SoftwareX article template Version 4 (November 2023)

Before you complete this template, a few important points to note:

- This template is for an original SoftwareX article. If you are submitting an update to a software article that has already been published, please use the Software Update Template found on the Guide for Authors page.

- The format of a software article is very different to a traditional research article. To help you write yours, we have created this template. We will only consider software articles submitted using this template.

- It is mandatory to publicly share the code/software referred to in your software article. You'll find information on our software sharing criteria in the SoftwareX Guide for Authors.

- It's important to consult the Guide for Authors when preparing your manuscript; it highlights mandatory requirements and is packed with useful advice.

Still got questions? Email our editorial team at softwarex@elsevier.com.

Now you are ready to fill in the template below. As you complete each section, please carefully read the associated instructions. All sections are mandatory, unless marked optional. Once you have completed the template, delete these instructions. In addition, please delete the instructions in the template (the text written in italics).

gamma_flow: Guided Analysis of Multi-label spectra by Matrix Factorization for Lightweight Operational Workflows

Viola Rädle[a,*], Tilman Hartwig[a], Benjamin Oesen[a], Emily Alice Kröger[b],
Julius Vogt[b], Eike Gericke[b], Martin Baron[b]

[a]*Application Lab for AI and Big Data, German Environmental Agency, Leipzig, Germany*
[b]*Federal Office for Radiation Protection, Berlin, Germany*

Abstract

Ca. 100 words. The abstract is followed by a maximum of six keywords and some mandatory and optional metadata.

Your main body of text (sections 1-5 below) should be a maximum 6 pages in total (excluding metadata, tables, figures, references) with a 3000-word limit (we ask that more priority is placed on the word limit versus the page count). Though we strictly insist on the author following the template, in exceptional circumstances, we can be flexible with the page numbers and word limit. In such cases, it should be discussed with the managing editor or publisher prior to submission. All queries regarding the same can be reached at softwarex@elsevier.com.

Keywords: Python, Gamma spectroscopy, Non-negative Matrix Factorization, Classification, Denoising, Spectral Deconvolution

Metadata

The ancillary data table 1 is required for the sub-version of the codebase. Please replace the italicized text in the right column with the correct information about your current code and leave the left column untouched.

Optionally, you can provide information about the current executable software version filling in the left column of Table 2. Please leave the first column as it is.

---

*Corresponding author: raedle.htwk@web.de

Nr.	Code metadata description	Metadata
C1	Current code version	For example v42
C2	Permanent link to code/repository used for this code version	For example: `https://github.com/mozart/mozart2`
C3	Permanent link to Reproducible Capsule	For example: `https://codeocean.com/capsule/0270963/tree/v1`
C4	Legal Code License	All software and code must be released under one of the pre-approved licenses listed in the Guide for Authors, such as Apache License, GNU General Public License (GPL) or MIT License. Write the name of the license you've chosen here.
C5	Code versioning system used	For example: svn, git, mercurial, etc. (put none if none is used)
C6	Software code languages, tools, and services used	For example: C++, python, r, MPI, OpenCL, etc.
C7	Compilation requirements, operating environments & dependencies	
C8	If available Link to developer documentation/manual	For example: `http://mozart.github.io/documentation/`
C9	Support email for questions	

Table 1: Code metadata (mandatory)

1. Motivation and significance

In this section, we want you to introduce the scientific background and the motivation for developing the software.

- *Explain why the software is important and describe the exact (scientific) problem(s) it solves.*

- *Indicate in what way the software has contributed (or will contribute in the future) to the process of scientific discovery; if available, please cite a research paper using the software.*

- *Provide a description of the experimental setting. (How does the user use the software?)*

- *Introduce related work in literature (cite or list algorithms used, other software etc.).*

Nr.	(Executable) software metadata description	Please fill in this column
S1	Current software version	For example 1.1, 2.4 etc.
S2	Permanent link to executables of this version	For example: `https://github.com/combogenomics/DuctApe/releases/tag/DuctApe-0.16.4`
S3	Permanent link to Reproducible Capsule	
S4	Legal Software License	List one of the approved licenses
S5	Computing platforms/Operating Systems	For example Android, BSD, iOS, Linux, OS X, Microsoft Windows, Unix-like , IBM z/OS, distributed/web based etc.
S6	Installation requirements & dependencies	
S7	If available, link to user manual - if formally published include a reference to the publication in the reference list	For example: `http://mozart.github.io/documentation/`
S8	Support email for questions	

Table 2: Software metadata (optional)

2. Software description

Describe the software. Provide enough detail to help the reader understand its impact.

2.1. Software architecture

Give a short overview of the overall software architecture; provide a pictorial overview where possible; for example, an image showing the components. If necessary, provide implementation details.

2.2. Software functionalities

Present the major functionalities of the software.

2.3. Sample code snippets analysis (optional)

3. Illustrative examples

Provide at least one illustrative example to demonstrate the major functions of your software/code.

Optional*: you may include one explanatory video or screencast that will appear next to your article, in the right hand side panel. Please upload any video as a single supplementary file with your article. Only one MP4 formatted, with 150MB maximum size, video is possible per article. Recommended video dimensions are 640 x 480 at a maximum of 30 frames / second. Prior to submission please test and validate your .mp4 file at* `http: // elsevier-apps. sciverse. com/ GadgetVideoPodcastPlayerWeb/ verification` *. This tool will display your video exactly in the same way as it will appear on ScienceDirect.*

4. Impact

This is the main section of the article and reviewers will weight it appropriately. Please indicate:

- *Any new research questions that can be pursued as a result of your software.*

- *In what way, and to what extent, your software improves the pursuit of existing research questions.*

- *Any ways in which your software has changed the daily practice of its users.*

- *How widespread the use of the software is within and outside the intended user group (downloads, number of users if your software is a service, citable publications, etc.).*

- *How the software is being used in commercial settings and/or how it has led to the creation of spin-off companies.*

Please note that points 1 and 2 are best demonstrated by references to citable publications.

5. Conclusions

[1]

Acknowledgements

Optional. You can use this section to acknowledge colleagues who don't qualify as a co-author but helped you in some way.

References

[1] J. A. Kulesza, T. R. Adams, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, T. P. Burke, A. R. Clark, R. A. A. Forster III, J. F. Giron, T. S. Grieve, C. J. Josey, R. L. Martz, G. W. McKinney, E. J. Pearson, M. E. Rising, C. J. C. Solomon Jr., S. Swaminarayan, T. J. Trahan, S. C. Wilson, A. J. Zukaitis, MCNP® Code Version 6.3.0 Theory & User Manual, Tech. Rep. LA-UR-22-30006, Los Alamos National Laboratory (LANL), Los Alamos, NM (United States) (Sep. 2022). `doi:10.2172/1889957`.

References

[1] Use this style of ordering. References in-text should also use a similar style.

If the software repository you used supplied a DOI or another Persistent IDentifier (PID), please add a reference for your software here. For more guidance on software citation, please see our guide for authors or this article on the essentials of software citation by FORCE 11, of which Elsevier is a member.

Reminder: Before you submit, please delete all the instructions in this document, including this paragraph. Thank you!