Learning the Evolution of the Universe in N-body Simulations
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Background
- Numerical simulations that reconstruct the full evolution of the Universe are needed to understand the physics of large cosmological surveys down to non-linear scales, but snapshots of a simulated Universe at a large number of times need substantial storage.
- The goal of this work is to predict the N-body simulations at an intermediate cosmological time step given two widely separated snapshots using deep neural network. This work would greatly reduce the storage requirement and allow us to reconstruct the cosmic history from far fewer snapshots of the Universe.

Data
- Our dataset consists of cosmological N-body simulations from the QUIJOTE simulation. Each simulation follows the evolution of 512³ particles in a box of 1 (Gpc/h)³ volume at various time steps (redshift, z).
- We use 101 simulations: 80 for training, 20 for validation, and 1 for testing.
- Our input are displacement $S$ and velocity vectors $v$ of each particle at different redshifts. Our target is the displacement vector of each particle at an intermediate redshift.

Method
Neural Network
We adopt a V-Net type network with 3 stages of resolutions linked in a "V" shape, taking two downsampling and two upsampling layers:

- We use the Adam optimizer with learning rate 0.0001, $\beta_1$, $\beta_2$ = 0.9, 0.999, and reduce the learning rate by half when there is no improvement after three training epochs.
- We train the neural network to minimize the MSE loss as $\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} (S_i - S_i^{\text{truth}})^2$, where $N$ is the total number of particles, $S_i$ and $S_i^{\text{truth}}$ are the predicted and target displacement vector of the i-th particle.

Benchmark: Cubic Hermite Interpolation $S$ at an intermediate redshift predicted with Cubic Hermite interpolator is set as benchmark against which we compare our results of the neural network.

The coefficients of the polynomial are determined by requiring the polynomial matches $S$ and its derivative $dS/dz = -v/H(z)$ at both input redshifts.

Results for Four Statistics
We use the neural network and the cubic Hermite interpolator to predict the $z = 1$ displacement field from two snapshots at $z = 2$ and $z = 0$.

2D density field
Density projections over a region of 100 × 100 × 30 (h⁻¹ Mpc)³ at $z = 1$ for the Quijote simulation (left), V-Net (middle), and cubic Hermite interpolation (right).

Power spectrum
The top panels show the power spectra of the displacement and the density fields. To countify the accuracy, we use the Pearson correlation coefficient $r(k) = \frac{P_X(k)}{\sqrt{P(k) P_{\text{Truth}}(k)}}$, where $P_X(k)$ is the cross-power spectrum between the predicted $P(k)$ the power spectrum from the simulation $P_{\text{Truth}}(k)$.

Bispectrum
Equilateral ($k_1 = k_2 = k_3 = k$) bispectrum is calculated by multiplying the amplitude of three modes that form a closed triangle ($k_1 + k_2 + k_3 = 0$).

Dark Matter Halos
Dark matter halos are gravitationally bound structures where galaxies form and live, identified using the the FOF halo finder with linking length $b = 0.2$, and minimum particle number 20. We compute the halo mass function which quantifies the abundance of dark matter halos.

Conclusion
Our neural networks can learn to interpolate between the output of N-body simulations. It achieves high accuracy on the four statistics, outperforming the benchmark, indicating that deep learning is an accurate alternative to running large simulations to model the dynamical evolution of the Universe.