

# Simulated Annealing — Part 2

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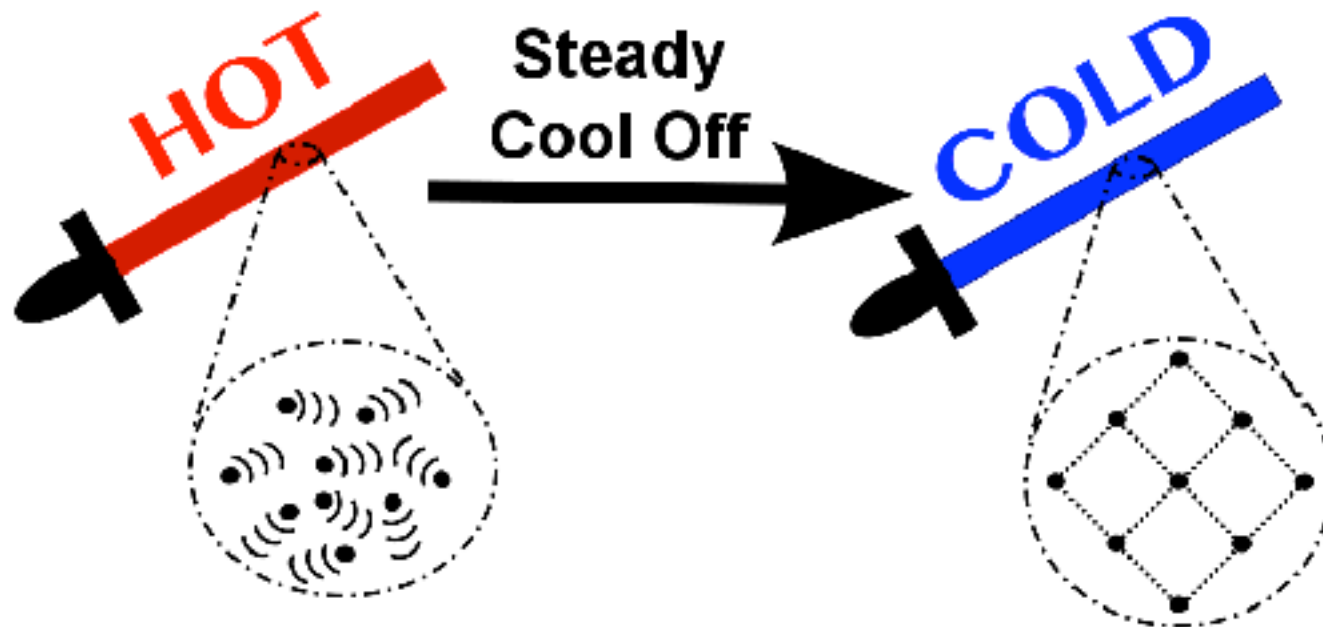
# Simulated Annealing

Simulated Annealing (assuming maximisation)

1. current\_solution = generate initial solution randomly
2. Repeat:
  - 2.1 rand\_neighbour = generate random neighbour of current\_solution
  - 2.2 If  $\text{quality}(\text{rand\_neighbour}) \leq \text{quality}(\text{current\_solution})$  {
    - 2.2.1 With some probability,**  
current\_solution = rand\_neighbour
  - } Else current\_solution = rand\_neighbour
  - 2.3 Reduce probability**
- Until a maximum number of iterations

# Metallurgy Annealing

- A blacksmith heats the metal to a very high temperature.
- When heated, the steel's atoms can move fast and randomly.



- The blacksmith then lets it cool down slowly.
- If cooled down at the right speed, the atoms will settle in nicely.
- This makes the sword stronger than the untreated steel.





# Probability Function

Probability of accepting a solution of equal or worse quality, inspired by thermodynamics:

$$e^{\Delta E/T}$$

$$\Delta E = \text{quality}(\text{rand\_neighbour}) - \text{quality}(\text{current\_solution})$$

( $\leq 0$ )

Assuming maximisation...

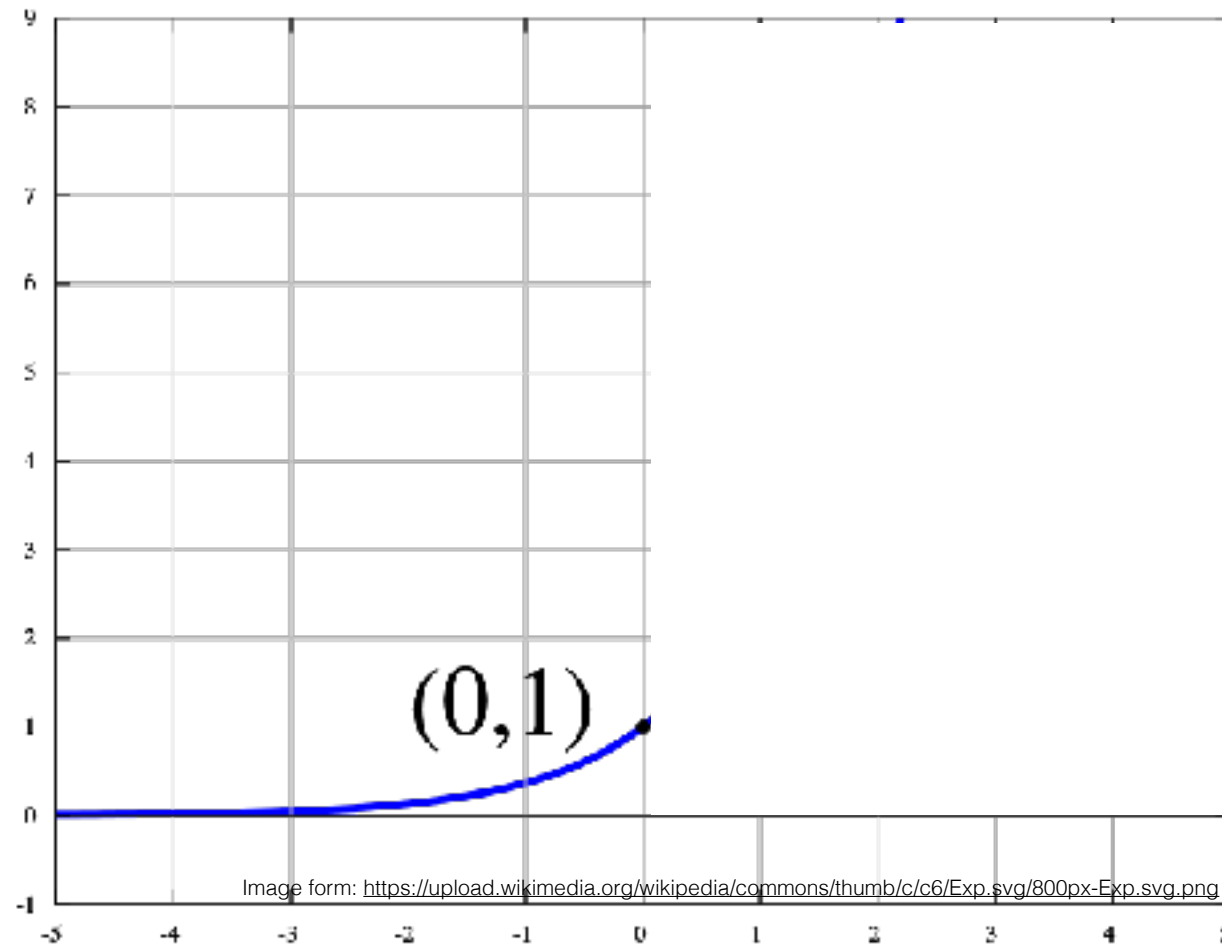
$$T = \text{temperature}$$

( $> 0$ )

$$e = 2.71828\dots$$

# Exponential Function

$$e^{(\leq 0) \Delta E/T}$$

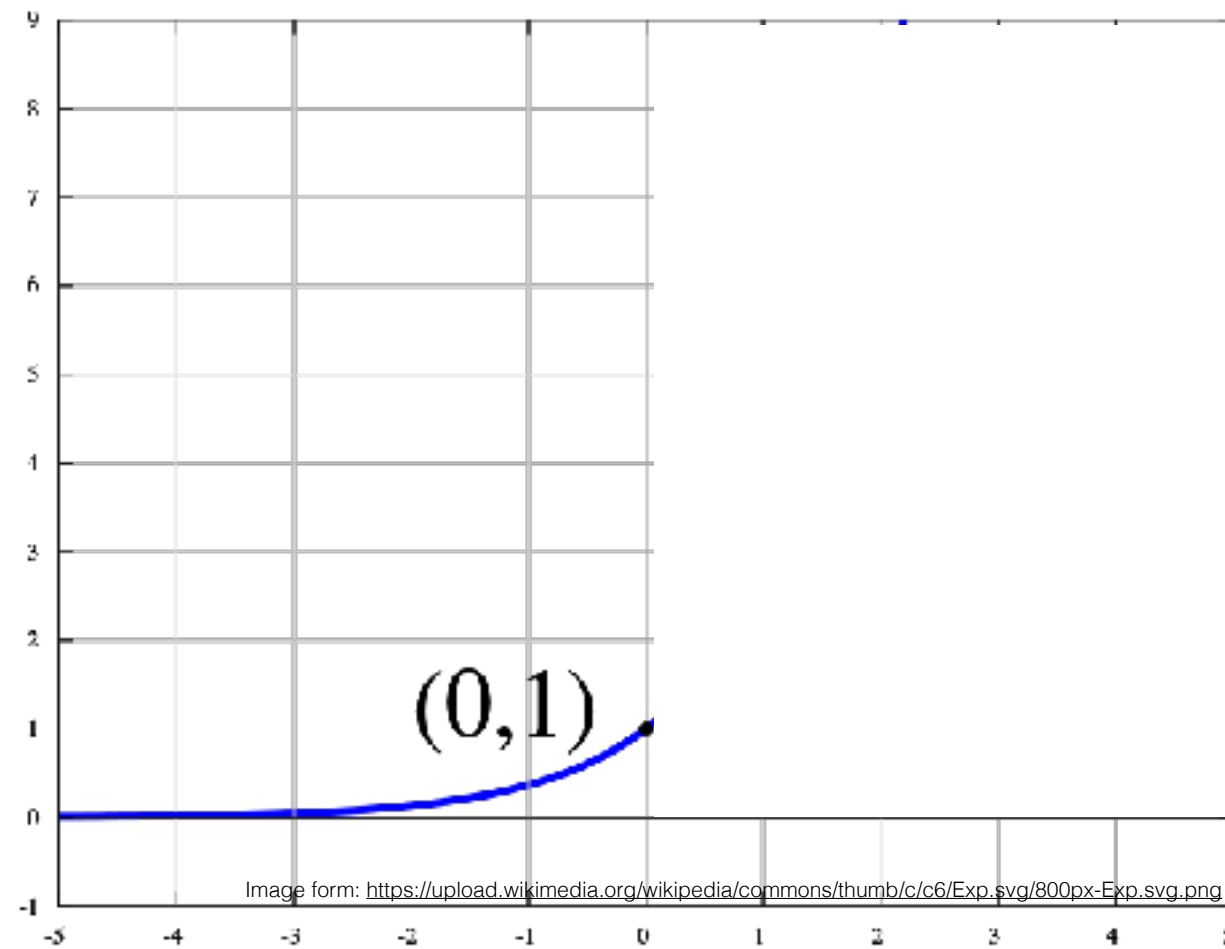


$$\Delta E/T$$

# Exponential Function

$$e^{\Delta E/T}$$

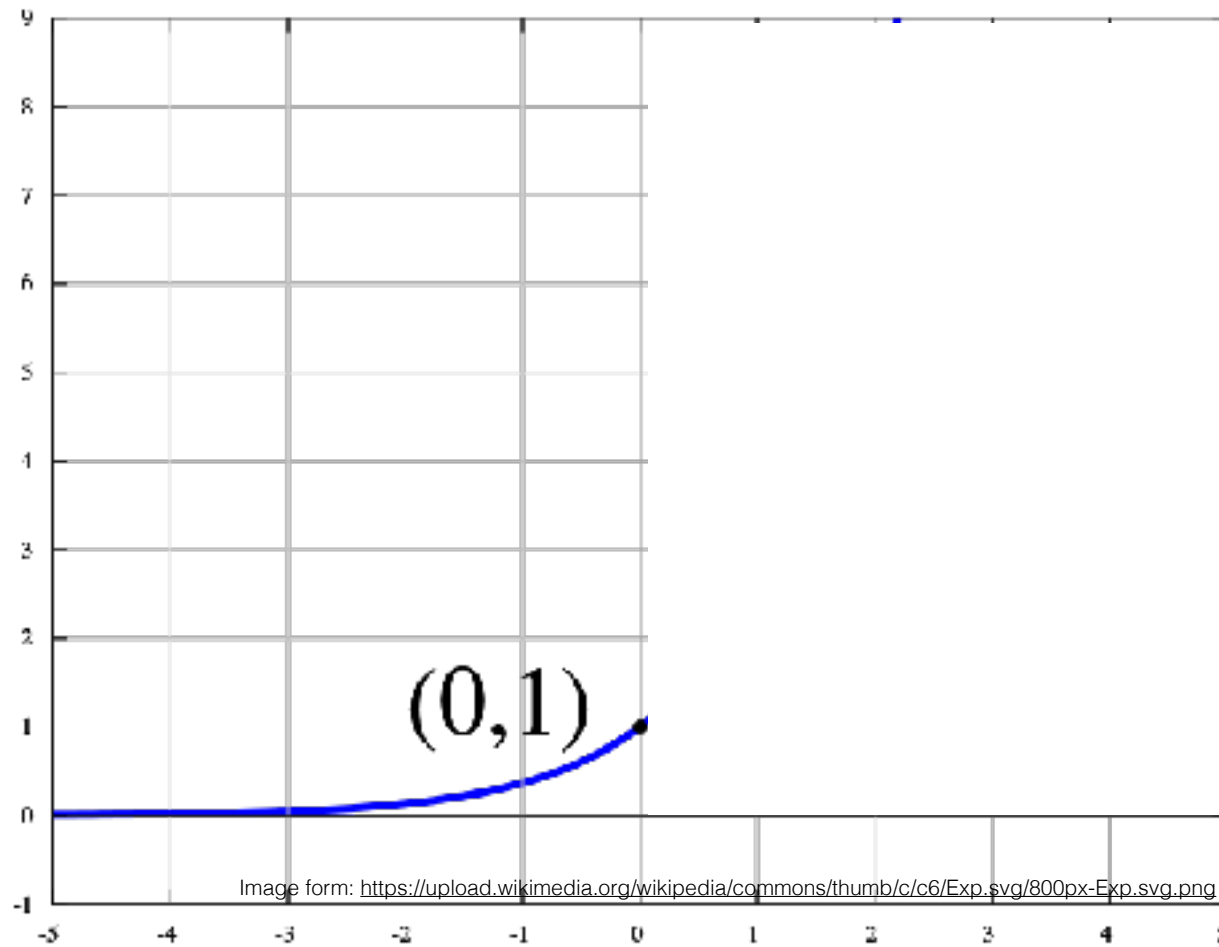
$e^{\Delta E/T}$



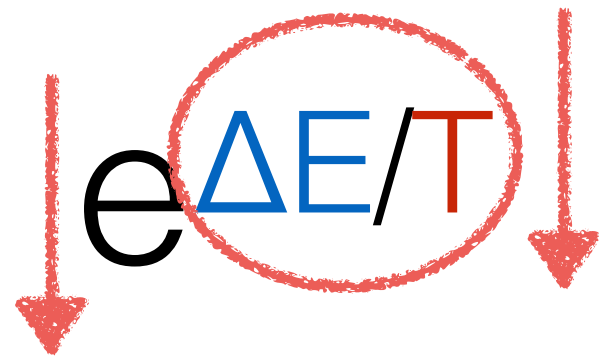
$$\Delta E/T$$

# Exponential Function

$$e^{\Delta E/T}$$



$$\Delta E/T$$



But never  
reaches  
zero



# How Does $\Delta E$ Affect the Probability?

Probability of accepting a solution of equal or worse quality:

$$e^{-\Delta E/T}$$

$\Delta E = \text{quality}(\text{rand\_neighbour}) - \text{quality}(\text{current\_solution})$   
( $\leq 0$ )

Assuming maximisation...

$T = \text{temperature}$   
( $> 0$ )

The worse the neighbour is in comparison to the current solution,  
the less likely to accept it.

# How Does $\Delta E$ Affect the Probability?

Probability of accepting a solution of equal or worse quality:

But never reaches zero

$$e^{\Delta E / T}$$

$\Delta E = \text{quality}(\text{rand\_neighbour}) - \text{quality}(\text{current\_solution})$   
( $\leq 0$ )

Assuming maximisation...

$T = \text{temperature}$   
( $> 0$ )

We always have some probability to accept a bad neighbour, no matter how bad it is.

# How Does $\Delta E$ Affect the Probability?

Probability of accepting a solution of equal or worse quality:

$$e^{-\Delta E / T}$$

$\Delta E = \text{quality}(\text{rand\_neighbour}) - \text{quality}(\text{current\_solution})$

$\Delta E$  ( $\leq 0$ )

Assuming maximisation...

$T = \text{temperature}$   
( $> 0$ )

The better the neighbour is, the more likely to accept it.

# How Should the Probability be Set?

- **Probability to accept solutions with much worse quality should be lower.**
  - **We don't want to be dislodged from the optimum.**
- High probability in the beginning.
  - More similar effect to random search.
  - Allows us to **explore** the search space.
- Lower probability as time goes by.
  - More similar effect to hill-climbing.
  - Allows us to **exploit** a hill.

# How Does $T$ Affect the Probability?

Probability of accepting a solution of **equal or worse quality**:



$$e^{\frac{\Delta E}{T}}$$

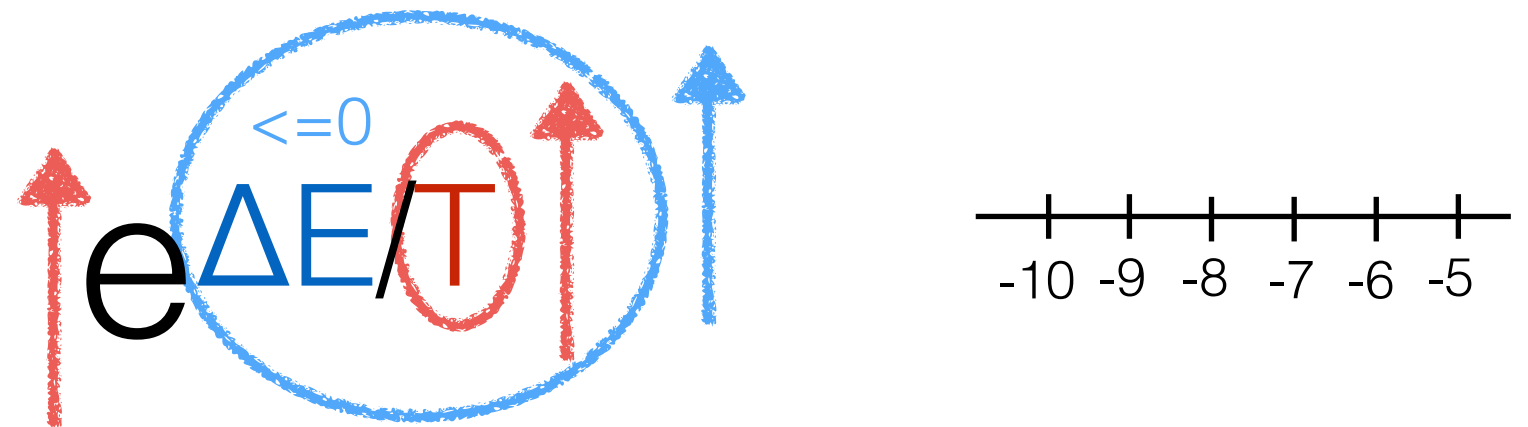
$\Delta E = \text{quality}(\text{rand\_neighbour}) - \text{quality}(\text{current\_solution})$   
( $\leq 0$ )

Assuming maximisation...

$T = \text{temperature}$   
( $> 0$ )

# How Does $T$ Affect the Probability?

Probability of accepting a solution of equal or worse quality:



The diagram shows the formula  $e^{\Delta E / T}$  for the probability of accepting a worse solution. The entire formula is enclosed in a blue hand-drawn circle. Above the circle, the text " $\leq 0$ " is written in blue. To the left of the circle, a red arrow points upwards. To the right of the circle, a blue arrow points upwards. Further to the right, a horizontal number line is shown with tick marks at -10, -9, -8, -7, -6, and -5.

$$\Delta E = \text{quality}(\text{rand\_neighbour}) - \text{quality}(\text{current\_solution})$$

( $\leq 0$ )

Assuming maximisation...

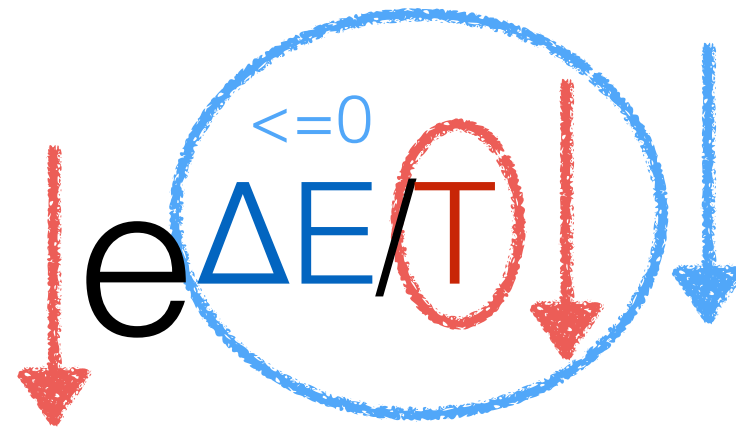
$T$  = temperature  
( $> 0$ )

If  $T$  is higher, the probability of accepting the neighbour is higher.



# How Does $T$ Affect the Probability?

Probability of accepting a solution of equal or worse quality:



A diagram illustrating the probability formula  $e^{-\Delta E/T}$ . The expression is enclosed in a blue hand-drawn circle. Above the circle, the text " $\leq 0$ " is written in blue. A red hand-drawn circle highlights the denominator  $T$ . A red arrow points down from the left towards the expression, and a blue arrow points down from the right towards the expression.

$$\Delta E = \text{quality}(\text{rand\_neighbour}) - \text{quality}(\text{current\_solution})$$

( $\leq 0$ )

Assuming maximisation...

$T$  = temperature  
( $> 0$ )

If  $T$  is lower, the probability of accepting the neighbour is lower.

# How Does $T$ Affect the Probability?

Probability of accepting a solution of equal or worse quality:

Diagram illustrating the condition for a superconductor:  $\Delta E/T \leq 0$ . The expression is enclosed in a blue circle, with a red circle around the  $T$ . Red and blue arrows point downwards on either side.

$$\Delta E = \text{quality}(\text{rand\_neighbour}) - \text{quality}(\text{current\_solution})$$

( $\leq 0$ )

Assuming maximisation...

T = temperature  
( $>0$ )

So, reducing the temperature over time would reduce the probability of accepting the neighbour.

# How Should the Temperature be Set?

- High probability in the beginning.
  - More similar effect to random search.
  - Allows us to **explore** the search space.

T should start high.

- Lower probability as time goes by.
  - More similar effect to hill-climbing.
  - Allows us to **exploit** a hill.

T should reduce slowly over time.



Image from: <http://static.comicvine.com/uploads/original/13/130470/2931473-151295.jpg>

# How to Set and Reduce **T**?

- T starts with an initially high pre-defined value (parameter of the algorithm).
- There are different update rules (schedules)...
- Update rule:
  - $T = \alpha T$ ,  
 $\alpha$  is close to, but smaller than, 1  
e.g.,  $\alpha = 0.95$

# Simulated Annealing

Simulated Annealing (assuming maximisation)

Input: initial temperature  $T_i$

1. current\_solution = generate initial solution randomly

**2.  $T = T_i$**

3. Repeat:

3.1 rand\_neighbour = generate random neighbour of current\_solution

3.2 If quality(rand\_neighbour)  $\leq$  quality(current\_solution) {

**3.2.1 With probability  $e^{\Delta E/T}$ ,**

current\_solution = rand\_neighbour

} Else current\_solution = rand\_neighbour

**3.3  $T = \text{schedule}(T)$**

Until a maximum number of iterations

# Simulated Annealing

Simulated Annealing (assuming maximisation)

Input: initial temperature  $T_i$ , minimum temperature  $T_f$

1. current\_solution = generate initial solution randomly

**2.  $T = T_i$**

3. Repeat:

3.1 rand\_neighbour = generate random neighbour of current\_solution

3.2 If quality(rand\_neighbour)  $\leq$  quality(current\_solution) {

**3.2.1 With probability  $e^{\Delta E/T}$ ,**

current\_solution = rand\_neighbour

} Else current\_solution = rand\_neighbour

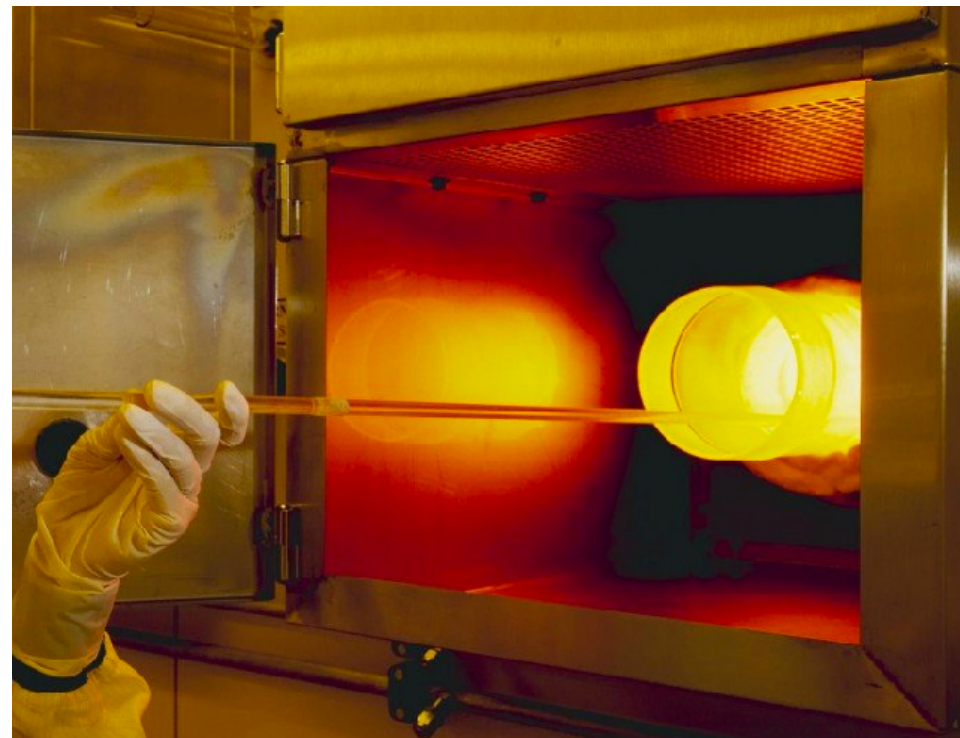
**3.3  $T = \text{schedule}(T)$**

**until a minimum temperature  $T_f$  is reached or  
until the current solution “stops changing”**



# Local Search

- Simulated annealing can also be considered as a local search, as it allows to move only to neighbour solutions.
- However, it has mechanisms to try to escape from local optima.



# Optimality

Is simulated annealing guaranteed to find the optimum?

- Simulated annealing is **not** guaranteed to find the optimum **in a reasonable amount of time**.
- Whether or not it will find the optimum depends on the termination criteria and the schedule.
- If we leave simulated annealing to run indefinitely, it is guaranteed to find an optimal solution, depending on the schedule used.
- However the time required for that can be prohibitive — even more than the time to enumerate all possible solutions using brute force.
- Therefore, the advantage of simulated annealing is that it can frequently obtain good (near optimal) solutions, by escaping from several poor local optima in a reasonable amount of time.

# Time and Space Complexity

- Time complexity:
  - We will run more or less iterations depending on the schedule and minimum temperature / termination criterion.
  - It is possible to compute the [time complexity to reach the optimal solution](#), but it varies depending on the problem and may be even worse than the brute force time complexity, as mentioned in the previous slide.
- Space complexity:
  - Depends on how the design variable is represented in the algorithm.

# Summary

- The probability of accepting neighbouring solutions of equal or worse quality than the current solution is inspired by metallurgy annealing.
- A “temperature” is used to control how low the probability is.
- A schedule is used to reduce the “temperature” over time.
- The worse a neighbour is, the lower the chances of accepting it.

## Next

- Dealing with constraints.