Sampling states of spin models using generative neural networks

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Motivation

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- Supervised and Reinforcement learning compared
- Temperature dependent networks

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- Hamiltonian:

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- Two dimensional case with $J = 1$ shows a continuous phase transition at $\beta_c = 1/2 \ln\left(1 + \sqrt{2}\right) \approx 0.44$

Generative neural networks

- Randomly generate samples $\mathbf{s}$ using neural networks
- Goal: Distribution of $\mathbf{s}$ should equal the Boltzmann-Distribution

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- Asymptotically unbiased expectation values estimated by

Reweighting A. M. Ferrenberg, R. H. Swendsen, 1988; K. A. Nicoli, N. Strodthoff et al., 2020

$$\langle \mathcal{A} \rangle \approx \frac{1}{M} \sum_{\mathbf{s} \sim q} \frac{p(\mathbf{s})}{q(\mathbf{s})} \mathcal{A}(\mathbf{s}) \approx \frac{\sum_{\mathbf{s} \sim q} \mathcal{A}(\mathbf{s}) e^{-\beta \mathcal{H}(\mathbf{s})}/q(\mathbf{s})}{\sum_{\mathbf{s} \sim q} e^{-\beta \mathcal{H}(\mathbf{s})}/q(\mathbf{s})}$$

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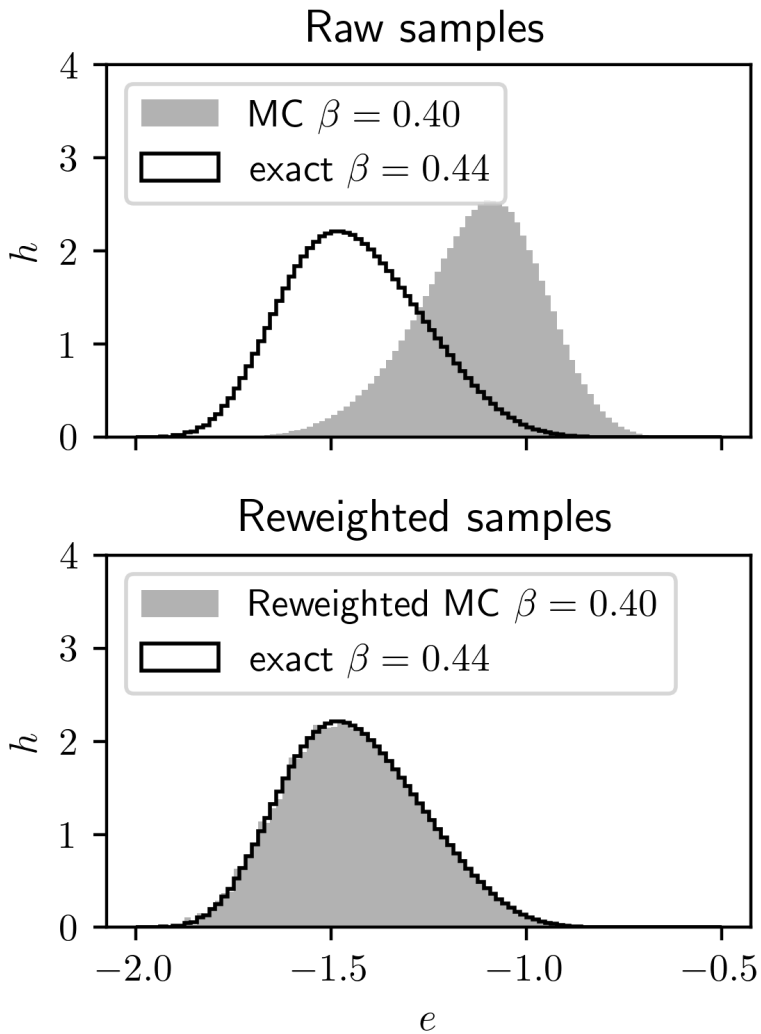
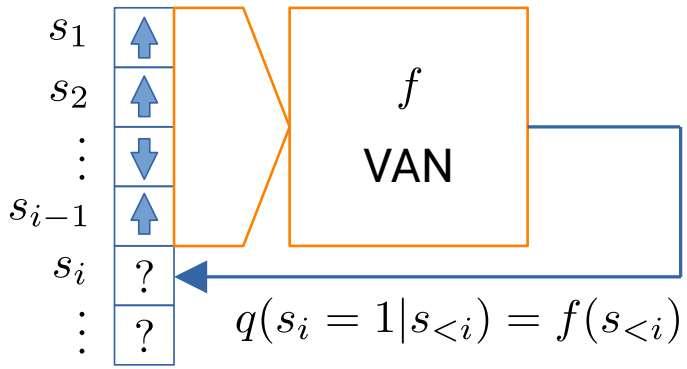


Variational autoregressive networks (VANs)



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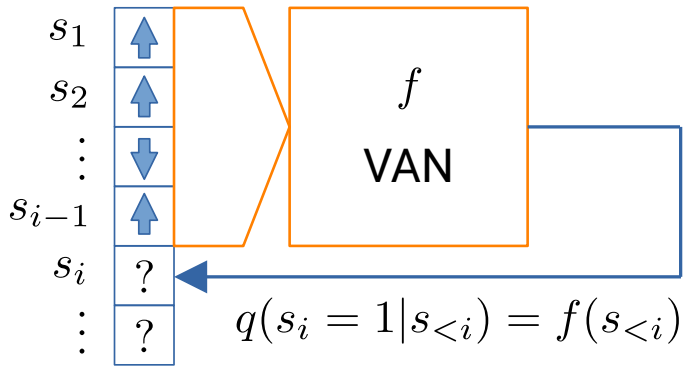

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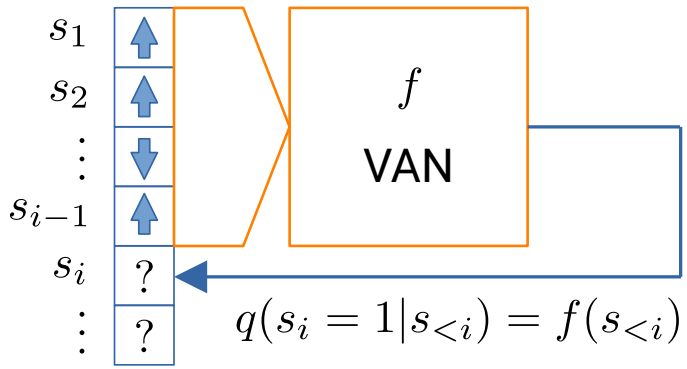

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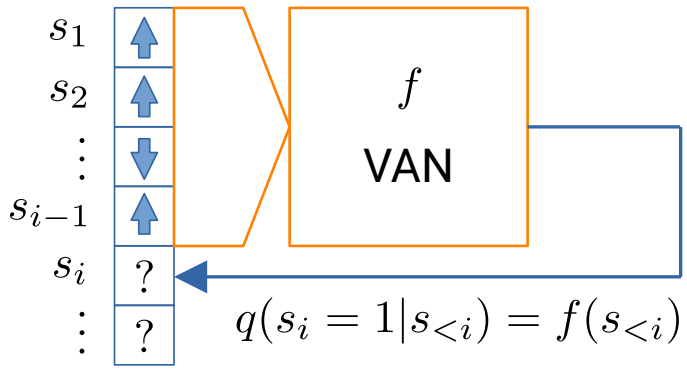

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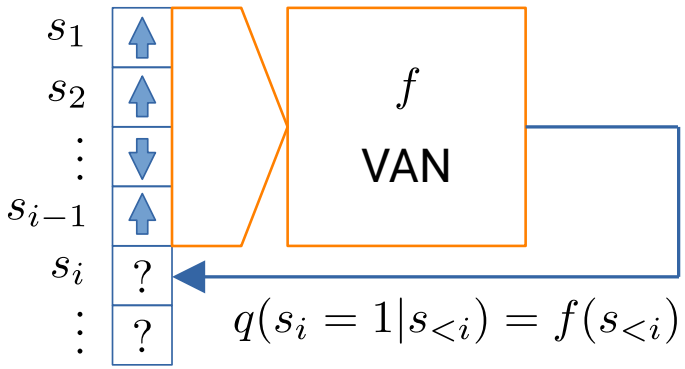

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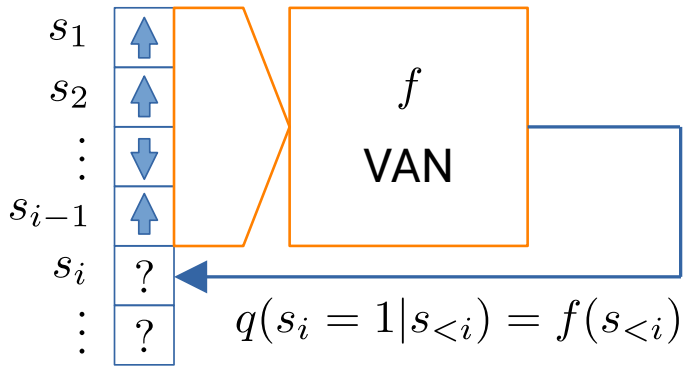

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5. Return s and $q(\mathrm{s}) = \prod_{i=1}^{N} q(s_i|s_{<i})$

VAN architecture

- Causal convolutional layers to fulfill the autoregressive property

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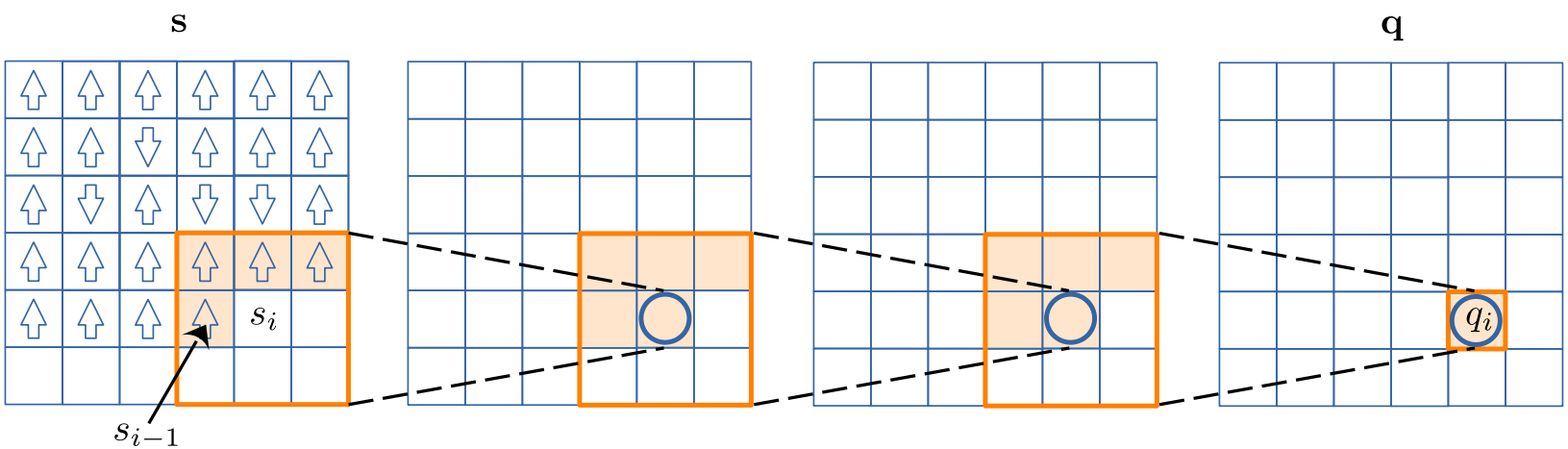

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Reinforcement learning

- The network generates a batch of samples
- Kullback-Leibler divergence is a measure of deviations between distributions
- Minimize $D_{\mathrm{KL}}(q \| p)$:

$$D_{\mathrm{KL}}(q \| p) \propto \sum_{\mathbf{s} \sim q} \log \left(\frac{q(\mathbf{s})}{p(\mathbf{s})} \right)$$

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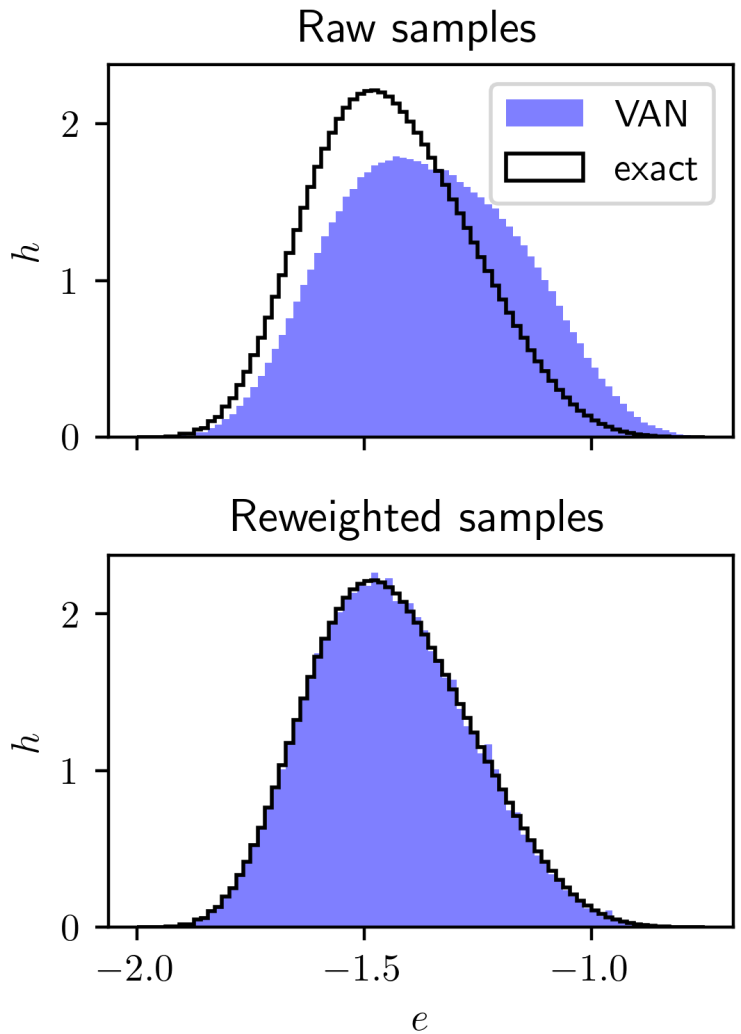
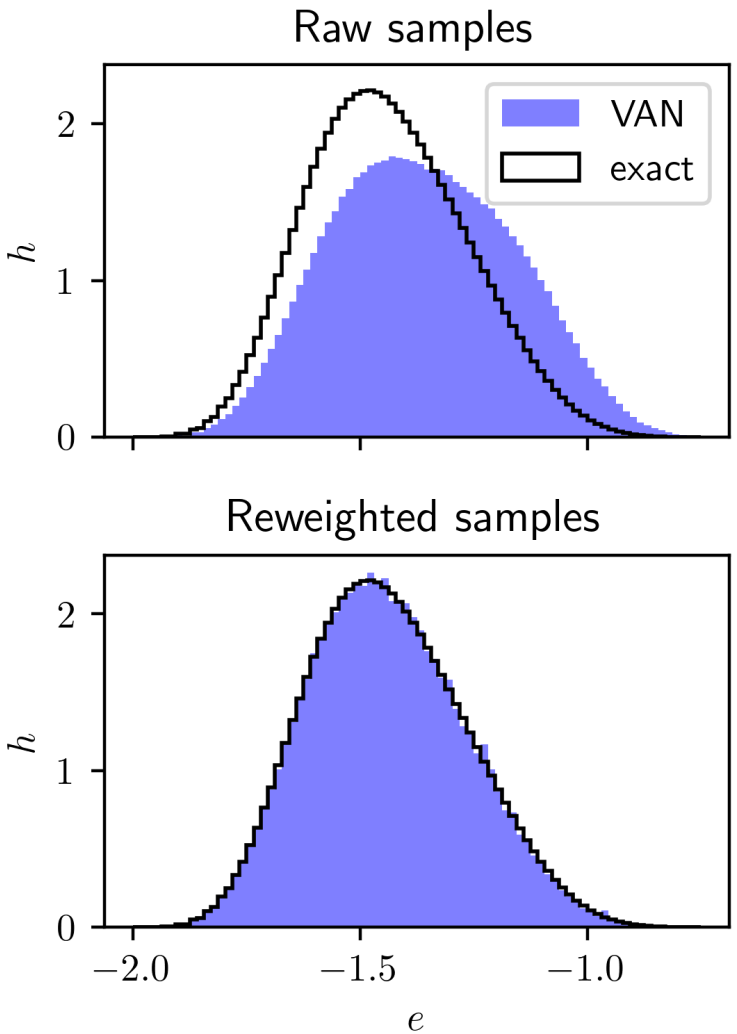


Energy histogram of sampled states

- VAN supervised trained for $L = 16$ and $\beta = 0.44$
- Estimates for $\langle e \rangle$ obtained from 10^6 samples:

Exact	$-1.4477...$
Raw samples	-1.3679
Reweighted	-1.4465 ± 0.0027
Relative error	8.5×10^{-4}



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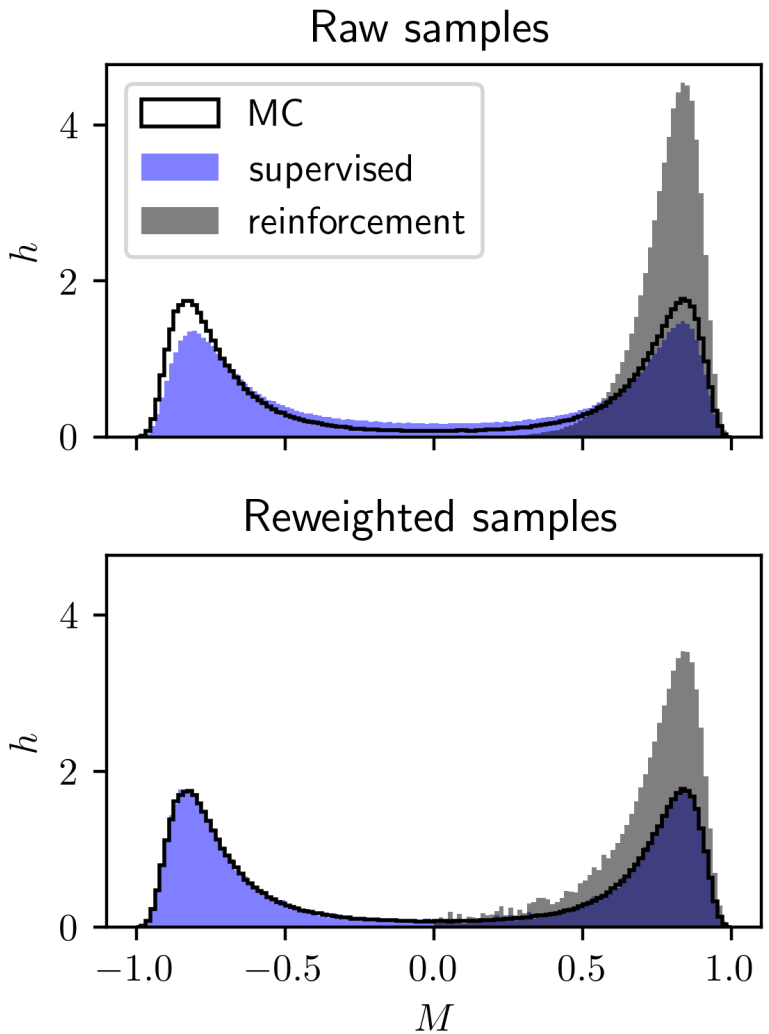

Supervised and Reinforcement Learning

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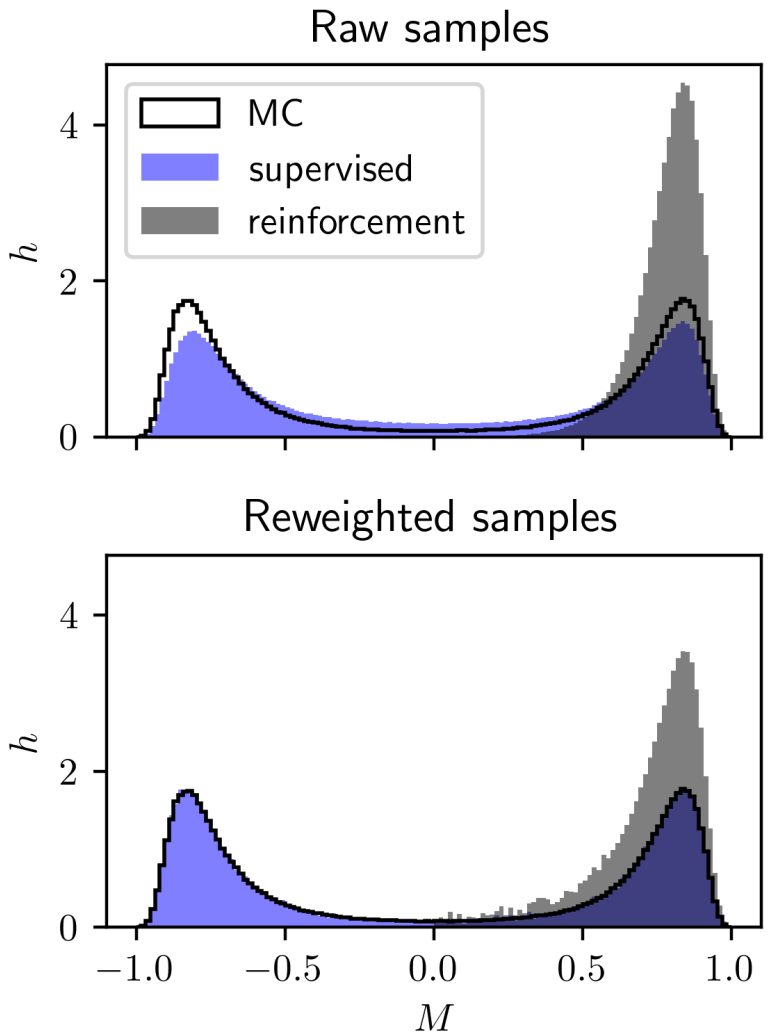
- Reinforced trained VAN does not require training data, but not capturing entire phase space
- Might be problematic for more complex systems



Observables from temperature dependent VANs

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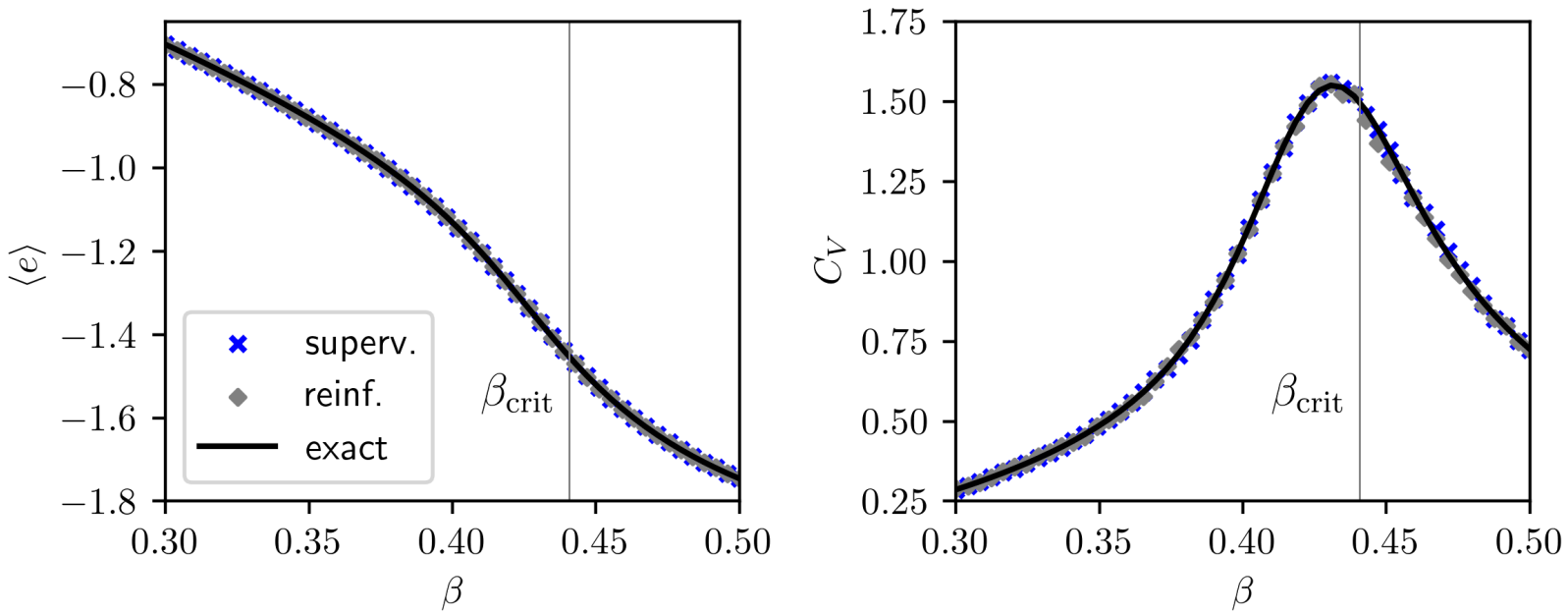
- Precise results for $\langle e \rangle$ and C_V in temperature range



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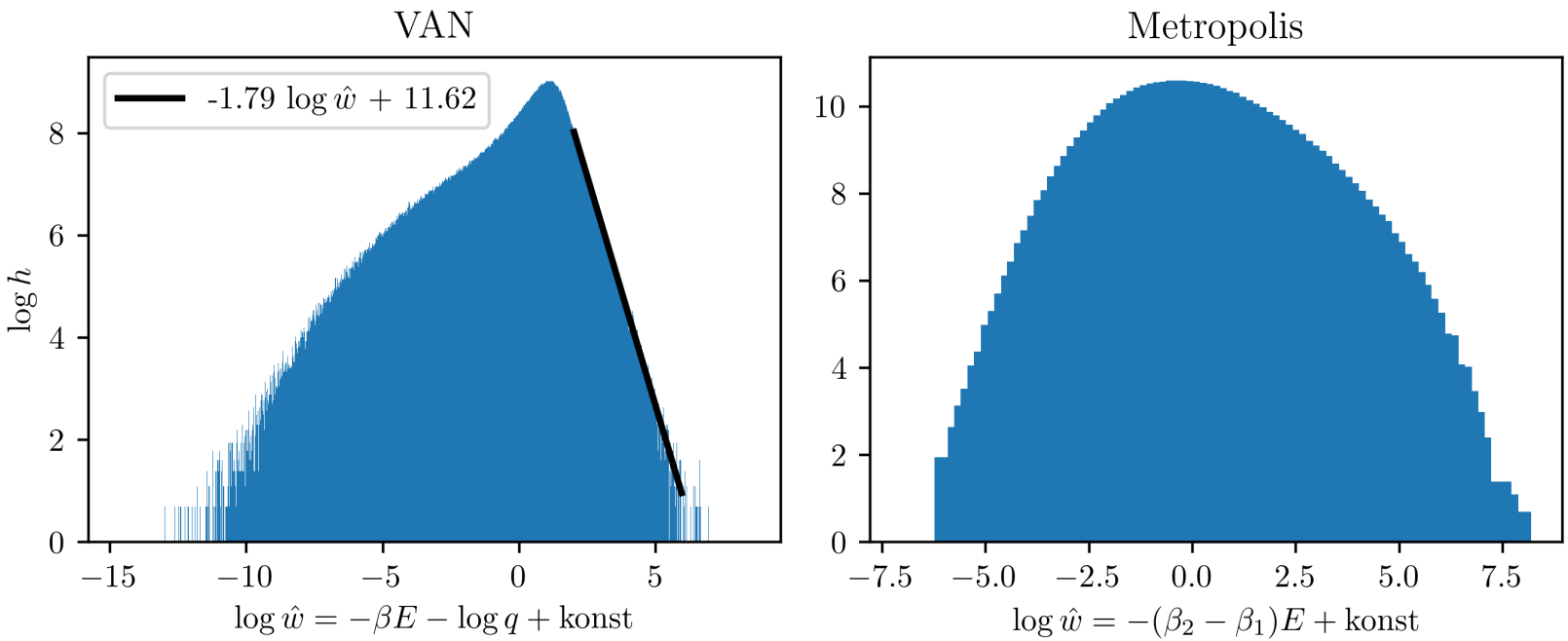
VAN
-1.79 log ŵ + 11.62
log h
log ŵ = −βE − log q + konst
Metropolis
log ŵ = −(β2 − β1)E + konst

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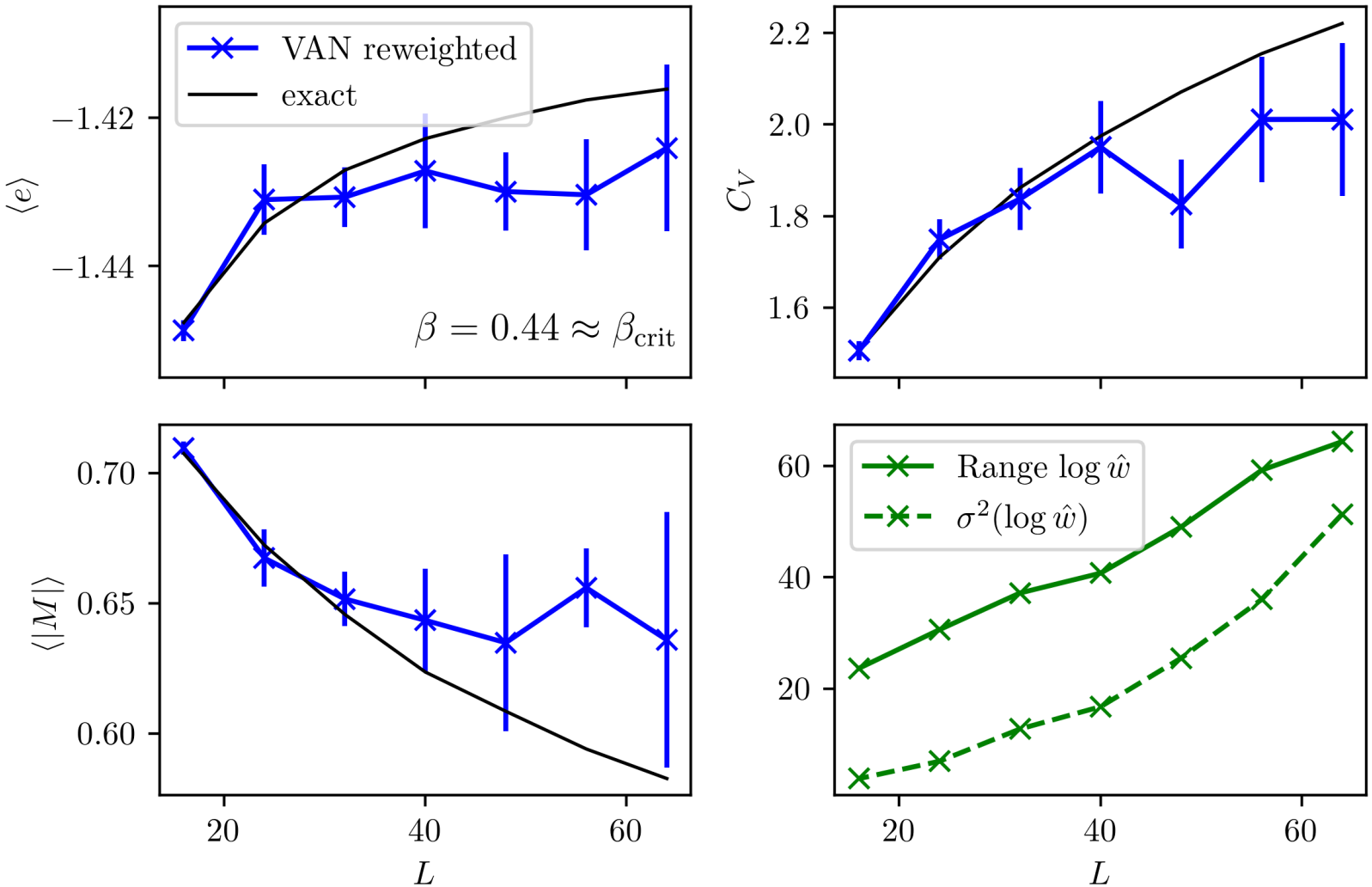
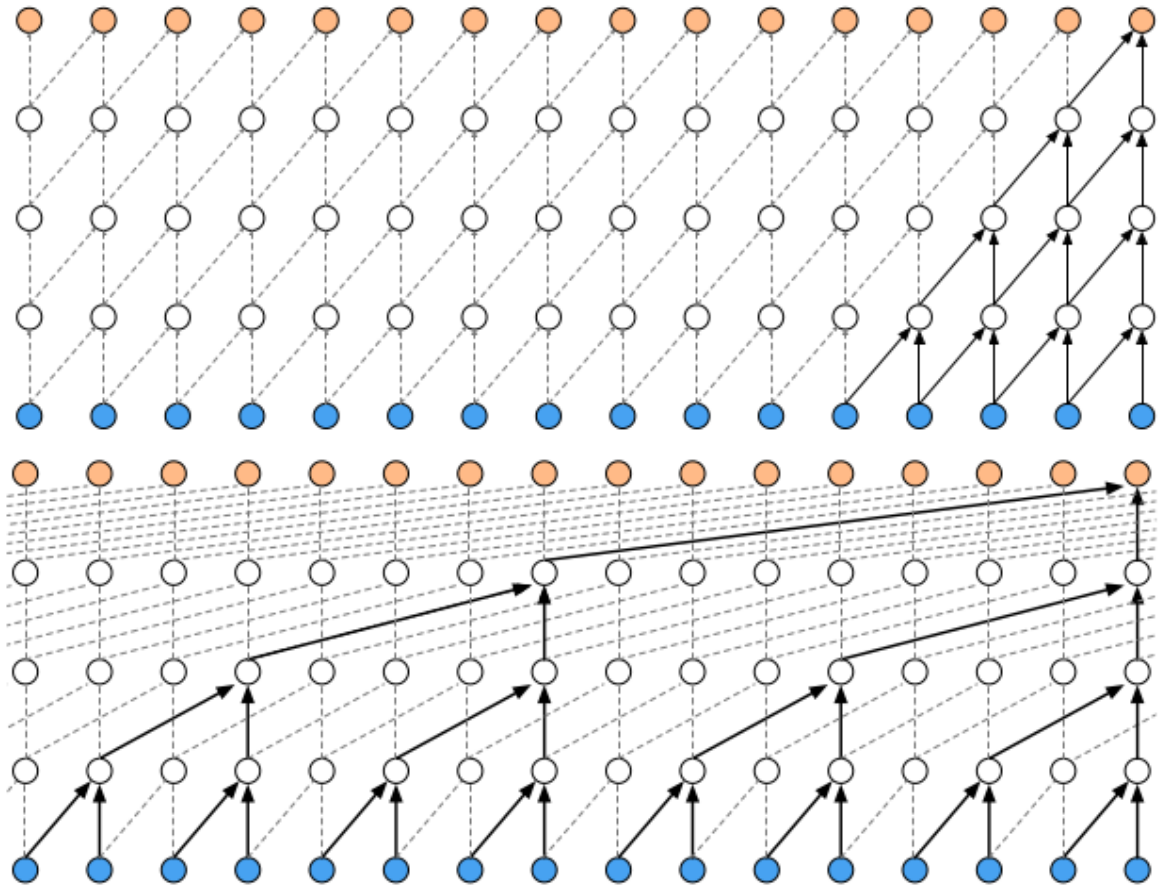

VAN reweighted
exact
$\beta = 0.44 \approx \beta_{\text{crit}}$
$\langle e \rangle$
−1.42
−1.44
C_V
2.2
2.0
1.8
1.6
$\langle |M| \rangle$
0.70
0.65
0.60
Range $\log \hat{w}$
$\sigma^2(\log \hat{w})$
60
40
20
20
40
60
L
L

Discussion



A. van den Oord, S. Dieleman, H.Zen et. al, 2016