Variational Gibbs Inference for Statistical Model Estimation from Incomplete Data

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informatics

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

Statistical models and the missing data issue

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- Statistical models $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ of complex phenomena are a key component of many important tasks in machine learning.

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- And are typically fitted via maximum-likelihood estimation (MLE)

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

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Expectation Maximisation (EM)

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Issue with Monte Carlo EM

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

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

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Variational inference (VI)

- $\forall \boldsymbol{x}_\mathsf{o} \in \mathcal{D}$ specify a $f_{\boldsymbol{\phi}}(\boldsymbol{x}_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \in \mathcal{Q}(\boldsymbol{\phi})$.
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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.

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Amortised VI

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

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	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	$f_{\boldsymbol{\phi}}(x^3_1, x^3_2, x^3_3 \mid x^3_4)$
$\vdots$		$\vdots$			$\vdots$

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Disadvantages of VI

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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).

Overview

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Variational Gibbs Inference: Core idea

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.

Variational Gibbs Inference: Core idea

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

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

   where $\boldsymbol{\pi}(j \mid \mathrm{idx}(\boldsymbol{m}))$ is the selection probability for the j-th dimension of a Gibbs sampler.

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     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 $q_{\boldsymbol{\phi}_j}(x_j \mid \boldsymbol{x}_{\mathrm{m}\smallsetminus j}, \boldsymbol{x}_\mathrm{o})$.

Variational Gibbs Inference: Persistent chains

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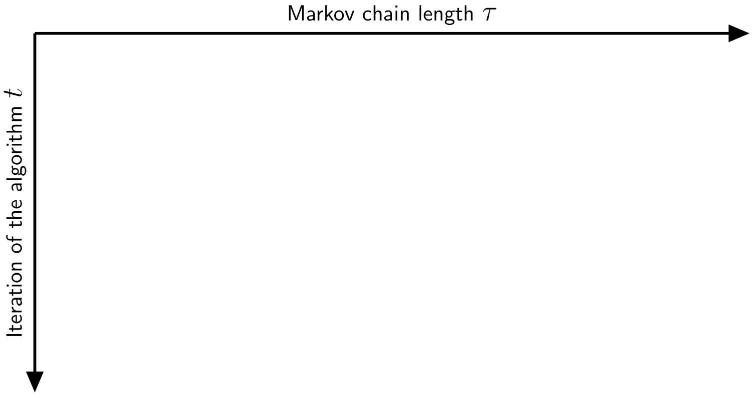

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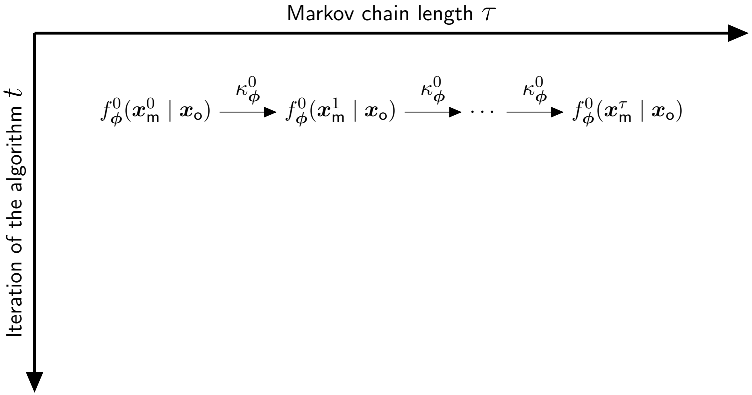

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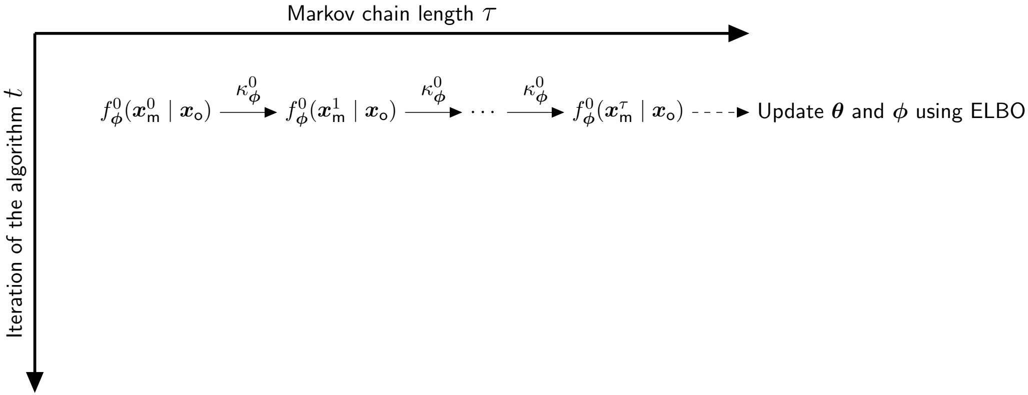

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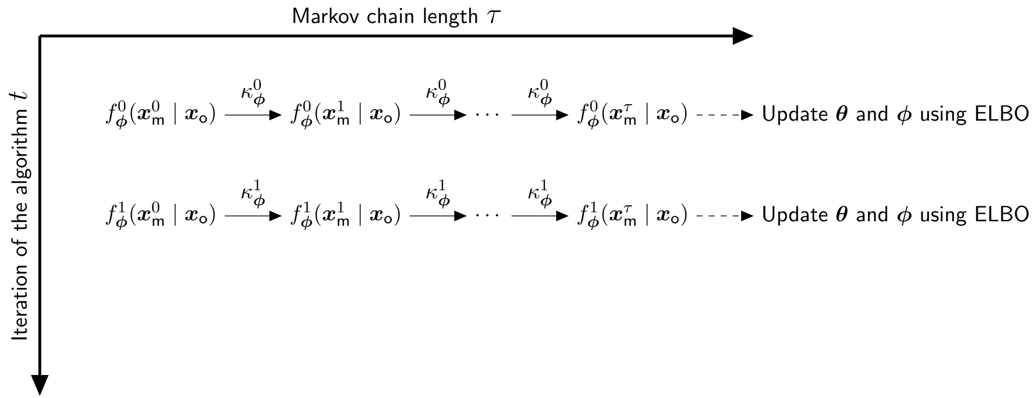


Variational Gibbs Inference: Persistent chains

Markov chain length τ

Iteration of the algorithm t

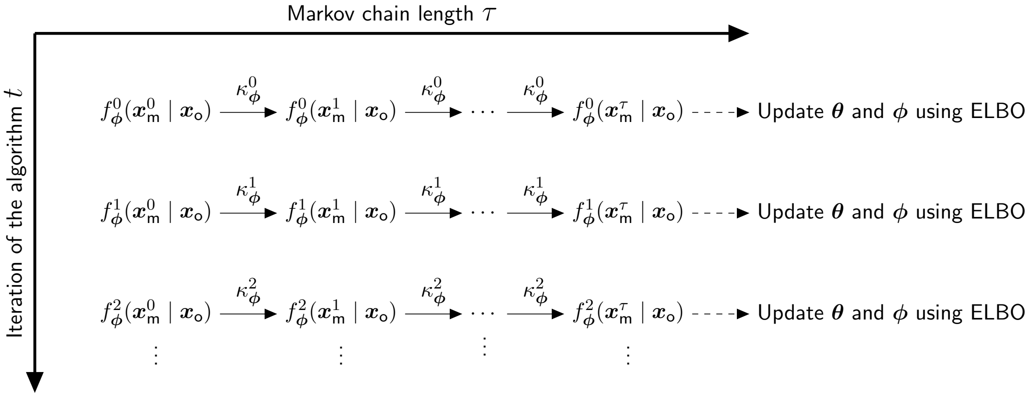
$$f^0_\phi(\boldsymbol{x}^0_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \xrightarrow{\kappa^0_\phi} f^0_\phi(\boldsymbol{x}^1_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \xrightarrow{\kappa^0_\phi} \cdots \xrightarrow{\kappa^0_\phi} f^0_\phi(\boldsymbol{x}^\tau_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \dashrightarrow \text{Update } \boldsymbol{\theta} \text{ and } \phi \text{ using ELBO}$$

$$f^1_\phi(\boldsymbol{x}^0_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \xrightarrow{\kappa^1_\phi} f^1_\phi(\boldsymbol{x}^1_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \xrightarrow{\kappa^1_\phi} \cdots \xrightarrow{\kappa^1_\phi} f^1_\phi(\boldsymbol{x}^\tau_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \dashrightarrow \text{Update } \boldsymbol{\theta} \text{ and } \phi \text{ using ELBO}$$

$$f^2_\phi(\boldsymbol{x}^0_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \xrightarrow{\kappa^2_\phi} f^2_\phi(\boldsymbol{x}^1_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \xrightarrow{\kappa^2_\phi} \cdots \xrightarrow{\kappa^2_\phi} f^2_\phi(\boldsymbol{x}^\tau_\mathsf{m} \mid \boldsymbol{x}_\mathsf{o}) \dashrightarrow \text{Update } \boldsymbol{\theta} \text{ and } \phi \text{ using ELBO}$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

- Sampling long Markov chains at each iteration t of the algorithm is costly.



Variational Gibbs Inference: Persistent chains

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- Sampling long Markov chains at each iteration t of the algorithm is costly.
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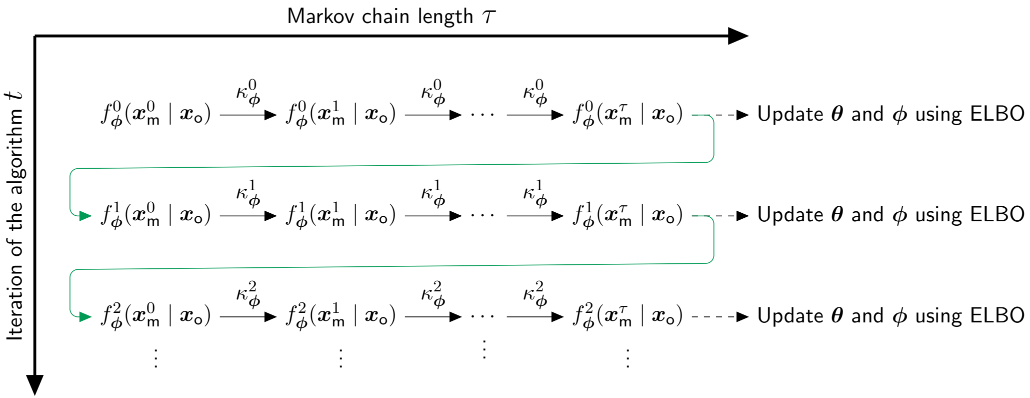
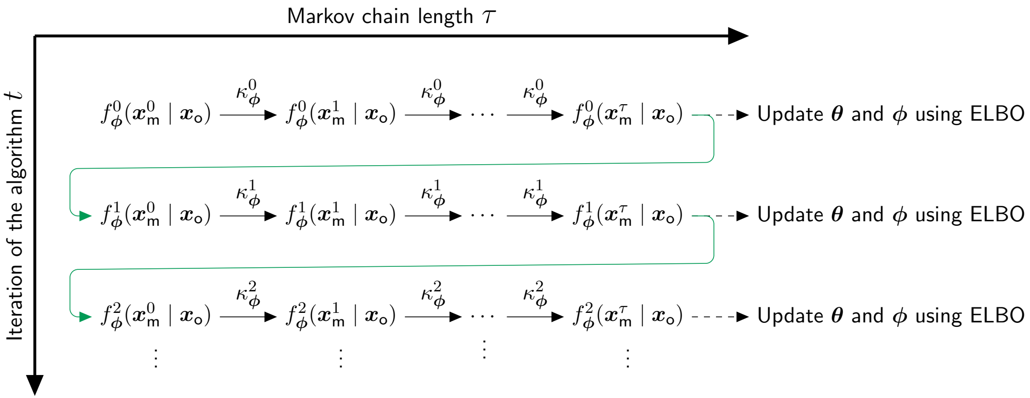


Variational Gibbs Inference: Persistent chains

- 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.



Variational Gibbs Inference: "Cutting" chains

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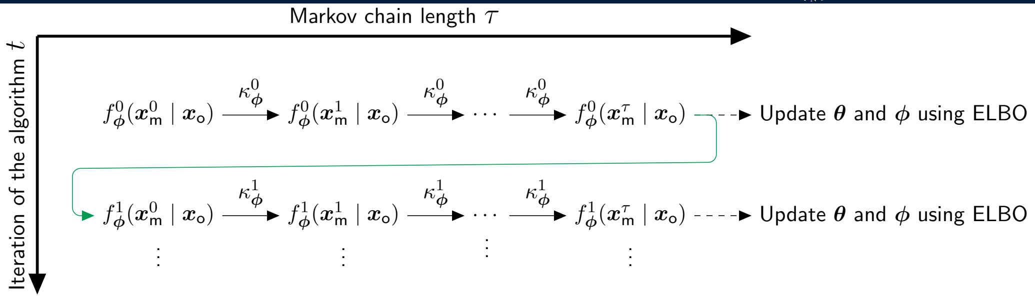

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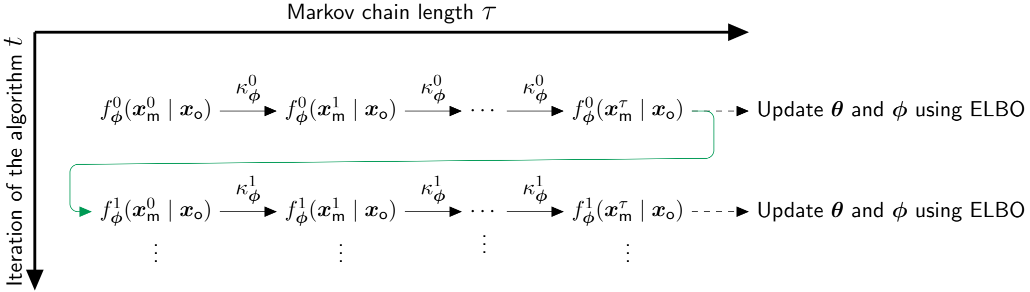

- Computing the marginal density $f^t_{\boldsymbol{\phi}}(\boldsymbol{x}^\tau_{\mathsf{m}} \mid \boldsymbol{x}_{\mathsf{o}})$ of a Markov chain remains intractable:

$$f^t_{\boldsymbol{\phi}}(\boldsymbol{x}^\tau_{\mathsf{m}} \mid \boldsymbol{x}_{\mathsf{o}}) = \int f^t_{\boldsymbol{\phi}}(\boldsymbol{x}^0_{\mathsf{m}} \mid \boldsymbol{x}_{\mathsf{o}}) \prod_{h=0}^{\tau-1} \kappa_{\boldsymbol{\phi}}(\boldsymbol{x}^{h+1}_{\mathsf{m}} \mid \boldsymbol{x}_{\mathsf{o}}, \boldsymbol{x}^h_{\mathsf{m}}) \, \mathrm{d}\boldsymbol{x}^0_{\mathsf{m}} \ldots \mathrm{d}\boldsymbol{x}^{\tau-1}_{\mathsf{m}}.$$

Variational Gibbs Inference: “Cutting” chains

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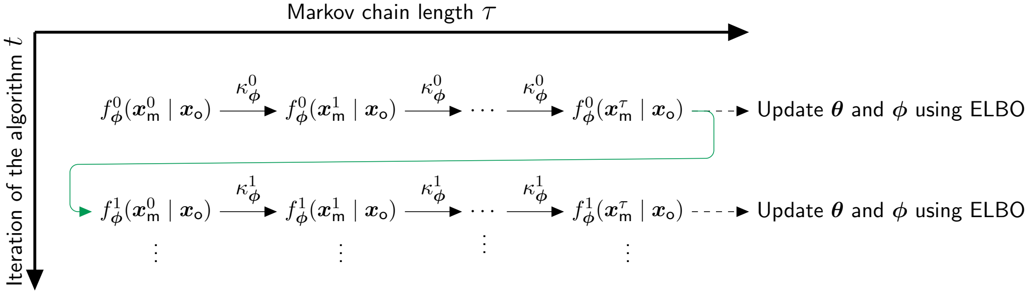

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- So how can we optimise the parameters ϕ of the kernel κ_ϕ?

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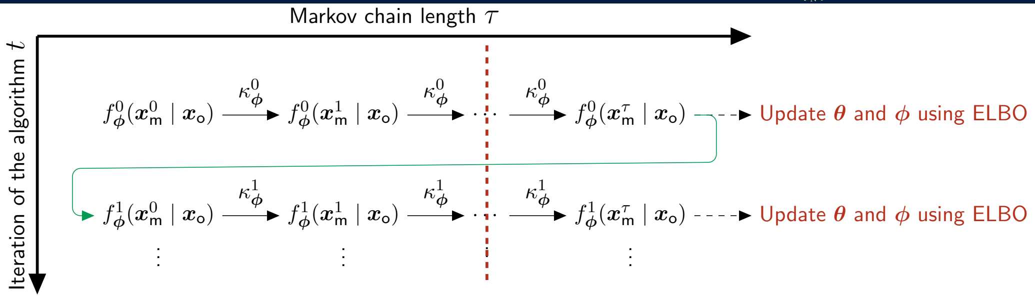

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- So how can we optimise the parameters ϕ of the kernel κ_ϕ?
- Instead of optimising ϕ over the full length of the Markov chains, we "cut" the chains just before the last transition and optimise over the last step of the chain.

Variational Gibbs Inference: Learning objective

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

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

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- We only need samples from penultimate step of the Markov chain f^{t-1}.

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Variational Gibbs Inference: Learning objective

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- 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:

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

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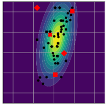
- The fitted $\kappa_{\boldsymbol{\phi}}$ approximates the Gibbs kernel with the stationary distribution $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathsf{m}} \mid \boldsymbol{x}_{\mathsf{o}})$.

Algorithm 1 Variational Gibbs inference

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



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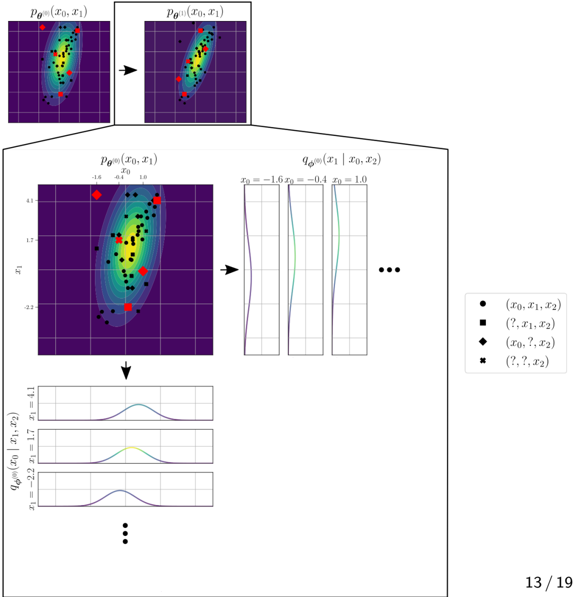
7: **end for**



Variational Gibbs Inference: Algorithm

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  Persist the imputations in $\mathcal{B}_K$ to $\mathcal{D}_K$

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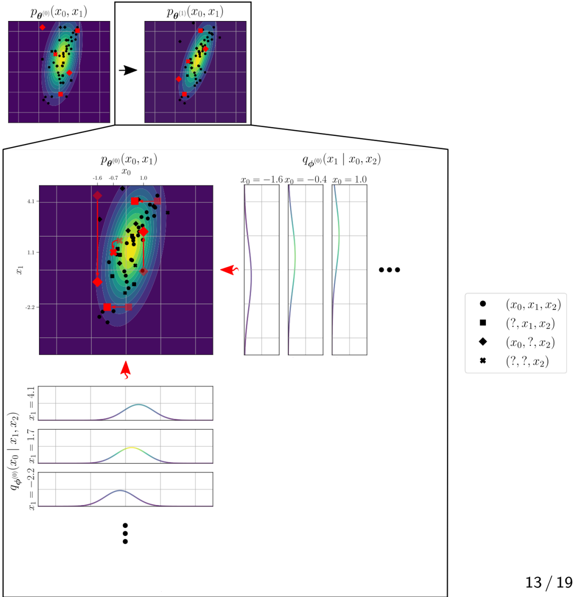

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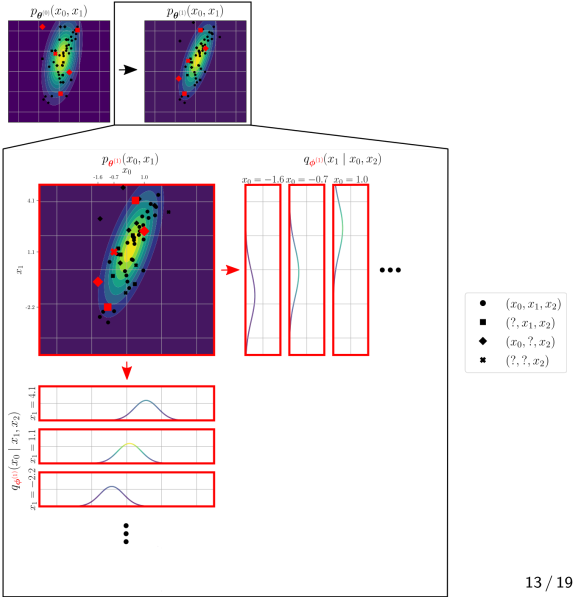

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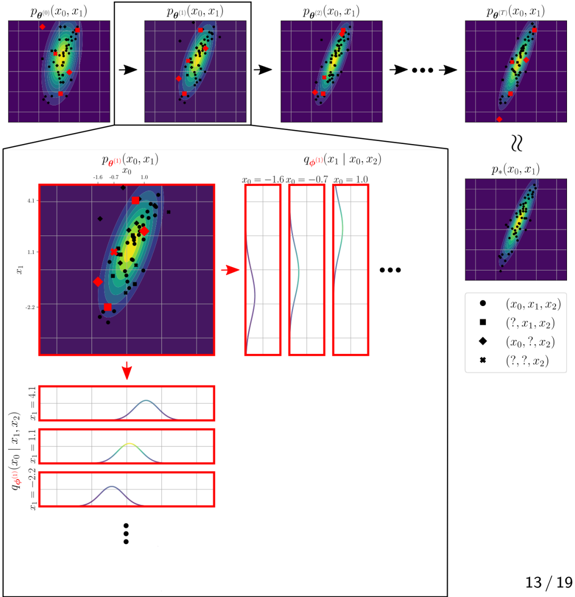

Variational Gibbs Inference: Summary

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- Direct fitting by marginalising the missing variables x_m ?

Variational Gibbs Inference: Summary

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Variational Gibbs Inference: Summary

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- 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)

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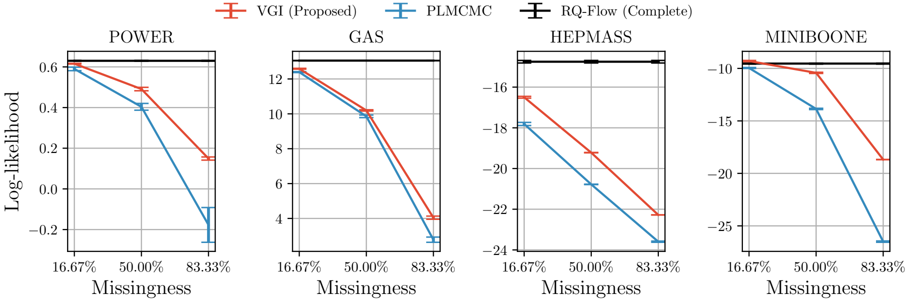

Variational Gibbs Inference: Results (VAE)

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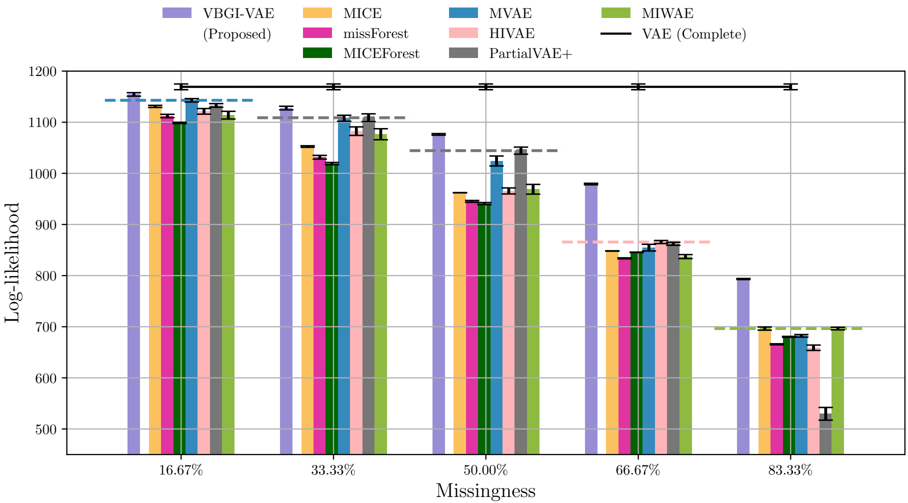

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Summary

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  - Achieves good performance on normalising flow and VAE estimation, compared to other methods.

Thank you for listening.
Questions?

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