A Hybrid Quasi-Random Sampling Method for Three-Body Initial Conditions

Methodology Description

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Overview

This method generates initial conditions for a planar, equal-mass three-body system. The core idea is to fix one particle and sample the second from a well-defined space using a low-discrepancy sequence to ensure uniform coverage.

- Fix particle 1 at $p_1 = (1, 0, 0)$ on the unit sphere.
- Sample particle 2, p_2, quasi-uniformly from the 3-D hemisphere defined by $\{x \leq 0, x^2 + y^2 + z^2 \leq 1\}$.
- Set particle 3 as $p_3 = -(p_1 + p_2)$ to keep the center of mass at the origin for the equal-mass case.
- Initialize all velocities to 0.
- Use a low-discrepancy (e.g., Sobol or Halton) sequence instead of a pseudorandom generator so every finite batch covers the space evenly.

Choose a low-discrepancy engine

The choice of engine and its parameters are crucial for implementation.

- **Dimension**: Use a 4-dimensional engine if you plan to include global scaling and rotation; a 3-dimensional engine is sufficient for only sampling the hemisphere.
- **Engine Call**: A single call to the engine yields a vector $(u_1, u_2, u_3, u_4) \in (0, 1)^d$, where d is the dimension.
- **Scrambling**: It is recommended to enable scrambling (e.g., `qmc.Sobol(scramble=True)`). This feature preserves determinism while breaking any residual lattice artifacts in the sequence.

0.1 Map Sobol numbers → hemisphere sample

The generated quasi-random numbers in the unit hypercube must be mapped to the desired physical coordinates.

Direction on the unit sphere

1. Set the polar angle θ using $\cos\theta = 1 - 2u_1$. This ensures a uniform distribution for $\theta \in [0, \pi]$ with respect to solid angle.
2. Set the azimuthal angle $\phi = 2\pi u_2$, which is uniform for $\phi \in [0, 2\pi)$.
3. To enforce the $x \leq 0$ constraint, check the sign of $\cos\phi$. If $\cos\phi > 0$, the point lies in the wrong hemisphere. Mirror it by replacing ϕ with $(\phi + \pi) \pmod{2\pi}$. This preserves uniformity without resorting to inefficient rejection sampling.

4. Form the final unit direction vector d:

$$d = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

Radial distance inside the unit ball

To ensure the sample is uniform by volume, the radial distance r is calculated from u_3 using the cube root, which corrects for the radial bias in spherical coordinates:

$$r = u_3^{1/3}$$

The raw position for the second particle is then $p_{2_0} = rd$.

Optional global scaling and rotation

To create a more general dataset, the entire configuration can be scaled and rotated.

- **Scale**: Let $s = s_{\min} + (s_{\max} - s_{\min})u_4$. For example, with $s \in [0.2, 1.2]$. Then update the positions: $p_1 \leftarrow s \cdot p_1$ and $p_2 \leftarrow s \cdot p_{2_0}$.
- **Rotation**: The entire system can be rotated about an axis (e.g., the z-axis by an angle ψ) to ensure complete isotropy. This may require a fifth Sobol coordinate.

Compute the third body and velocities

The final positions and velocities are set according to the system constraints.

- $p_3 = -(p_1 + p_2)$
- $v_1 = v_2 = v_3 = (0, 0, 0)$

Safeguards

Robust implementation requires safeguards against numerical instabilities.

- **Collision Avoidance**: Reject the sample and advance to the next Sobol index if any pairwise distance falls below a prescribed threshold ϵ. This avoids singularities from near-collisions.
- **Stratification**: Optionally, stratify the dataset by a physical invariant like total potential energy or angular momentum. After generating a large set of initial conditions, compute the desired property and thin the set to achieve a uniform distribution across target bins.

Why this hybrid method is superior

- It combines the clear geometry of a 2-D setup with the richer configurations of a full 3-D hemisphere.
- Low-discrepancy points minimize both "clumping" and "voids," which can reduce the variance of model loss gradients and improve generalization.
- Determinism allows for exact reproduction of the training set for ablation studies or for incremental dataset growth by simply continuing the Sobol sequence.