The 11th International Conference "Inverse Problems: Modeling and Simulation
26th May - 1st June 2024, Malta

Neural wave-based imaging with amortized uncertainty quantification

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An overview is given on solving high-dimensional Bayesian Inference with expensive nonlinear (wave-based) forward operators with applications in medical and seismic imaging. After improving MAP estimates with conditional Normalizing Flows (CNFs), a full characterization of the posterior will be given with Bayesian Variational Inference using Simulation-Based Inference. Two complementary techniques to close the amortization gap will be reviewed and evaluated on realistic medical and seismic imaging problems. One is amortized and based on recursive refinements [1] (by improving fiducial points, $\mathbf{x}_0$) of the score-based summary statistics [3, 4], $\bar{\mathbf{y}} = \nabla_{\mathbf{x}} \log p(\mathbf{y}|\mathbf{x})\big|_{\mathbf{x}_0}$, so that $p(\mathbf{x}|\bar{\mathbf{y}}) \approx p(\mathbf{x}|\mathbf{y})$ in

$$\hat{\theta} \ = \arg\min_{\theta} \frac{1}{M} \sum_{m=1}^{M} \left(\|f_\theta(\mathbf{x}^{(m)}; \bar{\mathbf{y}}^{(m)})\|_2^2 - \log |\det \mathbf{J}_{f_\theta}| \right)$$

where $f_\theta(\cdot;\cdot)$ is a CNF with weights θ and Jacobian, $\mathbf{J}_{f_\theta}$, while the other corrects the amortized CNF (obtained by forward KL) by minimizing the reverse KL

$$\underset{\mathbf{x}_{1:N},\boldsymbol{\phi}}{\text{minimize}} \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2\sigma^2} \|\mathcal{F}(\mathbf{x}_i) - \mathbf{y}^{\text{obs}}\|_2^2 + \\ \frac{1}{2\gamma^2} \|\mathbf{x}_i - f_{\hat{\boldsymbol{\theta}}}^{-1}\left(h_{\boldsymbol{\phi}}(\mathbf{z}_i); \bar{\mathbf{y}}^{\text{obs}}\right)\|_2^2 + \frac{1}{2}\|h_{\boldsymbol{\phi}}(\mathbf{z}_i)\|_2^2 - \log\left|\det \mathbf{J}_{h_{\boldsymbol{\phi}}}\right|.$$

with $\mathbf{z}_i \sim \mathcal{N}(0, \mathbf{I})$, $h_{\boldsymbol{\phi}}(\cdot)$, the correction NF, and $\mathbf{y}^{\text{obs}}$ the observed data.

References

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[4] Yin, Ziyi, et al. "WISE: full-Waveform variational Inference via Subsurface Extensions." arXiv preprint arXiv:2401.06230 (2023).