Solving high-dimensional parameter inference: marginal posterior densities & Moment Networks

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Highlights

- High-dimensional probability density estimation suffers from "curse of dimensionality"
- Propose direct estimation of lower-dimensional marginal posterior distributions
- *Marginal flow*: estimate joint-marginals of subsets of parameters
- Moment Networks: hierarchy of fast regression models compute increasing moments of lower-dimensional marginal posterior density
- Beyond likelihood-free inference: can also efficiently solve known MCMC problems
- Demo: high-dimensional inference: a) MCMC reference, b) Gravitational wave data model



(A) 100-dimensional data model with known reference distribution evaluated with 10⁷ MCMC samples. Direct 2D marginal posterior estimation using a masked autoregressive flow ensemble (left panel) and representation of 2D Moment Network result (right panel) both trained with 8×10^4 simulations.

Marginal flows

see Figure A

(B) Example simulated gravitational wave time series signals for the strain "+" polarization h+ with realistic LIGO-like noise.

LIGO-like gravitational wave time series

- (C) *Left panel:* Moment

the 1- σ per strain parameter.

Right panel: For each of contours are marginal posterior σ from MN (shaded orange) and MCMC (dashed green).

Cosmological applications

• Full $p(x|\theta)$ density estimation for data x and parameters θ intractable in high-dimension

• Make marginal densities the target of inference • Estimate marginal posterior probability density for pairs of parameters $\alpha, \beta \in \boldsymbol{\theta}$ by minimizing $-\sum_i \log q(\alpha_i, \beta_i | \mathbf{x}_i)$

• Result q is an estimate (e.g. with normalizing flow) of marginal posterior $p(\alpha, \beta | \mathbf{x})$ if training parameters $\boldsymbol{\theta}_i$ drawn from prior $p(\theta)$ and used to simulate x_i

Markov chain Monte Carlo (MCMC) validation:

Moment Networks



• Fig. B: two example simulated gravitational wave time series. The simplified signals (dashed orange) are ~0.12s intervals from the 1 second before a binary black hole merger

• Fig. C *left panel:* Moment Network estimate of the marginal mean and variance for each time step parameter • Fig. C *right panel:* validation case of similar complexity, but with known likelihood • Trained Moment Network accurately matches long-run MCMC chain, which validates our approach



Mapping the Universe: tractable simulation-based inference of high-dimensional cosmological fields & dark matter maps Robustness: Moment Networks use simpler architectures, reducing training failure risk and boosting inference speed **Cross-validation**: moments of estimated marginal posteriors should match those from Moment Networks Evading MCMC: Even when the likelihood can be sampled, marginal flows and Moment Networks still provide advantages, as many of the drawbacks of high-dimensional MCMC can be simply avoided

 Side-step the posterior density estimation problem Estimate location, scale, and covariance (and possibly) higher-order moments) of marginal posteriors • Network F(x) minimizes L_2 loss over distribution of possible training examples $\{x_i, \theta_i\}$

 $J_0 = \int \|\boldsymbol{\theta} - F(\boldsymbol{x})\|^2 \, p(\boldsymbol{x}, \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{\theta}$

• For observed data it forms a posterior mean estimate $F(\boldsymbol{x}_{obs}) = \langle \boldsymbol{\theta} \rangle_{\theta^{|_{\boldsymbol{x}^{obs}}}}$

• Functions F and G can combine to output posterior means, variances, and covariances for subsets of the full set of parameters

 $J_1 = \int \left\| (\boldsymbol{\theta} - F_{\text{fixed}}(\boldsymbol{x}))^2 - G(\boldsymbol{x}) \right\|^2 p(\boldsymbol{x}, \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{\theta}$