
Non-Canonical Hamiltonian Monte Carlo Algorithm for Two Particles

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Abstract

The abstract paragraph should be indented ½ inch (3 picas) on both the left- and right-hand margins. Use 10 point type, with a vertical spacing (leading) of 11 points. The word **Abstract** must be centered, bold, and in point size 12. Two line spaces precede the abstract. The abstract must be limited to one paragraph.

1 Submission of papers to NeurIPS 2018

NeurIPS requires electronic submissions. The electronic submission site is

<https://cmt.research.microsoft.com/NeurIPS2018/>

Please read the instructions below carefully and follow them faithfully.

1.1 Style

Papers to be submitted to NeurIPS 2018 must be prepared according to the instructions presented here. Papers may only be up to eight pages long, including figures. Additional pages *containing only acknowledgments and/or cited references* are allowed. Papers that exceed eight pages of content (ignoring references) will not be reviewed, or in any other way considered for presentation at the conference.

The margins in 2018 are the same as since 2007, which allow for ~15% more words in the paper compared to earlier years.

Authors are required to use the NeurIPS L^AT_EX style files obtainable at the NeurIPS website as indicated below. Please make sure you use the current files and not previous versions. Tweaking the style files may be grounds for rejection.

1.2 Retrieval of style files

The style files for NeurIPS and other conference information are available on the World Wide Web at

<http://www.neurips.cc/>

The file `neurips_2018.pdf` contains these instructions and illustrates the various formatting requirements your NeurIPS paper must satisfy.

The only supported style file for NeurIPS 2018 is `neurips_2018.sty`, rewritten for L^AT_EX 2_ε. **Previous style files for L^AT_EX 2.09, Microsoft Word, and RTF are no longer supported!**

The L^AT_EX style file contains three optional arguments: `final`, which creates a camera-ready copy, `preprint`, which creates a preprint for submission to, e.g., arXiv, and `nonatbib`, which will not load the `natbib` package for you in case of package clash.

New preprint option for 2018 If you wish to post a preprint of your work online, e.g., on arXiv, using the NeurIPS style, please use the `preprint` option. This will create a nonanonymized version of your work with the text “Preprint. Work in progress.” in the footer. This version may be distributed as you see fit. Please **do not** use the `final` option, which should **only** be used for papers accepted to NeurIPS.

At submission time, please omit the `final` and `preprint` options. This will anonymize your submission and add line numbers to aid review. Please *do not* refer to these line numbers in your paper as they will be removed during generation of camera-ready copies.

The file `neurips_2018.tex` may be used as a “shell” for writing your paper. All you have to do is replace the author, title, abstract, and text of the paper with your own.

The formatting instructions contained in these style files are summarized in Sections 2, 3, and 4 below.

2 General formatting instructions

The text must be confined within a rectangle 5.5 inches (33 picas) wide and 9 inches (54 picas) long. The left margin is 1.5 inch (9 picas). Use 10 point type with a vertical spacing (leading) of 11 points. Times New Roman is the preferred typeface throughout, and will be selected for you by default. Paragraphs are separated by 1/2 line space (5.5 points), with no indentation.

The paper title should be 17 point, initial caps/lower case, bold, centered between two horizontal rules. The top rule should be 4 points thick and the bottom rule should be 1 point thick. Allow 1/4 inch space above and below the title to rules. All pages should start at 1 inch (6 picas) from the top of the page.

For the final version, authors’ names are set in boldface, and each name is centered above the corresponding address. The lead author’s name is to be listed first (left-most), and the co-authors’ names (if different address) are set to follow. If there is only one co-author, list both author and co-author side by side.

Please pay special attention to the instructions in Section 4 regarding figures, tables, acknowledgments, and references.

3 Headings: first level

All headings should be lower case (except for first word and proper nouns), flush left, and bold.

First-level headings should be in 12-point type.

3.1 Headings: second level

Second-level headings should be in 10-point type.

3.1.1 Headings: third level

Third-level headings should be in 10-point type.

Paragraphs There is also a `\paragraph` command available, which sets the heading in bold, flush left, and inline with the text, with the heading followed by 1 em of space.

4 Citations, figures, tables, references

These instructions apply to everyone.



Figure 1: Sample figure caption.

4.1 Citations within the text

The `natbib` package will be loaded for you by default. Citations may be author/year or numeric, as long as you maintain internal consistency. As to the format of the references themselves, any style is acceptable as long as it is used consistently.

The documentation for `natbib` may be found at

<http://mirrors.ctan.org/macros/latex/contrib/natbib/natnotes.pdf>

Of note is the command `\citet`, which produces citations appropriate for use in inline text. For example,

```
\citet{hasselmo} investigated\dots
```

produces

Hasselmo, et al. (1995) investigated...

If you wish to load the `natbib` package with options, you may add the following before loading the `neurips_2018` package:

```
\PassOptionsToPackage{options}{natbib}
```

If `natbib` clashes with another package you load, you can add the optional argument `nonatbib` when loading the style file:

```
\usepackage[nonatbib]{neurips_2018}
```

As submission is double blind, refer to your own published work in the third person. That is, use “In the previous work of Jones et al. [4],” not “In our previous work [4].” If you cite your other papers that are not widely available (e.g., a journal paper under review), use anonymous author names in the citation, e.g., an author of the form “A. Anonymous.”

4.2 Footnotes

Footnotes should be used sparingly. If you do require a footnote, indicate footnotes with a number¹ in the text. Place the footnotes at the bottom of the page on which they appear. Precede the footnote with a horizontal rule of 2 inches (12 picas).

Note that footnotes are properly typeset *after* punctuation marks.²

4.3 Figures

All artwork must be neat, clean, and legible. Lines should be dark enough for purposes of reproduction. The figure number and caption always appear after the figure. Place one line space before the figure

¹Sample of the first footnote.

²As in this example.

Table 1: Sample table title

Part		
Name	Description	Size (μm)
Dendrite	Input terminal	~ 100
Axon	Output terminal	~ 10
Soma	Cell body	up to 10^6

caption and one line space after the figure. The figure caption should be lower case (except for first word and proper nouns); figures are numbered consecutively.

You may use color figures. However, it is best for the figure captions and the paper body to be legible if the paper is printed in either black/white or in color.

4.4 Tables

All tables must be centered, neat, clean and legible. The table number and title always appear before the table. See Table 1.

Place one line space before the table title, one line space after the table title, and one line space after the table. The table title must be lower case (except for first word and proper nouns); tables are numbered consecutively.

Note that publication-quality tables *do not contain vertical rules*. We strongly suggest the use of the booktabs package, which allows for typesetting high-quality, professional tables:

<https://www.ctan.org/pkg/booktabs>

This package was used to typeset Table 1.

5 Main Result

5.1 Algorithm Background

Consider the case we sample q from the distribution $\pi(q)$. From now, we consider the case as sampling the distribution $\pi(q_1, q_2) = \pi(q_1)\pi(q_2)$. (Copy and paste the target distribution) we assume q_1 and q_2 has the momentum, p_1 and p_2 , respectively, with $p_1, p_2 \sim N(0, I)$. Then the Hamiltonian is defined by $H(q_1, q_2, p_1, p_2) = U(q_1) + U(q_2) + \frac{1}{2}p_1^T p_1 + \frac{1}{2}p_2^T p_2$. We observe what happens to this assumption in non-canonical Hamiltonian dynamics with $A \in \mathbb{R}^{4n \times 4n}$. We denote A as

$$A = \left[\begin{array}{c|c} E & F \\ \hline -F^T & G \end{array} \right]$$

where

$$E = \left[\begin{array}{c|c} E_1 & E_2 \\ \hline E_3 & E_4 \end{array} \right] \in \mathbb{R}^{2n \times 2n},$$

$$F = \left[\begin{array}{c|c} F_1 & F_2 \\ \hline F_3 & F_4 \end{array} \right] \in \mathbb{R}^{2n \times 2n},$$

$$G = \left[\begin{array}{c|c} G_1 & G_2 \\ \hline G_3 & G_4 \end{array} \right] \in \mathbb{R}^{2n \times 2n}.$$

Lemma 1. If $G_1 = G_4 = E_1 = E_4 = 0$ and $G_2^T + G_3, E_2^T + E_3$ are 0, (in other words, E, G are *anti-symmetric* matrix). Then the *non-canonical* Hamiltonian dynamics preserves H .

proof. The non-canonical hamiltonian dynamics is following:

$$\frac{d}{dt} \begin{bmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} E_1 & E_2 & F_1 & F_2 \\ E_3 & E_4 & F_3 & F_4 \\ -F_1^T & -F_3^T & G_1 & G_2 \\ -F_2^T & -F_4^T & G_3 & G_4 \end{bmatrix} \begin{bmatrix} \nabla_{q_1} U(q_1) \\ \nabla_{q_2} U(q_2) \\ p_1 \\ p_2 \end{bmatrix}$$

Since $G_1 = G_4 = E_1 = E_4 = 0$,

$$\begin{bmatrix} E_1 & E_2 & F_1 & F_2 \\ E_3 & E_4 & F_3 & F_4 \\ -F_1^T & -F_3^T & G_1 & G_2 \\ -F_2^T & -F_4^T & G_3 & G_4 \end{bmatrix} \begin{bmatrix} \nabla_{q_1} U(q_1) \\ \nabla_{q_2} U(q_2) \\ p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} E_2 \nabla_{q_2} U(q_2) + F_1 p_1 + F_2 p_2 \\ E_3 \nabla_{q_1} U(q_1) + F_3 p_1 + F_4 p_2 \\ -F_1^T \nabla_{q_1} U(q_1) - F_3^T \nabla_{q_2} U(q_2) + G_2 p_2 \\ -F_2^T \nabla_{q_1} U(q_1) - F_4^T \nabla_{q_2} U(q_2) + G_3 p_1 \end{bmatrix}$$

Also, note that the poisson bracket is

$$\frac{dQ}{dt} = \sum_{i=1}^{2n} \frac{\partial Q}{\partial p_i} \frac{dp_i}{dt} + \sum_{i=1}^{2n} \frac{\partial Q}{\partial q_i} \frac{dq_i}{dt}$$

Therefore, putting previous evaluations,

$$\begin{aligned} \frac{dQ}{dt} = & (\nabla_{p_1} Q)^T (-F_1^T \nabla_{q_1} U(q_1) - F_3^T \nabla_{q_2} U(q_2) + G_2 p_2) + (\nabla_{p_2} Q)^T (-F_2^T \nabla_{q_1} U(q_1) - F_4^T \nabla_{q_2} U(q_2) + \\ & G_3 p_1) + (\nabla_{q_1} Q^T) (E_2 \nabla_{q_2} U(q_2) + F_1 p_1 + F_2 p_2) + (\nabla_{q_2} Q^T) (E_3 \nabla_{q_1} U(q_1) + F_3 p_1 + F_4 p_2). \end{aligned}$$

This can be re-expressed as

$$\begin{aligned} \frac{dQ}{dt} = & (\nabla_{p_1} Q)^T (-F_1^T \nabla_{q_1} U(q_1) - F_3^T \nabla_{q_2} U(q_2)) + (\nabla_{p_2} Q)^T (-F_2^T \nabla_{q_1} U(q_1) - \\ & F_4^T \nabla_{q_2} U(q_2)) + (\nabla_{q_1} Q^T) (F_1 p_1 + F_2 p_2) + (\nabla_{q_2} Q^T) (F_3 p_1 + F_4 p_2) + (\nabla_{p_1} Q)^T G_2 p_2 + \\ & (\nabla_{p_2} Q)^T G_3 p_1 + (\nabla_{q_1} Q^T) E_2 \nabla_{q_2} U(q_2) + (\nabla_{q_2} Q^T) E_3 \nabla_{q_1} U(q_1). \end{aligned}$$

Now, letting $Q = H$, we know

$$\begin{aligned} & (\nabla_{p_1} H)^T (-F_1^T \nabla_{q_1} U(q_1) - F_3^T \nabla_{q_2} U(q_2)) + (\nabla_{p_2} H)^T (-F_2^T \nabla_{q_1} U(q_1) - F_4^T \nabla_{q_2} U(q_2)) + \\ & (\nabla_{q_1} H^T) (F_1 p_1 + F_2 p_2) + (\nabla_{q_2} H^T) (F_3 p_1 + F_4 p_2) = 0. \end{aligned}$$

Therefore, it is enough to find the condition for

$$(\nabla_{p_1} H)^T G_2 p_2 + (\nabla_{p_2} H)^T G_3 p_1 + (\nabla_{q_1} H^T) E_2 \nabla_{q_2} U(q_2) + (\nabla_{q_2} H^T) E_3 \nabla_{q_1} U(q_1) = 0.$$

By assumption of H , this is equivalent to

$$\begin{aligned} & p_1^T G_2 p_2 + p_2^T G_3 p_1 + (\nabla_{q_1} U(q_1))^T E_2 \nabla_{q_2} U(q_2) + (\nabla_{q_2} U(q_2))^T E_3 \nabla_{q_1} U(q_1) \\ & = p_2^T (G_2^T + G_3) p_1 + (\nabla_{q_2} U(q_2))^T (E_2^T + E_3) \nabla_{q_1} U(q_1) = 0. \end{aligned}$$

Since $G_2^T + G_3$ and $E_2^T + E_3$ are zero, we completes the proof.

Lemma 2. We can make *leapfrog like integrator* in this dynamic system.

proof. We split our Hamiltonian into sub-Hamiltonians as follow :

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2} U(q_1) + \frac{1}{2} U(q_2) + (\frac{1}{2} p_1^T p_1 + \frac{1}{2} p_2^T p_2) + \frac{1}{2} U(q_2) + \frac{1}{2} U(q_1),$$

with $H_1 = \frac{1}{2} U(q_1)$, $H_2 = \frac{1}{2} U(q_2)$, $H_3 = \frac{1}{2} p_1^T p_1 + \frac{1}{2} p_2^T p_2$. Then, the corresponding non-canonical dynamics for each Hamiltonian are following :

$$H_1 : \frac{d}{dt} \begin{bmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} 0 & E_2 & F_1 & F_2 \\ E_3 & 0 & F_3 & F_4 \\ -F_1^T & -F_3^T & 0 & G_2 \\ -F_2^T & -F_4^T & G_3 & 0 \end{bmatrix} \begin{bmatrix} \nabla_{q_1} U(q_1) \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ E_3 \nabla_{q_1} U(q_1) \\ -F_1^T \nabla_{q_1} U(q_1) \\ -F_2^T \nabla_{q_1} U(q_1) \end{bmatrix}$$

$$H_2 : \frac{d}{dt} \begin{bmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} 0 & E_2 & F_1 & F_2 \\ E_3 & 0 & F_3 & F_4 \\ -F_1^T & -F_3^T & 0 & G_2 \\ -F_2^T & -F_4^T & G_3 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ \nabla_{q_2} U(q_2) \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} E_2 \nabla_{q_2} U(q_2) \\ 0 \\ -F_3^T \nabla_{q_2} U(q_2) \\ -F_4^T \nabla_{q_2} U(q_2) \end{bmatrix}$$

$$H_3 : \frac{d}{dt} \begin{bmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} 0 & E_2 & F_1 & F_2 \\ E_3 & 0 & F_3 & F_4 \\ -F_1^T & -F_3^T & 0 & G_2 \\ -F_2^T & -F_4^T & G_3 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} F_1 p_1 + F_2 p_2 \\ F_3 p_1 + F_4 p_2 \\ G_2 p_2 \\ G_3 p_1 \end{bmatrix}$$

which are all tractable. Therefore, for given $\epsilon > 0$, we can construct a leapfrog operator for H ,

$$\Phi_{H,\epsilon} = \Phi_{H_1,\epsilon} \circ \Phi_{H_2,\epsilon} \circ \Phi_{H_3,\epsilon} \circ \Phi_{H_2,\epsilon} \circ \Phi_{H_1,\epsilon}.$$

For time reversibility, we can add matrix flipping operators, which are volume preserving and self-inverse map. (Just have done in MHMC paper). So we completes the proof.

We observed if $F_2 = F_3 = 0$, this is the case we wanted for two-particle interaction sampling case. We have not found if there is a corresponding dynamic system in physics and which selection of E and G would be helpful.

6 Preparing PDF files

Please prepare submission files with paper size “US Letter,” and not, for example, “A4.”

Fonts were the main cause of problems in the past years. Your PDF file must only contain Type 1 or Embedded TrueType fonts. Here are a few instructions to achieve this.

- You should directly generate PDF files using `pdflatex`.
- You can check which fonts a PDF files uses. In Acrobat Reader, select the menu Files>Document Properties>Fonts and select Show All Fonts. You can also use the program `pdf fonts` which comes with `xpdf` and is available out-of-the-box on most Linux machines.
- The IEEE has recommendations for generating PDF files whose fonts are also acceptable for NeurIPS. Please see <http://www.emfield.org/icuwb2010/downloads/IEEE-PDF-SpecV32.pdf>
- `xfig` "patterned" shapes are implemented with bitmap fonts. Use "solid" shapes instead.
- The `\bbold` package almost always uses bitmap fonts. You should use the equivalent AMS Fonts:

```
\usepackage{amsfonts}
```

followed by, e.g., `\mathbb{R}`, `\mathbb{N}`, or `\mathbb{C}` for \mathbb{R} , \mathbb{N} or \mathbb{C} . You can also use the following workaround for reals, natural and complex:

```
\newcommand{\RR}{\mathbb{R}} %real numbers
\newcommand{\Nat}{\mathbb{N}} %natural numbers
\newcommand{\CC}{\mathbb{C}} %complex numbers
```

Note that `amsfonts` is automatically loaded by the `amssymb` package.

If your file contains type 3 fonts or non embedded TrueType fonts, we will ask you to fix it.

6.1 Margins in L^AT_EX

Most of the margin problems come from figures positioned by hand using `\special` or other commands. We suggest using the command `\includegraphics` from the `graphicx` package. Always specify the figure width as a multiple of the line width as in the example below:

```
\usepackage[pdftex]{graphicx} ...  
\includegraphics[width=0.8\linewidth]{myfile.pdf}
```

See Section 4.4 in the graphics bundle documentation (<http://mirrors.ctan.org/macros/latex/required/graphics/grfguide.pdf>)

A number of width problems arise when L^AT_EX cannot properly hyphenate a line. Please give LaTeX hyphenation hints using the \- command when necessary.

Acknowledgments

Use unnumbered third level headings for the acknowledgments. All acknowledgments go at the end of the paper. Do not include acknowledgments in the anonymized submission, only in the final paper.

References

References follow the acknowledgments. Use unnumbered first-level heading for the references. Any choice of citation style is acceptable as long as you are consistent. It is permissible to reduce the font size to `small` (9 point) when listing the references. **Remember that you can use more than eight pages as long as the additional pages contain *only* cited references.**

[1] Alexander, J.A. & Mozer, M.C. (1995) Template-based algorithms for connectionist rule extraction. In G. Tesauro, D.S. Touretzky and T.K. Leen (eds.), *Advances in Neural Information Processing Systems 7*, pp. 609–616. Cambridge, MA: MIT Press.

[2] Bower, J.M. & Beeman, D. (1995) *The Book of GENESIS: Exploring Realistic Neural Models with the GEneral NEural Simulation System*. New York: TELOS/Springer-Verlag.

[3] Hasselmo, M.E., Schnell, E. & Barkai, E. (1995) Dynamics of learning and recall at excitatory recurrent synapses and cholinergic modulation in rat hippocampal region CA3. *Journal of Neuroscience* **15**(7):5249-5262.