# Inference for Dynamic and Latent Variable Models via Plug-and-Play Automatically Differentiable Particle Filtering

**Kevin Tan**[a], **Giles Hooker**[a], **and Edward L. Ionides**[b,1]

This manuscript was compiled on November 2, 2023

**Automatic differentiation has driven recent advances in machine learing, including deep neural networks and Hamiltonian Markov Chain Monte Carlo methods. This progress has required simultaneous advances in algorithms, software and hardware. Partially observed nonlinear stochastic dynamic systems have proved resistant to these techniques; despite various attempts, widely applicable methods have not yet emerged. We present a new approach which is applicable to a general class of models, possesses a theoretical foundation, and is demonstrated to beat current state-of-the-art methods on a challenging scientific benchmark problem. Our algorithm is compatible with parallel computation on a graphical processing unit, and enjoys the plug-and-play property that its software implementation requires only a simulator for the scientific dynamic model as input (in addition to data, and a measurement model).**

Sequential Monte Carlo | Automatic Differentiation | Particle Filter | Markov Process | Maximum Likelihood

Many approaches to inference in highly nonlinear stochastic dynamical systems assume access to the probability density of next states given the current state.

This is a problem in some critical applications, such as disease modeling, where the models are complex enough that obtaining the density is intractable. However, the particle filter, a popular method for solving the filtering problem in partially-observed dynamical systems, does not require evaluation of the transition density of the latent Markov process, enabling an arbitrary model simulator to be plugged into the algorithm in a feature known as the plug-and-play property.

Still, maximum likelihood parameter estimation can be challenging, especially when the Monte Carlo variance of the evaluation is high and the number of parameters is not small. Existing methods like the improved iterated filtering algorithm of Ionides et. al. (1) converge quickly to a neighborhood of the MLE, but struggle to optimize the last few units of log-likelihood.

We propose a hybrid algorithm that u

Unlike IF2, we explicitly characterize our method's rate of convergence

Algorithmic differentiation potentially facilitates numerical optimization, but currently its use for particle filters is limited. We investigate ways to use algorithmic differentiation of particle filters within the confines of the plug-and-play property, with the goal of enhancing current inference capabilities for general POMP models.

**The issue:** Particle filters provide convenient approaches to evaluating the log-likelihood function for partially observed Markov process (POMP) models. However, using this evaluator to obtain a maximum likelihood parameter estimate can be challenging – especially when the Monte Carlo variance of the evaluation is high and the number of parameters is not small. Empirically, methods such as the improved iterated filtering algorithm (IF2) from Ionides et. al. (1) rapidly converge to a neighborhood of the optimum but struggle at finding the exact optimum due to Monte Carlo variance, even with an annealing random walk standard deviation.

A potential solution to this could lie in auto-differentiation (AD). This would allow for the use of first and second-order iterative optimization techniques. However, though AD could potentially facilitate numerical optimization, its use for plug-and-play particle filters has so far been limited. This is



## Significance Statement

Many scientific models involve highly nonlinear stochastic dynamical systems which can be observed only via noisy and incomplete measurements. Under the Markov assumption on system dynamics, previous work has provided methods of performing inference for these models. In particular, prior to this work, iterated filtering algorithms were the only class of algorithms for maximum likelihood estimation that did not require access to the system's transition probabilities, instead needing only a simulator of the system dynamics. We leverage recent advances in automatic differentiation to propose a hybrid algorithm that requires only a differentiable simulator for maximum likelihood estimation. Our new method outperforms previous approaches on a challenging problem in epidemiology.

Author affiliations: [a]University of Pennsylvania; [b]University of Michigan

Please provide details of author contributions here.

Please declare any competing interests here.

[1]To whom correspondence should be addressed. E-mail: ionides@umich.edu

potentially because particle filtering methods are inherently non-differentiable due to the resampling step that may take place in between iterations.

**The importance of the plug-and-play property:.** Performing inference in highly nonlinear stochastic dynamical systems is a challenging problem. Although many methods for inference assume access to the density of state transitions, this is often not available, especially in critical applications like epidemiology.

Basic particle filtering algorithms do not require evaluation of the transition density of the latent Markov process, in a feature known as the **plug-and-play property** (2) since it enables an arbitrary model simulator to be plugged into the algorithm. We investigate ways to use algorithmic differentiation of particle filters within the confines of the plug-and-play property, with the goal of enhancing current inference capabilities for general POMP models.

**Other potential applications:.** This has applications beyond the obvious one of learning model parameters via first or second-order optimization routines. For example, it could be a step towards developing very general Hamiltonian Monte Carlo methods for particle MCMC, as Rosato et. al. (3) do by using previous work such as (4, 5) (and we conjecture that the seed-fixing derivatives of Rosato et. al. are the same as these as an immediate consequence of section **??**) to differentiate the particle filter.

## Guide to using this template on Overleaf

Please note that whilst this template provides a preview of the typeset manuscript for submission, to help in this preparation, it will not necessarily be the final publication layout. For more detailed information please see the PNAS Information for Authors.

If you have a question while using this template on Overleaf, please use the help menu ("?") on the top bar to search for help and tutorials. You can also contact the Overleaf support team at any time with specific questions about your manuscript or feedback on the template.

**Author Affiliations.** Include department, institution, and complete address, with the ZIP/postal code, for each author. Use lower case letters to match authors with institutions, as shown in the example. PNAS strongly encourages authors to supply an ORCID identifier for each author. Individual authors must link their ORCID account to their PNAS account at www.pnascentral.org. For proper authentication, authors must provide their ORCID at submission and are not permitted to add ORCIDs on proofs.

**Submitting Manuscripts.** All authors must submit their articles at PNAScentral. If you are using Overleaf to write your article, you can use the "Submit to PNAS" option in the top bar of the editor window.

**Format.** Many authors find it useful to organize their manuscripts with the following order of sections: title, author line and affiliations, keywords, abstract, significance statement, introduction, results, discussion, materials and methods, acknowledgments, and references. Other orders and headings are permitted.

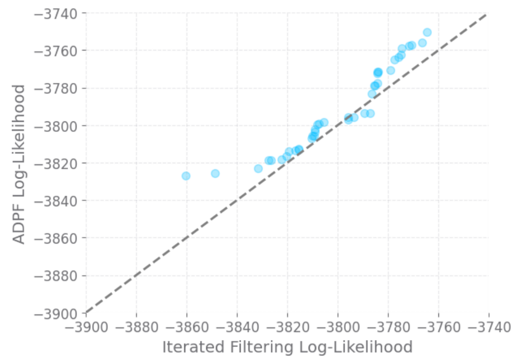


**Fig. 1.** Comparing the ADPF algorithm with IF2 on the Dacca model and data of (6)

**Table 1. Comparison of the fitted potential energy surfaces and ab initio benchmark electronic energy calculations**

| Species | CBS | CV | G3 |
|---|---|---|---|
| 1. Acetaldehyde | 0.0 | 0.0 | 0.0 |
| 2. Vinyl alcohol | 9.1 | 9.6 | 13.5 |
| 3. Hydroxyethylidene | 50.8 | 51.2 | 54.0 |

nomenclature for the TSs refers to the numbered species in the table.



**Manuscript Length.** A standard 6-page article is approximately 4,000 words, 50 references, and 4 medium-size graphical elements (i.e., figures and tables). The preferred length of articles remains at 6 pages, but PNAS will allow articles up to a maximum of 12 pages.

**References.** References should be cited in numerical order as they appear in text; this will be done automatically via bibtex,

**Data Archival.** PNAS must be able to archive the data essential to a published article. Where such archiving is not possible, deposition of data in public databases, such as GenBank, ArrayExpress, Protein Data Bank, Unidata, and others outlined in the Information for Authors, is acceptable.

**Language-Editing Services.** Prior to submission, authors who believe their manuscripts would benefit from professional editing are encouraged to use a language-editing service (see list at https://www.pnas.org/author-center/language-editing). PNAS does not take responsibility for or endorse these services, and their use has no bearing on acceptance of a manuscript for publication.

**Digital Figures.** EPS, high-resolution PDF, and PowerPoint are preferred formats for figures that will be used in the main manuscript. Authors may submit PRC or U3D files for 3D images; these must be accompanied by 2D representations in TIFF, EPS, or high-resolution PDF format. Color images must be in RGB (red, green, blue) mode. Include the font files for any text.

Images must be provided at final size, preferably 1 column width (8.7cm). Figures wider than 1 column should be sized to 11.4cm or 17.8cm wide. Numbers, letters, and symbols should be no smaller than 6 points (2mm) and no larger than 12 points (6mm) after reduction and must be consistent.

$$
\begin{aligned}
(x+y)^3 &= (x+y)(x+y)^2 \\
&= (x+y)(x^2+2xy+y^2) \\
&= x^3+3x^2y+3xy^3+x^3.
\end{aligned} \quad [1]
$$

Figures and tables should be labelled and referenced in the standard way using the `\label{}` and `\ref{}` commands.

Figure 1 shows an example of how to insert a column-wide figure. To insert a figure wider than one column, please use the `\begin{figure*}...\end{figure*}` environment. Figures wider than one column should be sized to 11.4 cm or 17.8 cm wide. Use `\begin{SCfigure*}...\end{SCfigure*}` for a wide figure with side legends.

**Tables.** Tables should be included in the main manuscript file and should not be uploaded separately.

**Single column equations.** Authors may use 1- or 2-column equations in their article, according to their preference.

To allow an equation to span both columns, use the `\begin{figure*}...\end{figure*}` environment mentioned above for figures.

Note that the use of the `widetext` environment for equations is not recommended, and should not be used.

**Supporting Information Appendix (SI).** Authors should submit SI as a single separate SI Appendix PDF file, combining all text, figures, tables, movie legends, and SI references. SI will be published as provided by the authors; it will not be edited or composed. Additional details can be found in the PNAS Author Center. The PNAS Overleaf SI template can be found here. Refer to the SI Appendix in the manuscript at an appropriate point in the text. Number supporting figures and tables starting with S1, S2, etc.

Authors who place detailed materials and methods in an SI Appendix must provide sufficient detail in the main text methods to enable a reader to follow the logic of the procedures and results and also must reference the SI methods. If a paper is fundamentally a study of a new method or technique, then the methods must be described completely in the main text.

***SI Datasets.*** Supply .xlsx, .csv, .txt, .rtf, or .pdf files. This file type will be published in raw format and will not be edited or composed.

***SI Movies.*** Supply Audio Video Interleave (avi), Quicktime (mov), Windows Media (wmv), animated GIF (gif), or MPEG files. Movie legends should be included in the SI Appendix file. All movies should be submitted at the desired reproduction size and length. Movies should be no more than 10MB in size.

## Materials and Methods

Please describe your materials and methods here. This can be more than one paragraph, and may contain subsections and equations as required.

**Subsection for Method.** Example text for subsection.

**ACKNOWLEDGMENTS.** Please include your acknowledgments here, set in a single paragraph. Please do not include any acknowledgments in the Supporting Information, or anywhere else in the manuscript.

1. EL Ionides, D Nguyen, Y Atchadé, S Stoev, AA King, Inference for dynamic and latent variable models via iterated, perturbed Bayes maps. *Proc. Natl. Acad. Sci. USA* **112**, 719—724 (2015).
2. C Bretó, D He, EL Ionides, AA King, Time series analysis via mechanistic models. *Annals Appl. Stat.* **3**, 319–348 (2009).
3. C Rosato, J Harris, J Panovska-Griffiths, S Maskell, Inference of stochastic disease transmission models using particle-mcmc and a gradient based proposal in *25th International Conference on Information Fusion (FUSION 2022).* (IEEE), pp. 1–8 (2022).
4. A Ścibior, F Wood, Differentiable particle filtering without modifying the forward pass. *arXiv:2106.10314* (2021).
5. G Poyiadjis, A Doucet, SS Singh, Particle approximations of the score and observed information matrix in state space models with application to parameter estimation. *Biometrika* **98**, 65–80 (2011).
6. AA King, EL Ionides, M Pascual, MJ Bouma, Inapparent infections and cholera dynamics. *Nature* **454**, 877–880 (2008).