Panel: Generative Flow Methods

Simone Bacchio
The Cyprus Institute

Maria Paola Lombardo
INFN Firenze

Daniel Hackett
MIT

Alberto Ramos
Valencia U., IFIC

Status & Prospects

Tour de table:

What is your feeling about ML and Generative Flow Methods in particular:

Incremental progress or a paradigm shift for Lattice?

Applications

- From gauge field generation to phenomenology – key applications that will benefit?
- What new applications/calculations will be enabled by Generative Flow Methods? Is there a USP?
- How will exascale HPC enable progress? What must the community consider?

Applications: in simulations

- Trivialize the theory and map uniform to target distribution (the goal but also very challenging)

- Map a simpler action/distribution to a more difficult one (e.g., lower beta to larger beta)

- Use the transformed action in HMC (i.e., as proposed by Luescher and investigated by Albandea et al.)

Challenges & Questions

Context: accuracy & precision:

Scalability; Expressiveness; Training robustness; Reliability metrics;
New computational/data management bottlenecks; Determination of cost and time to solution;

Towards an error budget in the "traditional" sense?

- Plethora of approaches or a few front-runners?
- Are there (new) tests that methods should/must pass?
- Can/should we quantify what a green HPC+ML lattice calculation is? Are we moving in the right & responsible direction?

Q & A

Introduction

In Lattice Gauge Theories, the expectation value of an observable is defined as

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U]\, \mathcal{O}(U)\ \exp(-S(U))$$

If the field is generated by the transformation $U = \mathcal{F}(V) \qquad D[U] = D[V]\det \mathcal{F}_*(V)$

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[V]\, \mathcal{O}(\mathcal{F}(V))\ \exp(-S_{\mathcal{F}}(V))$$

$$S_{\mathcal{F}}(V) = S(\mathcal{F}(V)) - \log\det \mathcal{F}_*(V)$$

Introduction

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathrm{D}[V]\, \mathcal{O}(\mathcal{F}(V))\, \exp(-S_{\mathcal{F}}(V))$$

$$\underbrace{S_{\mathcal{F}}(V)}_{-log(q)} = \underbrace{S(\mathcal{F}(V))}_{-log(p)} - \log\det \mathcal{F}_*(V)$$

Equivalent to the KL-divergence

Our goal, then, is to find a *flow*, $\mathcal{F}$, such that

- $S_{\mathcal{F}}(V)$ is easier to simulate with HMC (e.g. better autocorrelation) but force of $S_{\mathcal{F}}(V)$ is required
- $S_{\mathcal{F}}(V) \equiv S'(V)$, i.e. flows to a different action where it is easier to simulate (or already simulated)
- $S_{\mathcal{F}}(V) \equiv \mathrm{const}$, i.e. all configurations *V* have the same weight and they are uniformly distributed

→ Trivializing map, Lüscher, 2009! [0907.5491]