Meta-learning for stochastic gradient MCMC

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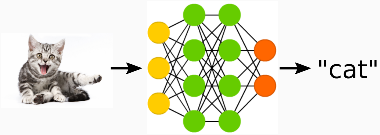
Bayesian neural networks 101

Goal: classifying different types of cats from images

- $\boldsymbol{x}$: input images; $\boldsymbol{y}$: output label
- build a neural network (with param. $\boldsymbol{\theta}$):
  $\hat{\boldsymbol{y}} = \mathrm{NN}_{\boldsymbol{\theta}}(\boldsymbol{x})$

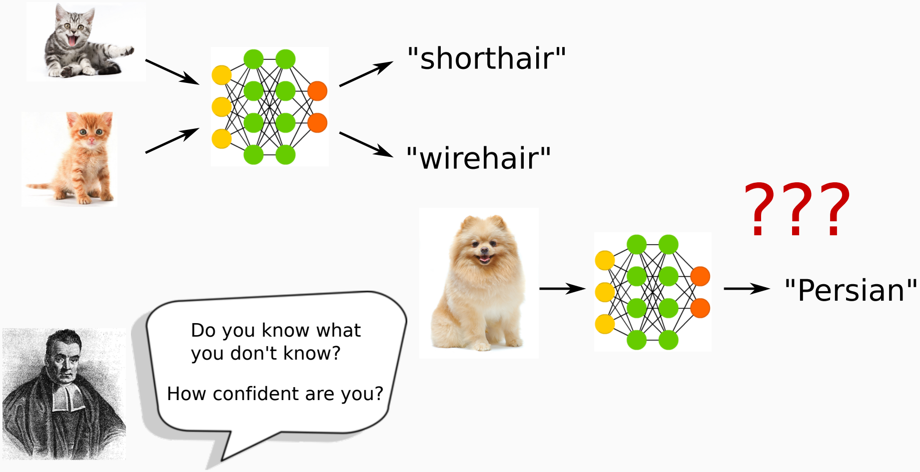


- find the best parameter $\boldsymbol{\theta}$ given a dataset $\mathcal{D} = \{(\boldsymbol{x}_n, \boldsymbol{y}_n)\}_{n=1}^{N}$:

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \log p(\boldsymbol{y}_n | \boldsymbol{x}_n, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$

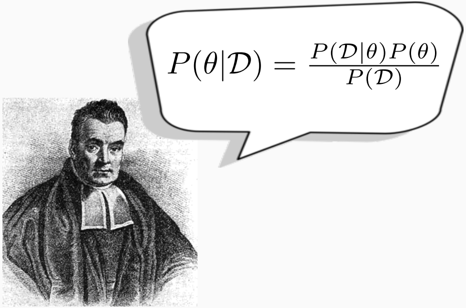
Maximum a posteriori (MAP)

Bayesian neural networks 101



Bayesian neural networks 101

Bayesian inference: given some function $F(\boldsymbol{\theta})$, want $\mathbb{E}_{p(\boldsymbol{\theta}|\mathcal{D})}\left[F(\boldsymbol{\theta})\right]$



- predictive mean

$$\hat{\boldsymbol{y}}_{\text{mean}} = \mathbb{E}_{p(\boldsymbol{\theta}|\mathcal{D})}\left[\text{NN}_{\boldsymbol{\theta}}(\boldsymbol{x})\right]$$

- predictive distribution

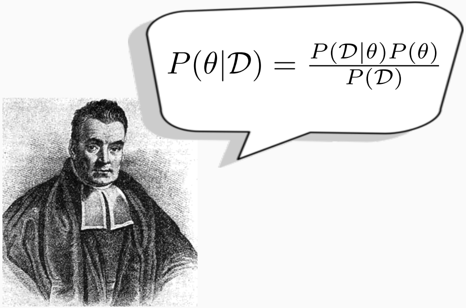
$$p(\boldsymbol{y}|\boldsymbol{x}, \mathcal{D}) = \mathbb{E}_{p(\boldsymbol{\theta}|\mathcal{D})}\left[p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta})\right]$$

- evaluate posterior

$$p(\boldsymbol{\theta} \in A|\mathcal{D}) = \mathbb{E}_{p(\boldsymbol{\theta}|\mathcal{D})}\left[\delta_A\right]$$

Bayesian neural networks 101

Bayesian inference: given some function $F(\boldsymbol{\theta})$, want $\mathbb{E}_{p(\boldsymbol{\theta}|\mathcal{D})}[F(\boldsymbol{\theta})]$



- Monte Carlo estimation:

$$\mathbb{E}_{p(\boldsymbol{\theta}|\mathcal{D})}[F(\boldsymbol{\theta})] \approx \frac{1}{K}\sum_{k=1}^{K} F(\boldsymbol{\theta}^k)$$

$$\boldsymbol{\theta}^k \sim p(\boldsymbol{\theta}|\mathcal{D}) \qquad \text{(intractable)}$$

- Stochastic gradient MCMC (SG-MCMC): efficient ways to (approximately) draw samples from $p(\boldsymbol{\theta}|\mathcal{D})$

From SGD to SG-MCMC

- The MAP problem can be rewritten as

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} U(\boldsymbol{\theta}),$$

$$p(\boldsymbol{\theta}|\mathcal{D}) \propto \exp[-U(\boldsymbol{\theta})], \quad -U(\boldsymbol{\theta}) = \sum_{n=1}^{N} \log p(\boldsymbol{y}_n|\boldsymbol{x}_n, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta})$$

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- In the MAP problem, we find $\boldsymbol{\theta}^*$ by gradient descent

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \nabla_{\boldsymbol{\theta}_t} U(\boldsymbol{\theta}_t),$$

$$-\nabla_{\boldsymbol{\theta}} U(\boldsymbol{\theta}) = \underbrace{\sum_{n=1}^{N} \nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{y}_n|\boldsymbol{x}_n, \boldsymbol{\theta})}_{\text{full gradient of LL}} + \nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta}), \quad \{(\boldsymbol{x}_m, \boldsymbol{y}_m)\}_{m=1}^{M} \sim \mathcal{D}^M$$

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- In the MAP problem, we find $\boldsymbol{\theta}^*$ by stochastic gradient descent (for big data)

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \nabla_{\boldsymbol{\theta}_t} \tilde{U}(\boldsymbol{\theta}_t),$$

$$-\nabla_{\boldsymbol{\theta}} \tilde{U}(\boldsymbol{\theta}) = \underbrace{\frac{N}{M} \sum_{m=1}^{M} \nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{y}_m|\boldsymbol{x}_m, \boldsymbol{\theta})}_{\text{stochastic gradient of LL}} + \nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta}), \quad \{(\boldsymbol{x}_m, \boldsymbol{y}_m)\}_{m=1}^{M} \sim \mathcal{D}^M$$

From SGD to SG-MCMC

- In the Bayesian inference problem, we need to (approximately) draw $\boldsymbol{\theta} \sim p(\boldsymbol{\theta}|\mathcal{D})$
- Big data: Stochastic gradient Langevin dynamics (SGLD)

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \nabla_{\boldsymbol{\theta}_t} \tilde{U}(\boldsymbol{\theta}_t) + \sqrt{2\eta}\boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

Welling and Teh (2011), Chen et al. (2014), Li et al. (2016), Chen et al. (2016)

From SGD to SG-MCMC

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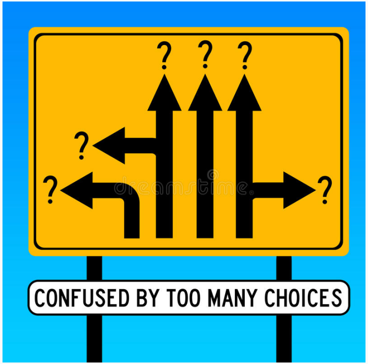
- SGLD = SGD + properly scaled Gaussian noise
- Other optimisation algorithms can be transformed into SG-MCMC samplers:
    - SGD + momentum $\rightarrow$ SGHMC; RMSprop $\rightarrow$ preconditioned SGLD; Adam $\rightarrow$ Santa

Welling and Teh (2011), Chen et al. (2014), Li et al. (2016), Chen et al. (2016)

“I’m bored of tuning my optimiser & sampler”

- Which SG-MCMC algorithm should I use?
- How do I tune the hyper-parameters?



Salimans et al. (2015), Song et al. (2017), Levy et al. (2018)

"I'm bored of tuning my optimiser & sampler"

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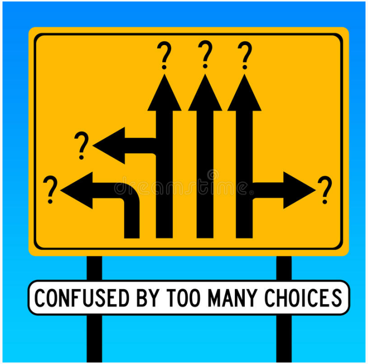
Learn it from data!

- Want a general solution for similar tasks
- Train on low-dim, generalise to high-dim



Salimans et al. (2015), Song et al. (2017), Levy et al. (2018)

Learning to learn

Meta-learning for optimisers:

- Define an optimiser with parameters ϕ:

$$\boldsymbol{z}_{t+1} = \boldsymbol{z}_t - \boldsymbol{f}_\phi(\boldsymbol{z}_t, H(\cdot))$$

- Run it on some training objective functions $H(\boldsymbol{z})$, provide learning signals to train ϕ
- Once learned, apply this optimiser to test objective functions

Andrychowicz et al. (2016), Li and Malik (2017), Wichrowska et al. (2017), Li and Turner (2018)

Learning to learn

Meta-learning for SG-MCMC: can we just naively

- Define a sampler with parameters ϕ:

$$\boldsymbol{z}_{t+1} = \boldsymbol{z}_t - \boldsymbol{f}_\phi(\boldsymbol{z}_t, H(\cdot), \boldsymbol{\epsilon}), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

- Run it on some training distributions $\pi(\boldsymbol{z}) \propto \exp[-H(\boldsymbol{z})]$, provide learning signals to train ϕ
- Once learned, apply this sampler to test distributions

Andrychowicz et al. (2016), Li and Malik (2017), Wichrowska et al. (2017), Li and Turner (2018)

Learning to learn

Meta-learning for SG-MCMC: can we just naively

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- Run it on some training distributions $\pi(\boldsymbol{z}) \propto \exp[-H(\boldsymbol{z})]$, provide learning signals to train ϕ
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Not quite yet! We need to make sure it is a valid sampler!

Andrychowicz et al. (2016), Li and Malik (2017), Wichrowska et al. (2017), Li and Turner (2018)

The complete framework: Ma et al. NIPS 2015

To sample from $\pi(\boldsymbol{z}) \propto \exp[-H(\boldsymbol{z})]$:

- Let's take the step-size $\eta \to 0$ and use exact gradient:

$$d\boldsymbol{z} = -\nabla_{\boldsymbol{z}} H(\boldsymbol{z}) dt + \sqrt{2} dW(t) \qquad \text{(Langevin dynamics)}$$

- $W(t)$ is a Wiener process
  (think about $dW(t)$ as some Gaussian noise with variance dt)
- Langevin dynamics is a special case of Itô diffusion

$$d\boldsymbol{z} = \boldsymbol{\mu}(\boldsymbol{z}) dt + \sqrt{2\boldsymbol{D}(\boldsymbol{z})} dW(t)$$

The complete framework: Ma et al. NIPS 2015

- Itô diffusion

$$d\boldsymbol{z} = \boldsymbol{\mu}(\boldsymbol{z})dt + \sqrt{2\boldsymbol{D}(\boldsymbol{z})}dW(t) \qquad (1)$$

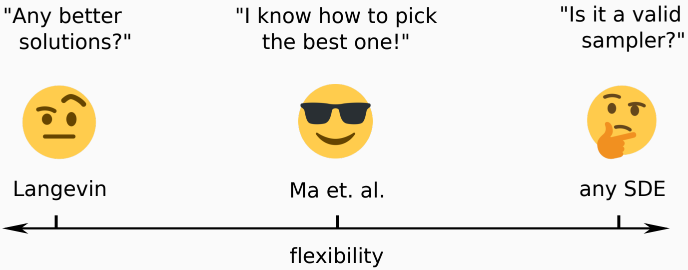
- To make sure $\pi(\boldsymbol{z}) \propto \exp[-H(\boldsymbol{z})]$ is a stationary distribution:

$$\boldsymbol{\mu}(\boldsymbol{z}) = -[\boldsymbol{D}(\boldsymbol{z}) + \boldsymbol{Q}(\boldsymbol{z})]\nabla_{\boldsymbol{z}} H(\boldsymbol{z}) + \boldsymbol{\Gamma}(\boldsymbol{z}), \quad \boldsymbol{\Gamma}(\boldsymbol{z})_i = \sum_{j=1}^{d} \frac{\partial}{\partial \boldsymbol{z}_j}[D_{ij}(\boldsymbol{z}) + Q_{ij}(\boldsymbol{z})] \qquad (2)$$

- $\boldsymbol{D}(\boldsymbol{z})$: diffusion matrix, PSD
- $\boldsymbol{Q}(\boldsymbol{z})$: curl matrix, skew-symmetric
- $\boldsymbol{\Gamma}(\boldsymbol{z})$: correction vector

Ma et al. (2015) completeness result: under some mild conditions
"Any Itô diffusion that has the unique stationary $\pi(\boldsymbol{z})$ is governed by (1)+(2)"

The complete framework: Ma et al. NIPS 2015



- Searching the best sampler within the complete framework:
  - Guaranteed to be correct
  - Retains the most flexibility
  - Only needs to learn how to parameterise $\boldsymbol{D}(\boldsymbol{z})$ and $\boldsymbol{Q}(\boldsymbol{z})$ matrices!

Our recipe: dynamics design

- Goal: train an SG-MCMC sampler to sample from $p(\boldsymbol{\theta}|\mathcal{D}) \propto \exp[-U(\boldsymbol{\theta})]$
- We augment the state space with momentum variable $\boldsymbol{p}$:

$$\boldsymbol{z} = (\boldsymbol{\theta}, \boldsymbol{p}), \quad \pi(\boldsymbol{z}) \propto \exp[-H(\boldsymbol{z})], \quad H(\boldsymbol{z}) = U(\boldsymbol{\theta}) + \frac{1}{2}\boldsymbol{p}^{\mathsf{T}}\boldsymbol{p}$$

- Recall the complete recipe

$$d\boldsymbol{z} = -[\boldsymbol{D}(\boldsymbol{z}) + \boldsymbol{Q}(\boldsymbol{z})]\nabla_{\boldsymbol{z}} H(\boldsymbol{z})dt + \boldsymbol{\Gamma}(\boldsymbol{z})dt + \sqrt{2}dW(t)$$

Our recipe: dynamics design

- Our recipe:

$$\boldsymbol{Q}(\boldsymbol{z}) = \begin{bmatrix} \mathbf{0} & -\boldsymbol{Q}_f(\boldsymbol{z}) \\ \boldsymbol{Q}_f(\boldsymbol{z}) & \mathbf{0} \end{bmatrix}, \quad \boldsymbol{D}(\boldsymbol{z}) = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{D}_f(\boldsymbol{z}) \end{bmatrix}, \quad \boldsymbol{\Gamma}(\boldsymbol{z}) = \begin{bmatrix} \boldsymbol{\Gamma}_{\boldsymbol{\theta}}(\boldsymbol{z}) \\ \boldsymbol{\Gamma}_{\boldsymbol{p}}(\boldsymbol{z}) \end{bmatrix}$$

$$\boldsymbol{Q}_f(\boldsymbol{z}) = \text{diag}[\boldsymbol{f}_{\phi_Q}(\boldsymbol{z})], \quad \boldsymbol{D}_f(\boldsymbol{z}) = \text{diag}[\alpha \boldsymbol{f}_{\phi_Q}(\boldsymbol{z}) \odot \boldsymbol{f}_{\phi_Q}(\boldsymbol{z}) + \boldsymbol{f}_{\phi_D}(\boldsymbol{z}) + c], \quad \alpha, c > 0$$

- Resulting update rules (rearrange terms & discretise & stochastic gradient):

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \overbrace{\eta \boldsymbol{Q}_f(\boldsymbol{z}_t)\boldsymbol{p}_t}^{\text{momentum SGD}} + \overbrace{\eta \boldsymbol{\Gamma}_{\boldsymbol{\theta}}(\boldsymbol{z}_t)}^{\text{correction}}$$

$$\boldsymbol{p}_{t+1} = \boldsymbol{p}_t - \underbrace{\eta \boldsymbol{D}_f(\boldsymbol{z}_t)\boldsymbol{p}_t}_{\textit{friction}} - \eta \boldsymbol{Q}_f(\boldsymbol{z}_t)\nabla_{\boldsymbol{\theta}_t}\tilde{U}(\boldsymbol{\theta}_t) + \eta \boldsymbol{\Gamma}_{\boldsymbol{p}}(\boldsymbol{z}_t) + \sqrt{\Sigma(\boldsymbol{z}_t)}\boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$\Sigma(\boldsymbol{z}_t) = 2\eta \boldsymbol{D}_f(\boldsymbol{z}_t) - \eta^2 \boldsymbol{Q}_f(\boldsymbol{z}_t)\boldsymbol{B}(\theta_t)\boldsymbol{Q}_f(\boldsymbol{z}_t), \quad \boldsymbol{B}(\theta_t) = \mathbb{V}[\nabla_{\boldsymbol{\theta}_t}\tilde{U}(\boldsymbol{\theta}_t)]$$

Our recipe: dynamics design

Designing $\boldsymbol{f}_{\phi_Q}(\boldsymbol{z})$ (responsible for the drift):
the i^{th} element is defined as

$$\boldsymbol{f}_{\phi_Q,i}(\boldsymbol{z}) = \beta + f_{\phi_Q}(\tilde{U}(\boldsymbol{\theta}), p_i)$$

- We want $\boldsymbol{f}_{\phi_Q}(\boldsymbol{z})$ to depend on the energy landscape:
  - Fast traversal through low-density regions
  - Better exploration in high-density regions
- But we don't want $\boldsymbol{\Gamma}_{\boldsymbol{\theta}}(\boldsymbol{z})$ to be too expensive!
  (using $\nabla_{\boldsymbol{\theta}} U(\boldsymbol{\theta})$ as input here leads to an extra term $\langle \nabla, \nabla_{\boldsymbol{\theta}} U(\boldsymbol{\theta}) \rangle$ in $\boldsymbol{\Gamma}_{\boldsymbol{\theta}}(\boldsymbol{z})$)

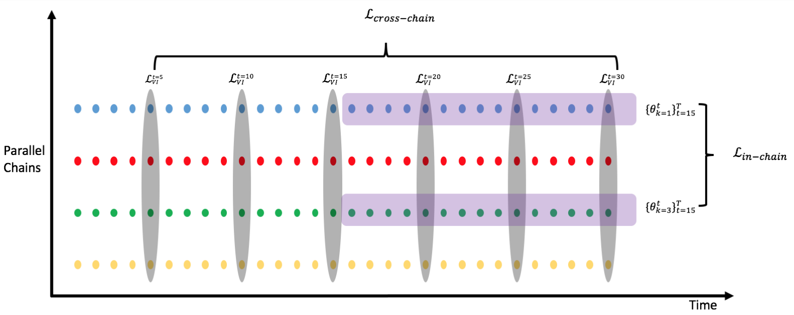
Our recipe: dynamics design

Designing $\boldsymbol{f}_{\phi_D}(\boldsymbol{z})$ (responsible for friction):
the i^{th} element is defined as

$$\boldsymbol{f}_{\phi_D,i}(\boldsymbol{z}) = f_{\phi_D}(\tilde{U}(\boldsymbol{\theta}), p_i, \partial_{\theta_i}\tilde{U}(\boldsymbol{\theta}))$$

- $\boldsymbol{\Gamma}_{\boldsymbol{p}}(\boldsymbol{z})$ only requires computing $\nabla_{\boldsymbol{p}} \boldsymbol{D}_{\boldsymbol{f}}(\boldsymbol{z})$
- ...so we can use the gradient information $\nabla_{\boldsymbol{\theta}} U(\boldsymbol{\theta})$
- prevent overshoot by "comparing" $\boldsymbol{p}$ and $\nabla_{\boldsymbol{\theta}} U(\boldsymbol{\theta})$

Our recipe: loss function design

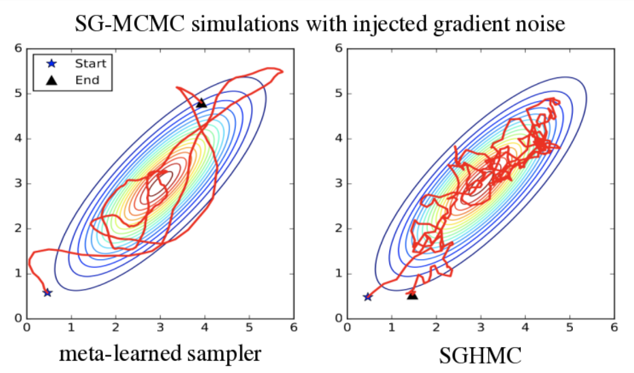


Use KL divergence $\mathrm{KL}[q(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D})]$ to define loss.

Define $q(\boldsymbol{\theta})$ *implicitly*: run parallel chains for several steps, then

- Cross-chain loss: at time t, collect samples across chains
- In-chain loss: for each chain, collect samples by *thinning*

A toy example



- trained on factorised Gaussians, tested on correlated Gaussians
- manually injected Gaussian noise to the gradients
  (and assume we don't know noise variance $\boldsymbol{B}(\theta)$)

Bayesian NN on MNIST

Goal: sample from BNN posterior

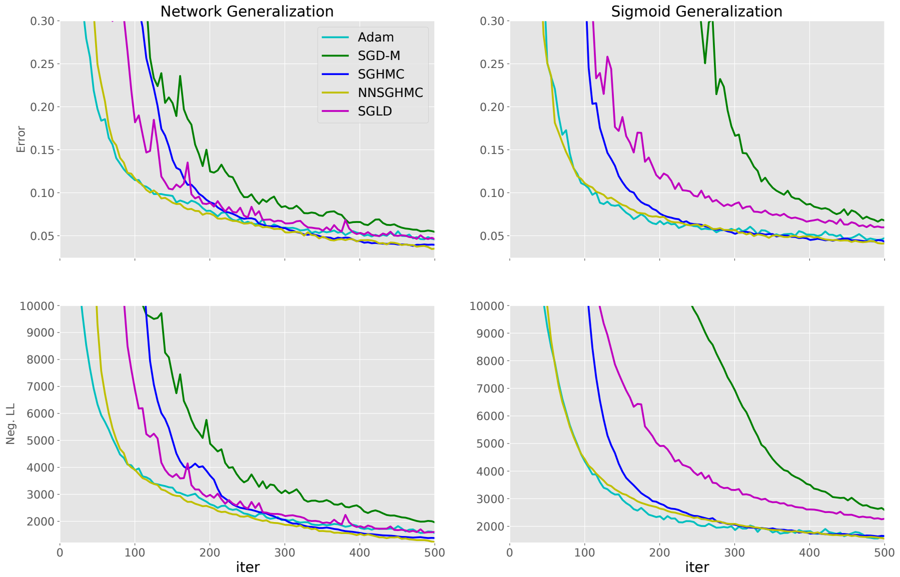
Training: meta sampler trained to sample from the posterior of a BNN (1-hidden layer, 20 hidden units, ReLU)

Three generalisation tests:

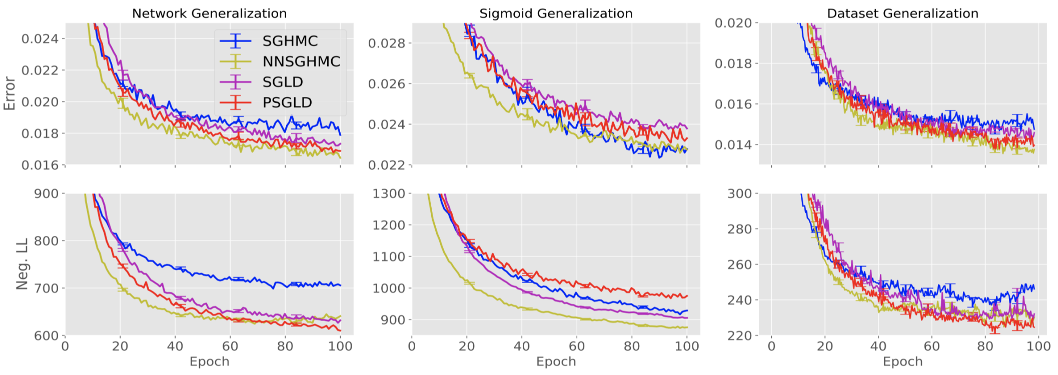
- to bigger network architecture: 2-hidden layer MLP (40 units, ReLU)
- to different activation function: 1-hidden layer MLP (20 units, Sigmoid)
- to different dataset: train on MNIST 0-4, test on MNIST 5-9

Also consider long-time horizon generalisation

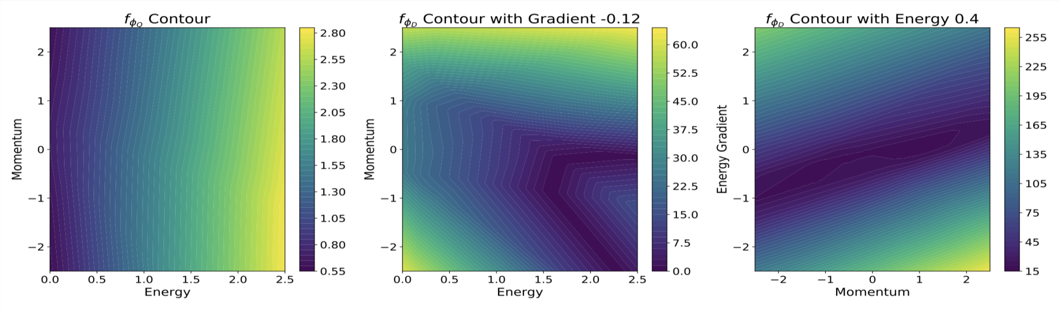
Bayesian NN on MNIST: speed improvements



Bayesian NN on MNIST: long-time generalisation



Bayesian NN on MNIST: understanding the learned sampler



$$Q_f(z) = \text{diag}[f_{\phi_Q}(z)], \quad D_f(z) = \text{diag}[\alpha f_{\phi_Q}(z) \odot f_{\phi_Q}(z) + f_{\phi_D}(z) + c]$$

- f_{ϕ_Q} (left): nearly linear wrt. energy (fast traversal, better exploration)
- f_{ϕ_D} (middle): decrease friction around high energy regions
- f_{ϕ_D} (right): increase friction when gradient & momentum "disagree" (prevent overshoot)

Summary

MCMC and meta-learning can be friends:

- MCMC can be improved using meta-learning
- Meta-learning works better when searching in a theoretically sound framework



Thank you!

Summary

MCMC and meta-learning can be friends:

- MCMC can be improved using meta-learning
- Meta-learning works better when searching in a theoretically sound framework

Future work:

- add in tempering, adaptive learning rate...
- meta-learn the Hamiltonian
- improving samplers for discrete variables



Thank you!

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