Zel'dovich test for GAN-universes

Motivation

There is a recent interest in using GANs for generating cosmological data (lensing images, CMB reconstruction etc.). Mustafa et al 2018 (Creating Virtual Universes Using Generative Adversarial Networks) discuss using GANs to generate weak lensing convergence maps. Their methodology involves a straightforward application of 2D Deep Convolutional GAN into convergence maps (which is a proxy for mass density from a particular line-of-sight direction). The validation of the newly generated maps is done via power spectrum and Minkowski functionals of the convergence maps.

We believe that a plain GAN (without any domain knowledge of cosmology) may not capture intricacies of nonlinear gravitational clustering. Power spectra (which is just a 1st order metric) and Minkowski functionals (which are topological/geometrical metrics that may be equivalent to the extracted convolutional features the CNNs are trained on) are not sufficient for benchmarking GAN's matter density generation.

Hence we propose an alternative scheme for generating and validating GANs applied in cosmological setting. This basically involves a first order collapse model *Zel'dovich approximation (ZA)* to generate and test the GAN pipelines. The steps are mentioned below:

1 Generating data

Generating the training set is similar to setting up cosmological initial conditions using ZA, i.e.,

1. For a cosmological model's initial power spectrum $P(k)$, generate displacement field $\mathbf{S}(\mathbf{q})$ using DFT. Use this to displace particles on regular grid. For future validation tests (explained later), we need to compute and save: (i) Initial matter density field $\overline{\rho}$ and (ii) spatial derivative of displacement field $\partial S_j/\partial q_i$.
2. Particles co-moving coordinates $\mathbf{x}$ and momenta $\mathbf{p}$ are given by ZA as

$$\mathbf{x} = \mathbf{q} + D(a)\mathbf{S}(\mathbf{q}); \quad \mathbf{p} = a^2\dot{x} \tag{1}$$

3. In the quasi-linear stage of evolution where the ZA is stopped, calculate the mass density field $\rho(\mathbf{x}, t)$. This will be our training data.

The above implementation already incorporated in HACC for creating ICs, so we can just use that directly. The generation should be fairly fast. We can either (i) generate one large ZA realization and divide into thousands of smaller boxes or (ii) generate a large number of small ZA realizations.

2 GAN Training

We could implement a 3D GAN, unlike the 2D version by Mustafa et al 2018. GANs are generally expensive, 3D will be even more expensive.

GAN training is unsupervised, i.e., the scalar field $\rho(\mathbf{x}, t)$ is both input and target.

Possible extension: mapping cosmological parameters to $\rho(\mathbf{x}, t)$ may be possible using conditional GANs.

3 Validation

Apart from the usual validation tests (power spectra, Minkowski functionals etc.), we can perform a full dynamical mapping test using ZA. An important caveat: while Eq. (1) could be used to map from Eulerian to Lagrangian coordinates of particles, the GAN pipeline uses scalar density fields, so we have to deal with mapping matter density field from final to initial timestep.

By applying mass conservation with ZA, we have:

$$\rho(\mathbf{x}, t) = \frac{\overline{\rho}}{\det(\partial x_j / \partial q_i)} = \frac{\overline{\rho}}{\det[\delta_{ij} + D(t) \times (\partial S_j / \partial q_i)]} \tag{2}$$

The GAN generated matter density field, $\rho_{GAN}(\mathbf{x}, t)$ should map to original $\overline{\rho}$, satisfying Eq. (2). The corresponding $P(k)$ and other initial parameters must match if the GAN captures dynamical evolution.

Conclusion

The Zel'dovich test (often used in IC validation) can be implemented for testing GAN generated cosmological density fields. ZA being exact at the initial stages of gravitational evolution makes it possible to retrace the GAN's *black-box* outputs, thus facilitating a comprehensive dynamical test.

In the future, this can be exploited in creating generative networks with cosmological domain knowledge, rather than training on convolutional features alone.