Continuous Normalizing Flows for Lattice QCD

based on Trivializing Maps

Dr. Simone Bacchio

Computational Scientist

CaSToRC, The Cyprus Institute

A work in collaboration with

Pan Kessel, Stefan Schaefer, Lorenz Vaitl

Funded by
PRACE-6IP, WP8 "Forward Looking Software Solutions".
Grant agreement ID: 823767, Project name: LyNcs.

Generative Models

$$\mathbf{x} = f(\mathbf{z}) \longrightarrow \log p_{\mathbf{x}}(\mathbf{x}) = \log p_{\mathbf{z}}(\mathbf{z}) - \log \det \left| \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \right|$$

➢ **First normalizing flows** arXiv:1505.05770

- Restrict functional form of *f* for simplified determinant
- Non-tractable analytic inverse of *f* → Not trainable on data

➢ **Autoregressive transformations** arXiv:1606.04934

- Use autoregressive models for lower-triangular Jacobian
- Expensive inverse of *f*, which requires *D* applications of *f*

➢ **Partitioned transformations** arXiv:1605.08803

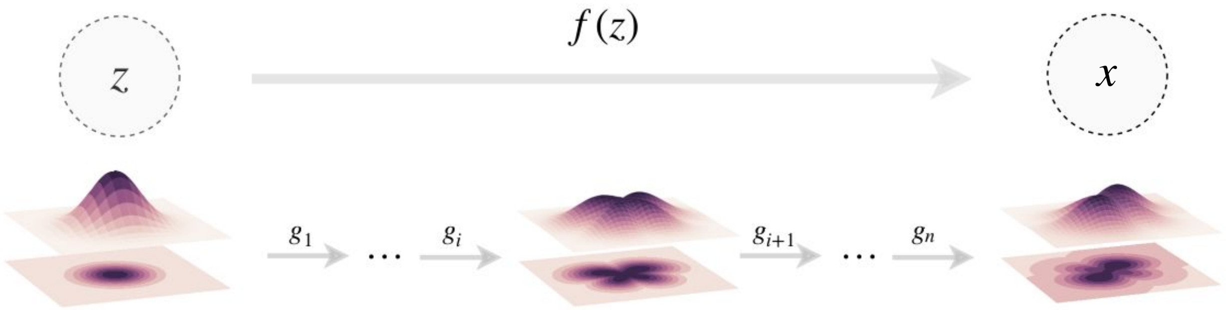
- Use partitioning and affine transformations for cheap *det* and inverse of *f*

➢ Cost of det ?

➢ Inverse of f?

From discrete to continuous

$$\mathbf{x} = f(\mathbf{z}) \longrightarrow \log p_{\mathbf{x}}(\mathbf{x}) = \log p_{\mathbf{z}}(\mathbf{z}) - \log \det \left| \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \right|$$



$$\mathbf{h}_{t+1} = \mathbf{h}_t + f(\mathbf{h}_t, \theta_t) \xrightarrow{?} \frac{d\mathbf{h}(t)}{dt} = f(\mathbf{h}(t), t, \theta)$$

From discrete to continuous

$$\mathbf{x} = f(\mathbf{z}) \longrightarrow \log p_{\mathbf{x}}(\mathbf{x}) = \log p_{\mathbf{z}}(\mathbf{z}) - \log \det \left| \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \right|$$

Neural Ordinary Differential Equations

arXiv:1806.07366

Ricky T. Q. Chen*, Yulia Rubanova*, Jesse Bettencourt*, David Duvenaud
University of Toronto, Vector Institute
{rtqichen, rubanova, jessebett, duvenaud}@cs.toronto.edu

$$\boxed{\frac{d\mathbf{z}}{dt} = f(\mathbf{z}(t), t)} \longrightarrow \log p(\mathbf{z}(t_1)) = \log p(\mathbf{z}(t_0)) - \int_{t_0}^{t_1} \mathrm{Tr}\left(\frac{\partial f}{\partial \mathbf{z}(t)} \right) dt$$

$$\longrightarrow \mathbf{x} = \mathbf{z}(t_1) = \mathbf{z}(t_0) + \int_{t_0}^{t_1} f(\mathbf{z}(t), t, \theta) dt$$

✓ *Tr cheaper*

✓ *No inverse required*

CNF for LFT

How to define $$\dot{U} \equiv \frac{dU}{dt} = f(U, t)$$???

where U is in $SU(N)$

ODEs on manifolds

$$\dot{U} = g(U)U$$ where $U \in$ Group, $\boxed{g \in \text{Algebra}}$

- g(U) must be element of the algebra
- Imposing Gauge invariance:

$$U_\mu(x) \to \Omega(x)U_\mu(x)\Omega^\dagger(x+\mu) \quad \Rightarrow \quad \boxed{g(U_\mu(x)) \to \Omega(x)g(U_\mu(x))\Omega^\dagger(x)}$$

- Strong constraints on g(U), **how to satisfy these properties?**

Lüscher's ansatz

$$g(U_\mu(x)) = \partial_{x,\mu}\tilde{S}(U)$$
$$\dot{U} = \left(\partial_{x,\mu}\tilde{S}(U)\right) U$$

arXiv:0907.5491

Trivializing maps, the Wilson flow and the HMC algorithm

Martin Lüscher

CERN, Physics Department, 1211 Geneva 23, Switzerland

where

$\tilde{S}(U) = \sum_i c_i W_i(U)$ and $W(U) = \sum_{x,\mu} \mathrm{Re}\,\mathrm{Tr}(U_\mu(x)\Sigma_\mu(x))$

Proof of properties

$$\partial_{x,\mu}\tilde{S}(U) = \sum_i c_i \sum_{y,\nu} \partial_{x,\mu}\mathrm{Tr}\big(U_\nu(y)\Sigma_\nu(y) + U_\nu^\dagger(y)\Sigma_\nu^\dagger(y)\big)$$

- **Is it element of the algebra?**

$$\begin{aligned} T_a\partial^a_{x,\mu}\mathrm{Tr}\big(U_\mu(x)\Sigma_\mu(x) + U_\mu^\dagger(x)\Sigma_\mu^\dagger(x)\big) &= T_a\mathrm{Tr}\big(T_aU_\mu(x)\Sigma_\mu(x) - \Sigma_\mu^\dagger(x)U_\mu^\dagger(x)T_a\big) \\ &\equiv T_a\mathrm{Tr}\big(T_a(U_\mu(x)\Sigma_\mu(x) - U_\mu^\dagger(x)\Sigma_\mu^\dagger(x))\big) \end{aligned}$$

$$M - M^\dagger = i\alpha_0 1 + \sum_b \alpha_b T_b \quad \Rightarrow \quad = T_a \sum_b \alpha_b \mathrm{Tr}(T_aT_b)$$

$$= -\frac{1}{2}T_a\sum_b \alpha_b\delta_{ab} = -\frac{1}{2}\sum_b \alpha_b T_b \qquad \square$$

Proof of properties

$$\partial_{x,\mu} \tilde{S}(U) = \sum_i c_i \sum_{y,\nu} \partial_{x,\mu} \mathrm{Tr}\left(U_\nu(y)\Sigma_\nu(y) + U_\nu^\dagger(y)\Sigma_\nu^\dagger(y)\right)$$

- **Does it transform as** $g(U_\mu(x)) \to \Omega(x) g(U_\mu(x)) \Omega^\dagger(x)$ **?**

$$\partial_{x,\mu} \mathrm{Tr}\left(U_\mu(x)\Sigma_\mu(x) + U_\mu^\dagger(x)\Sigma_\mu^\dagger(x)\right) = -\tfrac{1}{2}\left(U_\mu(x)\Sigma_\mu(x) - \Sigma_\mu^\dagger(x)U_\mu^\dagger(x) - i\alpha_0 1\right)$$

if $U_\mu(x)\Sigma_\mu(x)$ is a closed path, then

$$U_\mu(x) \to \Omega(x) U_\mu(x) \Omega^\dagger(x+\mu) \quad \Longrightarrow \quad \partial_{x,\mu} \tilde{S}(U) \to \Omega(x) \partial_{x,\mu} \tilde{S}(U) \Omega^\dagger(x)$$

$\square$

Lüscher's ansatz

$$g(U_\mu(x)) = \partial_{x,\mu}\tilde{S}(U)$$

$$\dot{U} = \left(\partial_{x,\mu}\tilde{S}(U)\right)U$$

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Lüscher ansatz satisfies all properties, but...

?

- Does the force of any gauge invariant quantity satisfy the properties?
- Are there more generic approaches to define g(U)?
- Is it Lüscher ansatz good enough to define a CNF?

Lüscher's ansatz

$$g(U_\mu(x)) = \partial_{x,\mu}\tilde{S}(U)$$

$$\dot{U} = \left(\partial_{x,\mu}\tilde{S}(U)\right) U$$

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$$\boxed{\frac{d\mathbf{z}}{dt} = f(\mathbf{z}(t), t)} \rightarrow \log p(\mathbf{z}(t_1)) = \log p(\mathbf{z}(t_0)) - \int_{t_0}^{t_1} \mathrm{Tr}\left(\frac{\partial f}{\partial \mathbf{z}(t)}\right) dt$$

$$\rightarrow \mathbf{x} = \mathbf{z}(t_1) = \mathbf{z}(t_0) + \int_{t_0}^{t_1} f(\mathbf{z}(t), t, \theta) dt$$

Reminder about CNF

Lüscher's ansatz

$$g(U_\mu(x)) = \partial_{x,\mu}\tilde{S}(U)$$

$$\dot{U} = \left(\partial_{x,\mu}\tilde{S}(U)\right)U$$

arXiv:0907.5491

Trivializing maps, the Wilson flow and the HMC algorithm

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- Another result from his work: **Lüscher already discovered CNFs!**

$$\log p(U(t_1)) = \log p(U(t_0)) - \int_{t_0}^{t_1} \mathcal{L}\tilde{S}(U)dt$$

where $$\mathcal{L}\tilde{S}(U) = -\sum_{x,\mu,a}\partial^a_{x,\mu}\partial^a_{x,\mu}\tilde{S}(U)$$

Laplacian of action

$$\mathcal{L}\tilde{S}(U) = -\sum_{x,\mu,a} \partial^a_{x,\mu}\partial^a_{x,\mu}\tilde{S}(U)$$

$$= -\sum_i c_i \sum_{x,\mu,a} \sum_{y,\nu} \partial^a_{x,\mu}\partial^a_{x,\mu} \mathrm{ReTr}\big(U_\nu(y)\Sigma_\nu(y)\big)$$

For loops w/o repeated links

$$= -\sum_i c_i \sum_{x,\mu,a} \mathrm{ReTr}\big(T^a T^a U_\mu(x)\Sigma_\mu(x)\big)$$

Laplacian of action

$$\mathcal{L}\tilde{S}(U) = -\sum_{x,\mu,a} \partial^a_{x,\mu}\partial^a_{x,\mu}\tilde{S}(U)$$

$$= -\sum_i c_i \sum_{x,\mu,a}\sum_{y,\nu} \partial^a_{x,\mu}\partial^a_{x,\mu} \mathrm{ReTr}\big(U_\nu(y)\Sigma_\nu(y)\big)$$

For loops w/o repeated links

$$= -\sum_i c_i \sum_{x,\mu,a} \mathrm{ReTr}\big(T^a T^a U_\mu(x)\Sigma_\mu(x)\big)$$

Using the completeness relation

$$= \frac{N^2-1}{2N}\sum_i c_i \sum_{x,\mu} \mathrm{ReTr}\big(U_\mu(x)\Sigma_\mu(x)\big) = \boxed{\frac{N^2-1}{2N}\tilde{S}(U)}$$

$$\sum_a T^a_{\alpha\beta}T^a_{\gamma\delta} = -\frac{1}{2}\left(\delta_{\alpha\delta}\delta_{\beta\gamma} - \frac{1}{N}\delta_{\alpha\beta}\delta_{\gamma\delta}\right) \Rightarrow \sum_a T^a_{\alpha\beta}T^a_{\beta\delta} = -\frac{N^2-1}{2N}\delta_{\alpha\delta}$$

Our work: from Trivializing Maps to CNF

1. Time-dependence in the coefficients

$$\tilde{S}(U) = \sum_i c_i(t) W_i(U)$$

2. Training of the coefficients via minimization of the KL divergence
3. Calculation of the gradients via back-propagation
4. Generic implementation for any Wilson loop
5. …

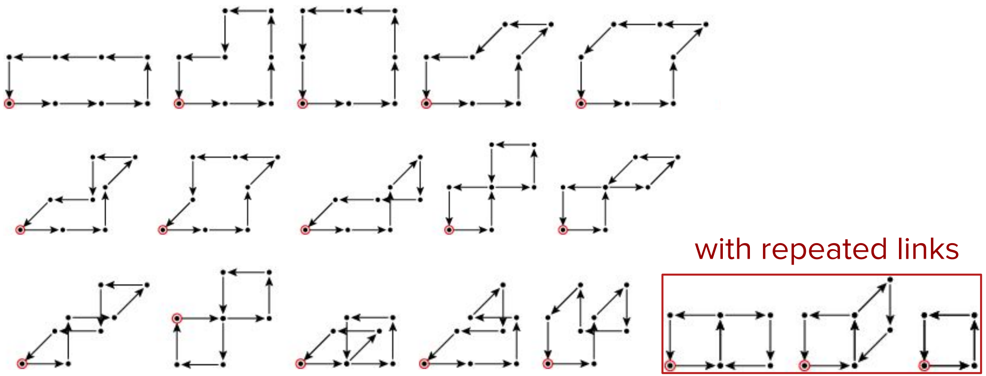
Mapping from uniform distribution:

$$L_{KL} = S_{\text{target}}(U_T) + \int_0^1 \mathcal{L}\tilde{S}(U_t)dt$$

Software

- Developed using Python and Lyncs-API
- Numpy implementation for S(N) in M-dimensions
- On GPU via Quda for SU(3) in 2/3/4-dimensions
- Logic for dealing with any-size closed loop

E.g. all unique geometries of length 8 in 3D

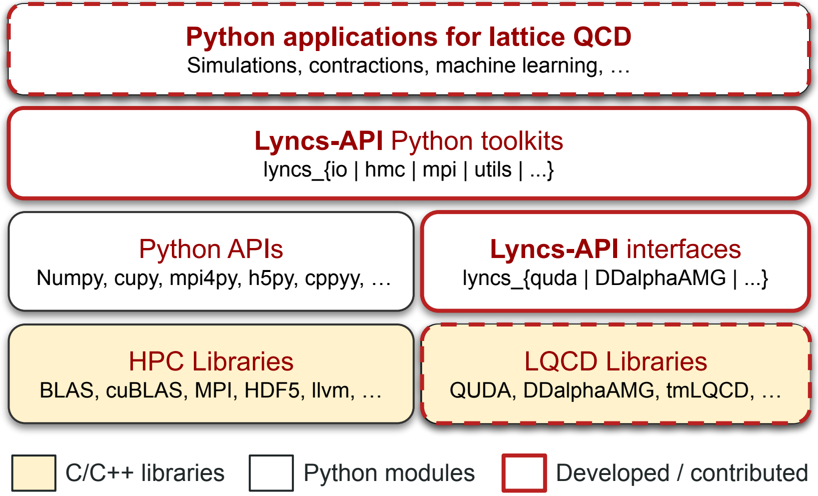


Lyncs-API

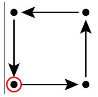
A Python API for Lattice QCD applications

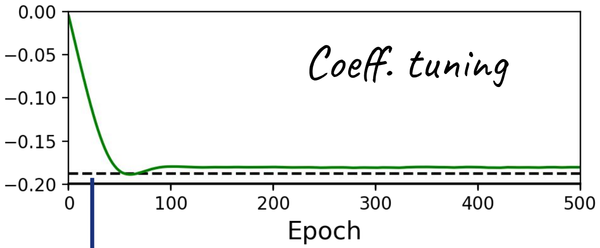
https://lyncs-api.github.io/ s.bacchio@gmail.com

Python ecosystem for Lattice QCD



First results





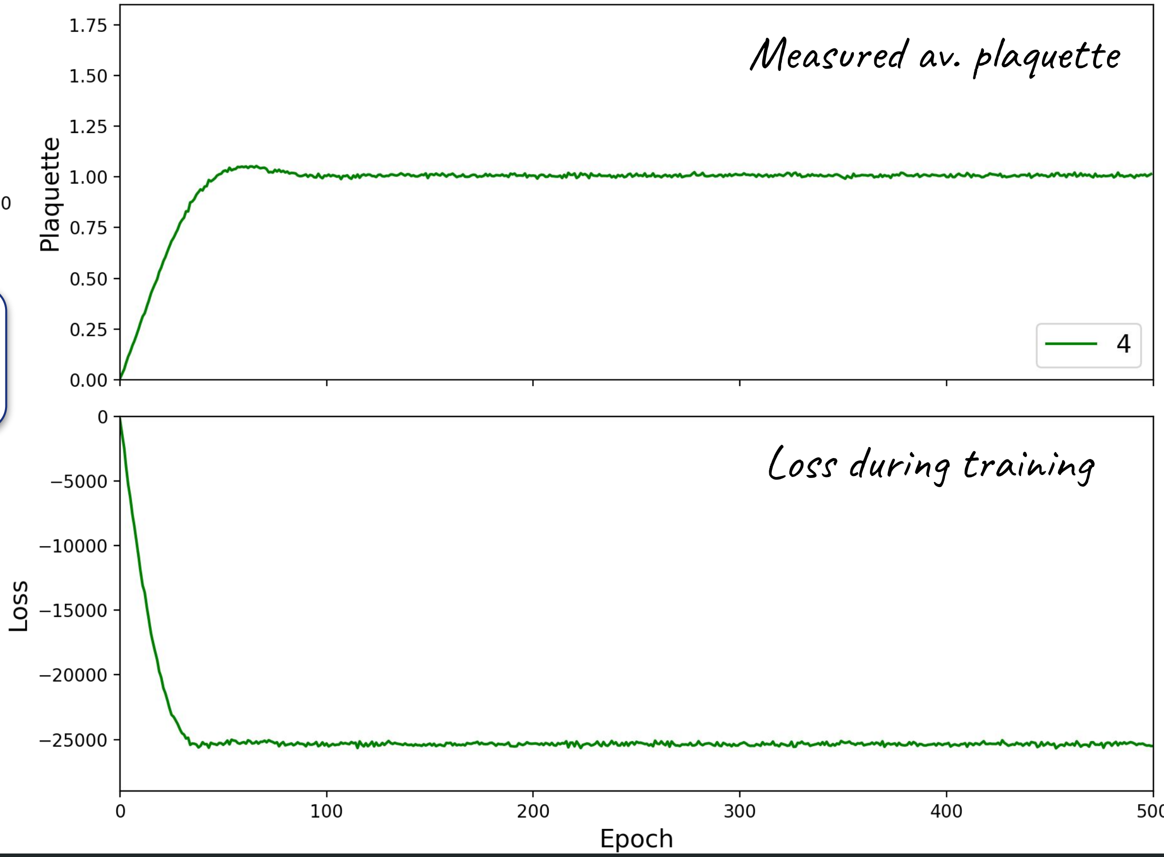
Wilson flow param.

$$\widetilde{S}^{(0)} = \left(-\frac{1}{32}\beta\right)\mathcal{W}_0 = \frac{3}{16}S_{\mathrm{w}}$$

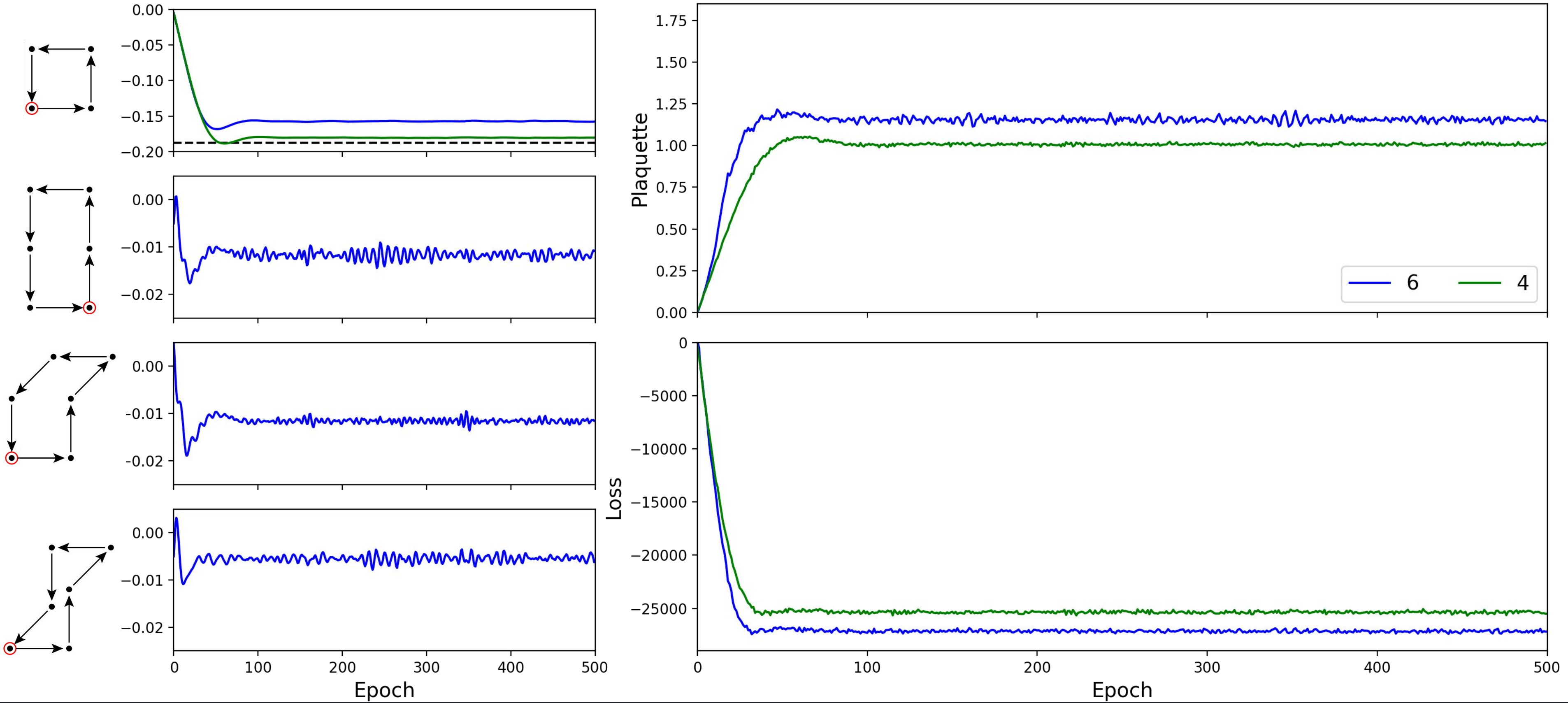
Setup

- Pure-gauge SU(3)
- Lattice size 16^4
- Coupling $\beta=6$
- No time depend.

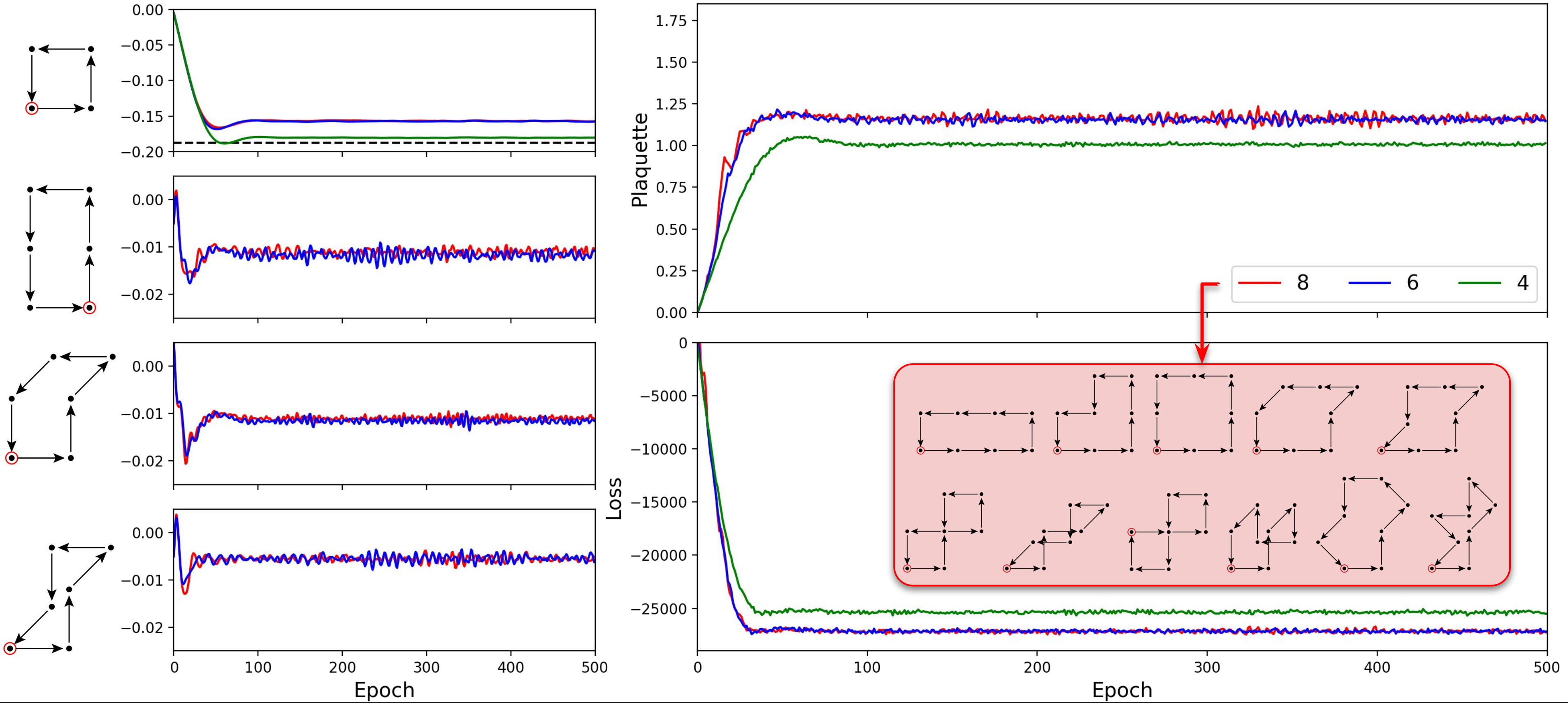
$$\tilde{S}(U) = \sum_i c_i(\cancel{t})W_i(U)$$



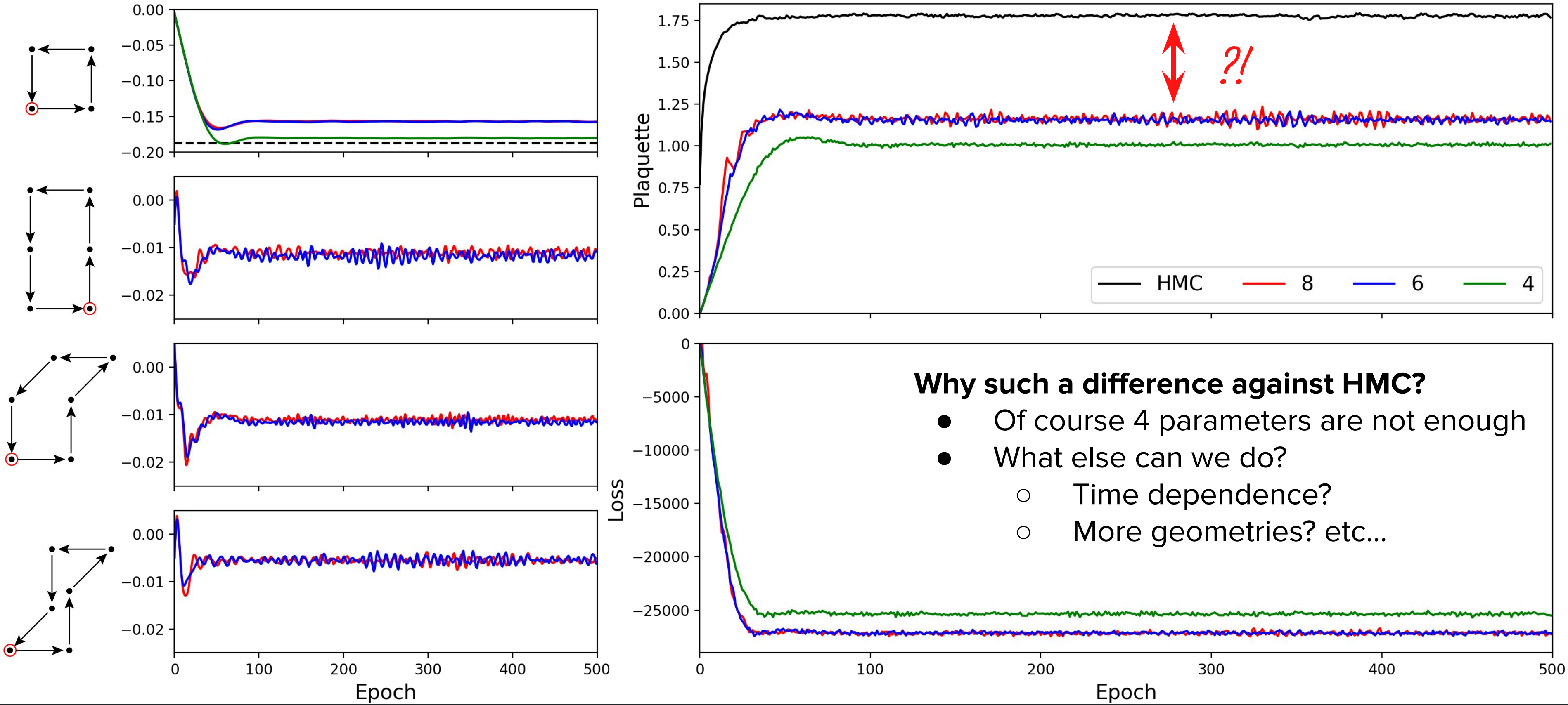
First results



First results



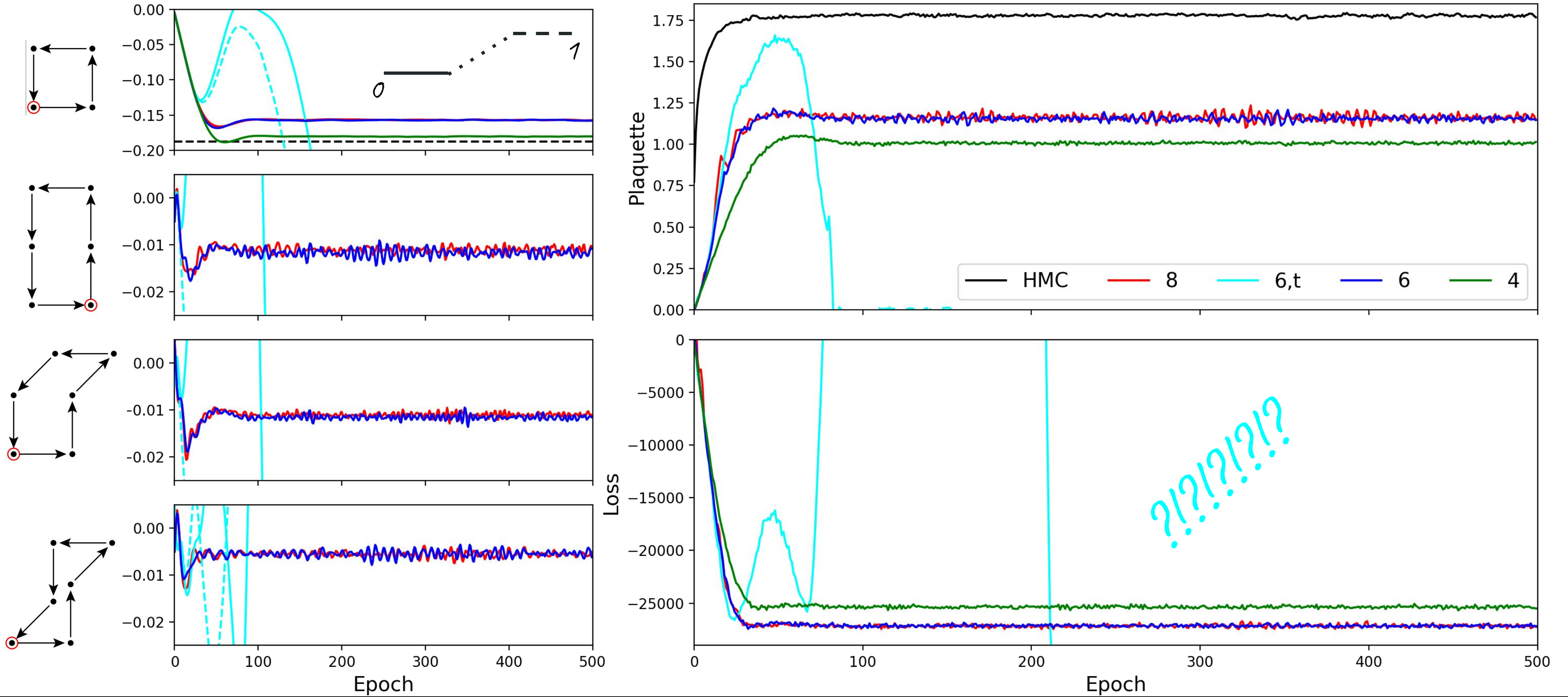
First results



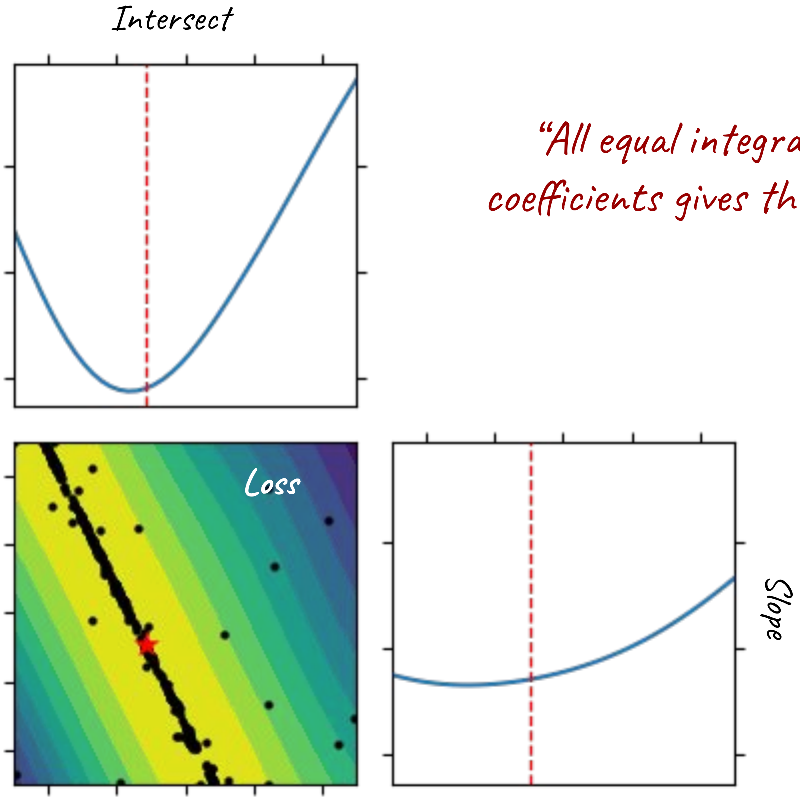
Why such a difference against HMC?

- Of course 4 parameters are not enough
- What else can we do?
    - Time dependence?
    - More geometries? etc...

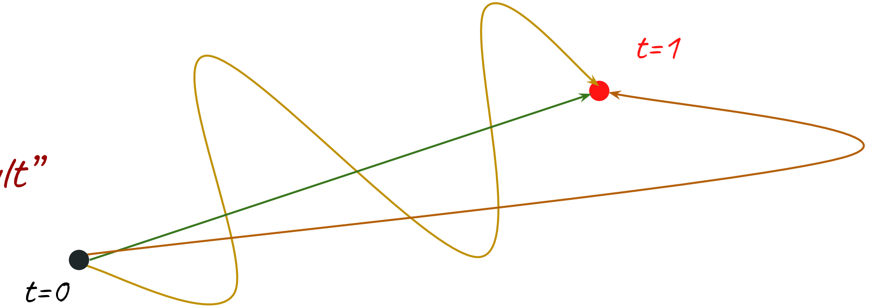
First results



Degeneracy of integral

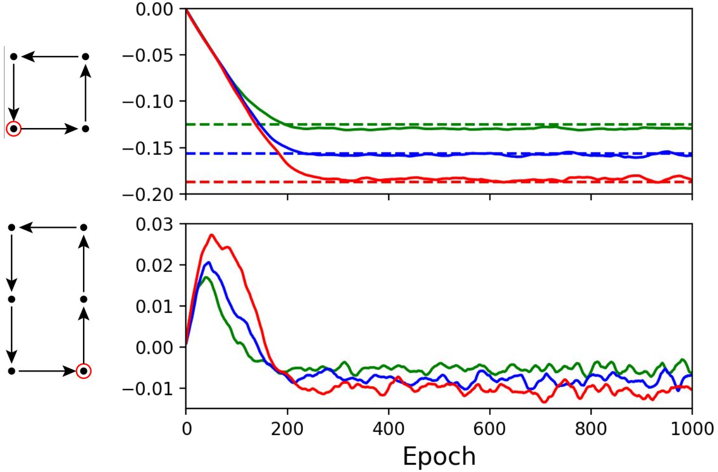


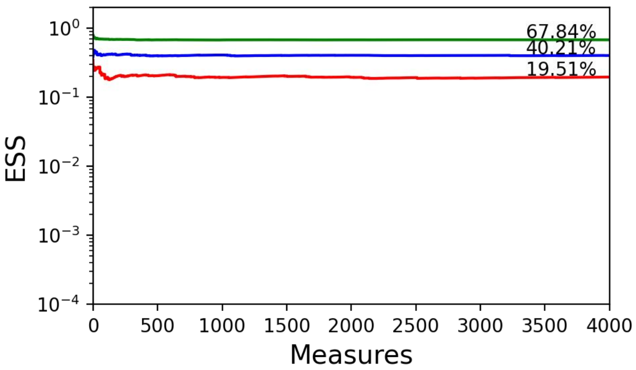
"All equal integrals over the coefficients gives the same result"

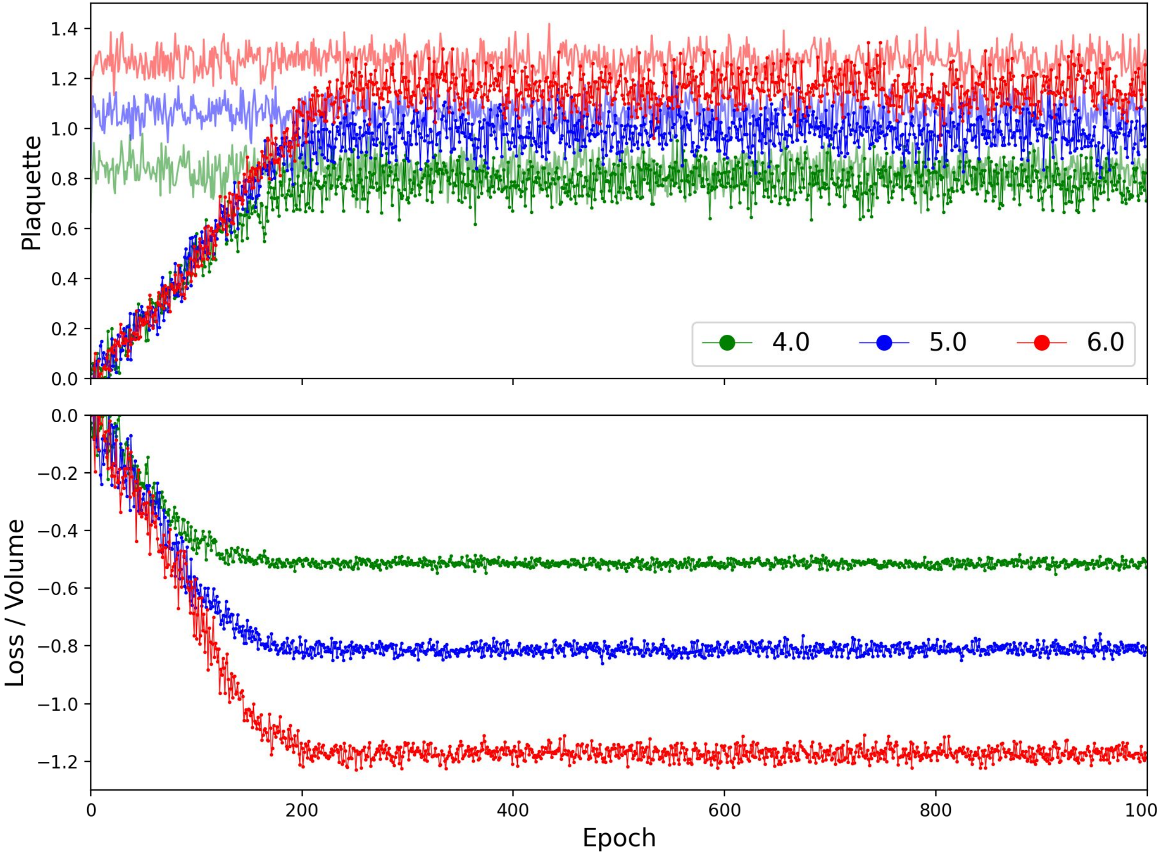


- Single-geometry integral is trivially degenerate
- Multiple-geometries integral is also degenerate:
  - Numerically tested for length 6... *Any proof?*
- Large coefficient introduce numerical instabilities
- Is constant enough? *Not really!*
- How to solve the problem? *We could improve it but not solve it*

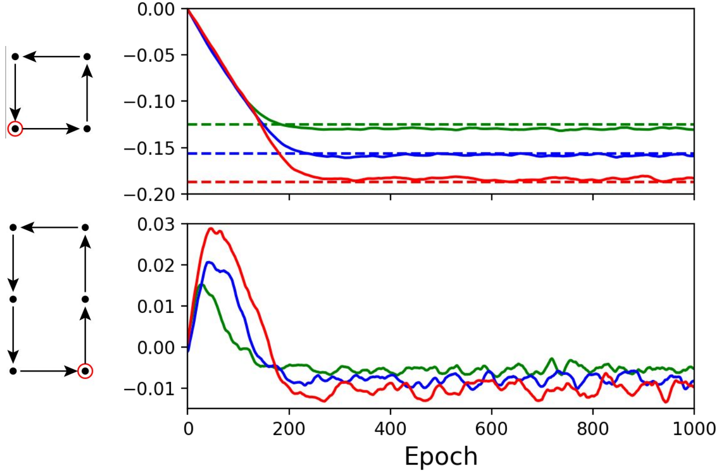
Let's be less ambitious: 4^2

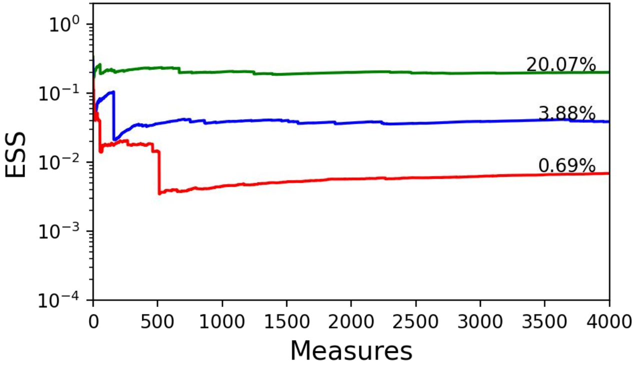


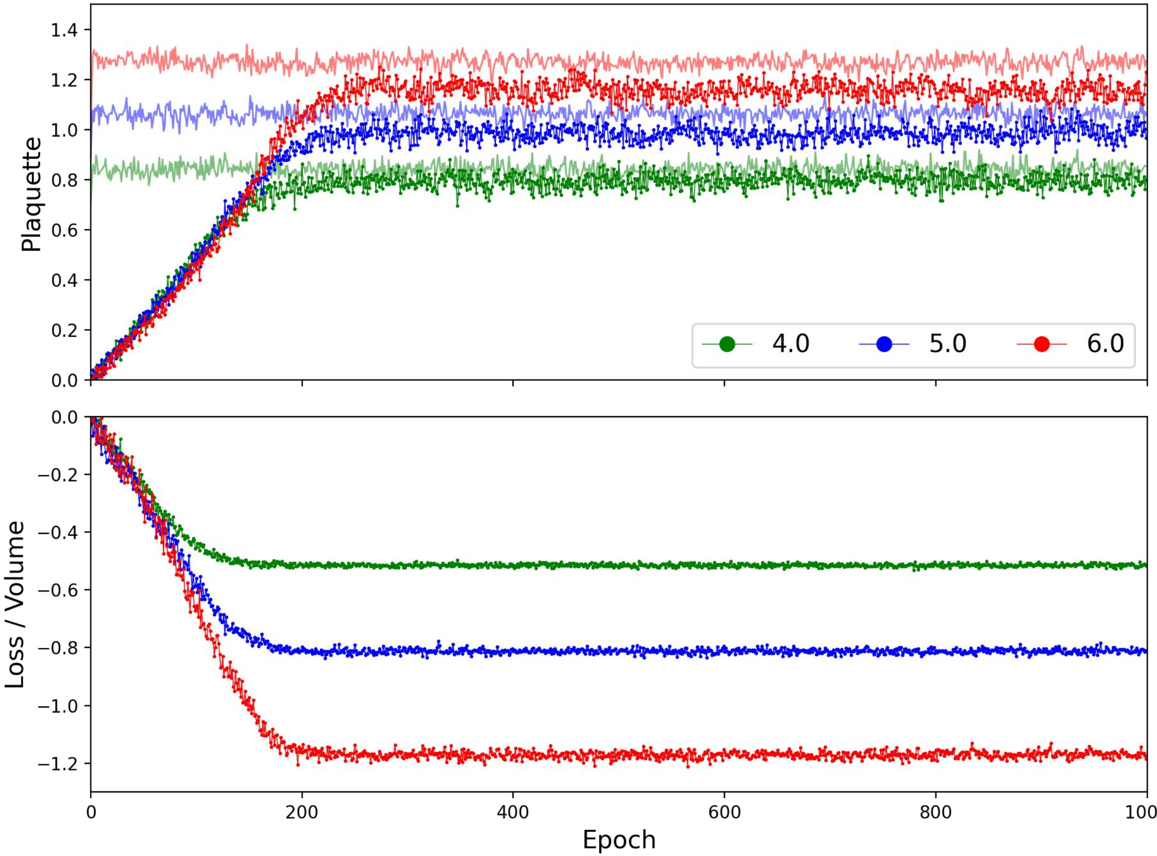




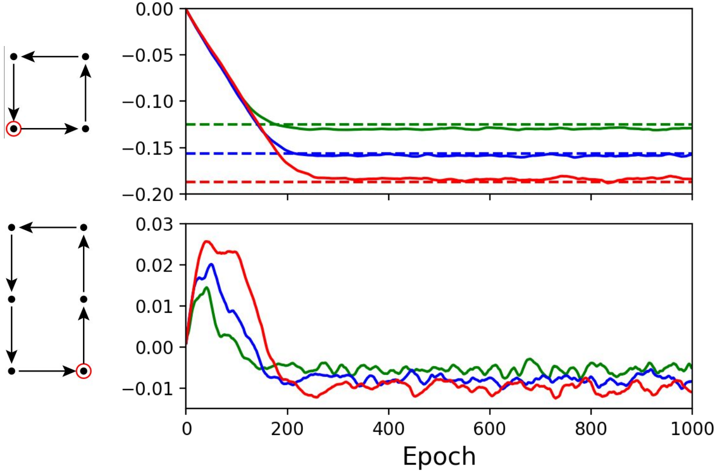
Let’s be less ambitious: 8^2

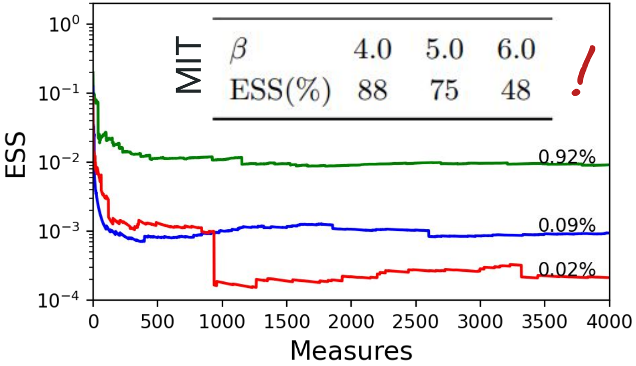




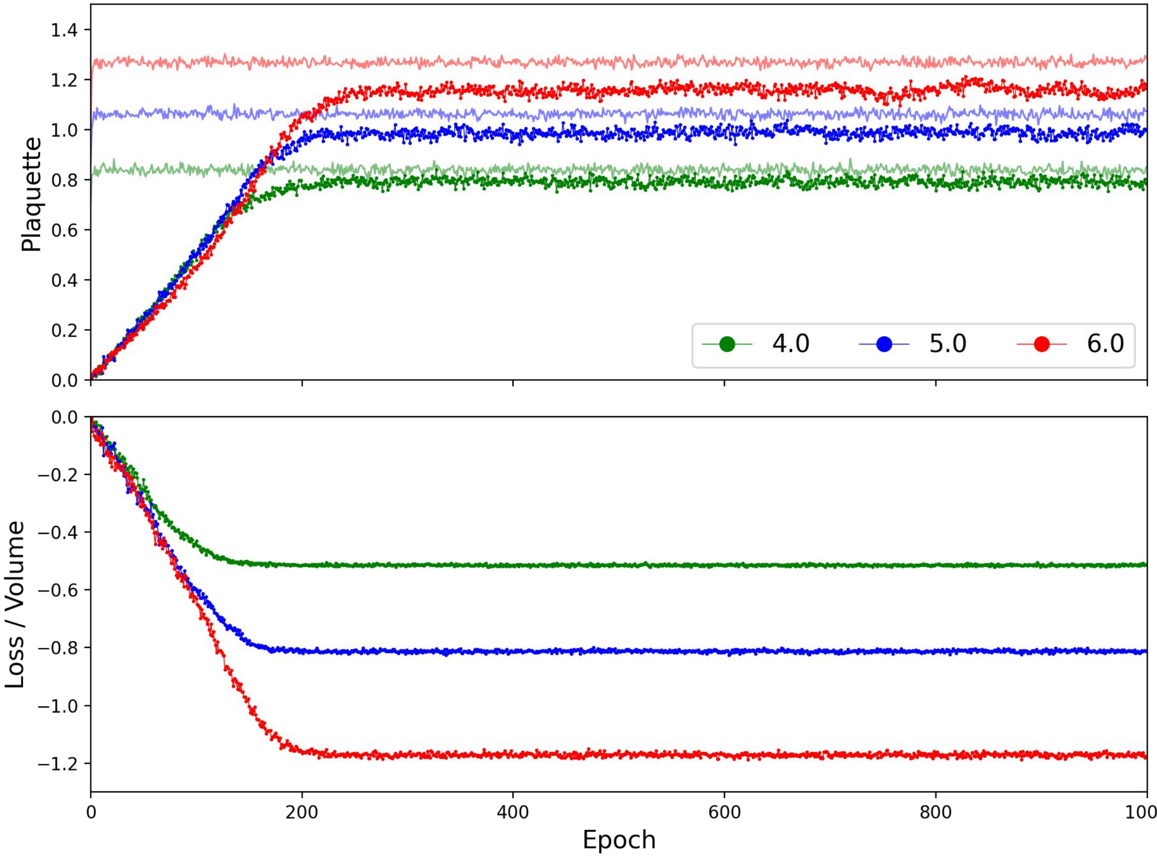


Let's be less ambitious: 16^2





MIT			
β	4.0	5.0	6.0
ESS(%)	88	75	48



What’s more? Loops with repeated links!

- **Issues:**
  - Much more difficult lagrangian
  - Product of traces and shifts

- **Questions:**
  - How to generalize them?
  - Will they help?

arXiv:0907.5491

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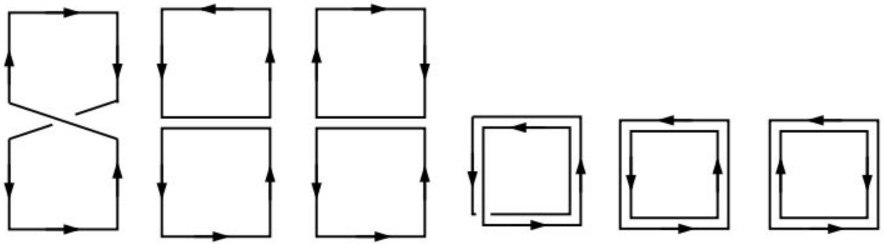
$$\mathfrak{L}_0\mathcal{W}_2 = \tfrac{31}{3}\mathcal{W}_2 + \mathcal{W}_4, \qquad \mathfrak{L}_0\mathcal{W}_5 = \tfrac{28}{3}\mathcal{W}_5 + 4\mathcal{W}_6,$$

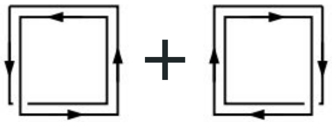
$$\mathfrak{L}_0\mathcal{W}_3 = 11\mathcal{W}_3 - \mathcal{W}_1, \qquad \mathfrak{L}_0\mathcal{W}_6 = \tfrac{28}{3}\mathcal{W}_6 + 4\mathcal{W}_5,$$

$$\mathfrak{L}_0\mathcal{W}_4 = \tfrac{31}{3}\mathcal{W}_4 + \mathcal{W}_2, \qquad \mathfrak{L}_0\mathcal{W}_7 = 12\mathcal{W}_7 + \text{constant}.$$



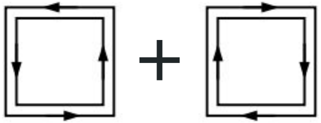
(2) (3) (4) (5) (6) (7)

Giving a closer loop



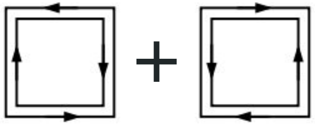
(5)

$$\mathrm{Re}\,\mathrm{Tr}(W^2)$$



(6)

$$\mathrm{Re}(\mathrm{Tr}(W))^2 - \mathrm{Im}(\mathrm{Tr}(W))^2$$



(7)

$$\mathrm{Re}(\mathrm{Tr}(W))^2 + \mathrm{Im}(\mathrm{Tr}(W))^2$$

$$\mathrm{Re}(\mathrm{Tr}(W))^2$$

$$\mathrm{Im}(\mathrm{Tr}(W))^2$$

Our work: from Trivializing Maps to CNF

1. Time-dependence in the coefficients

$$\tilde{S}(U) = \sum_i c_i(t) W_i(U)$$

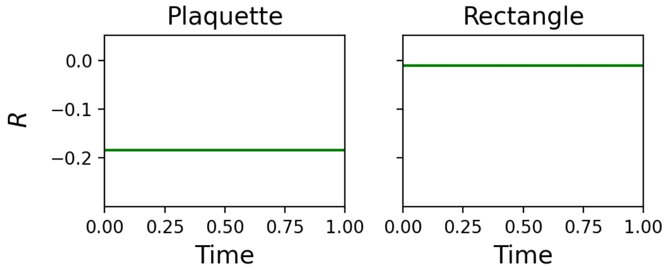
2. Training of the coefficients via minimization of the KL divergence
3. Calculation of the gradients via back-propagation
4. Generic implementation for any Wilson loop
5. Implementation of improved model:

Mapping from uniform distribution:

$$L_{KL} = S_{\text{target}}(U_T) + \int_0^1 \mathcal{L}\tilde{S}(U_t)dt$$

$$\tilde{S} = \sum_{i,l,m,n} c_{i,l,m,n}(t) \mathrm{Re}(W_{i,l})^m \mathrm{Im}(W_{i,l})^{2n} \quad \text{with} \quad W_{i,l} \equiv \mathrm{Tr}(W_i(U)^l)$$

Latest results: NMCMC, 16^2, β=6

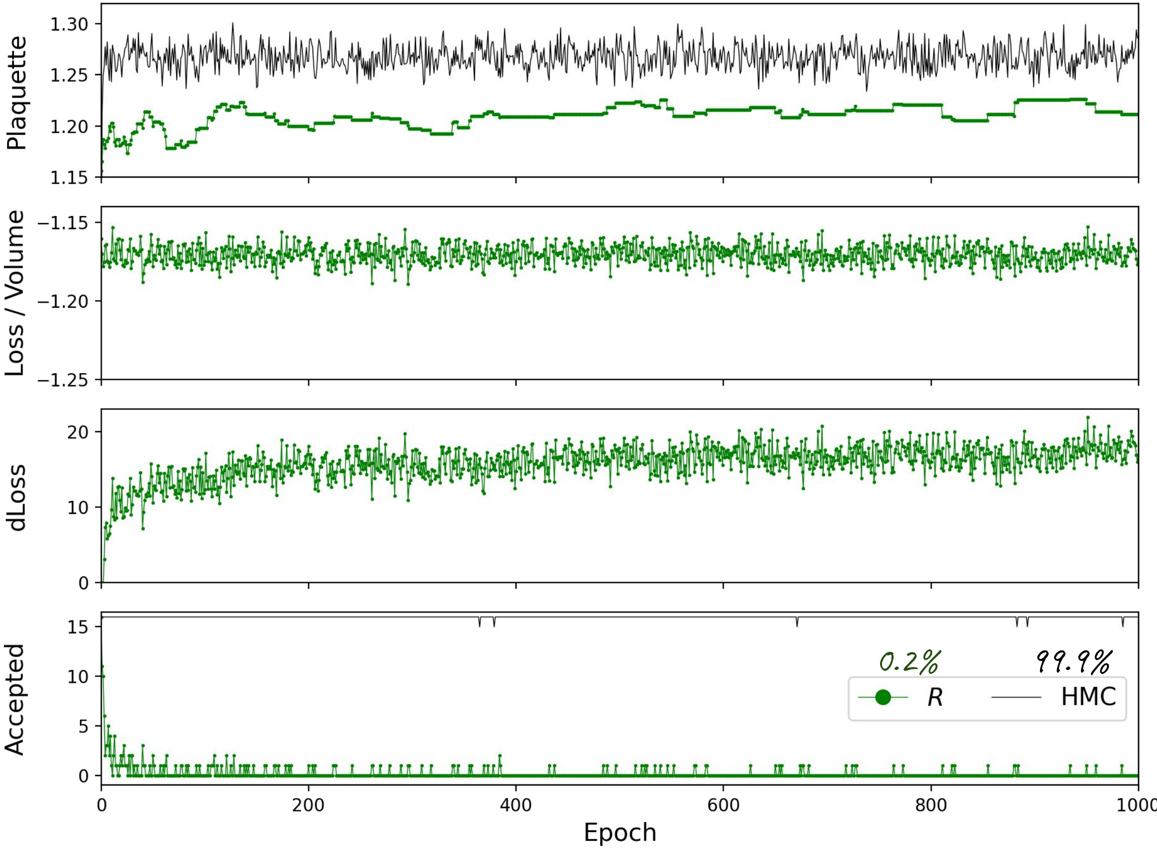


$$L_{KL} = S_{\text{target}}(U_T) + \int_0^1 \mathcal{L}\tilde{S}(U_t)dt$$

Acceptance probability:

$$\min\left(1, \frac{\exp(-L'_{KL})}{\exp(-L_{KL})}\right)$$

when sampling from uniform distribution



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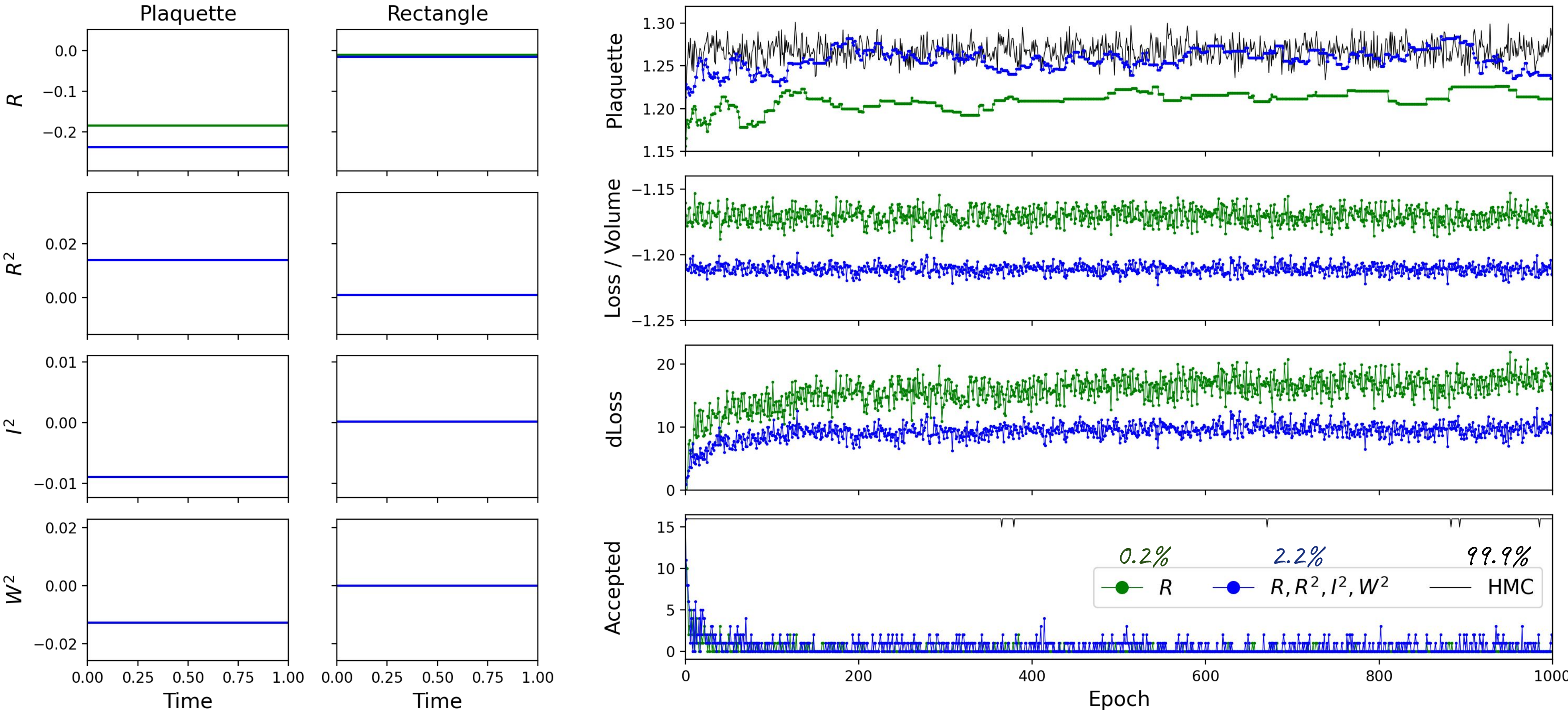
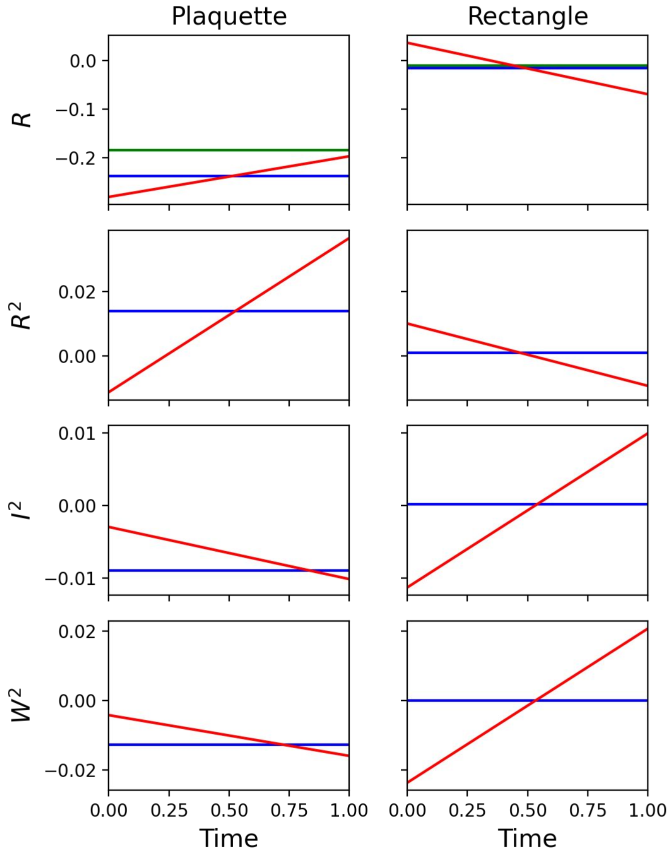
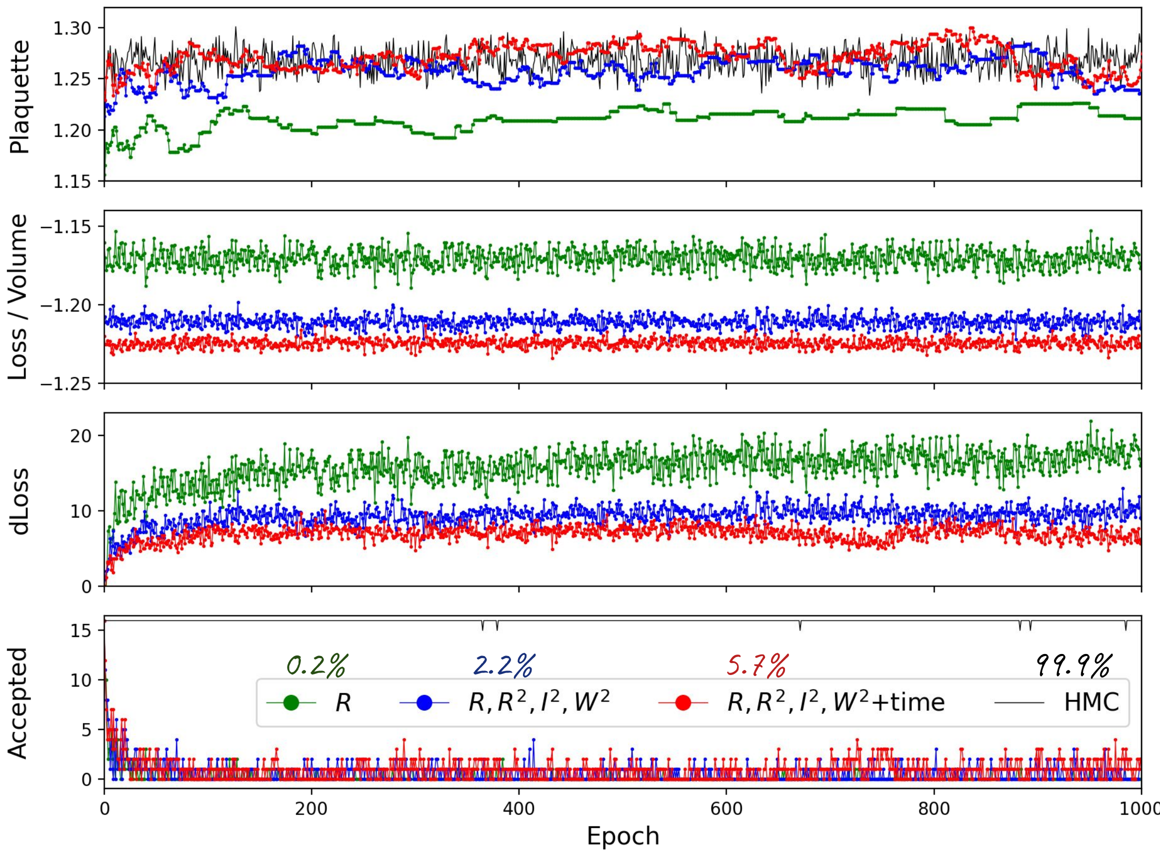


Latest results: NMCMC, 16^2, β=6





Conclusion

- Results for 16^2 at $\beta=6$:

ESS

0.02%	→	0.1%	→	0.5%	?	Goal ≳48%
2 params (plaq. + rect.)		**8 params** (plaq. + rect.) x (re,re^2,im^2,w^2)		**16 params** (plaq. + rect.) x (re,re^2,im^2,w^2) x 2 time (spline)		**O(10k) params?** [MIT, 2008.05456]

- Achievements:
  - ➢ Physical interpretation of parameters
  - ➢ Parameter transferring over volume
  - ➢ GPU and distributed implementation via QUDA
  - ➢ Generalization of Luesher approach
  - ➢ Parameter tuning via back propagation

- Open issues:
  - ➢ Sub-performing compared to normalizing flows
  - ➢ Manual implementation of models, not via ML libraries
  - ➢ Unstable tuning of time dependence due to degeneracy
  - ➢ Fermions not implemented yet, but doable
  - ➢ Integrator scaling when combining Lie groups and scalar

- Much more work to do and many idea... Working on first publication. Stay tuned!

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based on Trivializing Maps

Thank you for your attention!

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Runge-Kutta Integrators for scalar quantities

$$\frac{dy}{dt} = f(t, y)$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i$$

$$\begin{aligned}
k_1 &= f(t_n, y_n), \\
k_2 &= f(t_n + c_2 h, y_n + h(a_{21} k_1)), \\
k_3 &= f(t_n + c_3 h, y_n + h(a_{31} k_1 + a_{32} k_2)), \\
&\ \ \vdots \\
k_i &= f\left(t_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} k_j\right).
\end{aligned}$$

Butcher table

$$\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \dots & a_{1s} \\
c_2 & a_{21} & a_{22} & \dots & a_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\
\hline
 & b_1 & b_2 & \dots & b_s
\end{array}$$

Generic order 3

$$\alpha \neq 0, 2/3, 1$$

$$\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
\alpha & \alpha & 0 & 0 \\
1 & 1 + \frac{1-\alpha}{\alpha(3\alpha-2)} & -\frac{1-\alpha}{\alpha(3\alpha-2)} & 0 \\
\hline
 & \frac{1}{2} - \frac{1}{6\alpha} & \frac{1}{6\alpha(1-\alpha)} & \frac{2-3\alpha}{6(1-\alpha)}
\end{array}$$

Crouch-Grossman methods for Lie Groups

$$\dot{U} = g(U)U$$

$$\begin{aligned} k_i &= g(U^{(i)}) \\ U^{(i)} &= e^{h a_{i,i-1} k_{i-1}} \dots e^{h a_{i,1} k_1} U_n \\ U_{n+1} &= e^{h b_s k_s} \dots e^{h b_1 k_1} U_n \end{aligned}$$

order 1 : $\sum_i b_i = 1$

order 2 : $\sum_i b_i c_i = 1/2$

order 3 : $\sum_i b_i c_i^2 = 1/3 \quad \sum_{ij} b_i a_{ij} c_j = 1/6$

$\sum_i b_i^2 c_i + 2 \sum_{i<j} b_i c_i b_j = 1/3$

Butcher table

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \dots & a_{1s} \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\ \hline & b_1 & b_2 & \dots & b_s \end{array}$$

Example tables for order 3

$$\begin{array}{c|ccc} 0 & & & \\ -1/24 & -1/24 & & \\ 17/24 & 161/24 & -6 & \\ \hline & 1 & -2/3 & 2/3 \end{array}$$

$$\begin{array}{c|ccc} 0 & & & \\ 3/4 & 3/4 & & \\ 17/24 & 119/216 & 17/108 & \\ \hline & 13/51 & -2/3 & 24/17 \end{array}$$

How to combine scalars' and Lie groups' integration?

$$U_{n+1} = \left(\prod_{i=1}^{s} e^{hb_i k_i}\right) U_n$$

$$k_i = g(U^{(i)})$$

$$U^{(i)} = \left(\prod_{j=1}^{i-1} e^{ha_{ij} k_{i-1}}\right) U_n$$

- **Different coefficient from standard RK**

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i$$

$$k_i = f(U^{(i)}, y^{(i)})$$

$$y^{(i)} = y_n + h \sum_{j=1}^{i-1} a_{ij} k_j$$

- **Needed for:** Laplacian, gradients, etc..

?

- Currently we use O(3) for Lie groups, how does scalar integration scale?
- Can we have a scheme that has O(3) for both? Maybe with 4 steps?