Review of: "Annealed Stein Variational Gradient Descent for Improved Uncertainty Estimation in Full-Waveform Inversion"

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Potential competing interests: No potential competing interests to declare.

Review of "Annealed Stein Variational Gradient Descent for Improved Uncertainty Estimation in Full-Waveform Inversion" by Corrales et al.

Recommendation: Major revision. The manuscript presents an application of Annealed Stein Variational Gradient Descent (A-SVGD) to uncertainty quantification in Full-Waveform Inversion, but requires substantial improvements in its theoretical foundations, experimental validation, and reproducibility before it meets publication standards. A detailed assessment follows, with specific recommendations provided in the conclusion.

This review consists of three parts:

- 1. Content and scientific contribution assessment
- 2. Style and Presentation comments
- 3. Concluding recommendations

Part I: Content Review

This manuscript presents an application of Annealed Stein Variational Gradient Descent (A-SVGD) to Full-Waveform Inversion (FWI) for quantifying uncertainty in subsurface velocity models. Building upon the A-SVGD framework originally proposed by D'Angelo and Fortuin (2021), the authors evaluate its effectiveness compared to vanilla SVGD in addressing mode collapse and variance collapse issues that commonly arise in high-dimensional inverse problems.

Strengths

- The authors provide a thorough empirical evaluation comparing A-SVGD and vanilla SVGD in both single-scale and multi-scale FWI scenarios. Their detailed analysis effectively demonstrates the comparative advantages of the annealed approach.
- 2. The introduction of analysis techniques, specifically PCA and clustering, represents a potentially valuable contribution to understanding particle behavior and distribution.

Areas for Improvement

- 1. The numerical examples section would benefit from a clearer explanation of the true generative modelp(m|d) being approximated. The choice of A-SVGD over other Bayesian inference methods requires stronger justification. In particular, a comparison with established methods like the No-U-Turn Sampler^[1] would help demonstrate the computational advantages that A-SVGD offers for this specific application in FWI. A comparative discussion with alternative approaches would help readers better understand the method's advantages and appropriate use cases. The experimental validation could be more comprehensive. While statistical improvements are well-documented, their translation to geological meaningfulness requires more rigorous validation. Additional baseline comparisons and a more thorough discussion of hyperparameter selection would strengthen the experimental results.
- 2. The theoretical foundation of the analysis techniques requires further development. While PCA and clustering are well-explained mathematically, their geological significance and interpretation criteria remain unclear. The paper should better define what constitutes a geologically meaningful solution versus a non-physical one. Specifically, it should establish clear criteria for evaluating cluster quality from a geological perspective and demonstrate how practitioners can use PCA and clustering results to identify physically plausible solutions. This would make these analytical tools more practical for geophysical applications.
- 3. The manuscript lacks crucial information for reproducibility. While the authors describe their methodology and parameter settings, they do not provide access to the implementation code or data processing scripts. A public repository containing the code, synthetic data generation scripts, and example workflows would significantly enhance the paper's value to the research community and ensure reproducibility of the results. This is particularly important given the complex nature of the A-SVGD implementation and the various hyperparameter choices described in Section 3.2.

Part II: Style and Presentation

The manuscript is generally well-structured and follows a logical progression from theoretical background to practical implementation. However, several aspects of the presentation require attention to improve readability and clarity:

The mathematical notation in several equations needs refinement. For instance, in equation (3), the lack of spacing between "argmin" and "KL" reduces readability. A simple addition of proper spacing would make this expression clearer.

The bandwidth selection discussion, currently presented inline in the last paragraph of subsection 2.2, would benefit from a clearer format.

The presentation of equations (9) and (10) could be improved through better mathematical typesetting. For example, the current version of the cyclic schedule equation appears as $\alpha(I) = (mod(I, N/C)/(N/C))^{\circ}p$, whereas a more balanced

presentation with proper scaling of parentheses, such as $\alpha(I) = \left(\frac{1}{N/C}\right)^p$, would enhance readability.

The paper lacks proper attribution for the "median trick" used in bandwidth selection. This important algorithmic detail should be both cited and explained, giving readers context for this methodological choice.

There is an inconsistency in the citation style. The authors reference "Martin Ester, Hans-Peter Kriegel, Jörg Sander, Xiaowei Xu, et al." for the DBSCAN algorithm, but the original paper has exactly four authors, making the "et al." designation incorrect and potentially misleading.

Part III: Concluding Recommendations

The manuscript presents a valuable attempt to apply A-SVGD to uncertainty quantification in FWI. The thorough empirical evaluation and potential practical contributions to geophysical applications demonstrate merit. However, several significant issues must be addressed before the paper meets publication standards.

The major concerns include lack of reproducibility, insufficient theoretical justification, unclear geological interpretation criteria, and various presentation issues. These collectively indicate that substantial revision is required.

To improve the manuscript, the authors should:

First, strengthen the theoretical foundation and justification for their methodological choices, particularly regarding the selection of A-SVGD over alternative Bayesian inference methods.

Second, provide clear criteria for geological interpretation of their analytical tools, specifically defining what constitutes physically meaningful versus non-physical solutions.

Third, make their implementation publicly available through a code repository that includes their implementation, synthetic data generation scripts, and example workflows.

Fourth, address the noted presentation issues including mathematical notation, citation accuracy, and proper attribution of key algorithmic components.

Therefore, I recommend major revision before this manuscript can be considered for publication. While the work shows potential value to the field, the current version requires substantial improvements to meet publication standards..

References

1. Matthew D. Hoffman and Andrew Gelman. (2014). The No-U-Turn Sampler: Adaptively Setting Path Lengths in

<u>Hamiltonian Monte Carlo.</u> Journal of Machine Learning Research, vol. 15(1).