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ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ

Εισαγωγή σε μεθόδους Monte Carlo

Ενότητα 5: Η βελτιστοποίηση Monte Carlo

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Τμήμα Μαθηματικών και Εφαρμοσμένων Μαθηματικών

Optimization

❑ Basic Definitions:

- Differences between the numerical approach and the simulation approach to the problem
$$\max_{\theta \in \Theta} h(\theta)$$
lie in the treatment of the function h.

- In an optimization problem using deterministic numerical methods
  - The analytical properties of the target function (convexity, boundedness, smoothness) are often paramount.

- For the simulation approach
  - We are concerned with h from a probabilistic (rather than analytical) point of view.

Optimization: The Problem

- The problem

$$\max_{\theta \in \Theta} h(\theta)$$

- Deterministic numerical methods $\longrightarrow$ analytical properties

- Simulation approach $\longrightarrow$ probabilistic view.

    - This dichotomy is somewhat artificial
    - Some simulation approaches have no probabilistic interpretation

- Nonetheless, the use of the analytical properties of h plays a lesser role in the simulation approach.

Two Simulation Approaches

- Exploratory Approach
    - Goal: To optimize h by describing its entire range
    - Actual properties of h play a lesser role
- Probabilistic Approach
    - Monte Carlo exploits probabilistic properties of h
    - This approach tied to missing data methods

Stochastic Exploration

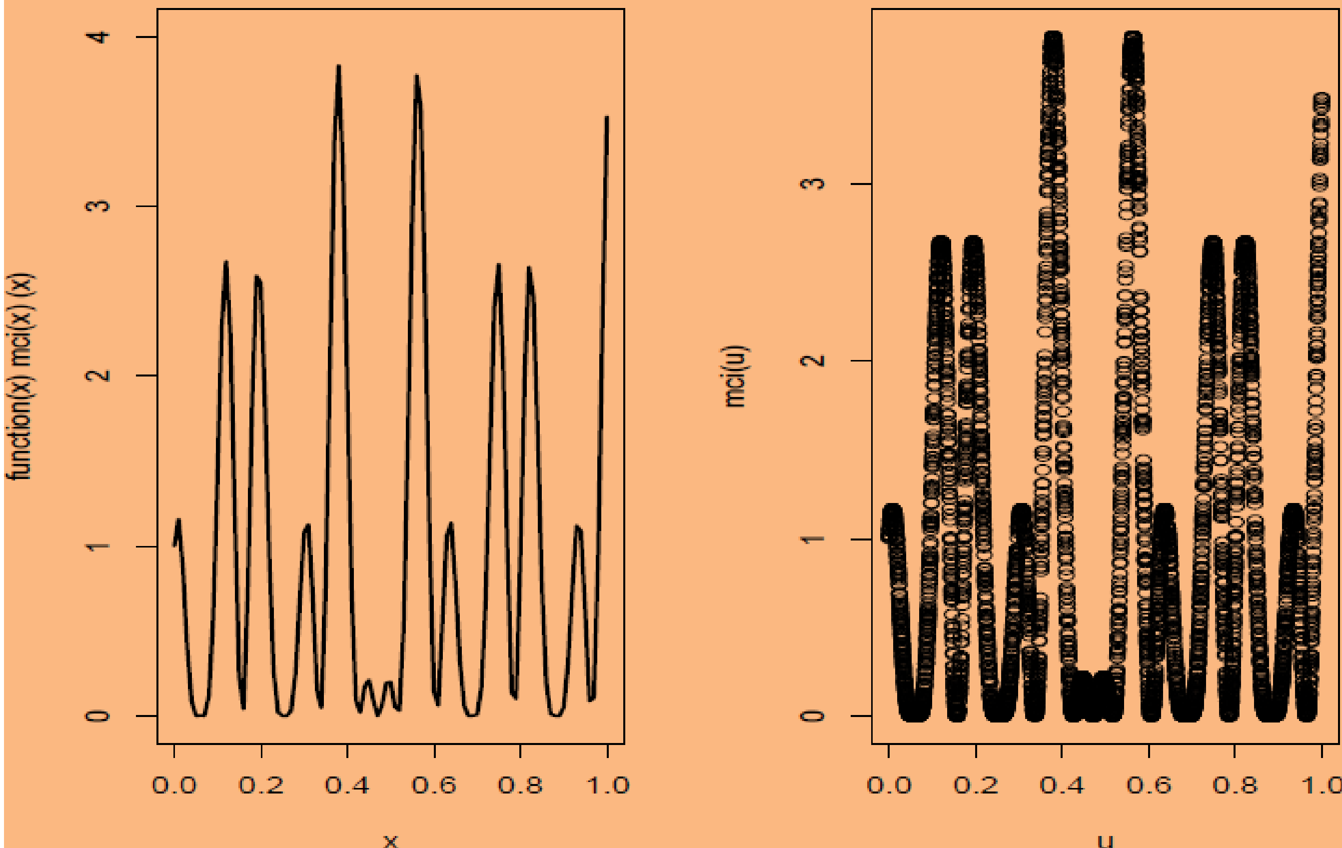
- A first approach is to simulate from a uniform distribution on Θ, $u_1, \ldots, u_m \sim \mathcal{U}_\Theta$,
- Use the approximation

$$h_m^* = \max(h(u_1), \ldots, h(u_m)).$$

- This method converges (as m goes to ∞), but it may be very slow since it does not take into account any specific feature of h.
- Distributions other than the uniform, which can possibly be related to h, may then do better.
- In particular, in setups where the likelihood function is extremely costly to compute the number of evaluations of the function h is best kept to a minimum.

Monte Carlo Maximization: A First Example

- Recall the function $h(x) = [\cos(50x) + \sin(20x)]^2$.
- we try our naïve strategy and simulate $u_1, \ldots, u_m \sim \mathcal{U}(0,1)$, and use the approximation $h^*_m = \max(h(u_1), \ldots, h(u_m))$

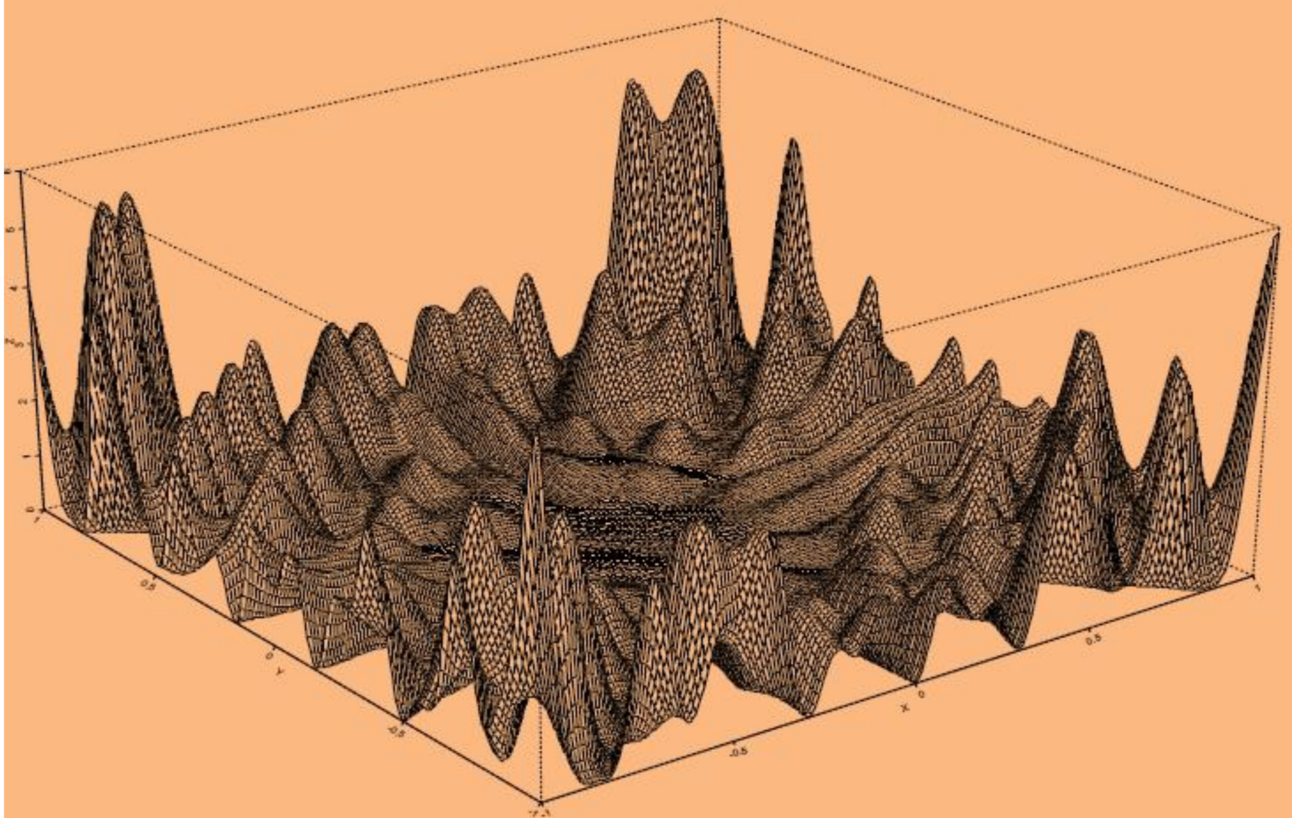


Monte Carlo: A Tough Minimization

- Consider minimizing

$$
\begin{aligned}
h(x,y) &= (x\sin(20y)+y\sin(20x))^2\cosh(\sin(10x)x) \\
&\quad + (x\cos(10y)-y\sin(10x))^2\cosh(\cos(20y)y)\ ,
\end{aligned}
$$

whose global minimum is 0, attained at $(x,y)=(0,0)$



Monte Carlo: A Tough Minimization

Properties

- Many local minima
- Standard methods may not find global minimum
- We can simulate from $\exp(-h(x,y))$
- Get minimum from $\min_i h(x_i, y_i)$
- Can use other methods...

Monte Carlo: A Tough Minimization

Deterministic Gradient Methods

- The *gradient method* is a deterministic numerical approach to the problem
$$\max_{\theta \in \Theta} h(\theta).$$
- It produces a sequence (θ_j) that converges to the maximum when
- ○ the domain $\Theta \subset \Re^d$
  ○ the function $(-h)$

  are both convex.
- The sequence (θ_j) is constructed in a recursive manner through
$$\theta_{j+1} = \theta_j + \alpha_j \nabla h(\theta_j) \ , \qquad \alpha_j > 0 \ ,$$

Here

○ ∇h is the gradient of h

○ α_j is chosen to aid convergence

Monte Carlo: A Tough Minimization

Stochastic Variant

- There are stochastic variants of the gradient method
- They do not always go along the steepest slope
- This is an advantage, as it can avoid local maxima and saddlepoints
- The best, and simple version is Simulated Annealing/Metropolis Algorithm

Simulated Annealing

- This name is borrowed from Metallurgy:
- A metal manufactured by a slow decrease of temperature (*annealing*) is stronger than a metal manufactured by a fast decrease of temperature.
- The fundamental idea of simulated annealing methods is that a change of scale, called *temperature*, allows for faster moves on the surface of the function h to maximize.
    - Rescaling partially avoids the trapping attraction of local maxima.
    - As T decreases toward 0, the values simulated from this distribution become concentrated in a narrower and narrower neighborhood of the local maxima of h

Simulated Annealing/Metropolis Algorithm

- **Basic Idea:**

- Simulation method proposed by Metropolis *et al.* (1953)
- Starting from θ_0, ζ is generated from

$$\zeta \sim \text{Uniform in a neighborhood of } \theta_0.$$

- The new value of θ is generated as

$$\theta_1 = \begin{cases} \zeta & \text{with probability } \rho = \exp(\Delta h/T) \wedge 1 \\ \theta_0 & \text{with probability } 1 - \rho, \end{cases}$$

  - $\Delta h = h(\zeta) - h(\theta_0)$
  - If $h(\zeta) \geq h(\theta_0)$, ζ is accepted
  - If $h(\zeta) < h(\theta_0)$, ζ may still be accepted
  - This allows escape from local maxima

Simulated Annealing/Metropolis Algorithm

Metropolis/Simulated Annealing Algorithm

- In its most usual implementation, the simulated annealing algorithm modifies the temperature T at each iteration
- It has the form

1. Simulate ζ from an instrumental distribution with density $g(|\zeta - \theta_i|)$;
2. Accept $\theta_{i+1} = \zeta$ with probability

$$\rho_i = \exp\{\Delta h_i / T_i\} \wedge 1;$$

   take $\theta_{i+1} = \theta_i$ otherwise.

3. Update T_i to T_{i+1}.

Simulated Annealing/Metropolis Algorithm

- **Important Comments:**

1. Simulate ζ from an instrumental distribution with density $g(|\zeta - \theta_i|)$;
2. Accept $\theta_{i+1} = \zeta$ with probability
$$\rho_i = \exp\{\Delta h_i / T_i\} \wedge 1;$$
take $\theta_{i+1} = \theta_i$ otherwise.
3. Update T_i to T_{i+1}.

- All positive moves accepted
- As $T \downarrow 0$
  - Harder to accept downward moves
  - No big downward moves
- Not a Markov Chain - difficult to analyze

Simulated Annealing/Metropolis Algorithm

❑ **Simple Example (as before):**

- Recall the function $h(x) = [\cos(50x) + \sin(20x)]^2$
- The specific algorithm we use is

  Starting at iteration t, the iteration is at $(x^{(t)}, h(x^{(t)}))$:

  1. Simulate $u \sim \mathcal{U}(a_t, b_t)$ where $a_t = \max(x^{(t)} - r, 0)$ and $b_t = \min(x^{(t)} + r, 1)$
  2. Accept $x^{(t+1)} = u$ with probability

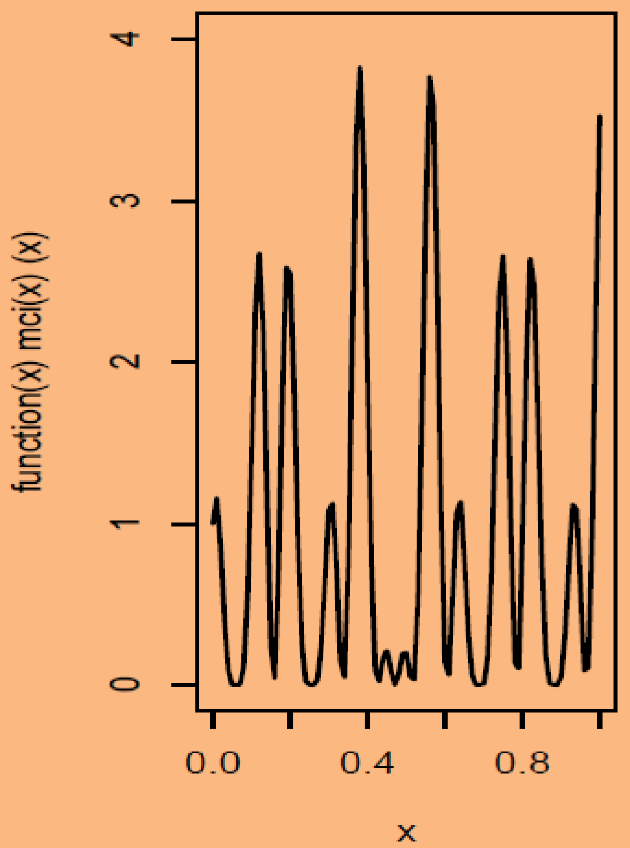
  $$\rho^{(t)} = \min\left\{\exp\left(\frac{h(u) - h(x^{(t)})}{T_t}\right), 1\right\},$$

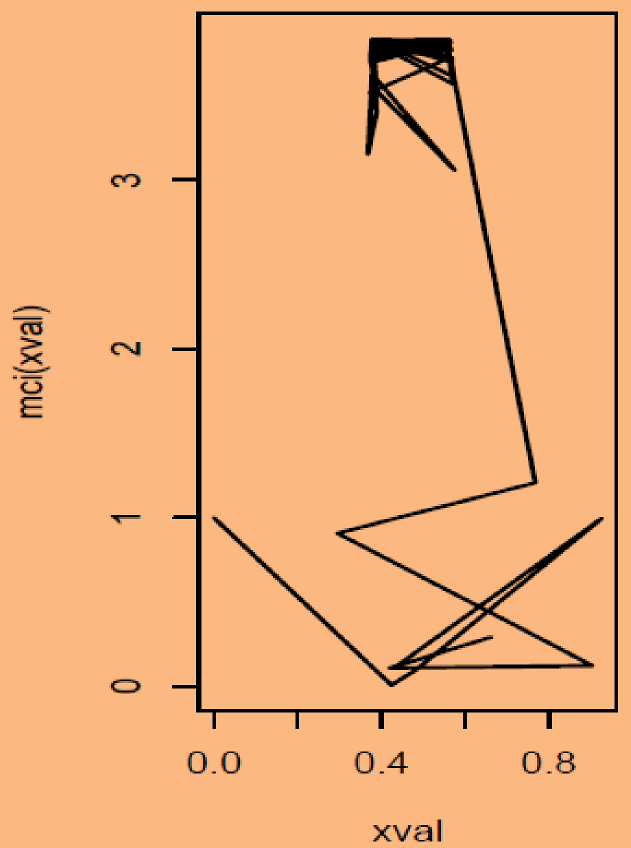
     take $x^{(t+1)} = x^{(t)}$ otherwise.
  3. Update T_t to T_{t+1}.

- ◦ The value of r controls the size of the interval around the current point (staying in $(0, 1)$)
- ◦ The value of T_t controls the cooling.

Simulated Annealing/Metropolis Algorithm

The Trajectory





- Left Panel is the function
- Right Panel is the Simulated Annealing Trajectory

Simulated Annealing

Simulated Annealing Property

- Theorem 5.7: Under mild assumptions, the Simulated Annealing algorithm is guaranteed to find the global maximum

❑ **Maximization problem (as before):**

Return to the difficult maximization

- Apply simulated Annealing
- Different choices of T_i
  - Results dependent on choice of T_i
  - $T_i \propto 1/\log(i+1)$ preferred

Simulated Annealing: Examples

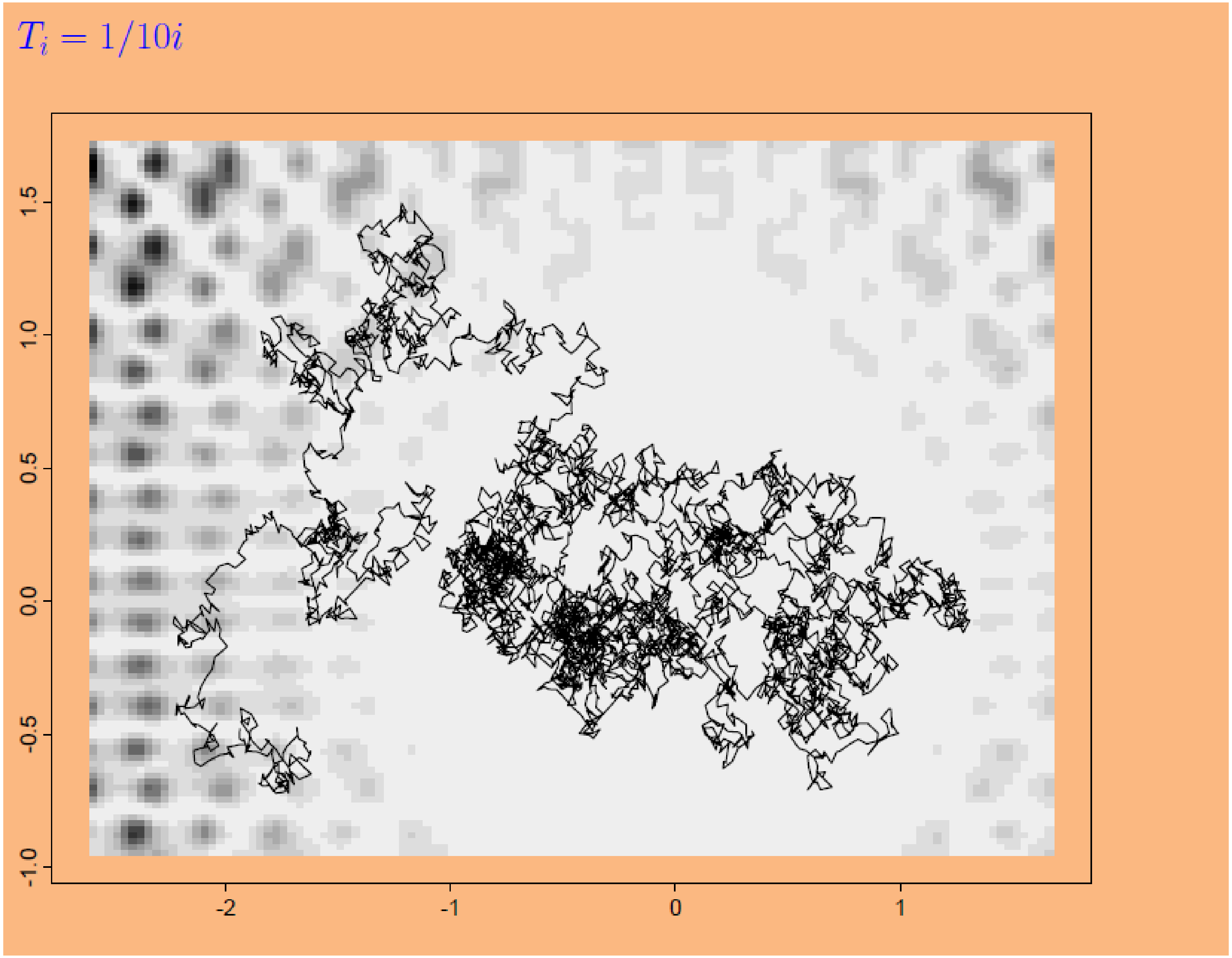
Simulated Annealing Runs

- $g \sim \text{Uniform}(-.1, .1)$
- Starting point $(0.5, 0.4)$

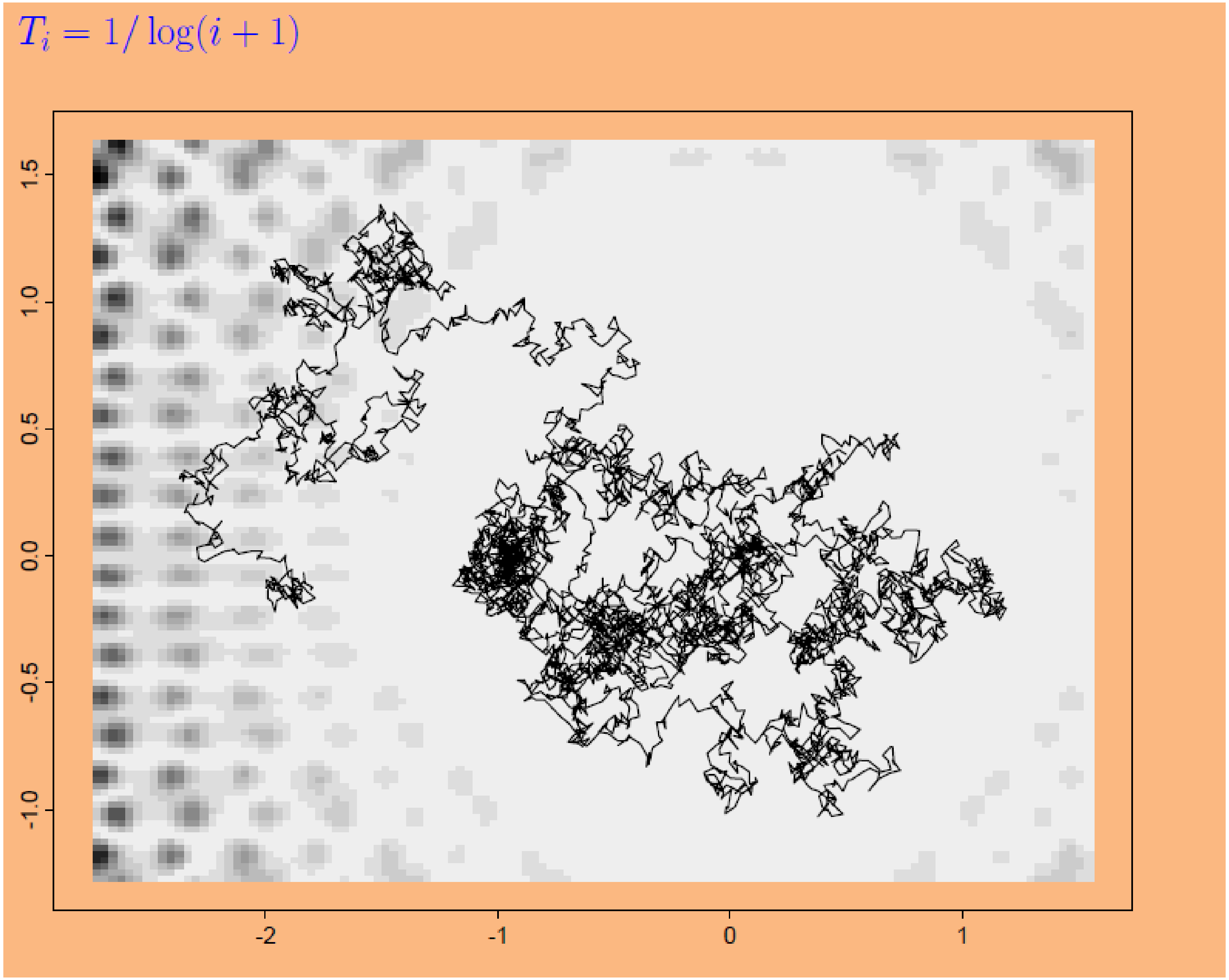
Case	T_i	θ_T	$h(\theta_T)$	$\min_t h(\theta_t)$	Accept. rate
1	$1/10i$	$(-1.94, -0.480)$	0.198	$4.02\,10^{-7}$	0.9998
2	$1/\log(1+i)$	$(-1.99, -0.133)$	3.408	3.823×10^{-7}	0.96
3	$100/\log(1+i)$	$(-0.575, 0.430)$	0.0017	4.708×10^{-9}	0.6888
4	$1/10\log(1+i)$	$(0.121, -0.150)$	0.0359	2.382×10^{-7}	0.71

- Case 3 explores "valley" near the minimum
- Recommended $T_i \approx \Gamma/\log(i+1)$ for large Γ

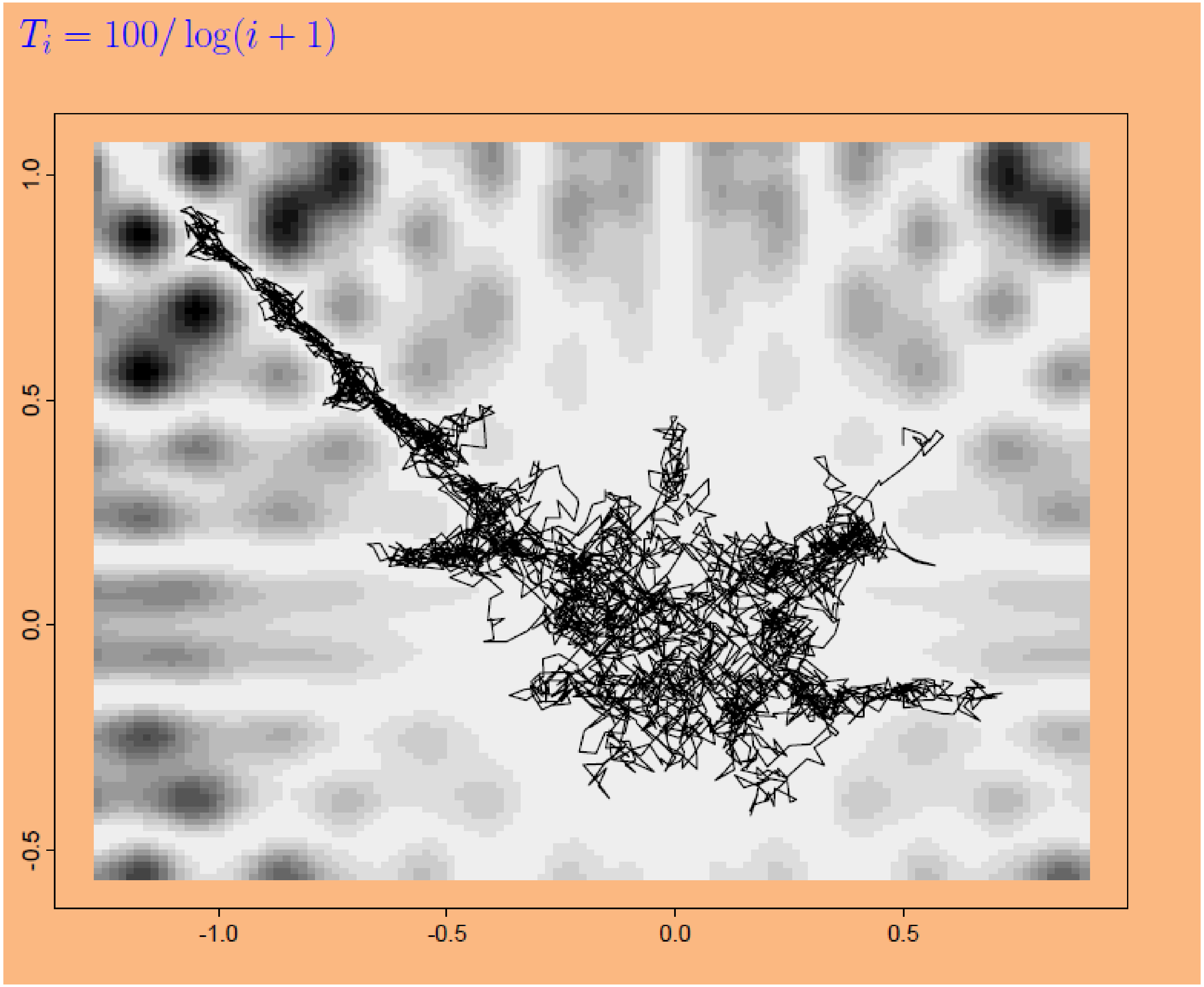
Simulated Annealing: Examples



Simulated Annealing: Examples



Simulated Annealing: Examples



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Τέλος Ενότητας

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Σημείωμα Αναφοράς

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