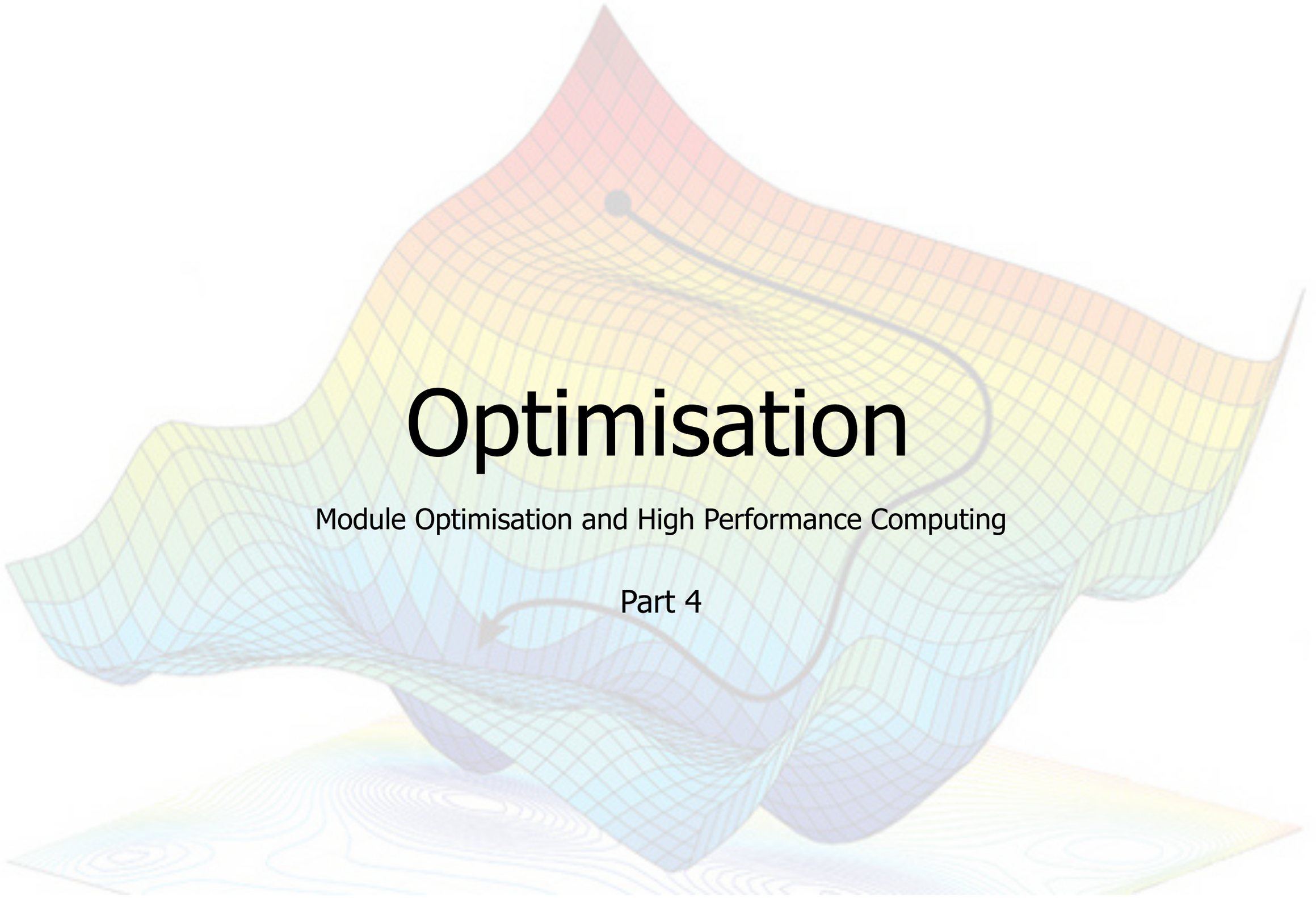
Zurich University of Applied Sciences
Institute of Computational Life Sciences



Optimisation

Module Optimisation and High Performance Computing

Part 4

Part 4

Stochastic Methods:

- Noisy Gradient Descent
- Simulated Annealing

Part 4

Stochastic Methods:

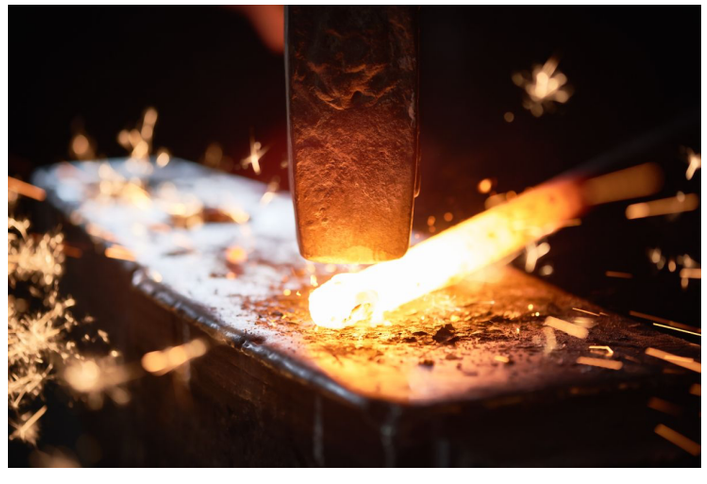
- Noisy Gradient Descent

- **Simulated Annealing**

Simulated Annealing

- **Simulated Annealing** borrows inspiration from **metallurgy**.

  Annealing is a process in which a material is heated and then cooled, making it more workable. **When hot, the atoms are more free to move around and tend to settle into better positions**. A slow cooling brings the material to an ordered, crystalline state. A fast, abrupt quenching causes defects because the material is forced to settle in its current condition.



- **Temperature** is used to control the degree of stochasticity during the randomised search.
  - The **temperature starts high**, allowing large jumps so that the process can freely move in the search space, with the hope that it will find a good region with the best local minimum.
  - The **temperature is then slowly brought down**, reducing the stochasticity and forcing the search to converge to a minimum.

- **Simulated Annealing** is often used on objective functions with many local minima due to its ability to escape such local minima.

Simulated Annealing

1. Start with an initial guess $\mathbf{x}_0$ and (high, but not too high) temperature $T = T_0$

2. Sample a candidate transition $\mathbf{x}_n \rightarrow \mathbf{x}'$ from a **transition distribution** $\mathscr{D}$

   In other words, generate a new candidate $\mathbf{x}'$ by making a small change to the current $\mathbf{x}_n$

3. Calculate the difference in the objective function $\Delta E = f(\mathbf{x}') - f(\mathbf{x}_n)$

4. Accept the move with probability:

$$\begin{cases} 1 & \text{if } \Delta E \leq 0 \\ e^{-\Delta E/T} & \text{if } \Delta E > 0 \end{cases}$$

   if the candidate $\mathbf{x}'$ is better, accept it

   if the candidate $\mathbf{x}'$ is worse, accept it with a probability that depends on the temperature T and the difference ΔE

   This acceptance probability, known as **Metropolis criterion**, allows the algorithm to escape from local minima if the temperature is high enough.

5. Reduce the temperature according to a **cooling schedule**

6. Iterate steps 2-5 until the system is frozen or another stopping criterion is met

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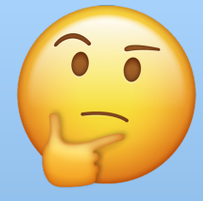

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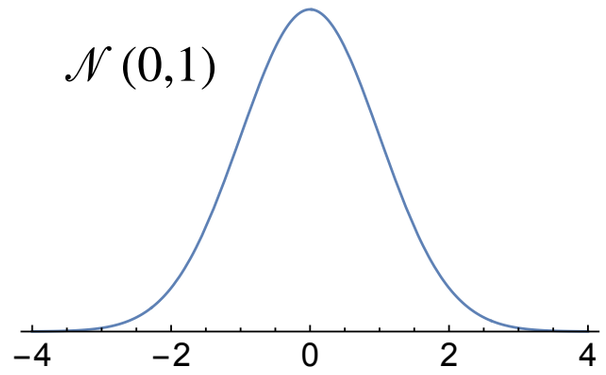
Simulated Annealing

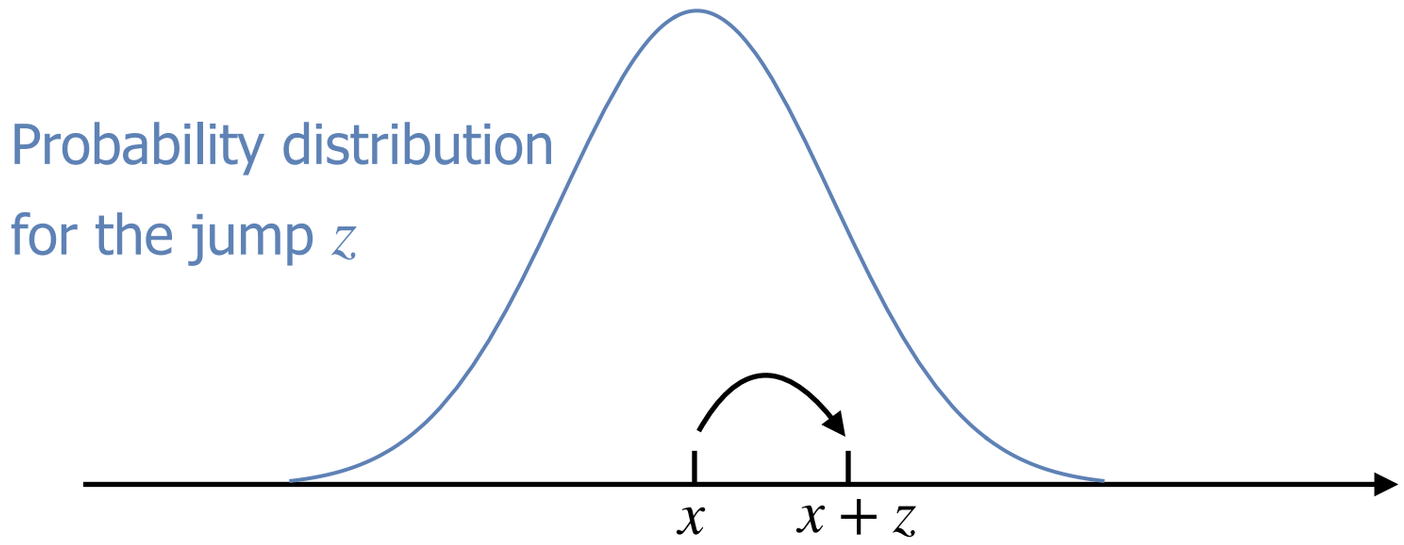
Let us consider first the simplest **univariate case**.

A quite popular transition distribution is a
zero-mean Gaussian distribution: $\mathscr{D} = \mathscr{N}(0,\sigma)$



We are in x and want to make a **random jump** from x to x':

$$x' = x + z \qquad z \sim \mathscr{D}$$

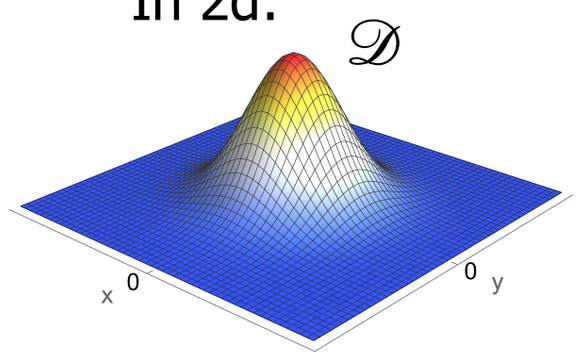


Simulated Annealing

The **multivariate** case is just a generalisation to multiple dimensions:

$$\mathscr{D} = \mathcal{N}\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right) \quad \text{with} \quad \boldsymbol{\mu} = \left[0, 0 \ldots, 0\right] \quad \text{and} \quad \boldsymbol{\Sigma} = \sigma\mathbf{I} = \begin{bmatrix} \sigma & 0 & \ldots & 0 \\ 0 & \sigma & \ldots & 0 \\ \vdots & \vdots & \ldots & \vdots \\ 0 & 0 & \ldots & \sigma \end{bmatrix}$$

In 2d:

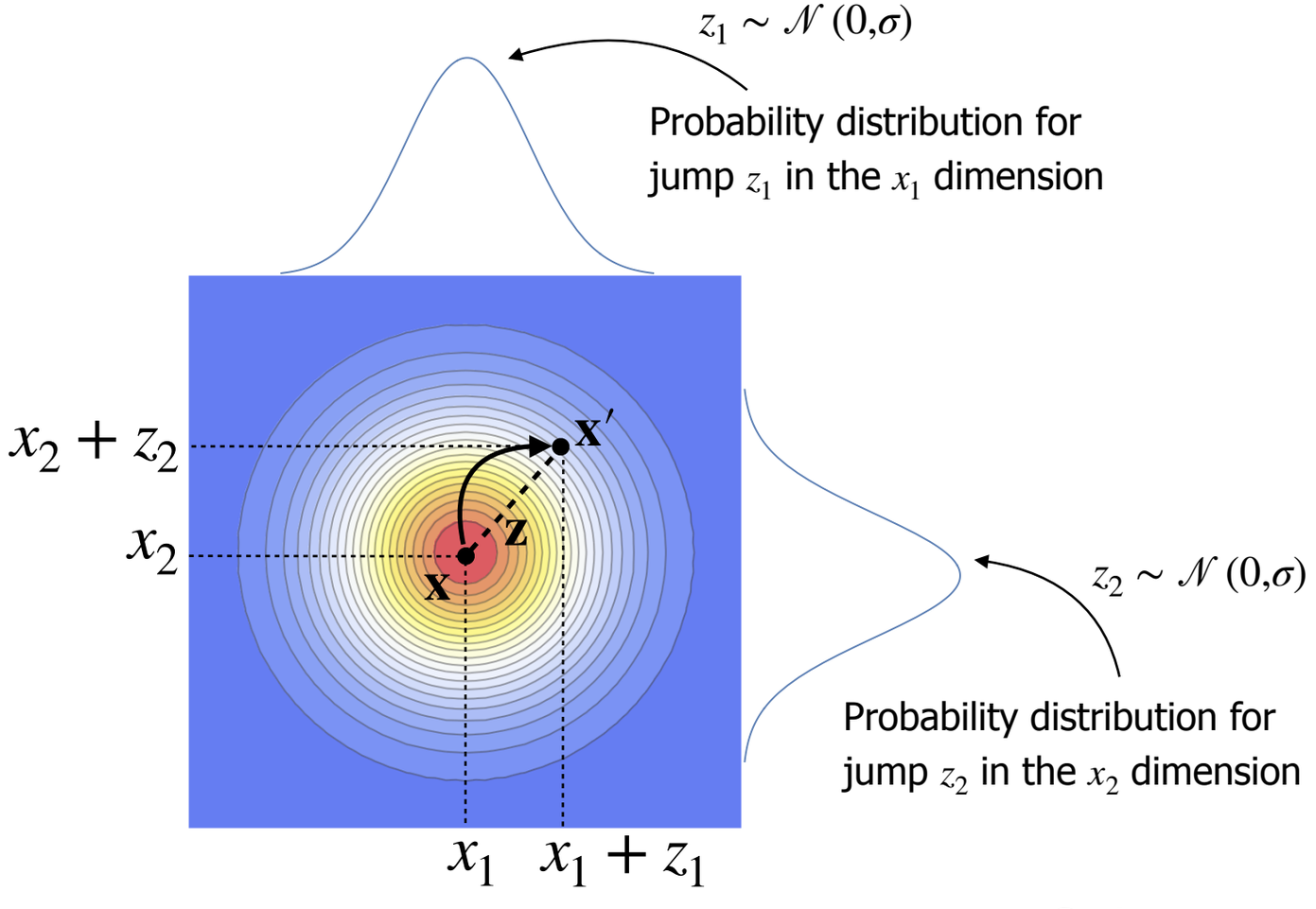


Random jump from $\mathbf{x}$ to $\mathbf{x}'$: $\mathbf{x}' = \mathbf{x} + \mathbf{z} \qquad \mathbf{z} \sim \mathscr{D}$

Example in 2d:

Current state: $\mathbf{x} = \left[x_1, x_2\right]$

Random jump: $\mathbf{z} = \left[z_1, z_2\right]$



Simulated Annealing

- The parameter σ specifies **how far one can jump**. **Critical parameter:** one should stay close to the current $\mathbf{x}$, but not too close.

- In Python, numpy provides an easy way to sample from multivariate distributions:

```python
import numpy as np
# --- Construct covariance matrix --- #
n_dims = 2                    # number of dimensions
means = np.full(n_dims, 0)    # array of mean values = [0,0,...,0]
sigma = 1                     # variance (the same for all dimensions)
covariance_matrix = np.diag(np.full(n_dims, sigma))  # diagonal covariance matrix (sigma*I)
# --- Sample from distribution --- #
z = np.random.multivariate_normal(means, covariance_matrix)
```

Simulated Annealing

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6. Iterate steps 2-5 until the system is frozen or another stopping criterion is met

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In physics the objective function to be minimised is an ENERGY

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GUEST EDITORS' INTRODUCTION

the Top 10 Algorithms of the 20th century

… the 10 algorithms with the greatest influence on the development and practice of science and engineering in the 20th century.

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection
- Fast Multipole Method

(in chronological order)

JACK DONGARRA
University of Tennessee and Oak Ridge National Laboratory
FRANCIS SULLIVAN
IDA Center for Computing Sciences

Simulated Annealing

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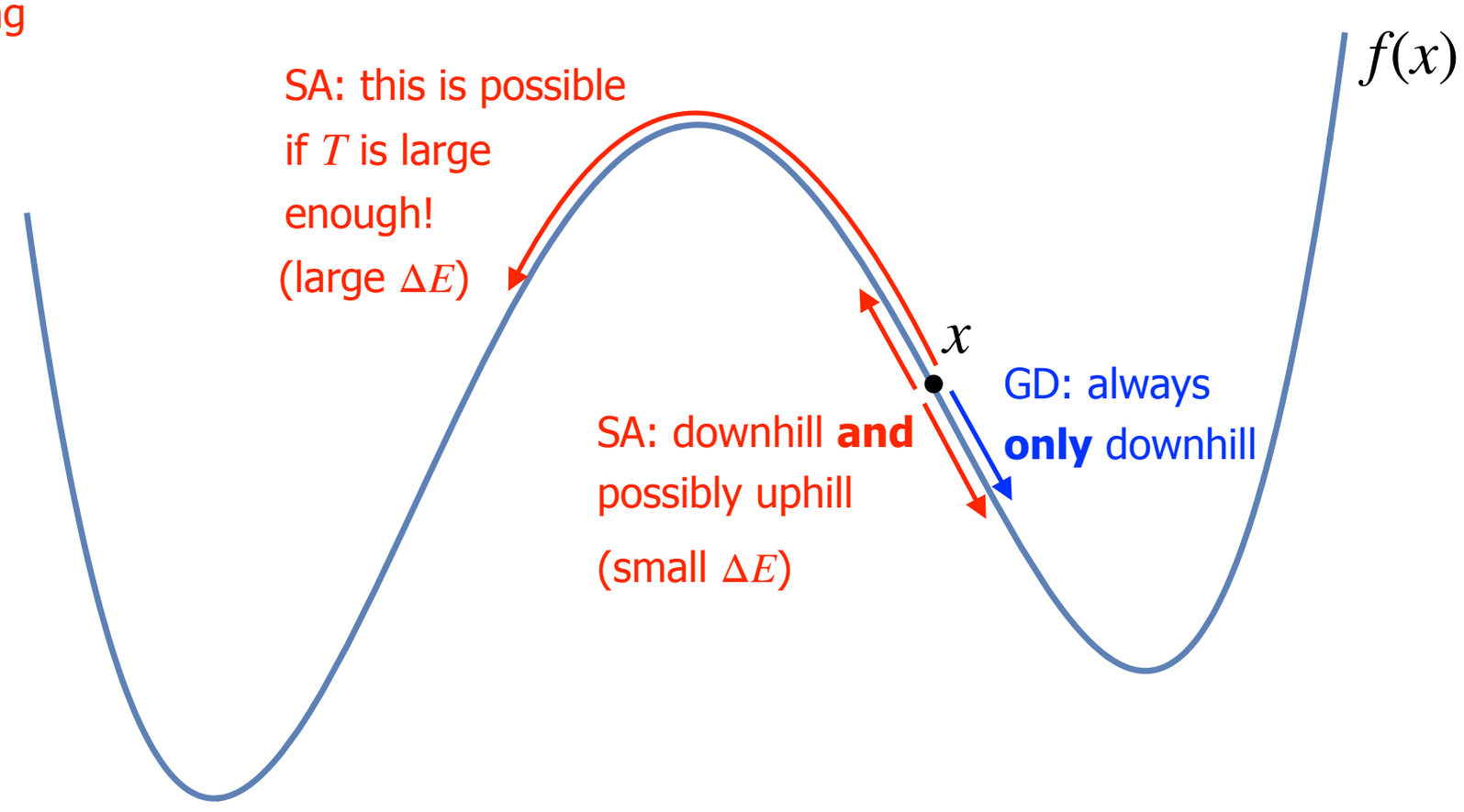
SA = Simulated Annealing

GD: Gradient Descent



Simulated Annealing

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Practically, how can it be implemented?

- Given current x_n and the proposal x', calculate $\Delta E = f(\mathbf{x}') - f(\mathbf{x}_n)$
- Generate a random number $s \in [0, 1)$

```
s = np.random.rand()
```

- `If` $e^{-\Delta E/T_n} \geq s$ accept the move: $x_{n+1} = x'$
- `else` reject it (and stay where you are): $x_{n+1} = x_n$

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The algorithm will not converge if we keep the temperature high

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Simulated Annealing

- The temperature parameter T controls the acceptance probability. An **annealing/cooling schedule** is used to slowly bring down the temperature as the algorithm progresses.
- The temperature T must be brought down to **ensure convergence**.
- If it is brought down too quickly, the search may not cover adequately the search space.
- Common annealing schedules are:
  - $T_n = T_0\left(1 - \frac{n}{n_{\max}}\right)$ $n_{\max}$ = max number of iterations
  - Logarithmic: $T_n = \frac{T_0 \ln 2}{\ln(n+1)}$ Efficient at finding global minima, but slow

    B. Hajek, "Cooling Schedules for Optimal Annealing", Mathematics of Operations Research, 1988
  - Exponential: $T_{n+1} = \gamma T_n$ $\gamma \in (0,1)$ Practically: $0.8 \leq \gamma \leq 0.99$
  - Fast annealing: $T_n = \frac{T_1}{n}$ H. Szu and R. Hartley, "Fast Simulated Annealing", Physics Letters A, 1987

Simulated Annealing

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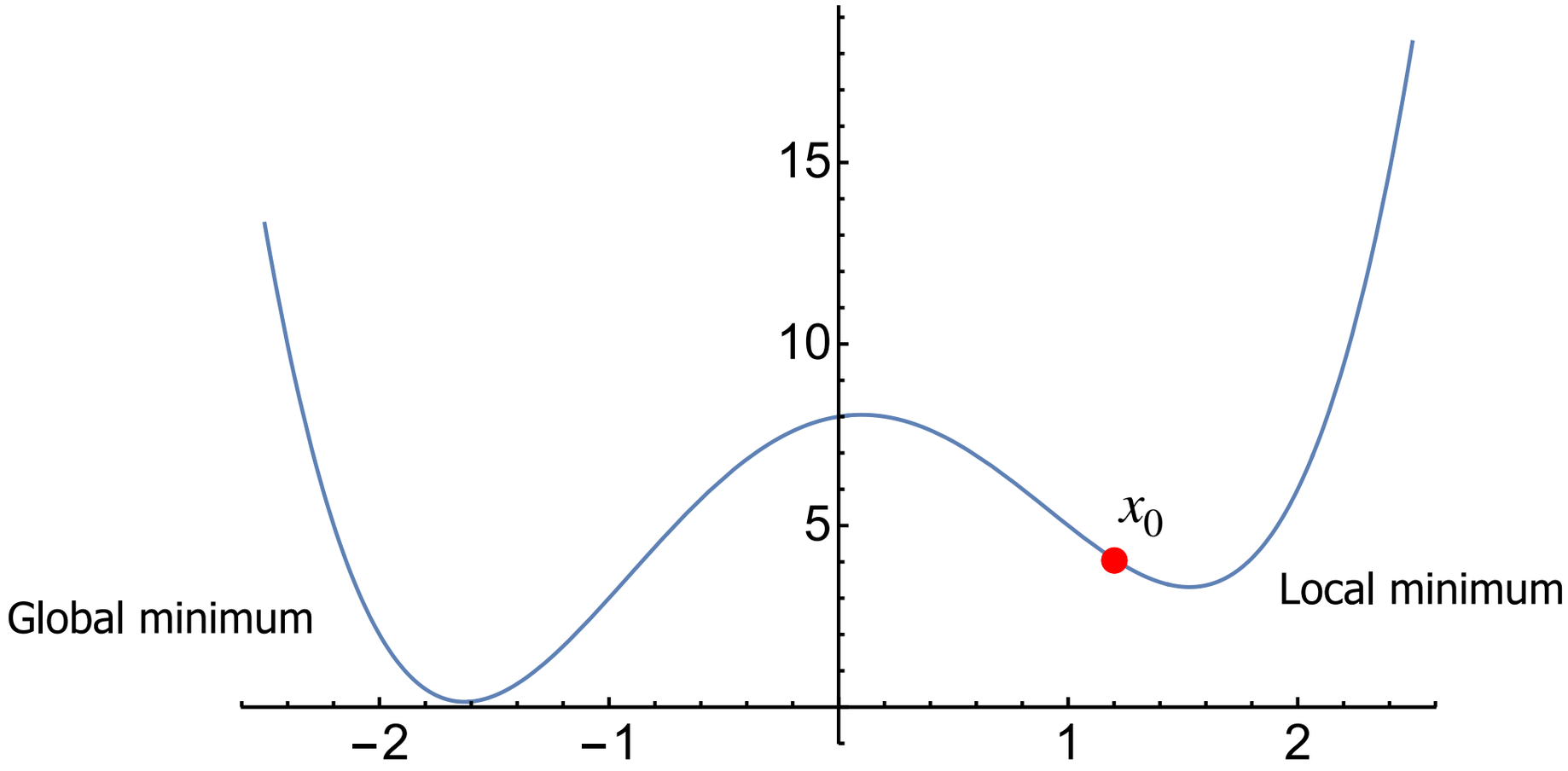
Simulated Annealing

- Consider the univariate objective function $f(x) = x^4 - 5x^2 + x + 8$
- and a start point $x_0 = 1.2$
- Optimisation problem: $\min_x f(x)$



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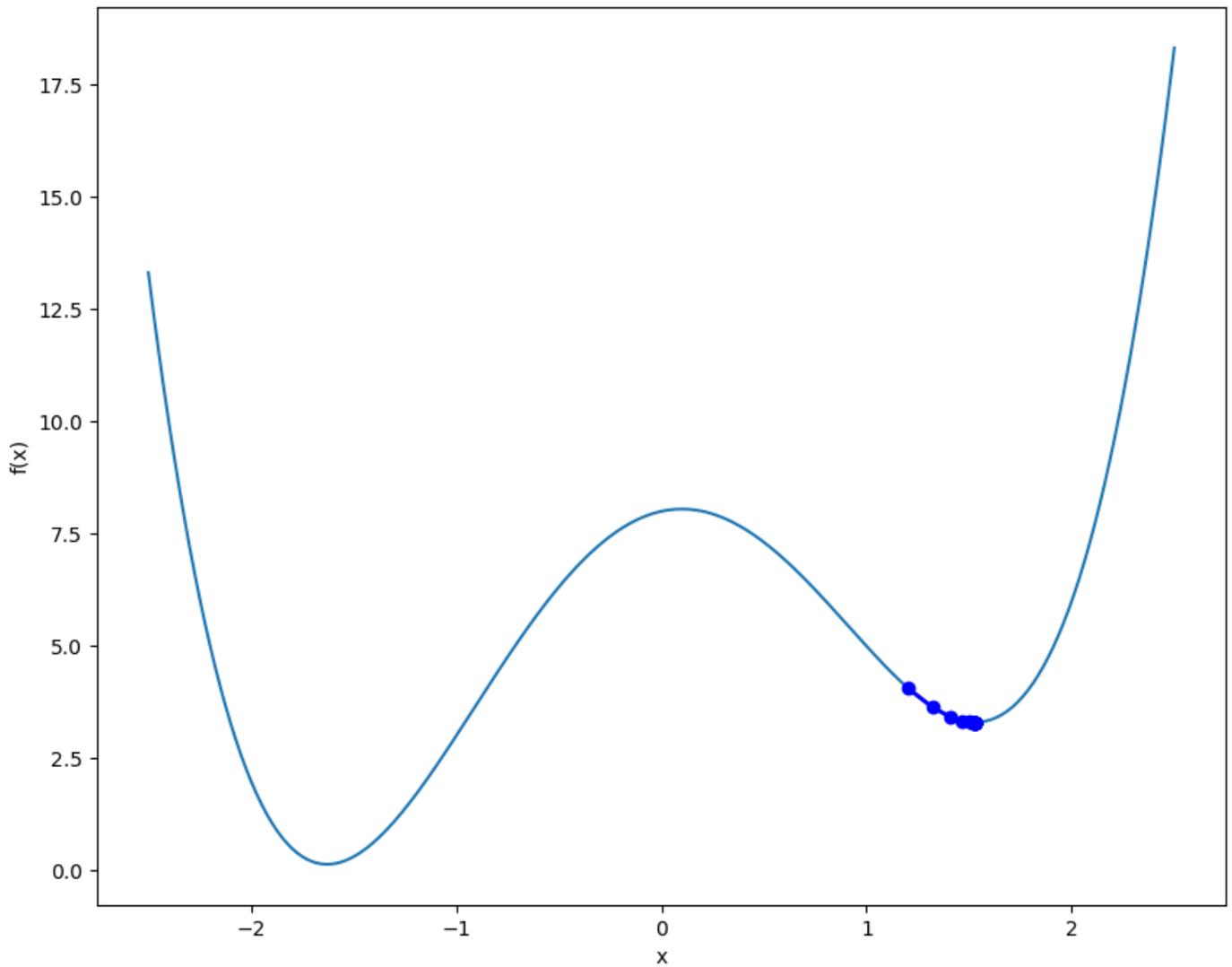
Gradient Descent finds the **local minimum**



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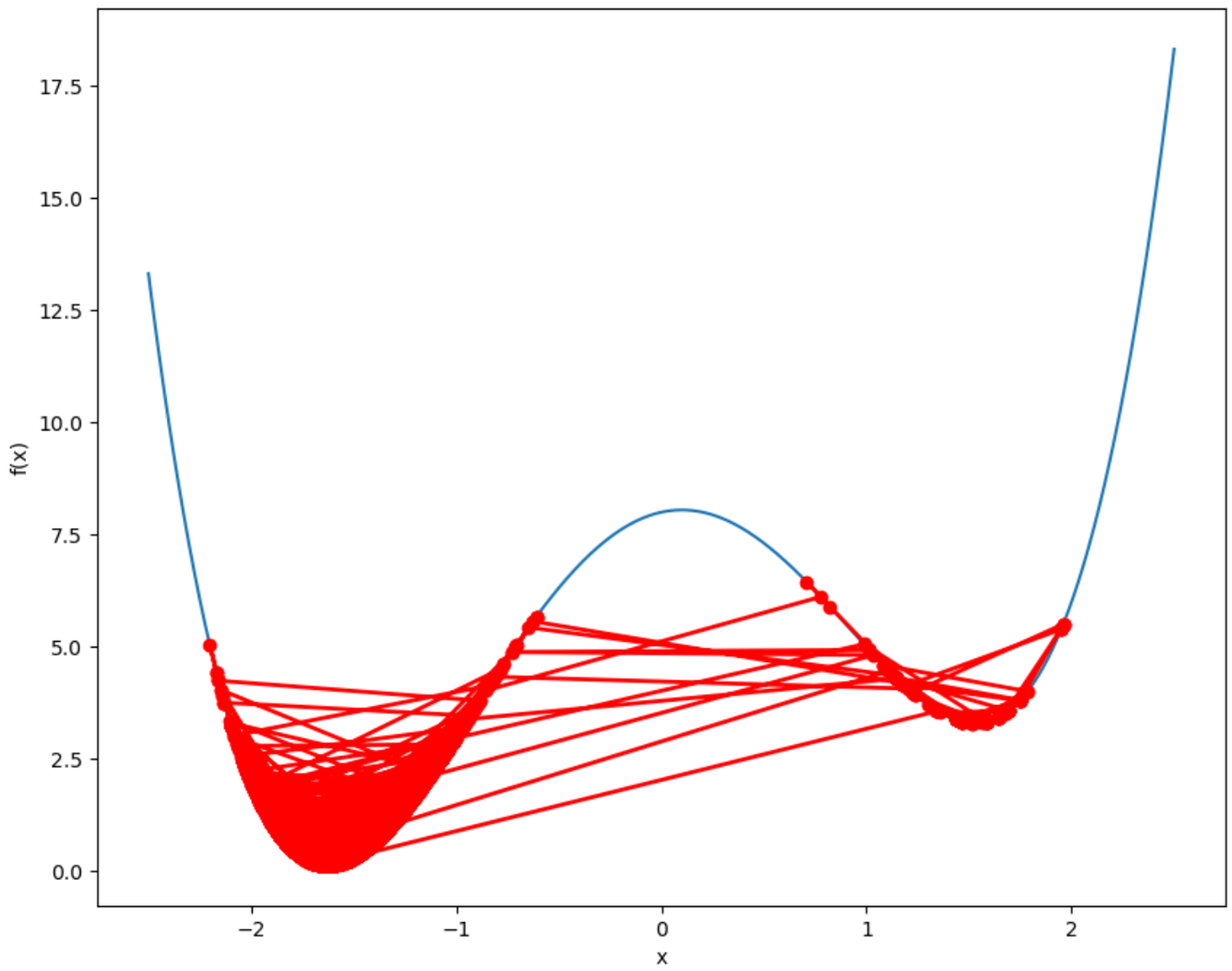
Simulated Annealing explores the whole space and finds the **global minimum**



$T_0 = 1.0$

$\sigma = 1.0$

`max_iter = 2e4`

Simulated Annealing

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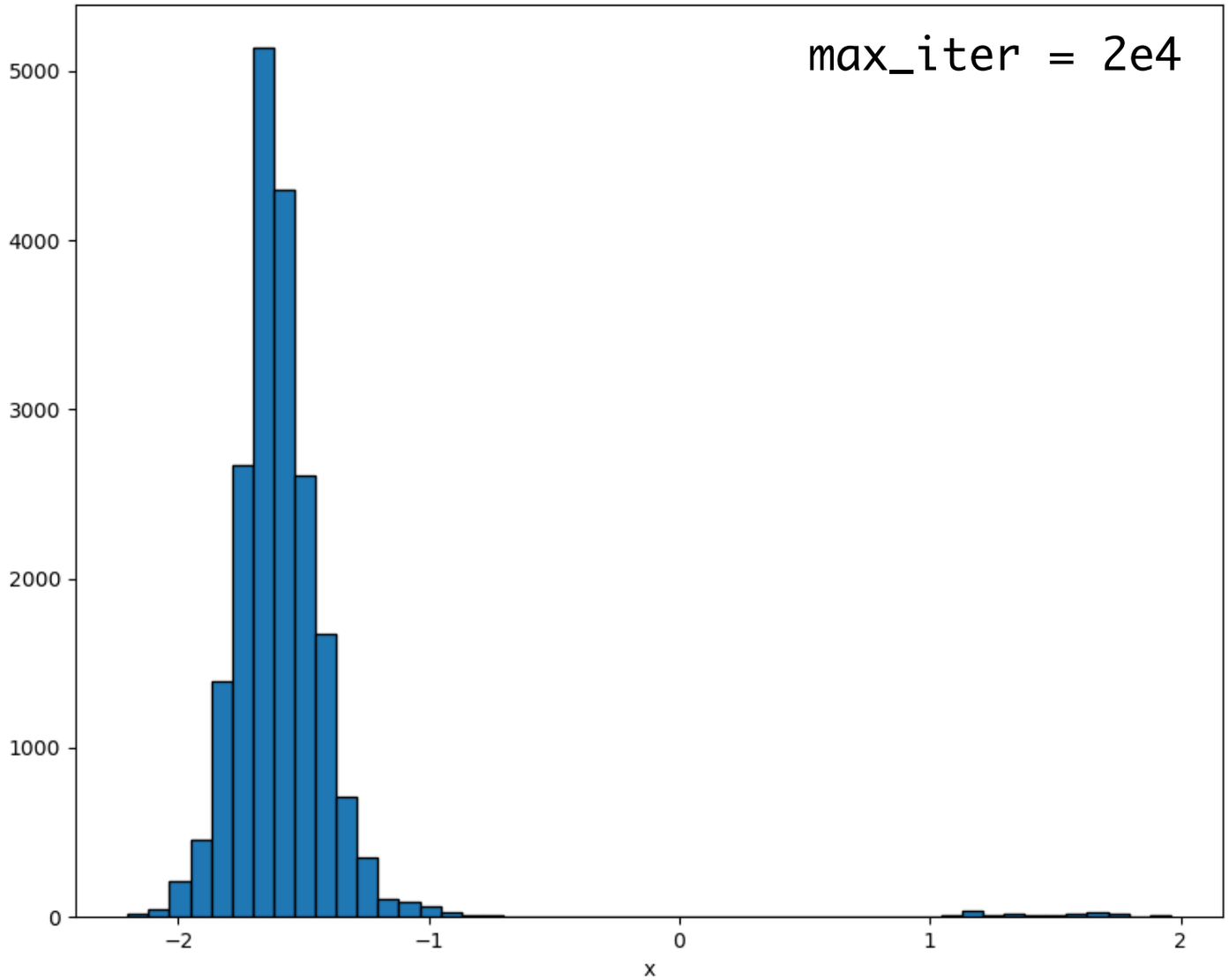
- **Plot the histogram**!

  It helps visualise how the algorithm samples the search space and converges to the **global** minimum.

Monte Carlo Sampling



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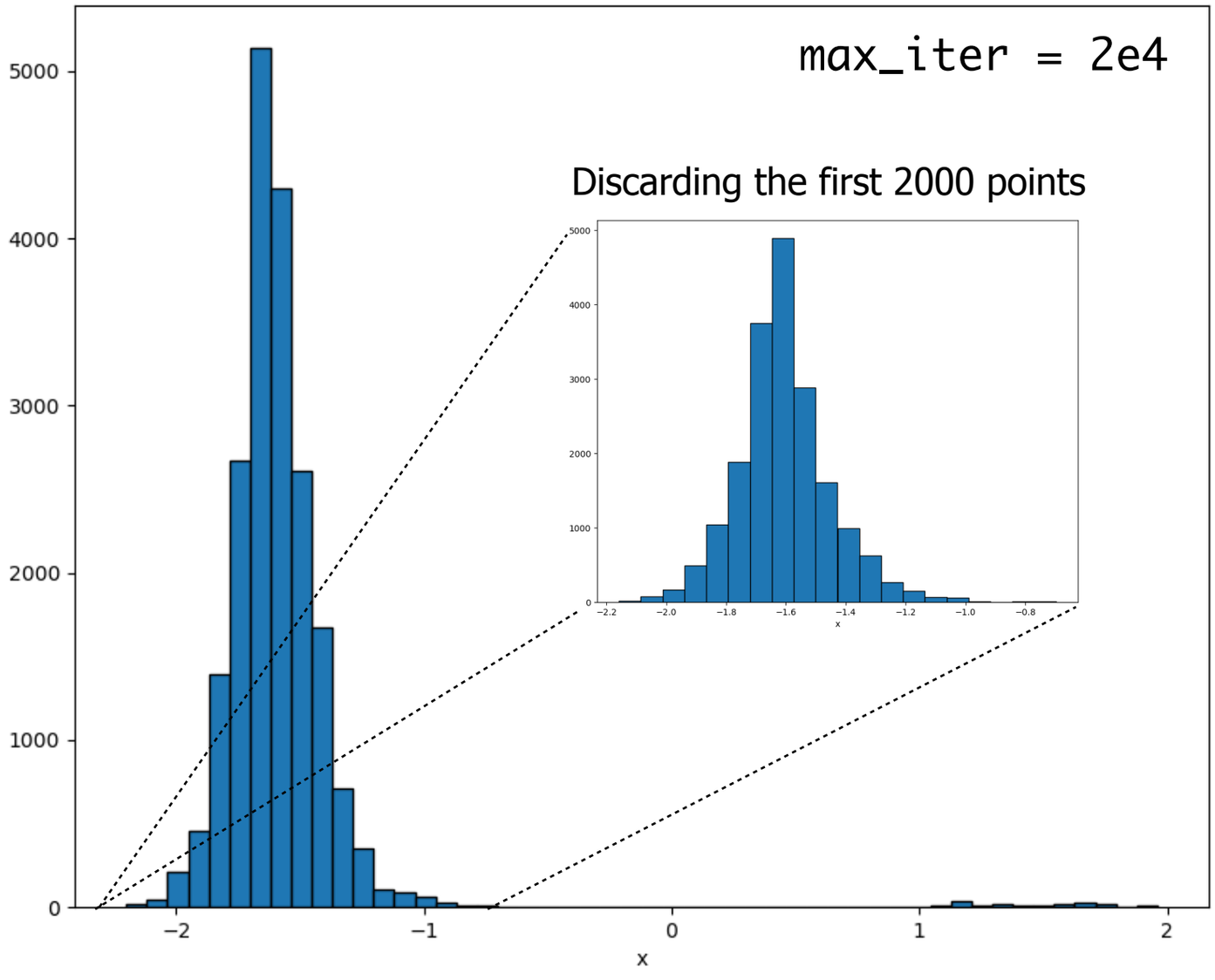
Monte Carlo Sampling

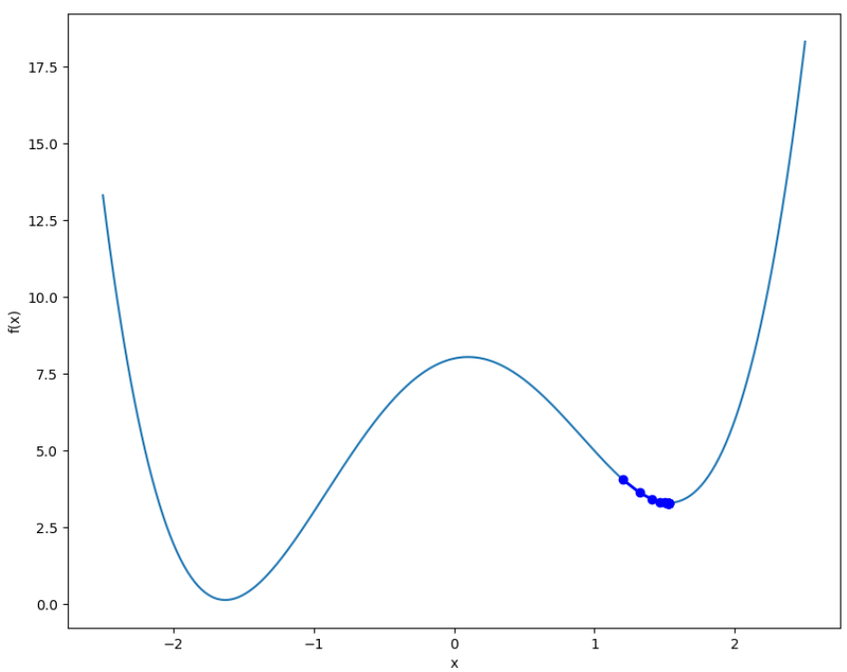
Mean over the dominant peak: $\bar{x} \approx -1.60$

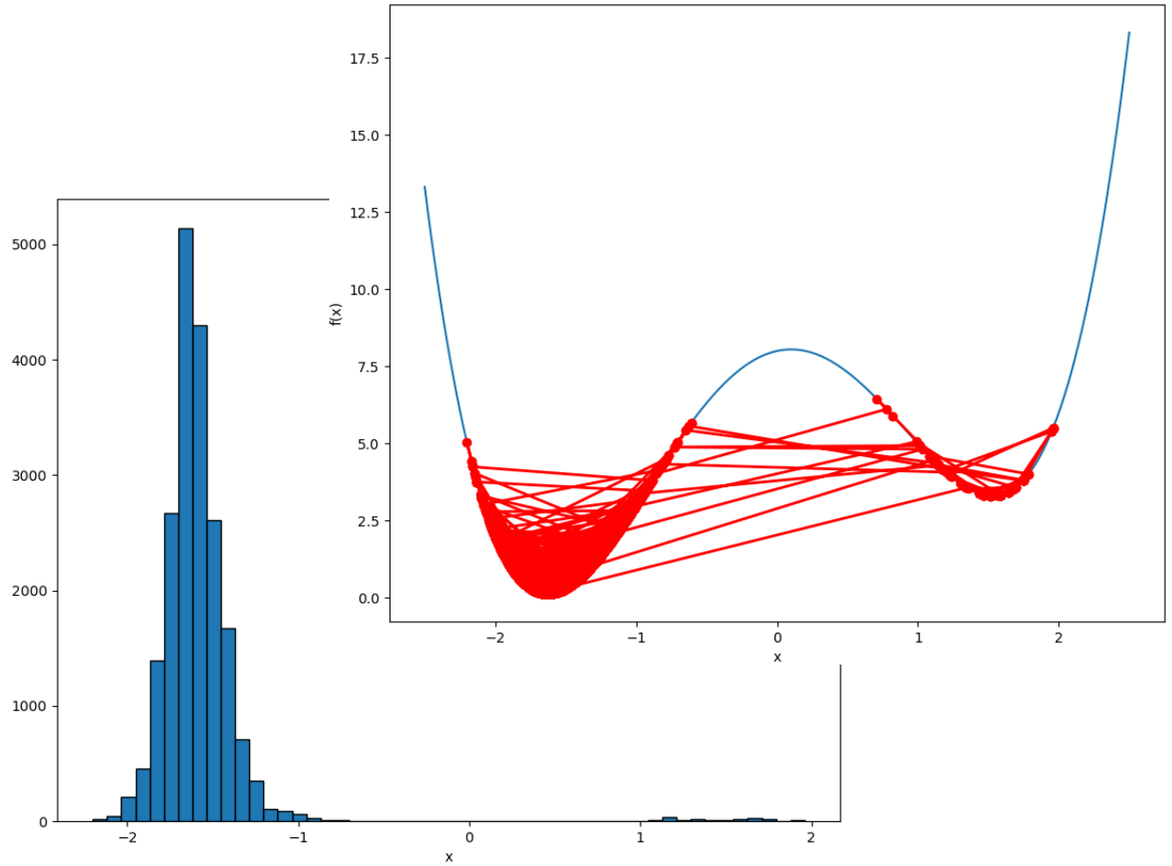


Simulated Annealing

- **Gradient Descent** is a **deterministic gradient-based** optimisation algorithm, suitable for smooth, differentiable functions, efficient for finding **local minima**, especially in convex problems.

- **Simulated Annealing** is a **probabilistic sampling-based** optimisation algorithm, suitable for a wide range of problems, including non-differentiable and non-convex functions, capable of finding **global minima** by escaping local minima through probabilistic moves.





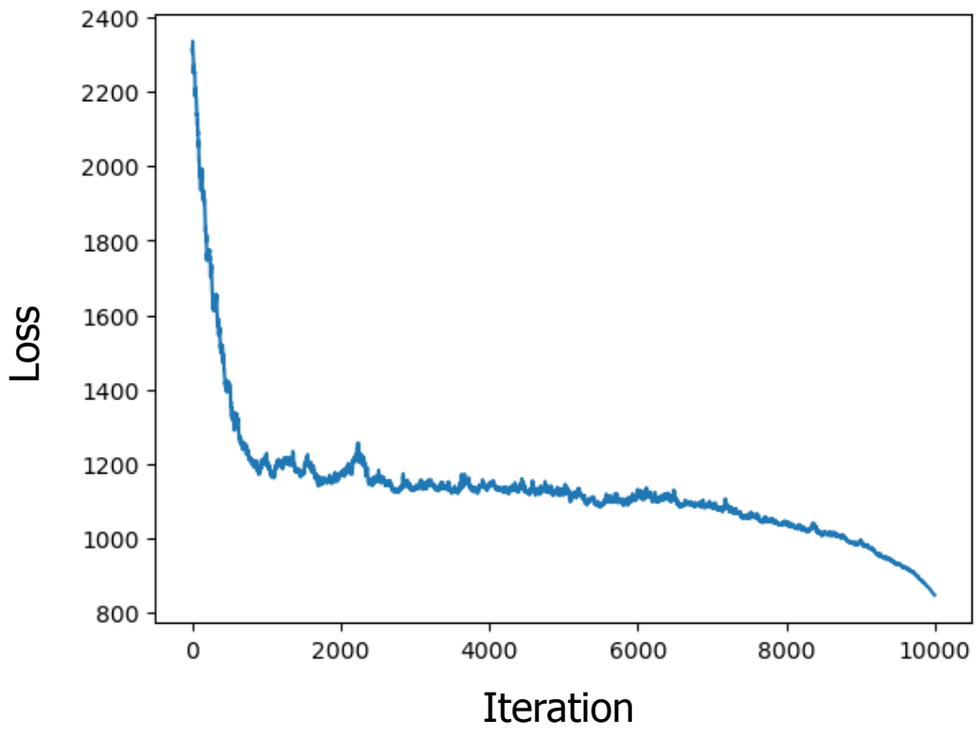
Simulated Annealing

```python
def simulated_annealing(x0, T0, sigma, f, n_iter = 2.5e5, burn_in = 2e5):

    x = x0.copy()  # initialize x
    T = T0         # initialize T
    n_params = x0.shape[0]  # number of parameters to be optimized

    # Means and covariance matrix for the jump distribution -> multivariate normal with mean 0 and standard deviation sigma
    means = np.full(n_params, 0)
    cov_matrix = np.diag(np.full(n_params, sigma))

    # Size of the output array after burn_in
    size_out = int(n_iter - burn_in)
    v = np.zeros((size_out, n_params))

    iter_counter = 0
    print("Initial loss:", f(x))
    # Start main loop
    while iter_counter < n_iter:
        iter_counter += 1;
        x_old = x;
        x_proposal = x_old + np.random.multivariate_normal(means, cov_matrix )
        DeltaE = f(x_proposal) - f(x_old)
        # Metropolis accept/reject step
        if np.exp(-np.clip(DeltaE/T,-100,100)) >= np.random.rand():
            x = x_proposal
        else:
            x = x_old
        # Update temperature according to schedule
        T = T0*(1-iter_counter/n_iter)
        # Keep track of the algorithm state
        if iter_counter%10000 == 0:
            print("Iteration ", iter_counter, " - Temperature:", T, "Loss:", f(x))
        if iter_counter > burn_in:
            v[iter_counter-int(burn_in)-1, :] = x

    return v
```

Loss function

- Run SA for different values of T_0 and σ, and look at the evolution of the loss (objective) function (e.g., MSE).

```
T0 = 1
sigma = 1
outSA = simulated_annealing(x0, T0, sigma, mse, n_iter = 2.5e5, burn_in = 2e5)

plt.figure()
mse_curve = np.apply_along_axis(mse, 1, outSA)
plt.plot(mse_curve)
plt.show(block=False)
```



Loss function

- Run SA for different values of T_0 and σ, and look at the evolution of the loss (objective) function (e.g., MSE). **Which one would you consider the "best"?**