UNIVERSITY OF AMSTERDAM

Report

Charged Particles in a Circle

Optimizing Particle Configurations with Simulated Annealing

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Abstract

In this report, we apply simulated annealing methods to optimize the two-dimensional distribution of identically charged particles on an in a circular potential well with infinitely tall walls.

1 Introduction

Simulated annealing is an optimization method that is inspired by the natural process of crystal formation in materials (Kirkpatrick, Gelatt, & Vecchi, 1983). The target function is minimized by allowing for random fluctuations in the system state and accepting mostly steps that improve the solution and some which worsen it. These increasing steps deteriorate the solution in the short term but improve the chances of finding a global minimum. Analogously to a physical system cooling down and becoming stable, the rate of accepting steps that worsen the solution is periodically decreased.

1.1 Theory of Simulated Annealing

Applied to a continuous optimization problem, simulated annealing minimizes the energy E of a system with states $x \in S \subset \mathbb{R}^n$, that is, finding

$$x^* = argmin_{x \in S} E(x)$$

The method works by repeatedly selecting neighboring states $\hat{x}$, and observing their change on the system energy. If the new energy $E(\hat{x})$ is lower than $E(x)$, the system is changed to the new state. In contrast to many local optimization methods, even steps whose energy is higher than $E(x)$ are sometimes accepted. The acceptance rate of steps that increase the energy is set by the system temperature T, which is adjusted according to a non-increasing cooling schedule. The

simulated annealing procedure is described in Algorithm 1.

Algorithm 1 Simulated Annealing Algorithm

```
Choose initial state x, initial temperature T
while not stopping condition do
    Select a neighbor x' of x
    Compute ΔE = E(x') − E(x)
    Accept x' with probability p = e^{−ΔE/T}
    Decrease T according to the cooling schedule
end while
```

At a constant temperature, the series of system states can be viewed as a Markov chain. With an infinite temperature, all steps are accepted, so the stationary distribution of the system is uniform over all states. Conversely, with a temperature of 0, the only stationary states are the global minima. The challenge in applying simulated annealing is choosing a cooling schedule and neighboring procedure that ensure sufficient exploration of the state space without doing too much unnecessary work.

1.2 Charged Particles on a Circle

We will now introduce the optimization problem to be solved in this report: A number of particles of equal charge are confined to a circular potential well with infinitely high walls. The system state is given by the locations $x = (x_1, ..., x_N) \in \mathbb{R}^{2N}$ where each $x_i \in \mathbb{R}^2$ is the location of particle i on the plane. The forces between particles are described by pairwise electrostatic repulsion, which is inversely proportional to the square of particle distances:

$$F(x_i, x_j) = \frac{x_i - x_j}{||x_i - x_j||_2^3}$$

The total potential energy of the system is thus given by

$$E(x) = \frac{1}{2} \sum_{i \neq j} \frac{1}{||x_i - x_j||_2}$$

This problem of the optimal configuration of charged particles on a circle is well studied and has been solved for up to 80 particles (Nurmela, 1998). A previous work applying simulated annealing to the problem (Wille & Vennik, 1985) with a very rudimentary cooling and neighboring procedures successfully generated configurations with very low energies for up to 23 particles, but did not always find the optimal configuration. This report intends to improve these results by testing the performance of different cooling schedules and neighboring procedures.

1.3 Related Work

Foundational studies in charge optimization, simulated annealing, and Monte Carlo methods provide critical insights for this research:

1. *The Thomson Problem* by Altschuler et al. (1997) explores minimal energy configurations of charges on a sphere, offering optimization principles applicable to circular boundaries. This study adopts similar energy minimization approaches to analyze confined particle systems (?, ?).
2. *Simulated Annealing* by Kirkpatrick et al. (1983) introduces a cooling-based optimization framework, forming the basis for the cooling schedules employed here. These schedules guide the convergence of particle configurations toward minimal energy states (?, ?).
3. *Monte Carlo Methods in Statistical Physics* by Binder (1978) outlines stochastic techniques for sampling configurations, integral to our implementation of particle perturbations and exploration of the configuration space (?, ?).

These works collectively inform the simulation design and optimization methods applied in this study, enabling effective exploration of minimal energy configurations for charged particles within a circular boundary.

2 Methods

2.1 Cooling Schedules

To ensure convergence to the global minimum, the cooling schedule must satisfy certain theoretical con-

ditions. These are:

- $T_{n+1} < T_n$: The temperature must decrease monotonically over iterations.
- $T \to 0$ as $n \to \infty$: The temperature must asymptotically approach zero to allow the system to stabilize.
- T_n decreases at an appropriate rate: The cooling must be slow enough to ensure sufficient exploration of the state space and prevent premature convergence.

When these conditions are met, the Markov Chain Monte Carlo process underlying simulated annealing guarantees that the stationary distribution converges to the global minimum. The schedules explored in this work are as follows:

1. **Reference Schedule** ((Wille & Vennik, 1985)):

$$T_{\text{new}} = \begin{cases} 0.95 \cdot T, & \text{if steps\_until\_decrease} = 0, \\ T, & \text{otherwise.} \end{cases}$$

   A classic schedule using periodic temperature reduction.

2. **Exponential Cooling Schedule**:

$$T_{\text{new}} = 0.999 \cdot T$$

   Reduces temperature by a fixed multiplicative factor.

3. **Sigmoid Cooling Schedule**:

$$T_{\text{new}} = T \cdot \frac{1}{1 + \exp\left(\frac{\text{step} - 5000}{1000}\right)}$$

   Gradual cooling, transitioning smoothly near a midpoint.

4. **Inverse Square Root Cooling Schedule**:

$$T_{\text{new}} = \frac{T}{\sqrt{\text{step} + 1}}$$

   Decreases temperature inversely with the square root of the step.

5. **Cosine Annealing Cooling Schedule**:

$$T_{\text{new}} = 0.5 \cdot T \cdot \left(1 + \cos\left(\frac{\pi \cdot \text{step}}{10000}\right)\right)$$

   Implements periodic cooling with cosine-based oscillations.

Here, T is the temperature, T_{new} the updated temperature, and *step* the current process step.

2.2 Neighboring procedure

For any particle configuration x, a neighboring state $\hat{x} = (x1, ..., x_{i=1}, x_i + \Delta x, x_{i+1}, ..., x_n)$ can be reached by slightly shifting the location of one particle. If the particle is moved outside of the circle, we project the updated location back onto the boundary to ensure our new state is valid. Since Δx is a local movement, it makes sense to view it in polar coordinates. A neighboring procedure then consists of a strategy for selecting a direction θ and magnitude r of Δx. One natural choice for the direction is to follow the sum of all forces acting on the particle. Following only this strategy, however, is not enough to explore the state space, so selecting a uniform random direction is also considered.

The step size r decides how much the state is changed in each step. To allow the state to get very close to a local minimum towards the end of the simulation, r can be decreased with the temperature. In this work, we consider the following four step size schedules:
A constant step size:

$$r = 0.1$$

Scaling the step size as the square root of the temperature:

$$r = \sqrt{T}$$

Selecting r from a uniform distribution:

$$r \sim U(0, 1)$$

Selecting r from a uniform distribution and scaling

with the temperature:

$$r \sim \sqrt{T} \cdot U(0,1)$$

2.3 Experimental Setup

2.3.1 Finding Optimal Particle Configurations

This study explores the optimization of particle configurations within a circular boundary by progressively increasing the system's complexity. The methodology involves three stages:

1. **Stage 1**: Small Systems (Up to 11 Particles).
   Simulations were conducted for systems with up to 11 particles. Key metrics such as the number of particles within the boundary (floating particles) and total system energy were recorded to evaluate the algorithm's effectiveness.

2. **Stage 2**: Transitional Case (12 Particles).
   The system's behavior was analyzed for 12 particles, a transitional configuration where the optimization algorithm faced increased complexity. This stage was used to assess the robustness and adaptability of the approach.

3. **Stage 3**: Larger Systems.
   Simulations were extended to systems containing up to 50 particles, with results analyzed to detect trends and identify *"magic numbers"* — particle counts yielding notable configurations.

Each simulation with varying particle sizes was run for a total of 100,000 steps and 50 runs to ensure sufficient exploration and convergence to optimal configurations. To quantify the algorithm's performance, the following metrics were collected for each simulation:

- *Floating Particles:* The number of particles located within the boundary ($r < 0.99$).

- *System Energy:* The total energy, computed as the sum of inverse pairwise distances between particles.

- *Optimal Configuration Likelihood:* The proportion of simulation runs where the number of floating particles matches the configuration with the lowest recorded energy for each particle count.

The simulations utilized the *paper cooling schedule* and the *square root step size schedule*, as these strategies ensured diverse exploration of configurations and efficient convergence, and their detailed descriptions have been provided in Section 2.1 and 2.2 respectively. We hope and hypothesize that, with this experimental setup and our model, we can outperform the Willes/Vernik paper in positional configurations.

2.3.2 Cooling Schedules Setup

Cooling schedules play a critical role in simulated annealing. In this study, we explore various cooling schedules and their characteristics, detailed in subsection 2.1.
We evaluate the following aspects:

- *Temperature Convergence:* How quickly does the temperature approach 0?

- *Energy Convergence:* How quickly does the system's energy approach its minimum?

- *Lowest Energy:* Which schedule achieves the lowest energy, indicating the most optimal solution?

Energy and temperature values are plotted over time across multiple runs to account for stochasticity. The optimal schedule is determined by comparing the final energy levels across runs, with the schedule yielding the lowest overall energy deemed the most effective.

2.3.3 Markov Chain Length

Using a cooling schedule that performed well in the experiments of section 2.3.2, we apply our annealing algorithm to the problem with 50 particles and analyze the effect of the Markov chain length on the final energy values and the likelihood of finding the global minimum.

2.3.4 Neighboring Procedure

With the best performing cooling schedule and an adequate markov chain length determined in the previous sections, we compare the different neighboring strategies described in section 2.2. For this, we first evaluate the resulting energies when the step direction is chosen randomly with a likelihood ρ, and along the sum of all forces acting on the particle with a likelihood $1 - \rho$ for different ρ. With the optimal mix of direction strategies, we then compare the energies of simulations using the different step size schedules. We use a Mann-Whitney U test to distinguish the distributions of the converged energies.

3 Results

3.1 Optimizing Particle Configurations

Table 1 shows the optimal energies, floating particles, and likelihoods for selected particle counts. Floating particles first appear at 12 particles, increasing gradually. Visual analysis indicates that energy increases consistently with particle count.

Figure 1 illustrates the visual representation of the optimal configurations for particle counts 11, 12, and 50, effectively highlighting the transition state at 12 particles.

Figure 2 depicts the two best n=50 solutions against the two worst n=50 solutions, both with steps 100.000 and 50 runs, as explained in the Methods. Its clear that the worse performing ones (meaning energy high) can shift in the placement of particles more, and not have massive differences in energy levels.

Table 1: Optimal Energies and Configurations for Selected Particles

Particles	**Optimal Energy**	**Floating Particles**	**Likelihood**
9	59.85	0	0.26
10	77.25	0	0.10
11	97.19	0	0.80
12	119.15	1	1.00
13	143.62	1	0.94
14	170.69	1	0.40
15	200.45	1	0.10
16	232.90	1	0.02
17	267.64	2	0.30
18	305.01	2	0.02
19	344.99	3	0.70
20	387.26	3	0.36
21	432.40	3	0.08
22	480.26	4	0.72
23	530.42	4	0.30
24	583.51	4	0.12
25	639.36	5	0.56
30	958.23	7	0.60
35	1344.75	9	0.60
40	1800.36	11	0.66
45	2325.04	13	0.42
50	2919.59	16	0.60

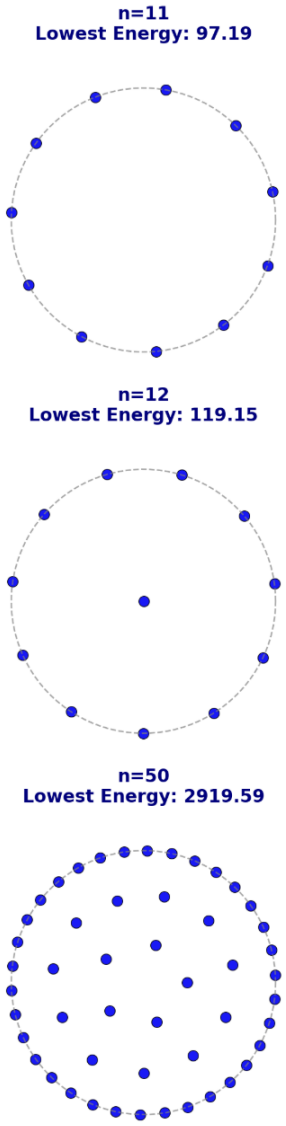

Figure 1: The optimal configurations at 11, 12 and 50 particles.

3.2 Cooling Schedules

In figure 3 we see the comparison for different cooling schedules. The energy levels and temperature are plotted over time. Some interesting observations:

- *Paper & Exponential Cooling Schedules:* These two schedules are closely related, with the primary difference being that the paper cooling schedule updates every 100 steps, while the exponential schedule updates continuously. When comparing the final energies, the zoomed-in plot suggests that the paper cooling schedule performs better than the constantly adapting exponential schedule.

- *Sigmoid Cooling Schedule:* The sigmoid cooling schedule exhibits slow temperature changes initially, followed by more significant adjustments later. While it converges relatively quickly, it produces poor best solutions and has a large standard deviation.

- *Inverse Square Root Cooling Schedule:* This schedule converges very quickly, with the temperature dropping rapidly toward zero. However, it tends to produce less-than-optimal solutions and relatively large standard deviations.

- *Cosine Annealing Cooling Schedule:* This schedule delays its temperature decrease, converging later due to its late approach toward zero.

3.2.1 Direct comparison of cooling schedules

To directly compare the different cooling schedules we can compare the final step of each schedule, a box plot of these steps is visible in figure 4. Here The paper cooling schedule seems to perform the best on average. To confirm this we have performed a Mann-Whitney U test, since the data is not normally distributed. These result show as shown in table 2 that the results are significant in comparison to the other schedules except the exponential cooling schedule.

Table 2: Mann-Whitney U Test results comparing `paper_cooling_schedule` against other schedules.

Schedule	U-Statistic	p-Value
exponential	5183.0	0.66
sigmoid	7380.0	$6.09 * 10^{-9}$
inverse sqrt	4030.0	0.017
cosine annealing	7996.0	$2.5 * 10^{-13}$

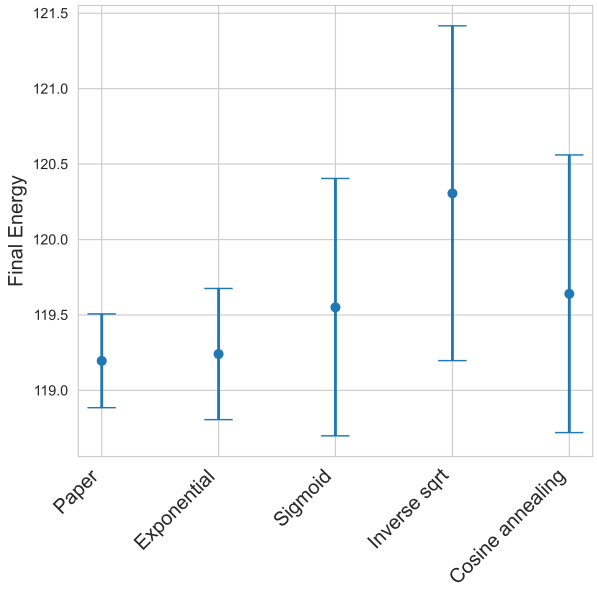

Figure 4: Boxplot of final step: Mean Energies with Std Deviation for each schedule. (On particle 12, with 10000 steps and 50 runs)

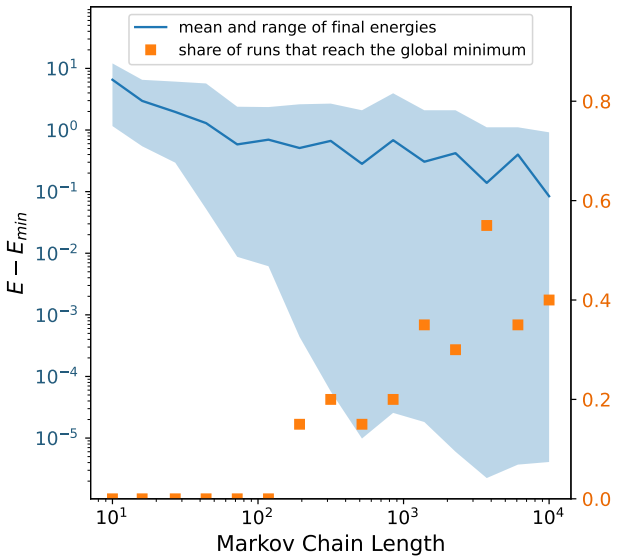

Figure 5: Impact of Markov chain length on range and mean of approximation errors $E - E_{min}$ and likelihood of converging to the global optimum E_{min} for 50 particles

3.3 Markov Chain Length

We simulate 20 runs with the exponential cooling schedule and various Markov chain lengths on 50 particles. The error of our approximation and the likelihood of finding the optimum are plotted in Figure 5. An increasing Markov chain length both improves the likelihood of reaching the global optimum as well as reducing the mean error of the approximation. While a chain length of about 300 is enough to have runs reaching the global minimum, even at the highest chain lengths of 10^4 there are still runs that converge to significantly worse local minima. In the next experiments, we choose a chain length of 1000 as a reasonable trade off between solution quality and simulation runtime.

3.4 Neighboring Procedure

We first compare the different strategies for choosing the direction Δx. For this, we simulate 50 runs each for different values of $\rho = \text{P(random direction)} = 1 - \text{P(force direction)}$. Figure 6 shows the mean approximation errors with 95 percent confidence intervals for three different particle numbers. At $\rho = 0$, the approximation error is significantly worse than all other values of ρ. With 22 particles, the error is smaller for very small and very large ρ while for 50 particles, the error is minimal for $\rho \approx 0.2$. In general, the approximation quality is almost indistinguishable with $0.1 < \rho < 0.9$, meaning that most combinations including both strategies perform similarly well.

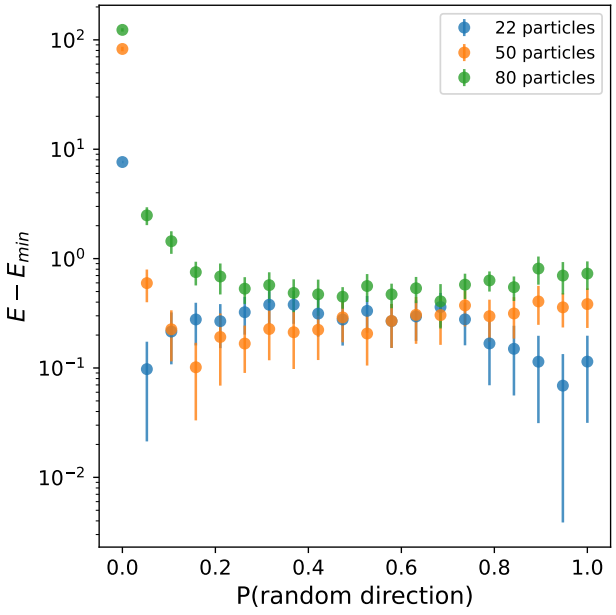

Figure 6: Caption

Setting ρ to 0.2,

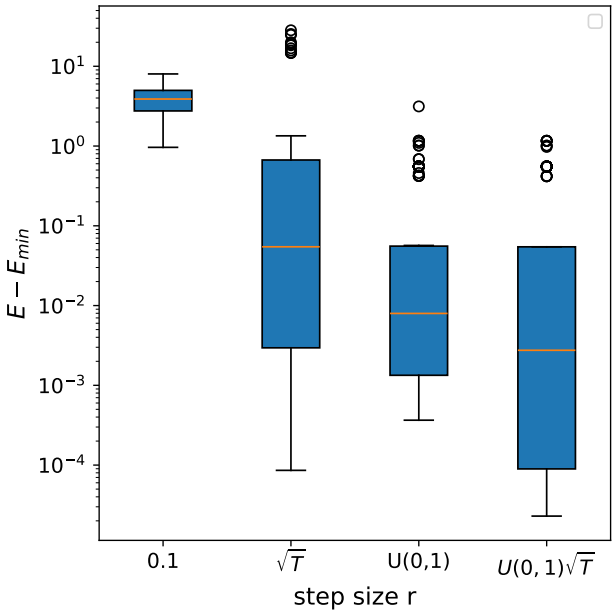

Figure 7: Caption

4 Discussion

4.1 Optimal Particle Configurations

Our exploration of optimal particle configurations reveals interesting trends as the number of particles increases. For systems with up to 11 particles, there are no floating particles in the optimal configurations, indicating that all particles are tightly arranged along the boundary. However, the system enters a transitional phase at 12 particles, where floating particles begin to appear (as shown visually in Figure 1). Beyond this point, the number of floating particles continues to increase with particle count, as shown in corresponding Table 1.

For larger systems, such as 50 particles, we observe significant variability in the number of floating particles, ranging from 15 to 18 in the worst-case scenarios (examples depicted in Figure 2). Despite this positional variability, the energy difference between the best and worst configurations remains relatively small. This consistency aligns with the expectations given our large number of simulation steps (100.000), ensuring convergence.

These findings build upon and contrast with earlier referenced studies, such as those by (Wille & Vennik, 1985), which achieved configurations with very low energy but were not always optimally laid out. Their methods, while effective in exploring low-energy states, sometimes led to suboptimal particle arrangements. Our approach explores a broader layout of configurations, leading to a more consistent identification of optimal or near-optimal positional configurations, even for larger particle systems.

5 Task distribution

References

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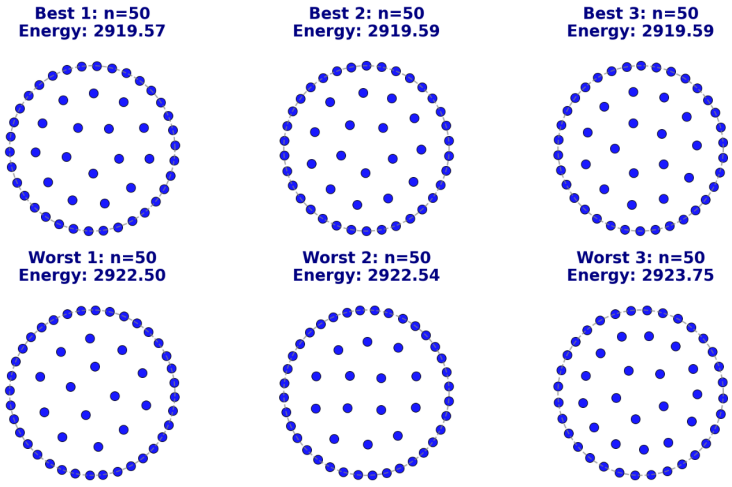

Figure 2: ....

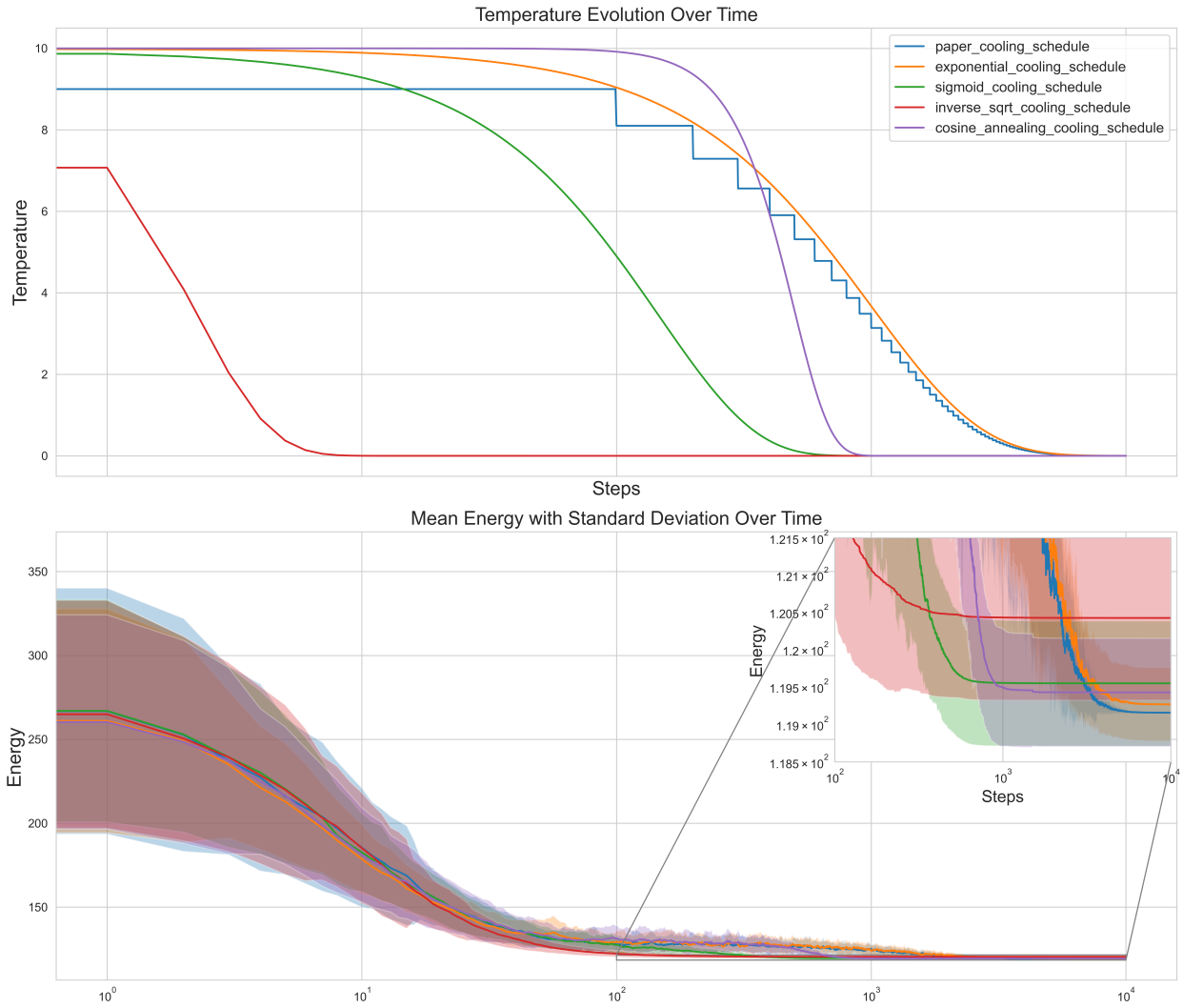

Figure 3: Comparison of different cooling schedules. On particle 12, with 10000 steps and 50 runs.