Variational Inference with Hamiltonian Monte Carlo

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Variational inference

Setting: Probabilistic model $p(x, z)$ with missing or latent variables z

- Quantity of interest: Marginal likelihood $p(x) = \int p(x, z)dz$
- Often not directly tractable
- Use a variational lower bound

$$\begin{aligned}\log p(x) &\geq \log p(x) - D_{KL}\left(q_\theta(z|x)||p(z|x)\right) \\ &= \mathbb{E}_{q_\theta(z|x)}\left[\log p(x, z) - \log q_\theta(z|x)\right] =: \mathcal{L}\end{aligned}$$

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Aim of this work: Improve the approximation

Markov Chain Monte Carlo (MCMC) methods

Objective: Generate samples from a complicated distribution $f_{\text{target}}(s)$

Idea: Create a Markov chain $(s_t)_{t \in \mathbb{N}}$, which converges to the target distribution

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Metropolis-Hastings algorithm: Produces such a Markov chain

1. Generate a proposal $\tilde{s}$ from some distribution $f_{\text{prop}}(\tilde{s}|s_{t-1})$ (with $f_{\text{prop}}(t|s) = f_{\text{prop}}(s|t)$)
2. Accept the proposal as the next state s_t with probability

$$p_{\text{accept}} = \min[1, \frac{f_{\text{target}}(\tilde{s})}{f_{\text{target}}(s_{t-1})}],$$

   otherwise set $s_t = s_{t-1}$.

Integrating MCMC into variational inference

Salimans et al. (2015): Interpret the Markov chain obtained in MCMC as a variational approximation

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$$\begin{aligned}
\log p(x) &\geq \mathcal{L} \\
&\geq \mathcal{L} - \mathbb{E}_{q(z_T|x)} \left[D_{KL} \left(q(z_0, \ldots, z_{T-1}|z_T, x) || r(z_0, \ldots, z_{T-1}|z_T, x) \right) \right] \\
&=: \mathcal{L}_{\text{aux}},
\end{aligned}$$

$\rightarrow$ Need to also learn a *reverse* model $r(z_0, \ldots, z_{T-1}|z_T, x)$

Hamiltonian Dynamics

- Reformulation of classical dynamics
- System state given by *position* z and *momentum* v

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- $U(z) = -\log p(x, z)$, the NLL of $p(z|x)$ upto additive constants
- $K(v) = (1/2)v^T M^{-1} v + C = -\log N(v|0, M)$, M called the mass matrix

Hamiltonian Dynamics - Numerical Solution

Leapfrog method:

- volume-preserving
- reversible
- approximate conservation of total energy

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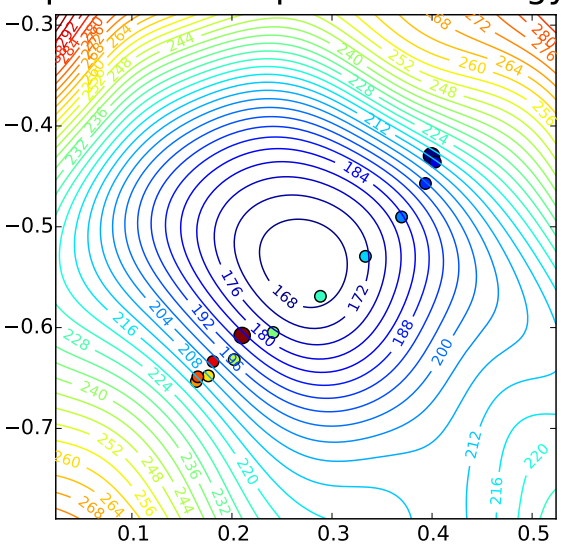
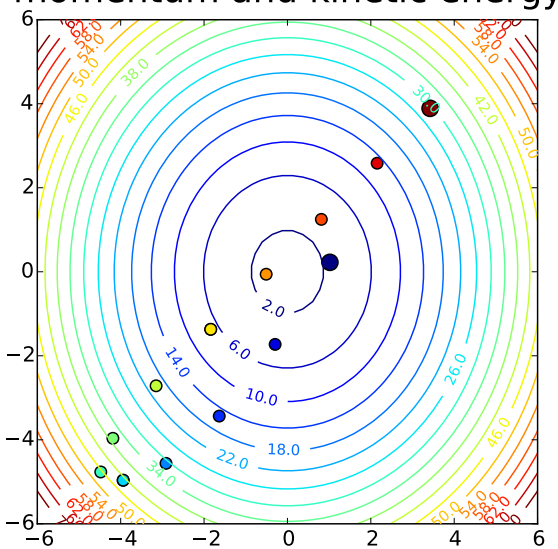
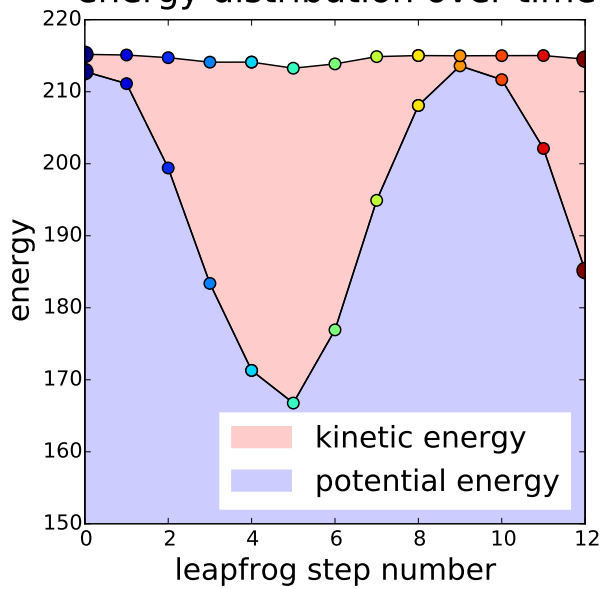
position and potential energy



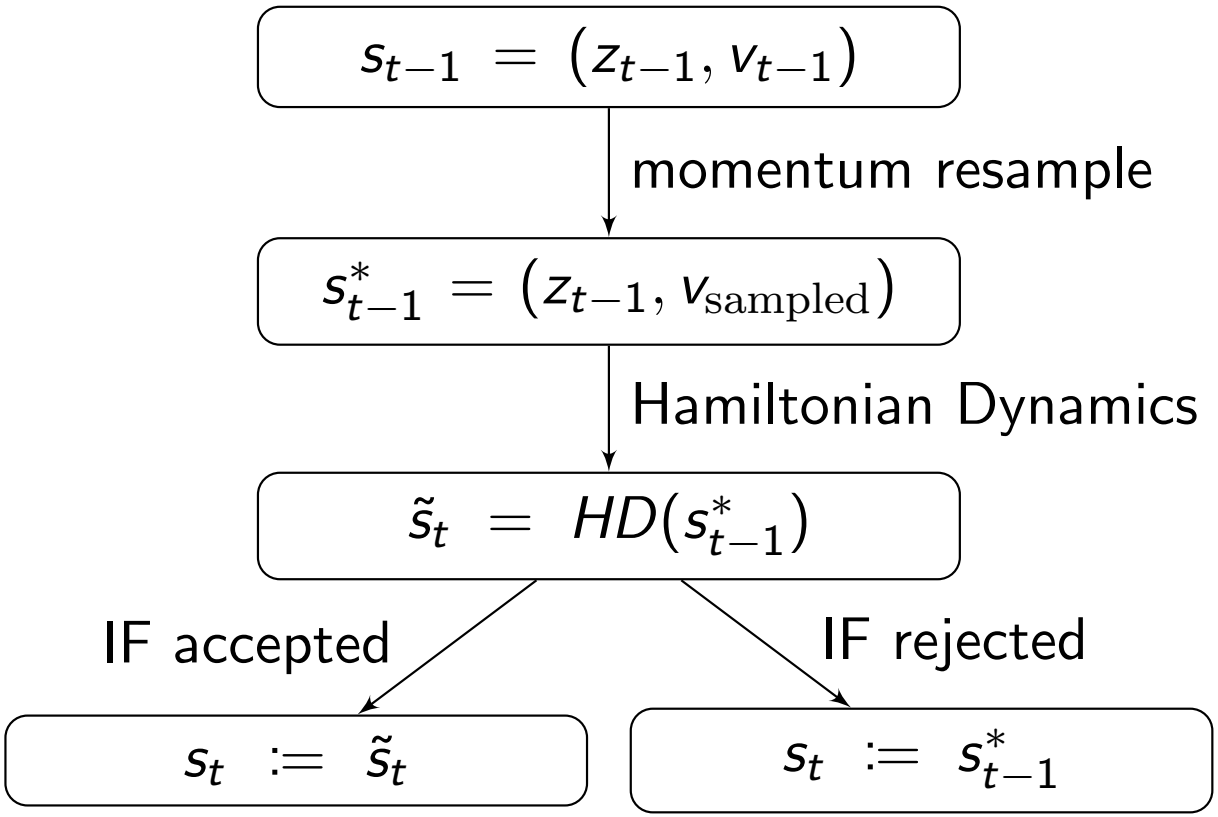
momentum and kinetic energy



energy distribution over time



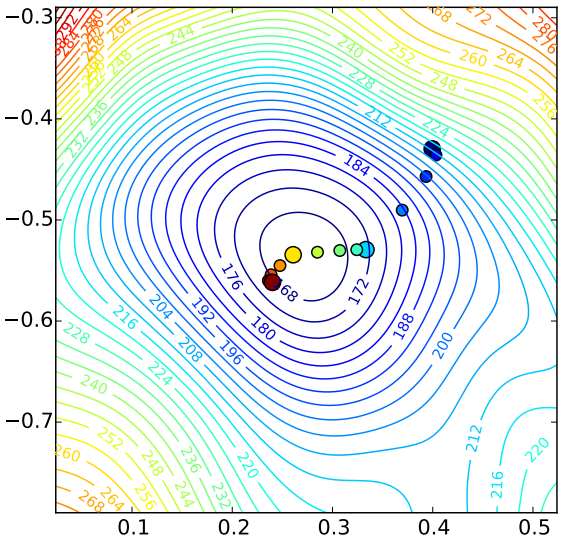
The Hamiltonian Monte Carlo (HMC) algorithm



$\rightarrow$ The constructed $(s_t)_{t \in \mathbb{N}}$ converges to $p(z|x) \cdot N(v|0, M)$

Visualizations of HMC

position and potential energy



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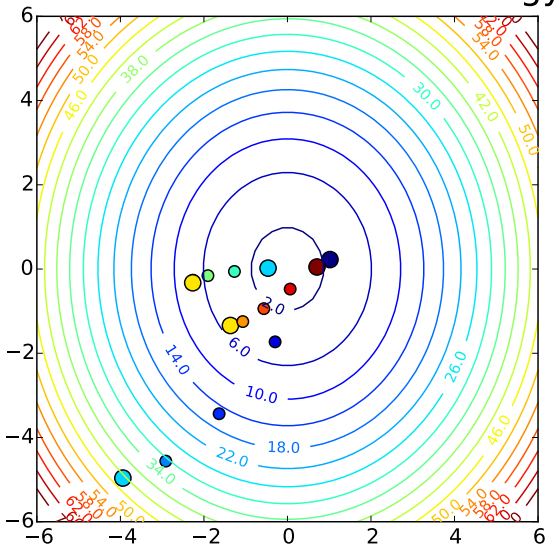

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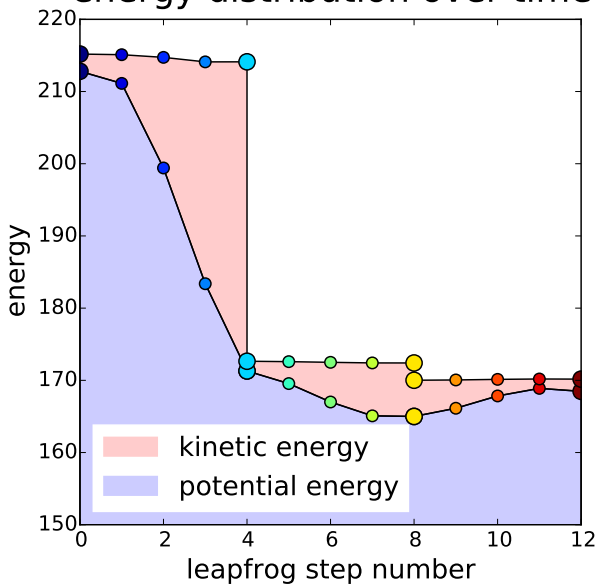

→ Momentum resampling leads to changes in total energy

→ Hamiltonian Dynamics explore the state spaces

Contributions

1. Include the acceptance step of the HMC algorithm in VI
2. Integrate partial momentum updates into lower bound
3. Make the kinetic energy input-dependent

Including the acceptance step

$$f_{S_t|S_{t-1},X}(s_t|s_{t-1},x)$$

$$= \sum_{a=0}^{1} \int f_{S_t,A,V_{\text{sampled}}|S_{t-1},X}(s_t,a,v|s_{t-1},x)dv$$

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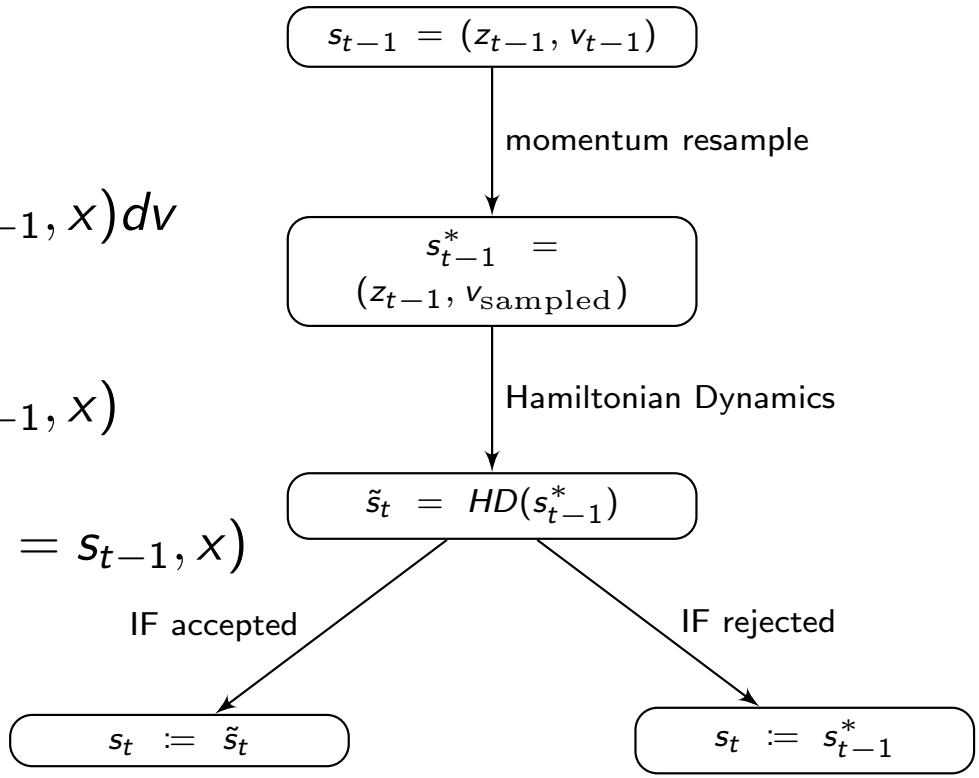
$$\cdot \mathbb{P}(A=a|V_{\text{sampled}}=v,S_{t-1}=s_{t-1},x)$$

$$\cdot f_{V_{\text{sampled}}|S_{t-1},X}(v|s_{t-1},x)dv$$



$\rightarrow$ With acceptance step: Asymptotic convergence is guaranteed

Partial momentum updates

In resampling step: Use weighted sum of current momentum and newly sampled momentum

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Effects:

- Particle tends to maintain its direction in the resampling step
- Avoids random walk behaviour
- Reduction of total energy is slower

$\rightarrow$ For sampling with HMC: Shown to be beneficial for short trajectories

Adaptive kinetic energy

Idea: Allow mass matrix M in the kinetic energy to depend on x

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Relevance: For trajectories of Hamiltonian Dynamics:

Change of mass matrix $\iff$ Rescaling of z-space

- Scaling too small $\rightarrow$ Large numerical errors
- Scaling too large $\rightarrow$ Slow exploration of the state space

$\rightarrow$ Input-dependent kinetic energy should improve convergence

Experimental setup

Variational Auto-Encoders on stochastically binarized MNIST digits

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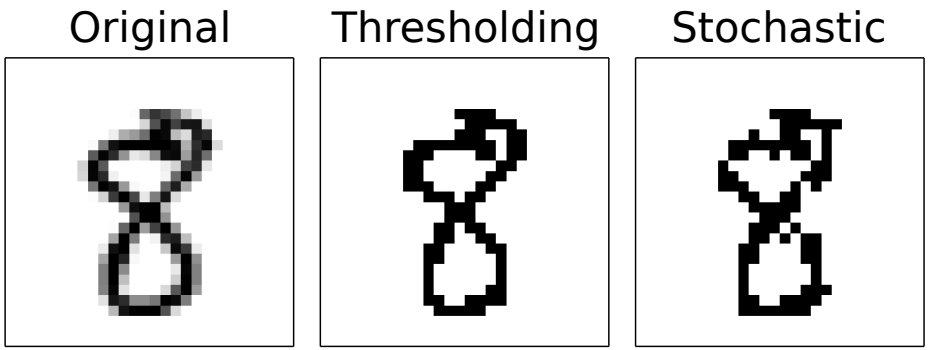
- Binarization: Want bilevel image to match Bernoulli modelling assumption



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Variational Auto-Encoders on stochastically binarized MNIST digits

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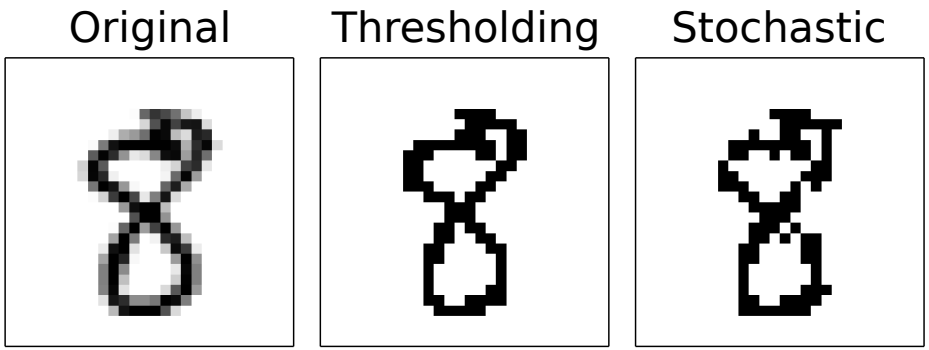

- Stochastic binarization: Randomly set pixel to 1 with probability given by its pixel value

- Effectively much larger dataset; similar effect to dropout regularization

Experimental results

Name	#HMC	#LF	Partial	M	Accept	$-\mathcal{L}_{\text{aux}}$	$-\log(p(x)) \approx$
Basic VI	0	0	-	-	-	92.35	88.27
HMCVI 1	1	12	-	Global	-	89.77	87.77
HMCVI 2	2	6	-	Global	-	89.83	87.53
HMCVI 3	3	4	-	Global	-	90.24	87.56
HMCVI 4	3	4	Yes	Global	-	90.15	87.49
HMCVI 5	3	4	-	NN	-	90.23	87.30
HMCVI 6	3	4	Yes	NN	-	89.72	87.44
HMCVI 7	3	4	-	Global	Yes	91.40	87.28
HMCVI 8	3	4	-	NN	Yes	???	???

$\rightarrow$ VI with HMC outperforms basic VI

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$\rightarrow$ Acceptance step improves the NLL

Future work

- More flexible reverse model
- Understand role of the auxiliary reverse model
- Speed up algorithm
- Allow other parameters to be input-dependent

Thank you for your attention

References

Neal, R. M. (2011). "MCMC using Hamiltonian dynamics". In: *Handbook of Markov Chain Monte Carlo*, pp. 113–162.

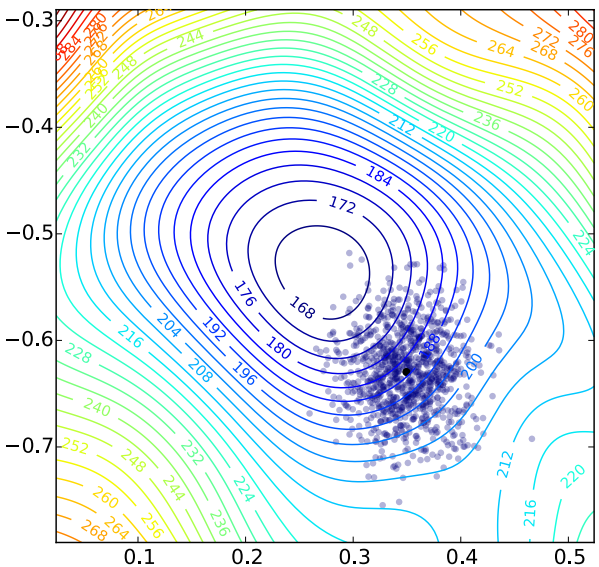
Salimans, T., D. P. Kingma, and M. Welling (2015). "Markov Chain Monte Carlo and Variational Inference: Bridging the Gap". In: *ICML 2015*.

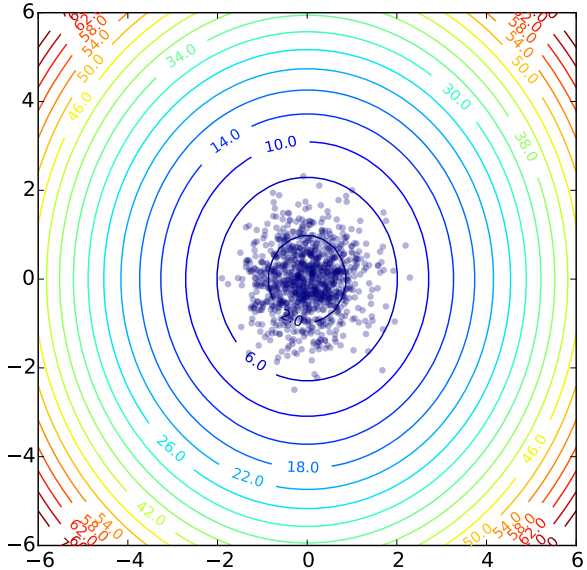
Visualizations of HMC (2)

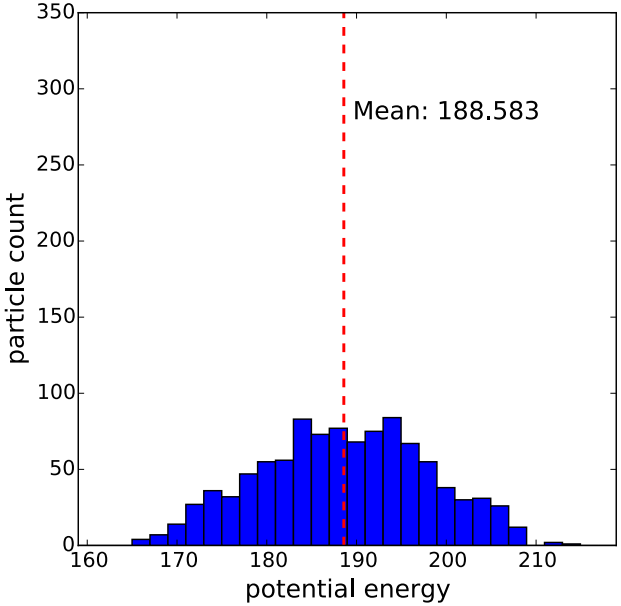
position and potential energy

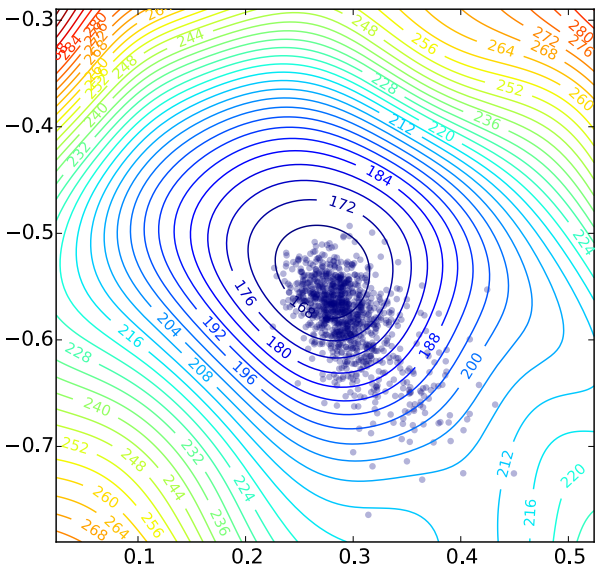
momentum and kinetic energy

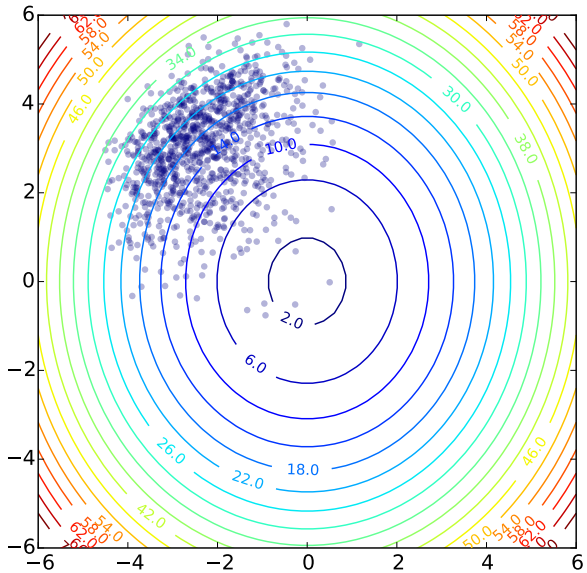
potential energy distribution

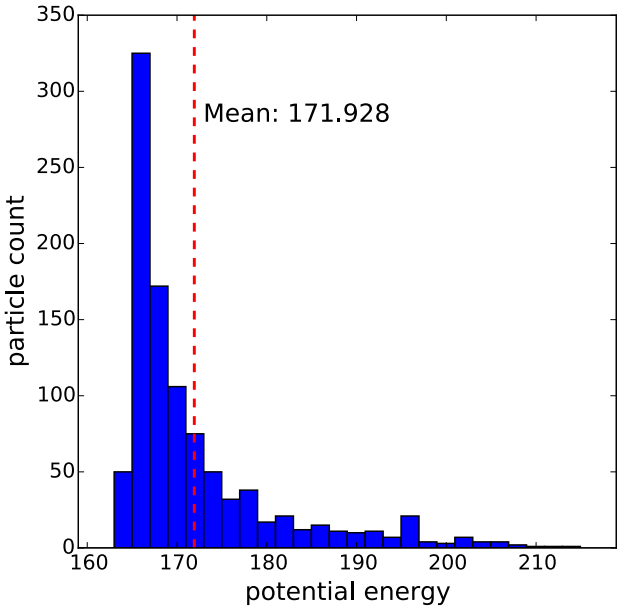












Potential energy of VAEs

Learnt latent representation of training data