Metropolis method in the canonical ensemble and simulated annealing

a general purpose global optimization algorithm
(Kirkpatrick S, Gelatt CD Jr, Vecchi MP
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Artificial intelligence…in 1983!

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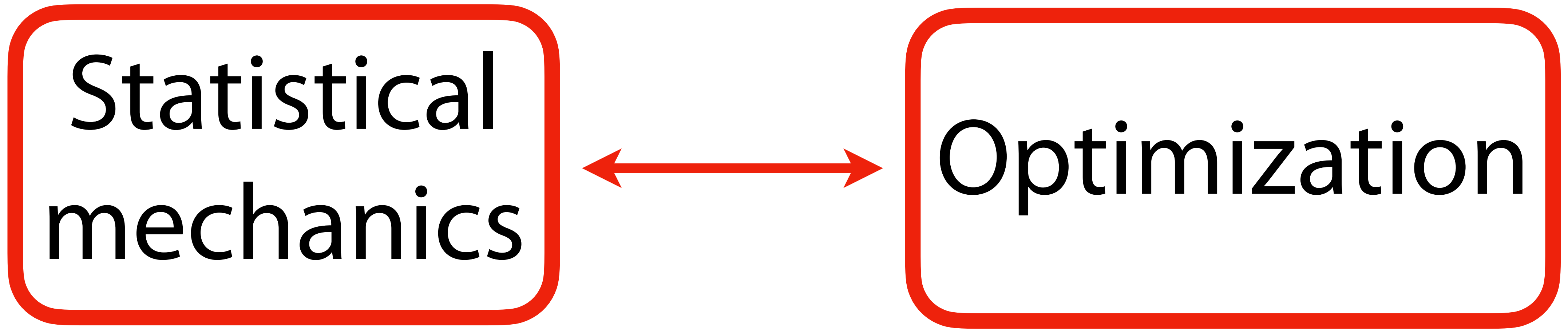
SCIENCE

Optimization by Simulated Annealing

S. Kirkpatrick, C. D. Gelatt, Jr., M. P. Vecchi

[...]

Simulation of the process of arriving at an optimal design by annealing under control of a schedule is an example of an evolutionary process modeled accurately by purely stochastic means. In fact, it may be a better model of selection processes in nature than is iterative improvement. Also, it provides an intriguing instance of "artificial intelligence," in which the computer has arrived almost uninstructed at a solution that might have been thought to require the intervention of human intelligence.



Metropolis and simulated annealing - I

- Stochastic search for global minimum. Monte Carlo optimization.

- The concept is based on the manner in which liquids freeze or metals recrystallize. Sufficiently high starting temperature and slow cooling are important to avoid freezing out in metastable states. A "cost function" is treated as the energy.

Metropolis and simulated annealing - II

- **Thermodynamic system at temperature T, energy E.**
- *Perturb configuration (generate a new one).*
- *Compute change in energy dE. If dE is negative the new configuration is accepted. If dE is positive it is accepted with a probability given by the Boltzmann factor :* $\exp(-dE/kT)$.
- *The process is repeated many times for good sampling of configuration space.*

(usual Metropolis procedure in the canonical ensemble)

- **then the temperature is slightly lowered and the entire procedure repeated, and so on, until a frozen state is achieved.**

Metropolis and simulated annealing - II

necessary:

- **Thermodynamic system at temperature T, energy E.**

usual Metropolis procedure in the canonical ensemble:

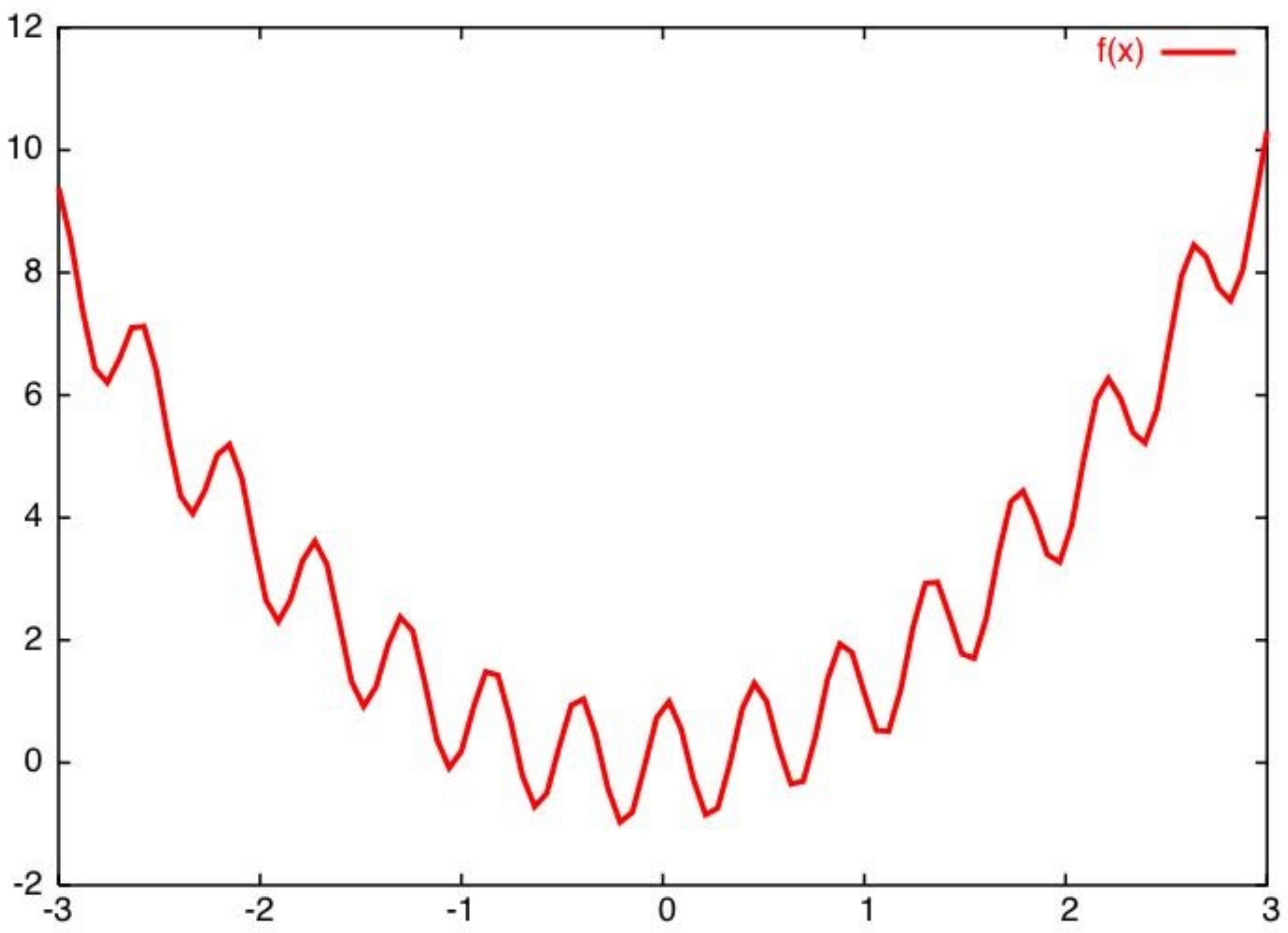
- *Perturb configuration (generate a new one).* ← a move generation strategy
- *Compute change in energy dE. If dE is negative the new configuration is accepted. If dE is positive it is accepted with a probability given by the Boltzmann factor : exp(-dE/kT).*
- *The process is repeated many times for good sampling of configuration space.* ← a freezing schedule
- **then the temperature is slightly lowered and the entire procedure repeated, and so on, until a frozen state is achieved.** ← a stopping criterion

Example

in **simulated_annealing.f90:**
minimization of

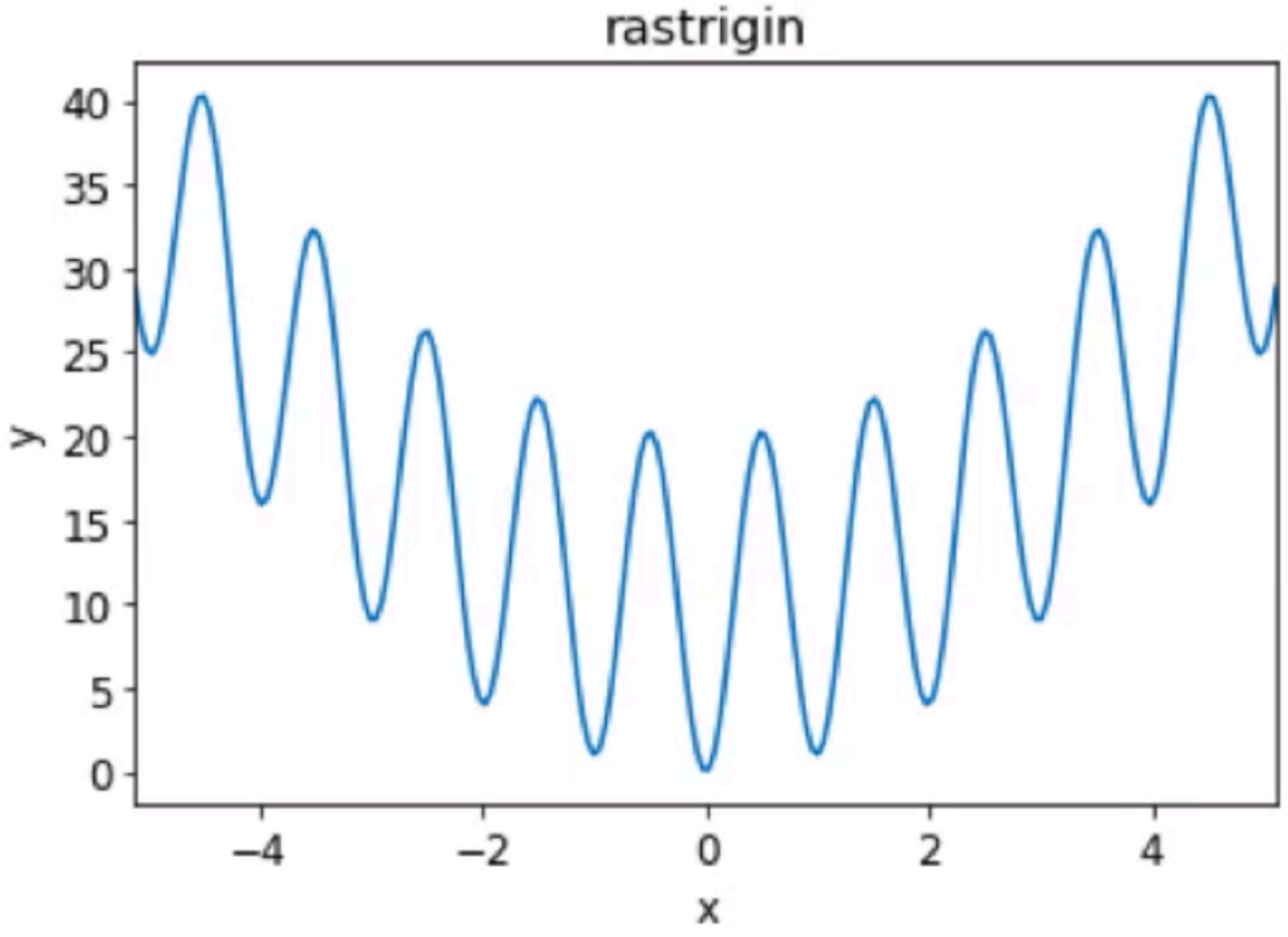
f(x)=(x+0.2)*x+cos(14.5*x-0.3)

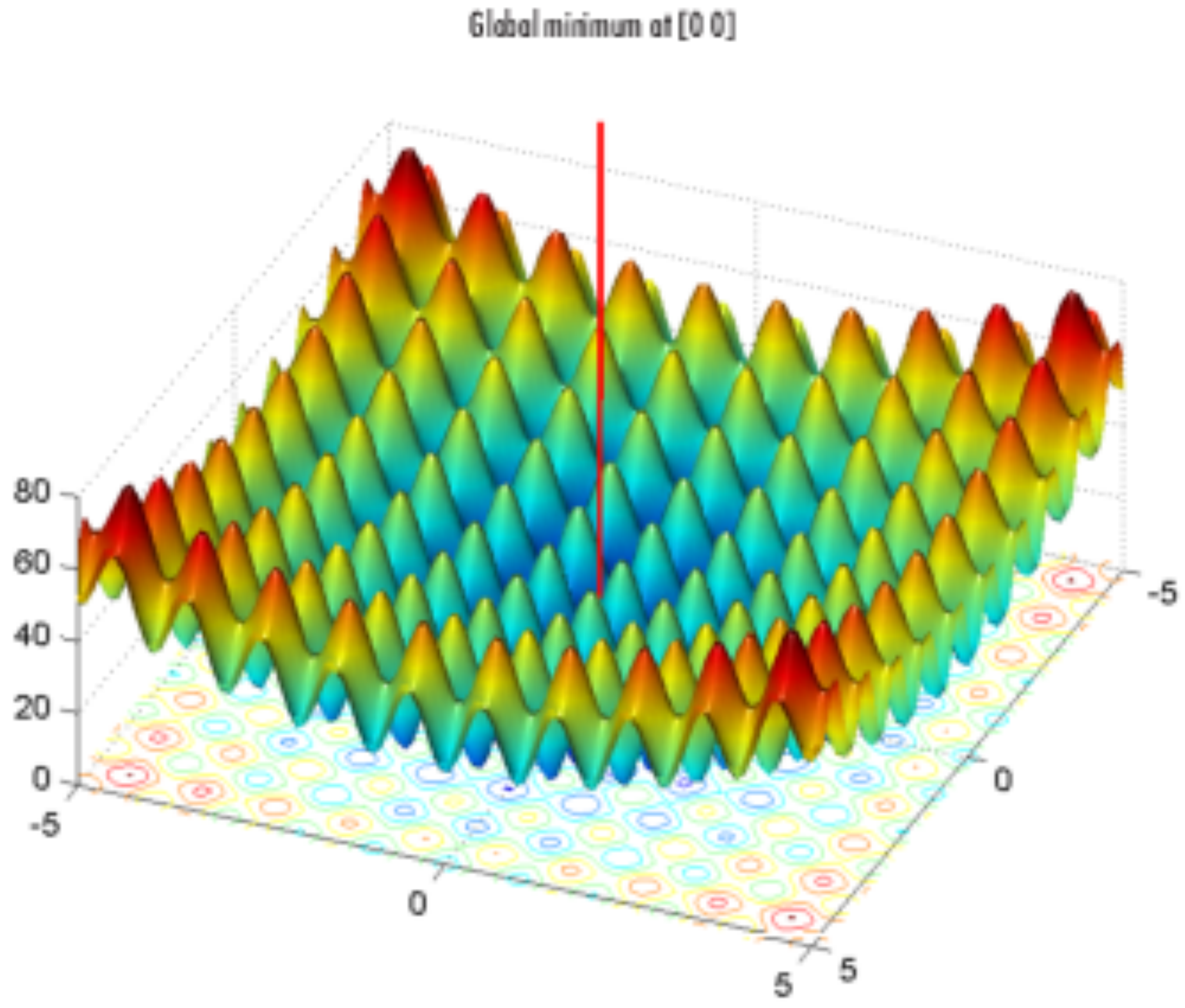
considered as an energy function and using a fictitious temperature



***Rastrigin function*:**

- non-convex *function* used as a performance test problem for optimization algorithm
- typical example of non-linear multimodal *function;*
- first proposed by *Rastrigin* as a 2-dimensional *function;* later generalized by Rudolph.





$$f(\boldsymbol{x}) = nA + \sum_{i=1}^{n}[x_i^2 - Acos(2\pi x_i)]$$

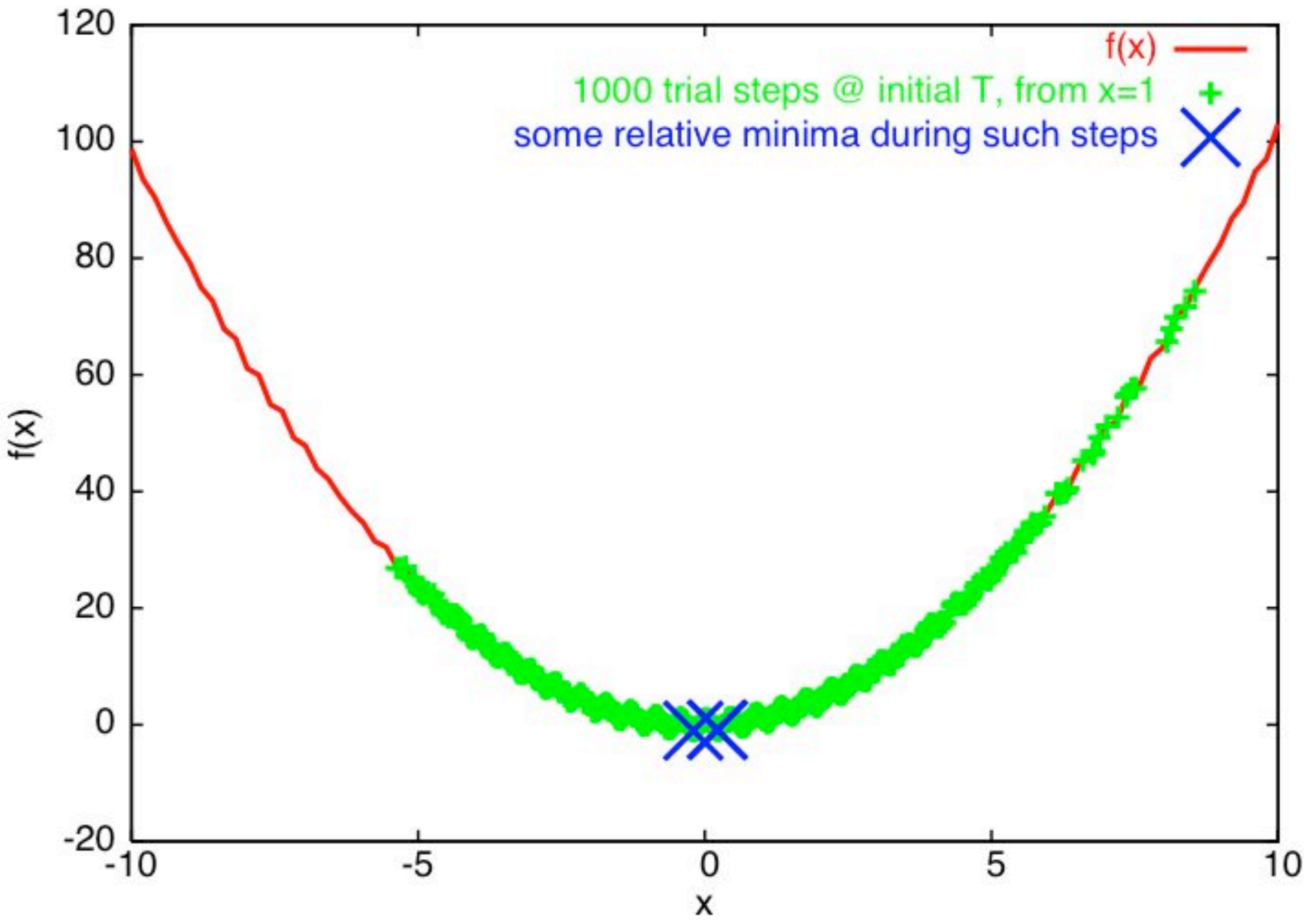
Function to be minimized: **f(x)** ; Starting point: **x, fx=f(x)**

Annealing schedule:	initial (high) temperature:	**temp**
	annealing temperature reduction factor:	**tfactor (<1)**
	number of steps per block:	**nsteps**
	'ad hoc' parameter for trial move:	**scale**

```
DO WHILE (temp > 1E-5) ! anneal cycle

  DO istep = 1, nsteps
    CALL RANDOM_NUMBER(rand) ! generate 2 random numbers; dimension(2) :: rand
    x_new = x + scale*SQRT(temp)*(rand(1) - 0.5) ! stochastic move
    fx_new = func(x_new) ! new object function value
    IF (EXP(-(fx_new - fx)/temp) > rand(2)) THEN ! success, save
      fx = fx_new
      x = x_new
    END IF
    IF (fx < fx_min) THEN
      fx_min = fx
      x_min = x
      PRINT '(3ES13.5)', temp, x_min, fx_min
    END IF
  END DO

  temp = temp * tfactor ! decrease temperature
END DO
```




```
initial T:   10 (K_B units)
initial x:       1.000000
initial f(x):    1.137208
```

```
final T:     2.50315E-01
final x:    -1.95067E-01
final f(x):-1.00088E+00
```