Variational Gibbs Inference for Statistical Model Estimation from Incomplete Data

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Topic of the talk

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Variational Gibbs Inference for Statistical Model Estimation from Incomplete Data

- General-purpose method for estimating statistical models from incomplete data.
- Journal of Machine Learning Research, 2023: jmlr.org/papers/v24/21-1373.html.
- Code: github.com/vsimkus/variational-gibbs-inference.
- Demo: nbviewer.org/github/vsimkus/variational-gibbs-inference/blob/main/notebooks/VGI_demo.ipynb.

Overview

1. Statistical models and the missing data issue
2. Some problems with direct estimation from incomplete data
3. Variational Gibbs Inference

Some modern statistical models

- Normalising flows

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}) = p(\boldsymbol{u}) \left|\det J_{T_{\boldsymbol{\theta}}}\right|^{-1},$$

$$\boldsymbol{x} = T_{\boldsymbol{\theta}}(\boldsymbol{u}), \quad T_{\boldsymbol{\theta}} = T_{\boldsymbol{\theta}}^{L} \circ \cdots \circ T_{\boldsymbol{\theta}}^{1},$$

  - $p(\boldsymbol{u})$ is a simple base distribution.
  - $T_{\boldsymbol{\theta}}^{l}$ are deterministic, invertible, and differentiable.

$p_{\boldsymbol{\theta}}(\boldsymbol{x}) =$ 

Image credit: *[Durkan et al., 2019]*

- Variational autoencoders (VAEs)

$$p_{\boldsymbol{\theta}}(\boldsymbol{x}) = \int p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z}) p_{\boldsymbol{\theta}}(\boldsymbol{z}) \, \mathrm{d}\boldsymbol{z}$$

  - $p_{\boldsymbol{\theta}}(\boldsymbol{z})$ is often a simple distribution such as standard Gaussian.
  - $p_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{z})$ is a simple distribution (e.g. Gaussian or Multinomial), parametrised via a neural network.

 $\sim p_{\boldsymbol{\theta}}(\boldsymbol{x})$

Image credit: *[Child, 2021]*

The missing data issue

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- The models $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ are specified for fully-observed data $\boldsymbol{x}$,
- And are typically fitted via maximum-likelihood estimation (MLE)

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \frac{1}{N} \sum_{i=1}^{N} \log p_{\boldsymbol{\theta}}(\boldsymbol{x}^i), \quad \text{where} \quad \boldsymbol{x}^i \in \mathcal{D}.$$

- Real-world data is often incomplete due to: non-response, sensor failure, occlusion, etc.
- What can we do?
- Denote $\boldsymbol{x}_{\mathrm{o}}$ and $\boldsymbol{x}_{\mathrm{m}}$ as the observed and missing elements of $\boldsymbol{x} = \boldsymbol{x}_{\mathrm{o}} \cup \boldsymbol{x}_{\mathrm{m}}$ (with $\boldsymbol{x}_{\mathrm{m}} \cap \boldsymbol{x}_{\mathrm{o}} = \varnothing$).

Options:

1. Discard data-points with missing values → loss of information, not sustainable, bias ✗
2. Impute-then-fit → selecting appropriate imputation method, imputation incongeniality ✗
3. Direct fitting by marginalising the missing variables $\boldsymbol{x}_{\mathrm{m}}$?

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Expectation Maximisation (EM)

- Marginalising the missing variables $\int p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathrm{o}}, \boldsymbol{x}_{\mathrm{m}})\,\mathrm{d}\boldsymbol{x}_{\mathrm{m}}$ is generally not tractable.
- What can we do if simplifying assumptions cannot be inserted?
- Expectation-maximisation (EM) (assuming ignorable missingness)

$$\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathrm{o}}) = \log \int f(\boldsymbol{x}_{\mathrm{m}} \mid \boldsymbol{x}_{\mathrm{o}}) \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathrm{o}}, \boldsymbol{x}_{\mathrm{m}})}{f(\boldsymbol{x}_{\mathrm{m}} \mid \boldsymbol{x}_{\mathrm{o}})}\,\mathrm{d}\boldsymbol{x}_{\mathrm{m}} \geqslant \mathbb{E}_{f(\boldsymbol{x}_{\mathrm{m}}|\boldsymbol{x}_{\mathrm{o}})}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathrm{o}}, \boldsymbol{x}_{\mathrm{m}})}{f(\boldsymbol{x}_{\mathrm{m}} \mid \boldsymbol{x}_{\mathrm{o}})}\right], \quad \text{“ELBO”}$$

  - **E-step:** Maximise w.r.t. $f(\boldsymbol{x}_{\mathrm{m}} \mid \boldsymbol{x}_{\mathrm{o}}^i)$ for $\forall \boldsymbol{x}_{\mathrm{o}}^i \in \mathcal{D}$: $f(\boldsymbol{x}_{\mathrm{m}} \mid \boldsymbol{x}_{\mathrm{o}}^i) = p_{\boldsymbol{\theta}^t}(\boldsymbol{x}_{\mathrm{m}} \mid \boldsymbol{x}_{\mathrm{o}}^i)$.
  - **M-step:** Maximise w.r.t. $\boldsymbol{\theta}$: $\boldsymbol{\theta}^{t+1} = \arg\max_{\boldsymbol{\theta}} \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}_{p_{\boldsymbol{\theta}^t}(\boldsymbol{x}_{\mathrm{m}}|\boldsymbol{x}_{\mathrm{o}}^i)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathrm{o}}^i, \boldsymbol{x}_{\mathrm{m}})\right]$
- Monte Carlo EM: Approximate the expectation using Monte Carlo average.
- Then, M-step corresponds to fitting $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ with completed data.

Issue with Monte Carlo EM

- Conditional sampling of $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathrm{m}} \mid \boldsymbol{x}_{\mathrm{o}})$ is generally intractable or inefficient.

Variational approximation to $p_{\boldsymbol{\theta}^t}(\boldsymbol{x}_\mathrm{m} \mid \boldsymbol{x}_\mathrm{o})$

Variational inference (VI)

- $\forall \boldsymbol{x}_\mathrm{o} \in \mathcal{D}$ specify a $f_{\boldsymbol{\phi}}(\boldsymbol{x}_\mathrm{m} \mid \boldsymbol{x}_\mathrm{o}) \in \mathcal{Q}(\boldsymbol{\phi})$.
- E-step: Maximise the ELBO w.r.t. $\boldsymbol{\phi}$.
- M-step: Sample $f_{\boldsymbol{\phi}}(\boldsymbol{x}_\mathrm{m} \mid \boldsymbol{x}_\mathrm{o})$ to approximate the expectation.

Amortised VI

- Parametrise $f_{\boldsymbol{\phi}}(\boldsymbol{x}_\mathrm{m} \mid \boldsymbol{x}_\mathrm{o})$ with a *single* neural network $\mathrm{NN}_{\boldsymbol{\phi}}(\boldsymbol{x}_\mathrm{o})$ for $\forall \boldsymbol{x}_\mathrm{o} \in \mathcal{D}$.

	d_1	d_2	d_3	d_4	$f_{\boldsymbol{\phi}}(\boldsymbol{x}^i_\mathrm{m} \mid \boldsymbol{x}^i_\mathrm{o})$
$\boldsymbol{x}^1$	x^1_1	?	x^1_3	x^1_4	$f_{\boldsymbol{\phi}}(x^1_2 \mid x^1_1, x^1_3, x^1_4)$
$\boldsymbol{x}^2$	?	x^2_2	x^2_3	?	$f_{\boldsymbol{\phi}}(x^2_1, x^2_4 \mid x^2_2, x^2_3)$
$\boldsymbol{x}^3$	?	?	?	x^3_4	$f_{\boldsymbol{\phi}}(x^3_1, x^3_2, x^3_3 \mid x^3_4)$
$\vdots$		$\vdots$			$\vdots$

Advantages of VI

- Choice of $\mathcal{Q}(\boldsymbol{\phi})$ is in our control.
- Turns inference to optimisation.
- Can fit using SGD.
- Efficient if $|\mathcal{D}|$ is small.

Disadvantages of VI

- Is inefficient if $|\mathcal{D}|$ is large.

Advantages of amortised VI

- Efficient for large $|\mathcal{D}|$.

Disadvantages of amortised VI

- Need one $f_{\boldsymbol{\phi}}(\boldsymbol{x}_\mathrm{m} \mid \boldsymbol{x}_\mathrm{o})$ for each pattern of missingness (2^M in total).

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Variational Gibbs Inference: Core idea

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Variational Gibbs Inference for Statistical Model Estimation from Incomplete Data, JMLR, 2023

- General-purpose method for estimating $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ from incomplete data.
- Efficient for large $|\mathcal{D}|$ and mitigates the need for 2^M conditional distributions.

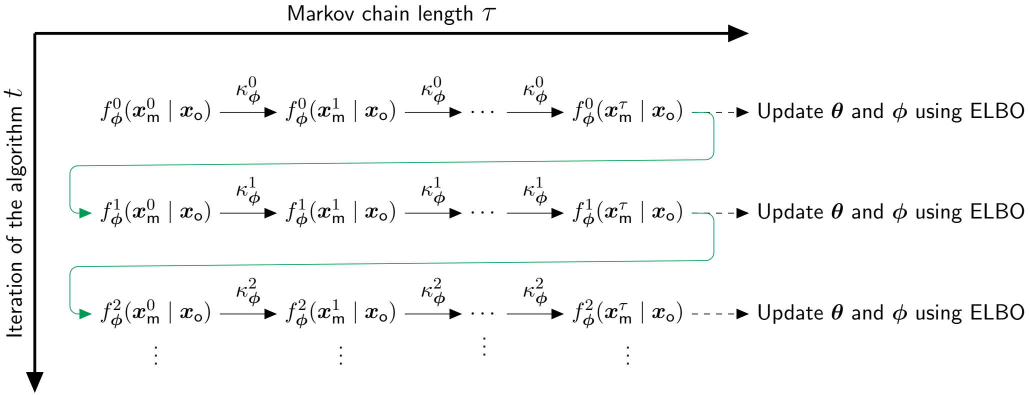
1. Core idea: Turn the 2^M conditional distribution problem into M conditional distributions.
2. To make $f^t_{\boldsymbol{\phi}}(\boldsymbol{x}_\mathrm{m} \mid \boldsymbol{x}_\mathrm{o})$ flexible:
   - Specify it to be the marginal of a Markov chain with a *learnable* kernel $\kappa_{\boldsymbol{\phi}}(\boldsymbol{x}^{\tau+1}_\mathrm{m} \mid \boldsymbol{x}_\mathrm{o}, \boldsymbol{x}^\tau_\mathrm{m})$.
3. To address the 2^M pattern problem:
   - We specify the kernel to be Gibbs (updates one dimension of $\boldsymbol{x}_\mathrm{m}$ at a time):

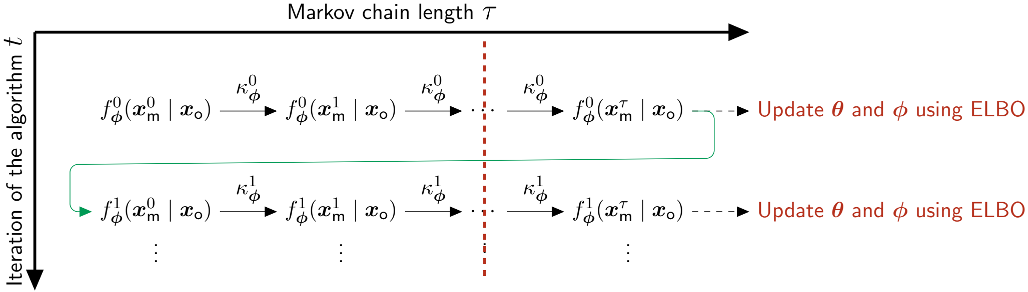
   $$\kappa_{\boldsymbol{\phi}}(\boldsymbol{x}^{\tau+1}_\mathrm{m} \mid \boldsymbol{x}^\tau_\mathrm{m}, \boldsymbol{x}_\mathrm{o}) = \mathbb{E}_{\boldsymbol{\pi}(j \mid \mathrm{idx}(\boldsymbol{m}))}\left[q_{\boldsymbol{\phi}_j}(x_j \mid \boldsymbol{x}^\tau_{\mathrm{m}\setminus j}, \boldsymbol{x}_\mathrm{o})\delta(\boldsymbol{x}^{\tau+1}_{\mathrm{m}\setminus j} - \boldsymbol{x}^\tau_{\mathrm{m}\setminus j})\right],$$

   where $\boldsymbol{\pi}(j \mid \mathrm{idx}(\boldsymbol{m}))$ is the selection probability for the j-th dimension of a Gibbs sampler.
   - Hence we have to learn only M variational Gibbs conditional $q_{\boldsymbol{\phi}_j}(x_j \mid \boldsymbol{x}_{\mathrm{m}\setminus j}, \boldsymbol{x}_\mathrm{o})$.

Variational Gibbs Inference: Persistent chains

- Sampling long Markov chains at each iteration t of the algorithm is costly.
- Use "persistent" chains: initialise the chains at the last state of the previous iteration.
- Can now use short chains, that is using small τ, at every iteration t.





- Computing the marginal density $f^t_\phi(x^\tau_m \mid x_o)$ of a Markov chain remains intractable:

$$f^t_\phi(x^\tau_m \mid x_o) = \int f^t_\phi(x^0_m \mid x_o) \prod_{h=0}^{\tau-1} \kappa_\phi(x^{h+1}_m \mid x_o, x^h_m)\, \mathrm{d}x^0_m \ldots \mathrm{d}x^{\tau-1}_m.$$

- So how can we optimise the parameters ϕ of the kernel κ_ϕ?
- Instead of optimising ϕ over the full length of the Markov chains, we "cut" the chains just before the last transition and optimise over the last step of the chain.

- Objective for learning $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$:

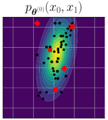
$$\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathsf{o}}) \geqslant \mathbb{E}_{\boldsymbol{\pi}(j|\mathrm{idx}(\boldsymbol{m}))f^{t-1}(\boldsymbol{x}_{\mathsf{m}\setminus j}|\boldsymbol{x}_{\mathsf{o}})q_{\boldsymbol{\phi}_j}(x_j|\boldsymbol{x}_{\mathsf{m}\setminus j},\boldsymbol{x}_{\mathsf{o}})}\left[\log \frac{p_{\boldsymbol{\theta}}(x_j, \boldsymbol{x}_{\mathsf{m}\setminus j}, \boldsymbol{x}_{\mathsf{o}})}{q_{\boldsymbol{\phi}_j}(x_j \mid \boldsymbol{x}_{\mathsf{m}\setminus j}, \boldsymbol{x}_{\mathsf{o}})}\right] + \text{Const.}$$

- We only need samples from penultimate step of the Markov chain f^{t-1}.
- Can optimise w.r.t. $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ using stochastic gradient ascent.
- Maximising the above w.r.t. $\boldsymbol{\phi}$ corresponds to minimising the KL divergence:

$$\mathbb{E}_{\boldsymbol{\pi}(j|\mathrm{idx}(\boldsymbol{m}))f^{t-1}(\boldsymbol{x}_{\mathsf{m}\setminus j}|\boldsymbol{x}_{\mathsf{o}})}\left[D_{\mathsf{KL}}(q_{\boldsymbol{\phi}_j}(x_j \mid \boldsymbol{x}_{\mathsf{m}\setminus j}, \boldsymbol{x}_{\mathsf{o}}) \,||\, p_{\boldsymbol{\theta}}(x_j \mid \boldsymbol{x}_{\mathsf{m}\setminus j}, \boldsymbol{x}_{\mathsf{o}}))\right]$$

- The fitted $\kappa_{\boldsymbol{\phi}}$ approximates the Gibbs kernel with the stationary distribution $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathsf{m}} \mid \boldsymbol{x}_{\mathsf{o}})$.

Variational Gibbs Inference: Algorithm



Algorithm 1 Variational Gibbs inference

1: **Create** K-times imputed data $\mathcal{D}_K$ using f_0

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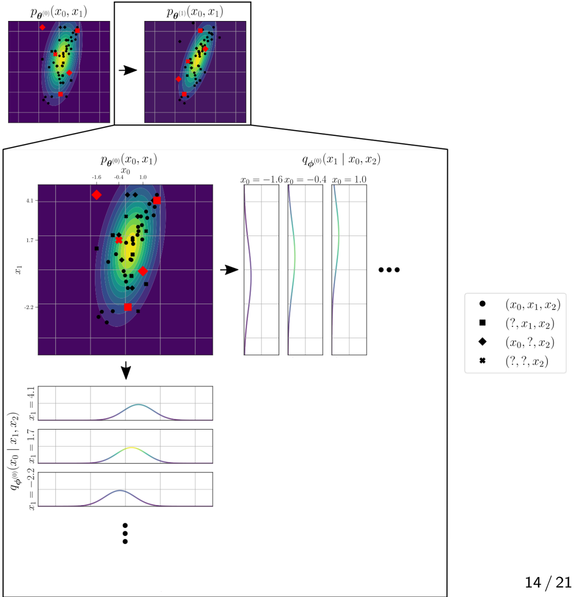
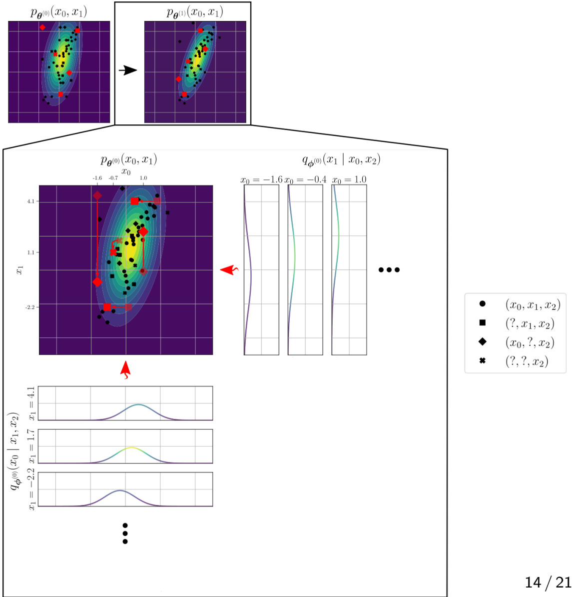
2: **for** t in $[1, \mathit{max\_epochs}]$ **do**
3: **Sample** mini-batch $\mathcal{B}_K$ from $\mathcal{D}_K$
7: **end for**



Variational Gibbs Inference: Algorithm

Algorithm 1 Variational Gibbs inference

Create K-times imputed data $\mathcal{D}_K$ using f_0
for t in $[1, \textit{max\_epochs}]$ **do**
  Sample mini-batch $\mathcal{B}_K$ from $\mathcal{D}_K$
  Update the imputations in $\mathcal{B}_K$:
  $\bar{\boldsymbol{x}}_{\mathrm{m}}^{(i,k)} \sim \mathrm{Gibbs}_{\tau}(\boldsymbol{x}_{\mathrm{o}}^{i}, \kappa_{\boldsymbol{\phi}}; \boldsymbol{x}_{\mathrm{m}}^{(i,k)}), \forall \boldsymbol{x}_{\mathrm{m}}^{(i,k)} \in \mathcal{B}_K$
  Persist the imputations in $\mathcal{B}_K$ to $\mathcal{D}_K$
end for



Variational Gibbs Inference: Algorithm

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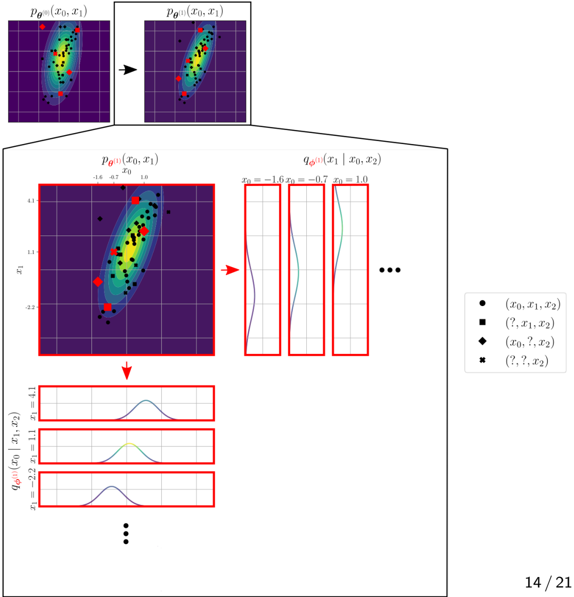
  Update $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ with SGA.
end for



Variational Gibbs Inference: Algorithm

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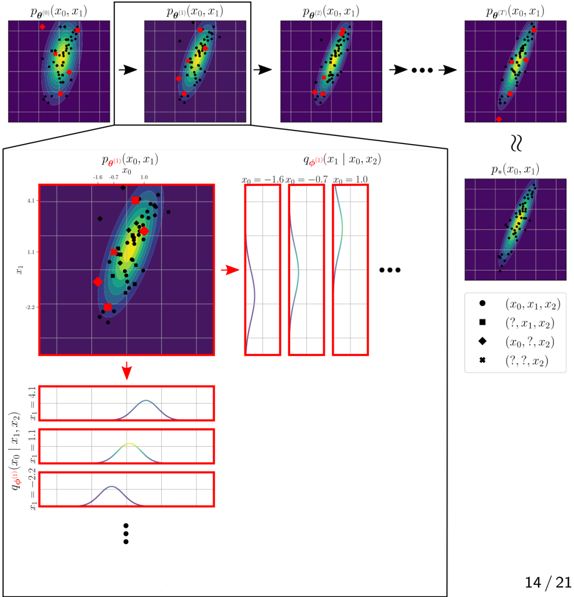
end for



Variational Gibbs Inference: Summary

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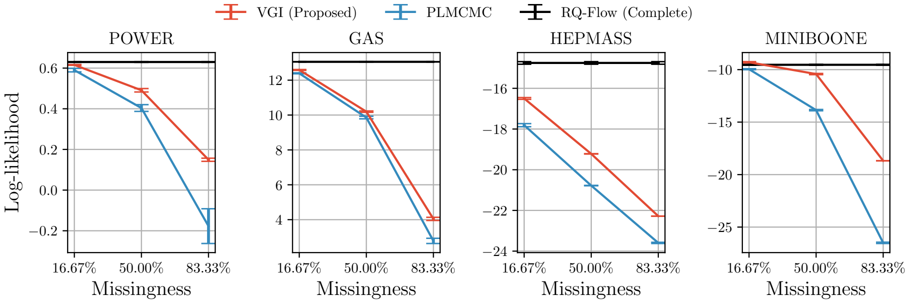
- Direct fitting by (approximately) marginalising the missing variables $\boldsymbol{x}_\mathrm{m}$ ✓

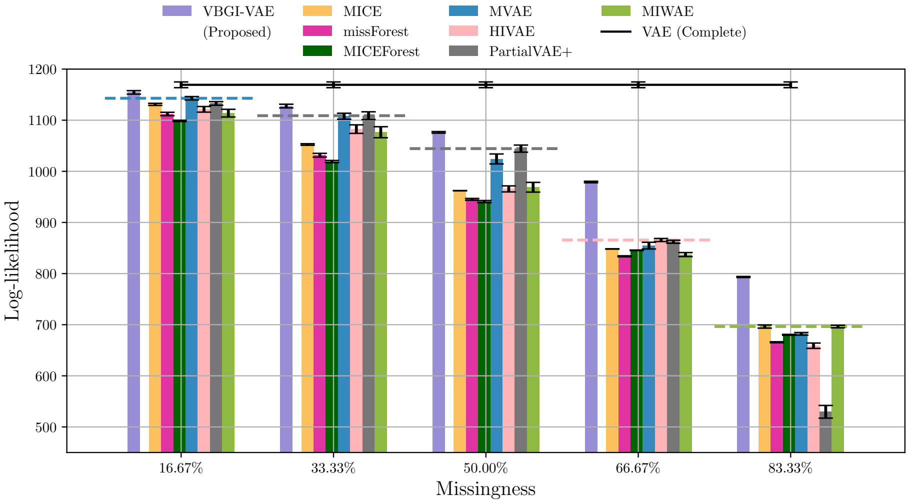
- General-purpose method for estimating $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ from incomplete data.
- Mitigated the need for 2^M conditional distributions to just M by representing the variational distribution via a learnable Gibbs kernel.
- Used "persistent" chains to efficiently sample imputations using the learnt Gibbs kernel.
- "Cut" the Markov chains to make optimisation of ϕ efficient.

Variational Gibbs Inference: Results (Flows)



	POWER	GAS	HEPMASS	MINIBOONE
Model parameters	∼2M	∼2M	∼1M	∼129K
Dimensionality	6	8	21	43

Variational Gibbs Inference: Results (VAE)



Model parameters: ∼682K. Dimensionality: 560.

Summary

- Statistical models and the missing data issue.
  - Modern models, such as normalising flows and VAEs, are very flexible.
  - But, they are formulated for complete data.
- Some problems with direct estimation from incomplete data.
  - Marginalisation $\int p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathsf{o}}, \boldsymbol{x}_{\mathsf{m}})\, \mathrm{d}\boldsymbol{x}_{\mathsf{m}}$ is generally intractable.
  - EM algorithm requires sampling conditionals $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathsf{m}} \mid \boldsymbol{x}_{\mathsf{o}})$ for $\forall \boldsymbol{x}_{\mathsf{o}} \in \mathcal{D}$, which is expensive.
  - Standard amortised VI requires 2^M variational distributions, which is inefficient.
- Variational Gibbs Inference.
  - General purpose method for model estimation from incomplete data.
  - Achieves good performance on normalising flow and VAE estimation, compared to other methods.

Thank you for listening.
Questions?

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