Stochastic normalizing flows as non-equilibrium transformations

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Based on:
M. Caselle, E. Cellini, A. N., M. Panero, JHEP 07 (2022) 015, [arXiv:2201.08862]

Normalizing flows and Jarzynski's equality?

Normalizing Flows

sample from a complex target distribution using neural network architectures

Jarzynski's equality in MCMC

computing ratios of Zs using stochastic out-of-equilibrium evolutions

$\Downarrow$

Stochastic Normalizing Flows

joint architecture of deterministic transformations (NFs) and a stochastic non-equilibrium trajectory towards the target distribution

Normalizing flows in lattice field theory

Configurations sampled sequentially in a Markov Chain are **autocorrelated**

$$\cdots \to \phi^{(t)} \to \phi^{(t+1)} \to \cdots \to \phi^{(t+n)} \sim p$$

When a critical point (e.g. continuum limit) is approached the autocorrelation diverges
$\to$ **critical slowing down**

What if every new configuration is sampled independently from the previous one?

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$\rightarrow$ 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]** ...

$\rightarrow$ strongly related to the idea of trivializing maps **[Lüscher; 2009]**, **[Bacchio et al.; 2022]**

Normalizing flows: structure

Normalizing flows are a deterministic mapping

$$g_\theta(y_0) = (g_N \circ \cdots \circ g_1)(y_0) \qquad\qquad y_0 \sim q_0$$

composed of N invertible transformations $\rightarrow$ the **coupling layers** g_i

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At each layer the field variables y are transformed

$$y_{n+1} = g_n(y_n)$$

e.g. affine transformations whose parameters are neural networks ($\rightarrow$ RealNVP architecture)

Generated distribution:

$$q_\theta(y_N) = q_0(g_\theta^{-1}(y_N)) \prod_n |\det J_n(y_n)|^{-1}$$

depends on the **prior** q_0 (e.g. a normal distribution) and on the Jacobian of each coupling layer

Normalizing flows: training and issues

training $\rightarrow$ iterative procedure that brings the generated distribution q_θ as close as possible to the target p

loss $\rightarrow$ quantity the training algorithm minimizes in order to reach the target

Typical choice is the **Kullback-Leibler** divergence: measure of the "similarity" between two distributions

$$\tilde{D}_{\mathrm{KL}}(q_\theta \| p) = \int \mathrm{d}\phi \, q_\theta(\phi) \left[\ln q_\theta(\phi) - \ln p(\phi)\right]$$

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Typical issues:

- **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 **[Hackett et al.; 2021]**, **[Abbott et al.; 2022]**
- **scalability**
  not clear how the training times scale when approaching the continuum limit **[Del Debbio et al.; 2021]**

Normalizing flows and the free energy

Compute v.e.v. with a reweighting step (not the only possibility: see independent MH)

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathrm{d}\phi \, \mathcal{O}(\phi) q_\theta(\phi) \frac{p(\phi)}{q_\theta(\phi)} = \frac{Z_0}{Z} \int \mathrm{d}\phi \, \underbrace{q_\theta(\phi)}_{\text{sample}} \underbrace{\mathcal{O}(\phi) \tilde{w}(\phi)}_{\text{measure}} = \frac{\langle \mathcal{O}(\phi) \tilde{w}(\phi) \rangle_{\phi \sim q_\theta}}{\langle \tilde{w}(\phi) \rangle_{\phi \sim q_\theta}}$$

and the with weight

$$\tilde{w}(\phi) = \exp\left(- \left\{ S[\phi] - S_0[g_\theta^{-1}(\phi)] - \log J \right\} \right) \sim \frac{p}{q_\theta}$$

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

$$Z = \int \mathrm{d}\phi \, \exp(-S[\phi]) = Z_0 \int \mathrm{d}\phi \, q_\theta(\phi)\tilde{w}(\phi) = Z_0 \langle \tilde{w}(\phi)\rangle_{\phi\sim q_\theta}$$

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And the loss:

$$\tilde{D}_{\mathrm{KL}}(q_\theta \| p) = -\langle \ln \tilde{w}(\phi)\rangle_{\phi\sim q_\theta} + \ln \frac{Z}{Z_0}$$

Jarzynski's equality in MCMC simulations

Free-energy differences (at equilibrium) directly calculated with an average over **non-equilibrium processes [Jarzynski; 1997]**:

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

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For an MCMC

- the stochastic evolution starts from a configuration sampled from q_0 and reaches the target p

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

- N intermediate MC steps each with a different transition probability $P_{\eta_n}(y_n \to y_{n+1})$ (i.e.: the action S_{η_n} changes)
- η_n is a **protocol** that interpolates the parameters of the theory between q_0 and p

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

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Along the process we compute the **work**

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

Works well also in LFT: the $\mathrm{SU}(3)$ equation of state in $(3+1)\mathrm{D}$ **[Caselle et al.; 2018]**

A common framework: Stochastic Normalizing Flows

We realized that Jarzynski's relation is the same formula used to extract Z in NFs:

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

as for deterministic mappings $\langle \dots \rangle_{\phi \sim q_\theta} = \langle \dots \rangle_{\mathrm{f}}$.

The "work" is simply

$$W(y_0, \dots, y_N) = S(y_N) - S_0(y_0) - Q(y_1, \dots, y_N) = -\ln \tilde{w}(\phi)$$

where the "heat" Q is

normalizing flows

$$y_0 \to y_1 = g_1(y_0) \to \dots \to y_N$$

$$Q = \sum_{n=0}^{N-1} \ln |\det J_n(y_n)|$$

stochastic non-equilibrium evolutions

$$y_0 \overset{P_{\eta_1}}{\to} y_1 \overset{P_{\eta_2}}{\to} \dots \overset{P_{\eta_N}}{\to} y_N$$

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

$$y_0 \to g_1(y_0) \overset{P_{\eta_1}}{\to} y_1 \to g_2(y_1) \overset{P_{\eta_2}}{\to} \dots \overset{P_{\eta_N}}{\to} y_N$$

$$Q = \sum_{n=0}^{N-1} S_{\eta_{n+1}}(y_{n+1}) - S_{\eta_{n+1}}(g_n(y_n)) + \ln |\det J_n(y_n)|$$

The proper KL divergence is

$$\tilde{D}_{\mathrm{KL}}(q_0 P_{\mathrm{f}} \| p P_{\mathrm{r}}) = \int \mathrm{d}y_0\, \mathrm{d}y_1 \ldots \mathrm{d}y_N\, q_0(y_0) P_{\mathrm{f}}[y_0, y_1, \ldots, y_N] \ln \frac{q_0(y_0) P_{\mathrm{f}}[y_0, y_1, \ldots, y_N]}{p(y_N) P_{\mathrm{r}}[y_N, y_{N-1}, \ldots, y_0]}$$

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

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

In general we have simply

$$\tilde{D}_{\text{KL}}(q_0 P_{\text{f}} \| p P_{\text{r}}) = \langle W \rangle_{\text{f}} + \ln \frac{Z}{Z_0}$$

If we go back to NFs: the same definition simplifies (using the change of variables theorem) to

$$\tilde{D}_{\text{KL}}(q_0 P_{\text{f}} \| p P_{\text{r}}) \rightarrow \tilde{D}_{\text{KL}}(q_\theta \| p) = -\langle \ln \tilde{w}(\phi) \rangle_{\phi \sim q_\theta} + \ln \frac{Z}{Z_0}$$

due to the deterministic nature of the mapping.

Testing SNFs in the 2D ϕ^4 model

Theory

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

target parameters $\kappa = 0.2$ and $\lambda = 0.022$ (as in **[Nicoli et al.; 2020]**): unbroken symmetry phase

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Goals

- can we train SNFs efficiently?
- can we improve both on NFs and on stochastic evolutions?

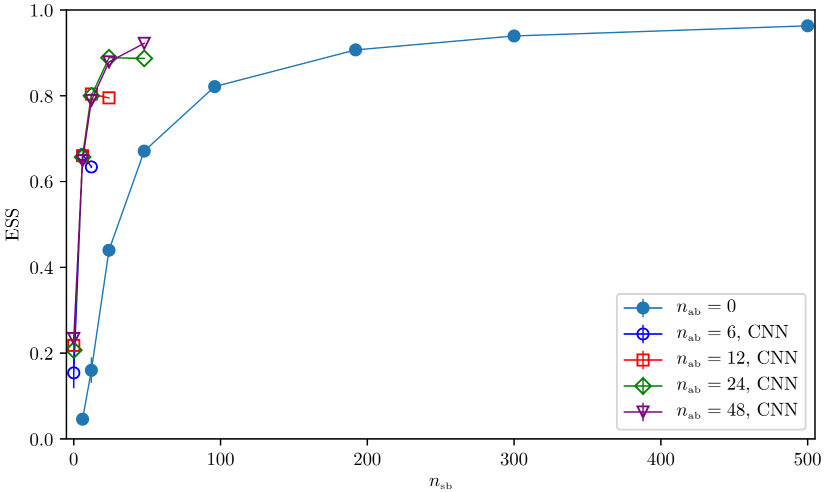
Metric

we use the Effective Sample Size to evaluate SNFs

$$\mathrm{ESS} = \frac{\langle \tilde{w} \rangle_f^2}{\langle \tilde{w}^2 \rangle_f}$$

Takes values between 0 and 1 (perfect training)

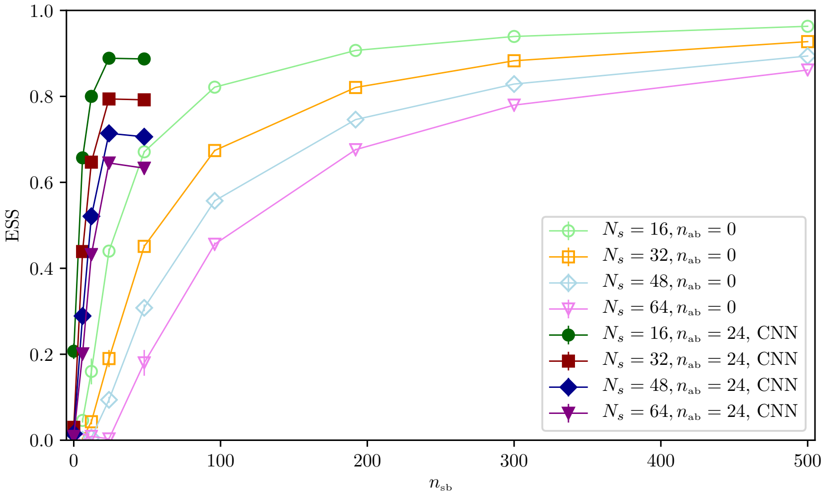
Comparing stochastic evolutions with (S)NFs on a $N_s \times N_t = 16 \times 8$ lattice,



on the x-axis: $n_{sb} = \#$ of stochastic updates

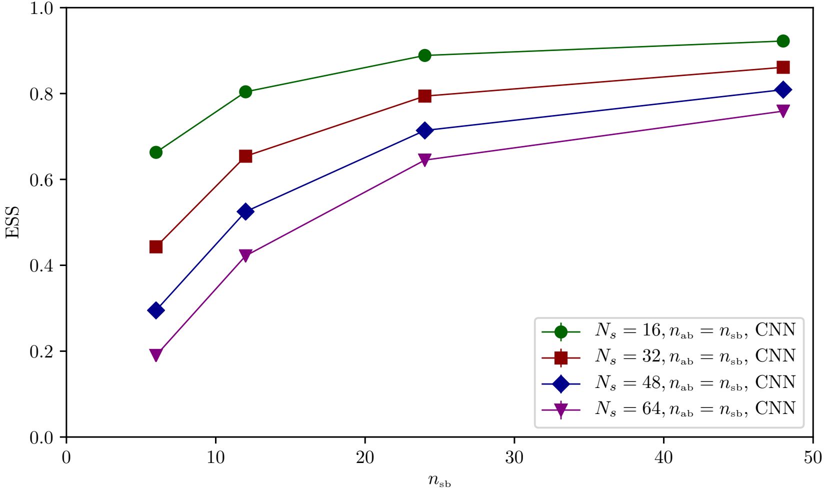
different colors: $n_{ab} = \#$ of coupling layers

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



Conclusions

The common framework between Jarzynski's equality and NFs is now explicit

General idea: use knowledge from non-equilibrium SM to create efficient SNFs

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SNFs vs. stochastic evolutions

- Jarzynski's equality provides a way to compute Z and $\langle O \rangle$ (which works well also in LGTs, see $\mathrm{SU}(3)$ e.o.s. **[Caselle et al.; 2018]**)
- SNFs might be an even better method!
- trade-off: training for less MCMC updates
- very interesting for thermodynamic applications (or similar)

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SNFs vs. normalizing flows

- improve scalability and interpretability?
- SNFs with CNNs and $n_{sb} = n_{ab}$ have a promising volume scaling at fixed training length
- training could be qualitatively "guided" towards the target by the protocol, but ultimately might also be limited by it

Thank you for your attention!

Normalizing flows: affine layers

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

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

- 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

Backpropagation

Also needed: an efficient way of computing the gradient of the loss with respect to the flow parameters θ

$$\nabla_\theta \tilde{D}_{\mathrm{KL}}(q_\theta \| p)$$

$\rightarrow$ **backpropagation** algorithm: the overall gradient is calculated combining the intermediate gradients at each layer n, which can be stored in memory during a forward pass through the flow

$$\nabla_\theta \mathcal{L} = \frac{\partial \mathcal{L}}{\partial y_N} \frac{\partial y_N}{\partial y_{N-1}} \dots$$

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

$$\frac{Z}{Z_0} = \langle \exp(-W) \rangle_f = \int \mathrm{d}y_0 \, \mathrm{d}y_1 \dots \mathrm{d}y_N \, q_0(y_0) \, P_\mathrm{f}[y_0, y_1, \dots, y_N] \, \exp(-W)$$

with

$$P_\mathrm{f}[y_0, y_1, \dots, y_N] = \prod_{n=0}^{N-1} P_{\eta_n}(y_n \to y_{n+1})$$

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

Some comparisons

	normalizing flows	stochastic evolutions	SNFs
preparation	training	setting the protocol η_n	both
forward prob. P_f	$P_\mathrm{f} = \prod_n P_n(y_n \to y_{n+1})$		
transition prob. P_n	$\delta(y_{n+1} - g_n(y_n))$	$P_{\eta_n}(y_n \to y_{n+1})$	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"	$W = S - S_0 - Q = -\ln \tilde{w}$		
"heat" Q	$\sum_{n=0}^{N-1} \ln \lvert \det J_n(y_n) \rvert$	$\sum_{n=0}^{N-1} S_{\eta_{n+1}}(y_{n+1}) - S_{\eta_{n+1}}(y_n)$	both
e.v. $\langle \mathcal{O} \rangle$	$\frac{\langle \mathcal{O}(y_N) \tilde{w}(y_N) \rangle_{y_N \sim q_\theta}}{\langle \tilde{w}(y_N) \rangle_{y_N \sim q_\theta}}$	$\frac{\langle \mathcal{O}(y_N) \exp(-W(y_0 \to y_N)) \rangle_\mathrm{f}}{\langle \exp(-W(y_0 \to y_N)) \rangle_\mathrm{f}}$	

Technical details

Stochastic evolution

- protocol interpolates linearly between a normal distribution ($\kappa = \lambda = 0$) and the target parameters
- heatbath algorithm for the stochastic updates

Coupling layers and NN

- neural networks in affine transformations are CNNs with 1 hidden layer, 3×3 kernel and 1 feature map
- also fully-connected networks were considered: 1 hidden layer and $\#$ neurons $= \#$ lattice sites
- affine layers uniformly distributed between MC updates

Related works

- Annealed Importance Sampling **[Neal; 1998]**: procedure equivalent to JE. Very popular in ML community. Used in SNF paper **[Wu et al.; 2020]**
- AIS $\rightarrow$ generalized in Sequential Monte Carlo (SMC) samplers. Also well known in ML.
- SNF idea reworked in CRAFT approach **[Matthews et al.; 2022]**
- **[Vaikuntanathan and Jarzynski; 2011]**: related approach with deterministic mappings on top of non-equilibrium transformations. No neural networks.

Taking cues from the $\mathrm{SU}(3)$ e.o.s.

Is there anything we can learn from out-of-equilibrium stochastic processes that we can apply to stochastic normalizing flows?

Relevant application: large-scale computation of the $\mathrm{SU}(3)$ equation of state **[Caselle et al.; 2018]**
goal: extract the pressure with Jarzynski's equality

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

evolution in β (inverse coupling) $\rightarrow$ changes lattice spacing a $\rightarrow$ changes temperature $T = 1/(aN_t)$ in $[\mathrm{f} = T_0 \rightarrow T]$ process

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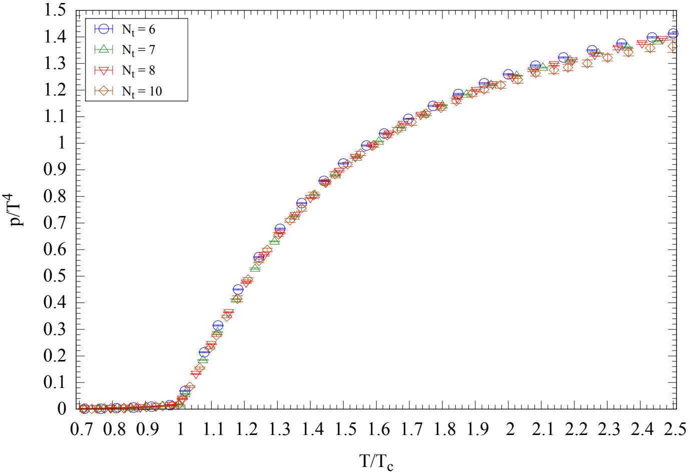
evolution in β (inverse coupling) $\rightarrow$ changes lattice spacing a $\rightarrow$ changes temperature $T = 1/(aN_t)$ in $[\mathrm{f} = T_0 \rightarrow T]$ process

Important difference: the prior is not a random distribution, but a thermalized Markov chain at a certain inverse coupling β_0 (or temperature T_0)

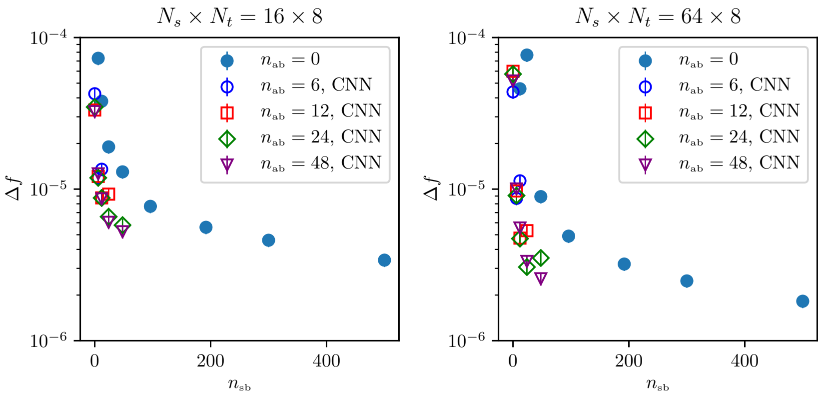
Observation: for systems with many d.o.f. (large volumes), Jarzynski's equality "converges" more easily to the right result when stochastic evolutions are very close to equilibrium (i.e. N is large, evolution is slow). "Easy" way to obtain reversibility.

SU(3) pressure in $(3+1)d$ across the deconfinement transition with Jarzynski's equality



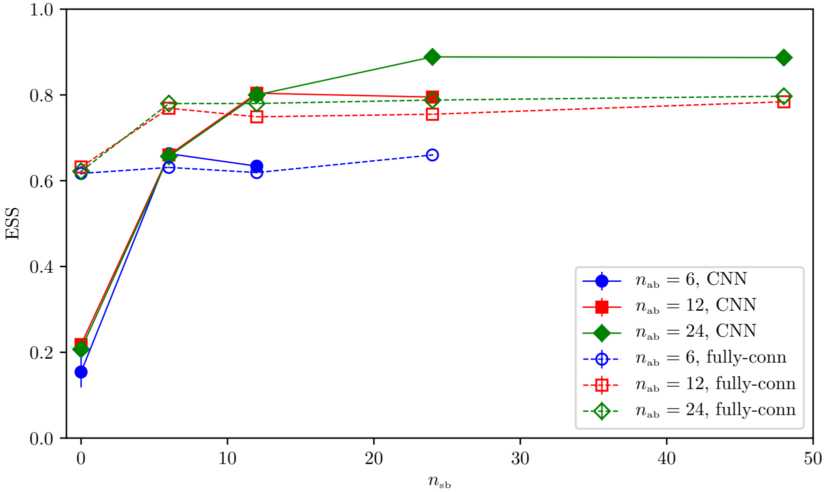
Does it work for SNFs?

More transparent comparison: error on the free-energy density

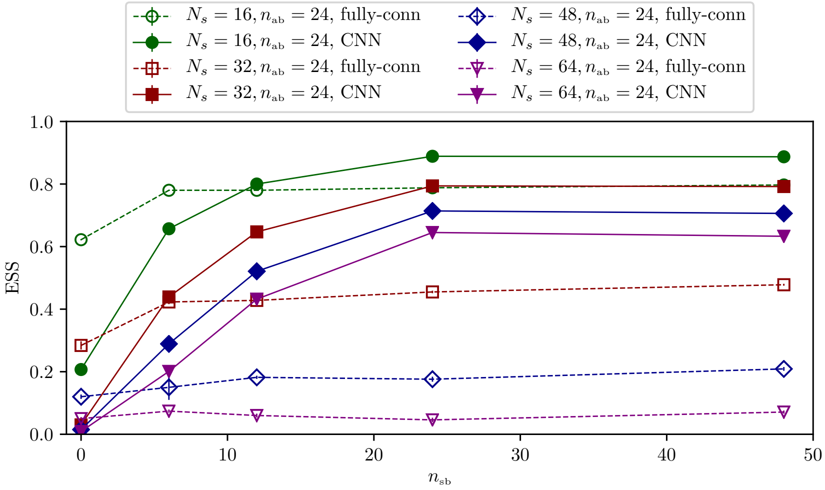


Overall computational cost difficult to assess

CNN vs fully-connected networks with $N_t \times N_s$ neurons, 16×8 lattice

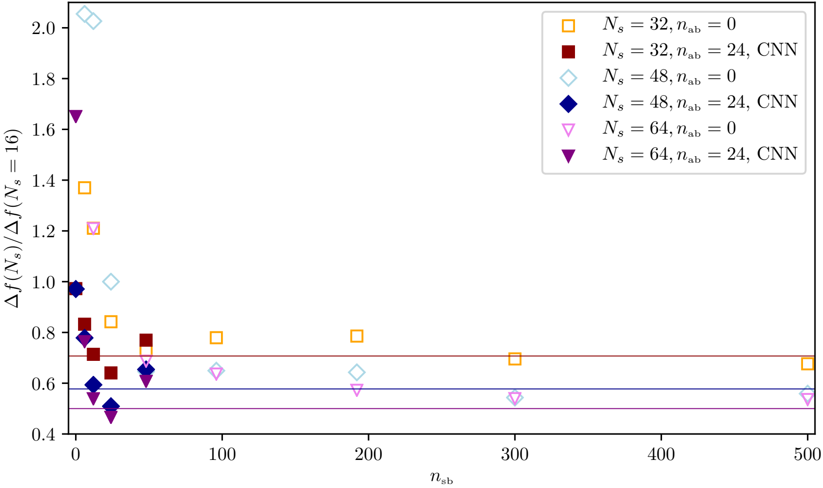


CNN vs fully-connected networks with $N_t \times N_s$ neurons, larger lattices



SNFs not necessarily convenient for any NFs: poor performance with fully-connected NNs

Error ratio



$N_s = 32, n_{ab} = 0$
$N_s = 32, n_{ab} = 24$, CNN
$N_s = 48, n_{ab} = 0$
$N_s = 48, n_{ab} = 24$, CNN
$N_s = 64, n_{ab} = 0$
$N_s = 64, n_{ab} = 24$, CNN
$\Delta f(N_s)/\Delta f(N_s = 16)$
n_{sb}
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0
100
200
300
400
500

The Second Law of Thermodynamics

We start from Clausius inequality

$$\int_A^B \frac{\mathrm{d}Q}{T} \leq \Delta S$$

that for isothermal transformations becomes

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

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

$$W \geq \Delta F$$

where the equality holds for reversible processes.

Moving from thermodynamics to statistical mechanics we know that the former relation (valid for a *macroscopic* system) becomes

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

JE and the Second Law

Starting from Jarzynski's equality

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

and using *Jensen's inequality*

$$\langle \exp x\rangle \geq \exp\langle x\rangle$$

(valid for averages on real x) we get

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

from which we have

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

In this sense Jarzynski's relation can be seen as a **generalization** of the Second Law.

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.