1
-1,-1, 1,-1, 1, 1,-1		-1,-1, 1,-1, 1,-1,-1
-1,-1,-1,-1,-1,-1, 1		-1, 1,-1,-1,-1,-1, 1

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Recombination

-1, 1, 1, 1,-1,-1, 1 → -1, 1, 1, 1, 1,-1, 1

1, 1,-1, 1,-1,-1,-1 → 1, 1,-1, 1,-1, 1,-1

1,-1,-1,-1, 1,-1, 1 → 1, 1,-1,-1, 1,-1, 1

-1,-1, 1,-1, 1, 1,-1 → -1,-1, 1,-1, 1,-1,-1

-1,-1,-1,-1,-1,-1, 1 → -1, 1,-1,-1,-1,-1, 1

-1, 1,-1,-1,-1,-1, 1 X -1,-1, 1,-1, 1,-1,-1

↓

-1, 1,-1,-1, 1,-1,-1

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Selection

-1, 1, 1, 1,-1,-1, 1	$F(s_1)$	→	-1, 1, 1, 1,-1,-1, 1
1, 1,-1, 1,-1,-1,-1	$F(s_2)$	→	1, 1,-1, 1,-1,-1,-1
1,-1,-1,-1, 1,-1, 1	$F(s_3)$		1, 1,-1, 1,-1,-1,-1
-1,-1, 1,-1, 1, 1,-1	$F(s_4)$		1, 1,-1, 1,-1,-1,-1
-1,-1,-1,-1,-1,-1, 1	$F(s_5)$	→	-1,-1,-1,-1,-1,-1, 1

$$P(\mathbf{s}^j) = \frac{\exp(F(\mathbf{s}^j)/T)}{\sum_{k=1}^{N} \exp(F(\mathbf{s}^k)/T)}$$

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Genetic algorithm demo

http://www-cse.uta.edu/~cook/ai1/lectures/applets/gatsp/TSP.html

Premature convergence

http://www.biology.arizona.edu/evolution/act/drift/frame.html