A new approach to simulating lattice field theories

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12th November 2023

INFN Theory Retreat in Santo Stefano Belbo

Past and present

PhD student in **Torino** (with M. Caselle and M. Panero)

- lattice gauge theory at non-zero temperature: SU(2) and SU(3) YM equation of state
- effective string theory: testing Nambu-Goto predictions
- algorithms: Jarzynski's equality

Post-doc in **DESY Zeuthen** (with S. Schaefer and R. Sommer)

- algorithms: multilevel for quark correlators
- phenomenology: QCD running coupling
- algorithms: finite-size scaling of gradient flow

Now: **post-doc** of the **Simons Collaboration on Confinement and QCD Strings** (local PI M. Caselle)

- effective string theory: beyond Nambu-Goto picture
- algorithms: Stochastic Normalizing Flows for gauge theories (with M. Caselle, M. Panero, A. Bulgarelli and E. Cellini)

How to compute the path integral in a lattice simulation?

Computing v.e.v. on the lattice

How do we compute expectation values in a lattice simulation?

After discretizing the theory of interest (in Euclidean spacetime), the path integral becomes

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \prod_i \mathrm{d}\phi_i \, \mathcal{O}(\phi) \exp(-S(\phi))$$

How do we compute expectation values in a lattice simulation?

After discretizing the theory of interest (in Euclidean spacetime), the path integral becomes

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \prod_i \mathrm{d}\phi_i \; \underbrace{\mathcal{O}(\phi)}_{\text{compute}} \; \underbrace{\exp(-S(\phi))}_{\text{sample}}$$

- use the Boltzmann distribution as a weight to sample numerically configurations of fields ϕ
- simply "measure" the observable by computing it on the configurations

$$\langle \mathcal{O} \rangle = \frac{1}{N_{\text{conf}}} \sum_{n=1}^{N_{\text{conf}}} \mathcal{O}(\phi^{(n)}), \qquad \phi^{(n)} \sim \exp(-S(\phi^{(n)}))$$

provided that the $\phi^{(n)}$ are effectively sampled according to Boltzmann distribution!

How do we sample from $\exp(-S)/Z$?

Markov Chain Monte Carlo

An elegant and reliable numerical recipe is provided by Markov Chain Monte Carlo **[Creutz; 1979]**

- Generate a (thermalized) Markov chain

$$\underbrace{\phi^{(0)} \stackrel{P_p}{\to} \phi^{(1)} \stackrel{P_p}{\to} \dots \stackrel{P_p}{\to}}_{\text{thermalization}} \underbrace{\phi^{(t)} \stackrel{P_p}{\to} \phi^{(t+1)} \stackrel{P_p}{\to} \dots \to \phi^{(t+N_{\text{conf}})}}_{\text{equilibrium}}$$

(setting $\exp(-S)$ as the equilibrium distribution)

- Measure $\mathcal{O}$ on sampled equilibrium configurations

MCMC algorithm of choice (Metropolis, heatbath, HMC) defined by the transition probability P_p

(details are unimportant for the sake of this presentation)

Critical slowing down

The configurations sampled sequentially in a Markov Chain are **autocorrelated**

$$\cdots \rightarrow \underbrace{\phi^{(t)} \rightarrow \phi^{(t+1)} \rightarrow \ldots}_{2\tau_{\text{int}}} \rightarrow \phi^{(t+n)}$$

Number of effectively independent configurations $= n/2\tau_{\text{int}}$

Critical slowing down: when a critical point is approached τ_{int} diverges

E.g. in the continuum limit $a \rightarrow 0$

$$\tau_{\text{int}} \simeq a^{-z}$$

where z depends on the algorithm and on the observable under study

Topological freezing: topological charge in YM has $z \simeq 5$ **[Schaefer, Sommer, Virotta; 2011]**

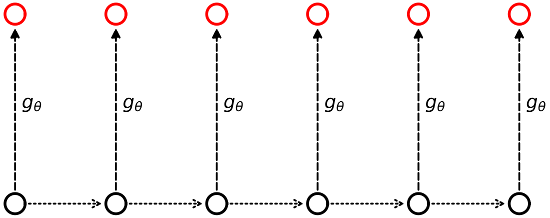
Trivializing and Normalizing flows

A different kind of sampling

Idea

Sample each new configuration (almost) independently from the previous one by construction

Trivializing map g_θ between a trivial base distribution and the "difficult" target



Wilson flow **[Lüscher; 2009]**: approximate trivializing map in Yang-Mills

Normalizing flows for lattice field theory

Normalizing Flows are a promising deep generative architecture that can provide a mapping between the target $p(\phi)$ with some tractable distribution $q_0(z)$

NFs are a diffeomorphism g_θ

$$g_\theta(\phi_0) = (g_{N_{cl}} \circ \cdots \circ g_1)(\phi_0) \qquad \phi_0 \sim q_0$$

composed of N_{cl} transformations $\rightarrow$ the **coupling layers** g_n

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Training: minimize the **Kullback-Leibler** divergence, a measure of the “similarity” between two distributions

$$\tilde{D}_{\mathrm{KL}}(q_\theta \| p) = \int \mathrm{d}\phi \, q_\theta(\phi) \log \frac{q_\theta(\phi)}{p(\phi)}$$

Sampling with Normalizing flows

Sampling

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathrm{d}\phi \, \mathcal{O}(\phi) q_\theta(\phi) \frac{p(\phi)}{q_\theta(\phi)} = \frac{1}{Z} \int \mathrm{d}\phi \, \underbrace{q_\theta(\phi)}_{\text{sample}} \underbrace{\mathcal{O}(\phi) \tilde{w}(\phi)}_{\text{measure}} = \frac{\langle \mathcal{O}(\phi) \tilde{w}(\phi) \rangle_{\phi \sim q_\theta}}{\langle \tilde{w}(\phi) \rangle_{\phi \sim q_\theta}}$$

with a weight

$$\tilde{w}(\phi) = \frac{p}{q_\theta}$$

Get Z directly by sampling from q_θ **[Nicoli et al.; 2020]**

$$Z = \int \mathrm{d}\phi \, p(\phi) = \int \mathrm{d}\phi \, q_\theta(\phi) \tilde{w}(\phi) = \langle \tilde{w}(\phi) \rangle_{\phi \sim q_\theta}$$

Issues with NFs

Incomplete list of recent works:

→ successfully applied in LFTs in 2d: ϕ^4 scalar field theory **[Albergo et al.; 2019]**, **[Kanwar et al.; 2020]**, **[Nicoli et al.; 2020]**, **[Del Debbio et al.; 2021]**, $\mathrm{SU}(N)$ **[Boyda et al.; 2020]**, fermionic theories **[Albergo et al.; 2021]**, $\mathrm{U}(1)$ and $\mathrm{SU}(N)$ with fermions **[Abbott et al.; 2022]**, Schwinger model **[Finkenrath et al.; 2022]**, **[Albergo et al.; 2022]**, first attempts in 4d **[Abbott et al.; 2023]**

→ strongly related to the idea of trivializing maps **[Lüscher; 2009]**, **[Bacchio et al.; 2022]**, **[Albandea et al.; 2023]**

- NFs effectively remove critical slowing in low dimensional theories
- training generally scales badly with volume and in the continuum limit
- quite complicated architectures for gauge theories

Non-equilibrium stochastic evolutions

The Second Law of Thermodynamics

Clausius inequality for an (isothermal) transformation from state A to state B

$$\frac{Q}{T} \leq \Delta S$$

If we use

$$\begin{cases} Q = & \Delta E - W \quad \text{(First Law)} \\ F \stackrel{\text{def}}{=} & E - ST \end{cases}$$

the Second Law becomes

$$W \geq \Delta F = F_B - F_A$$

where the equality holds for reversible processes.

Moving from thermodynamics to statistical mechanics we know that actually

$$\langle W \rangle_f \geq \Delta F = F_B - F_A$$

Jarzynski's equality and the Second Law

Jarzynski's equality [Jarzynski; 1997] is a beautiful result from non-equilibrium statistical mechanics

$$\left\langle \exp\left(-\frac{W}{T}\right)\right\rangle_f = \exp\left(-\frac{\Delta F}{T}\right)$$

valid for a given process f

Using Jensen's inequality $\langle \exp x \rangle \geq \exp\langle x \rangle$ we get

$$\langle W \rangle_f \geq \Delta F$$

Apart from the real world, it can be proved for several processes

→ most relevantly for us: **Markov Chain Monte Carlo** for lattice field theory

Jarzynski's equality in MCMC

Consider two distributions q_0 and p

$$q_0 = \exp(-S_0)/Z_0 \rightarrow \cdots \rightarrow p = \exp(-S)/Z$$

The ratio of partition functions is computed directly with an average over **non-equilibrium evolutions**

$$\frac{Z}{Z_0} = \langle \exp\left(-W\right) \rangle_f$$

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Over a single evolution:

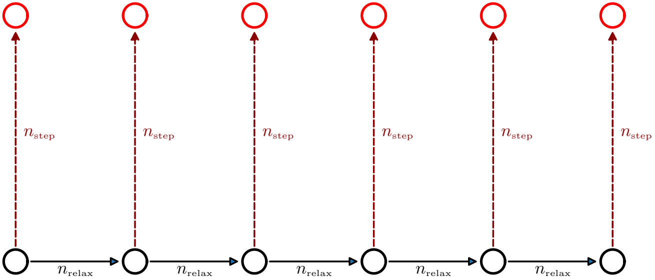
- update the system using regular MC updates over n_{step}
- but the transition probability changes along the evolution according to a **protocol** η_n that interpolates q_0 and p

$$q_0 \simeq e^{-S_{\eta_0}} \to e^{-S_{\eta_1}} \to \cdots \to p \simeq e^{-S}$$

- along the process we compute the **work**

$$W = \sum_{n=0}^{n_{\text{step}}-1} \left\{ S_{\eta_{n+1}}\left[\phi_n\right] - S_{\eta_n}\left[\phi_n\right] \right\}$$

A new paradigm: out-of-equilibrium stochastic evolutions



compute v.e.v. with

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O}(\phi) \exp(-W(\phi_0 \to \phi)) \rangle_{\mathrm{f}}}{\langle \exp(-W(\phi_0 \to \phi)) \rangle_{\mathrm{f}}}$$

Jarzynski's equality for lattice field theory

Several applications, spearheaded by the Torino group over the last few years

Compute ratios of partition functions:

- interface free-energy in the Z_2 gauge theory **[Caselle et al.; 2016]**
- $\mathrm{SU}(3)$ equation of state **[Caselle, Nada and Panero; 2018]**
- running coupling for $\mathrm{SU}(N)$ **[Francesconi, Panero and Preti; 2020]**
- entanglement entropy for Ising model in $2d$ and $3d$ **[Bulgarelli and Panero; 2023]**

But also just to sample difficult distributions:

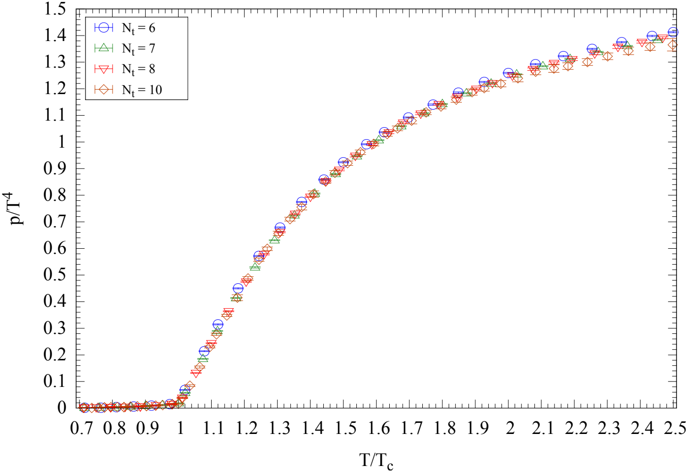
- sampling topological observables on periodic boundary conditions **[Bonanno, Nada and Vadacchino; 2023]**

SU(3) e.o.s. with Jarzynski's equality

Large-scale application: computation of the SU(3) equation of state **[Caselle et al.; 2018]**

Extract the pressure with Jarzynski's equality

$$\frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = \left(\frac{N_t}{N_s}\right)^3 \log\langle e^{-W_{\mathrm{SU}(N_c)}}\rangle_{\mathrm{f}}$$



A common framework: Stochastic Normalizing Flows

Jarzynski's equality is the same formula used to extract Z in NFs

$$\frac{Z}{Z_0} = \langle \tilde{w}(\phi) \rangle_{\phi \sim q} = \langle \exp(-W) \rangle_{\mathrm{f}}$$

Normalizing Flows

$$\phi_0 \to \phi_1 = g_1(\phi_0) \to \cdots \to \phi$$

$$-\log \tilde{w} = S(\phi) - S_0(\phi_0) - \log |\det J|$$

stochastic non-equilibrium evolutions

$$\phi_0 \overset{P_{\eta_1}}{\to} \phi_1 \overset{P_{\eta_2}}{\to} \ldots \overset{P_{\eta_{n_{\mathrm{step}}}}}{\to} \phi$$

$$W = S(\phi) - S_0(\phi_0) - Q$$

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Stochastic Normalizing Flows (introduced in **[Wu et al.; 2020]**)

$$\phi_0 \to g_1(\phi_0) \stackrel{P_{\eta_1}}{\to} \phi_1 \to g_2(\phi_1) \stackrel{P_{\eta_2}}{\to} \dots \stackrel{P_{\eta_{n_{\mathrm{step}}}}}{\to} \phi$$

$$W = S(\phi) - S_0(\phi_0) - Q - \log |\det J|$$

The proper loss we use for training is

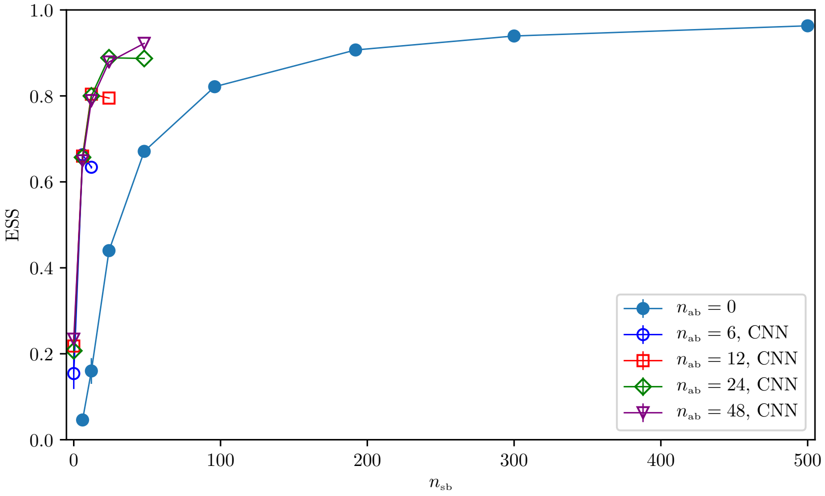
$$\tilde{D}_{\mathrm{KL}}(q_0 P_{\mathrm{f}} \| p P_{\mathrm{r}}) = \int \prod_{i=0}^{n_{\mathrm{step}}} \mathrm{d}\phi_i \, q_0(\phi_0) P_{\mathrm{f}}[\phi_0, \phi_1, \ldots, \phi] \log \frac{q_0(\phi_0) P_{\mathrm{f}}[\phi_0, \phi_1, \ldots, \phi]}{p(\phi) P_{\mathrm{r}}[\phi, \phi_{N-1}, \ldots, \phi_0]}$$

$\rightarrow$ measure of how reversible the process is!

Clear "thermodynamic" interpretation

$$\tilde{D}_{\mathrm{KL}}(q_0 P_{\mathrm{f}} \| p P_{\mathrm{r}}) = \underbrace{\langle W \rangle_{\mathrm{f}} + \log \frac{Z}{Z_0} \geq 0}_{\text{Second Law}}$$

Efficiency test on the $2d$ ϕ^4 scalar field theory



stochastic evolutions vs SNFs on a $N_s \times N_t = 16 \times 8$ lattice

SNFs for lattice field theory

- Theoretical common framework between Jarzynski's equality and NFs is now explicit
- SNFs can be trained!
- improvement over non-equilibrium evolutions: less MCMC updates used
- improvement over normalizing flows: limited training times, good scaling with volume
- perhaps non-equilibrium statistical mechanics can give us even more insights

What next?

SNFs already applied to sample **directly** the Nambu-Goto string on a lattice **[Caselle, Cellini and Nada; 2023]**

- main project of **E. Cellini**
- unfeasible to do numerically with a MCMC, SNFs best approach (and still challenging)
- allows to test NG and Effective String Theories directly, when analytic results are not available (string width)

New approach to sample lattice gauge theories

- SNFs for $\mathrm{SU}(3)$ gauge theory under development (with **A. Bulgarelli** and **E. Cellini**)
- final aim: mitigating (if not removing) topological freezing from lattice gauge theory simulations
- proof of concept in the CP^{N-1} model **[Bonanno, Nada and Vadacchino; 2023]**
- much less risky program! instead of building a trivializing map from the ground up, we **systematically improve** something that already works (non-equilibrium MC)

Thank you for your attention!

Out-of-equilibrium stochastic evolutions

Closer look at the average on the processes in the equality:

$$\frac{Z}{Z_0} = \langle \exp(-W) \rangle_f = \int \mathrm{d}\phi_0 \, \mathrm{d}\phi_1 \ldots \mathrm{d}\phi_N \, q_0(\phi_0) \, P_\mathrm{f}[\phi_0, \phi_1, \ldots, \phi_N] \, \exp(-W)$$

with

$$P_\mathrm{f}[\phi_0, \phi_1, \ldots, \phi_N] = \prod_{n=0}^{N-1} P_{\eta_n}(\phi_n \to \phi_{n+1})$$

- the *actual* probability distribution at each step is NOT the equilibrium distribution $\sim \exp(-S_{\eta_n})$: it's a non-equilibrium process!
- the $\langle \ldots \rangle_f$ average is taken over as many evolutions as possible (all independent from each other!)

Typical toy model for tests: ϕ^4 field theory in 2 dimensions in the unbroken symmetry phase

$$S(\phi) = \sum_{x \in \Lambda} -2\kappa \sum_{\mu=0,1} \phi(x)\phi(x+\hat{\mu}) + (1-2\lambda)\phi(x)^2 + \lambda\phi(x)^4$$

Protocol

η_n interpolates between the prior (normal distribution is recovered with $\kappa = \lambda = 0$) and target parameters $\kappa = 0.2$ and $\lambda = 0.022$

- linear protocol η_n
- heatbath algorithm for the stochastic updates
- n_{sb} = # of stochastic updates

Coupling layer

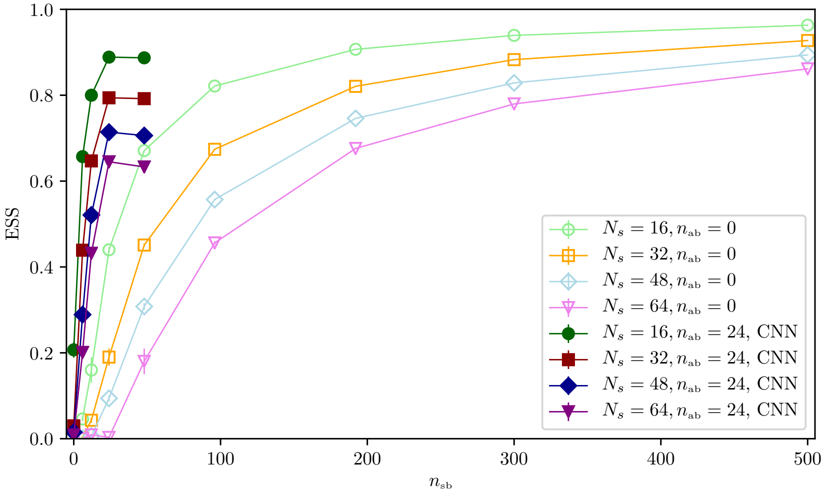
- using affine layers with CNNs
- n_{ab} = # of affine blocks

Metric

Effective Sample Size as metric to evaluate architectures

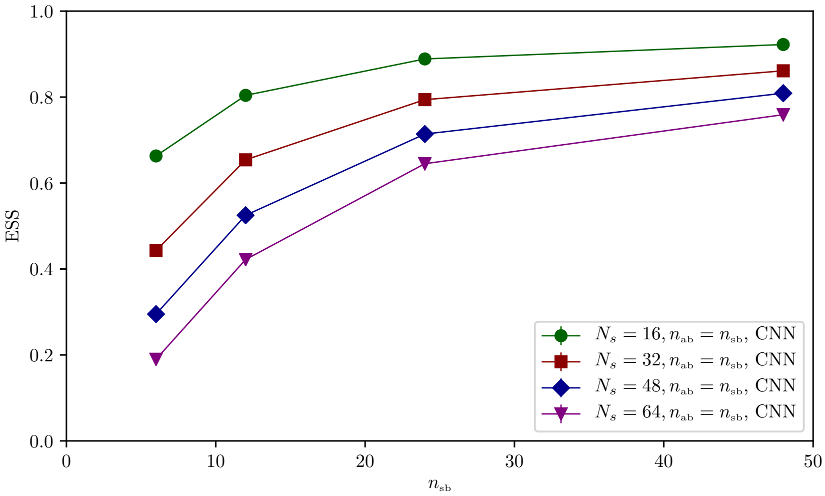
$$\text{ESS} = \frac{\langle \exp(-W) \rangle_f^2}{\langle \exp(-2W) \rangle_f}$$

Training length: 10^4 epochs for all volumes. Slowly-improving regime reached fast

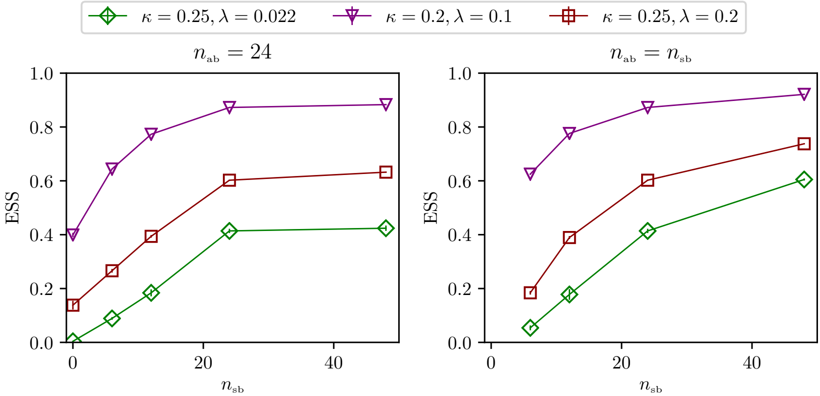


Interesting behaviour for all volumes: a peak for $n_{sb} = n_{ab}$?

SNFs with $n_{sb} = n_{ab}$ as a possible recipe for efficient scaling



More results in the unbroken phase



Stochastic evolutions/SNF/NF wrap-up

	normalizing flows	stochastic evolutions	SNFs
preparation	training	setting the protocol η_n	both
forward prob. P_{f}	$P_{\mathrm{f}} = \prod_n P_n(\phi_n \to \phi_{n+1})$		
transition prob. P_n	$\delta(\phi_{n+1} - g_n(\phi_n))$	$P_{\eta_n}(\phi_n \to \phi_{n+1})$	uses both
KL divergence	$\tilde{D}_{\mathrm{KL}}(q_\theta \| p)$	$\tilde{D}_{\mathrm{KL}}(q_0 P_{\mathrm{f}} \| p P_{\mathrm{r}})$	
"work"	$W = S - S_0 - Q = -\log \tilde{w}$		
"heat" Q	$\sum_{n=0}^{N-1} \log \lvert \det J_n(\phi_n) \rvert$	$\sum_{n=0}^{N-1} S_{\eta_{n+1}}(\phi_{n+1}) - S_{\eta_{n+1}}(\phi_n)$	both
e.v. $\langle \mathcal{O} \rangle$	$\frac{\langle \mathcal{O}(\phi_N) \tilde{w}(\phi_N) \rangle_{\phi_N \sim q_\theta}}{\langle \tilde{w}(\phi_N) \rangle_{\phi_N \sim q_\theta}}$	$\frac{\langle \mathcal{O}(\phi_N) \exp(-W(\phi_0 \to \phi_N)) \rangle_{\mathrm{f}}}{\langle \exp(-W(\phi_0 \to \phi_N)) \rangle_{\mathrm{f}}}$	

Crooks fluctuation theorem

Crooks theorem **[Crooks; 1998]**: another relation deeply connected with Jarzynski's equality

$$\frac{\mathcal{P}_F(W)}{\mathcal{P}_R(-W)} = e^{W-\Delta F}$$

The $\mathcal{P}_{F,R}$ indicate the probability distribution of the work performed in the forward and reverse realizations of the transformation.

JE is easily recovered by moving the $\exp(-W)$ and $\mathcal{P}_R$ factors and integrating in W on both sides.

$W_d = W - \Delta F$ is the **dissipated** work.

Transformations g_n must be invertible + the Jacobian has to be efficiently computable

A class of coupling layers called **affine layers** meets this criteria

- The variables ϕ are divided into two partitions A and B
- For each layer, one is kept "frozen" while the other is transformed following

$$g_n : \begin{cases} \phi_{\mathrm{A}}^{n+1} = \phi_{\mathrm{A}}^{n} \\ \phi_{\mathrm{B}}^{n+1} = e^{-s(\phi_{\mathrm{A}}^{n})} \phi_{\mathrm{B}}^{n} + t(\phi_{\mathrm{A}}^{n}) \end{cases}$$

- s and t are the neural networks where the trainable parameters θ are
- **RealNVP** architecture **[Dinh et al.; 2016]**

Natural choice for lattice variables: checkerboard (i.e. even-odd) partitioning

Affine block = even c. layer + odd c. layer

Some possible issues with NFs

- **multi-modal distributions**
  in the presence of multiple vacua the training procedure "picks" only one

  "mode-collapse": only one mode of the distribution is sampled by the flow

  see **[Hackett et al.; 2021]**

- **scalability**
  measurements of v.e.v. are statistically independent (no autocorrelation)

  not clear however how the training times scale when approaching the continuum limit

  comprehensive discussion in **[Del Debbio et al.; 2021]** and **[Abbott et al.; 2022]**