
Instructions for Paper Submissions to AISTATS 2021

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Abstract

Metabolites — organic molecules involved in or created by cellular metabolism — are ubiquitous in biological systems and are a rich source of drug candidates, targets, and disease biomarkers. Liquid chromatography tandem mass spectrometry (LC-MS/MS) is an increasingly common way of identifying new metabolites suitable for clinical deployment. Identifying chemical structures in LC-MS/MS spectra is a difficult and open problem. Here we propose a supervised topic modeling approach to identify modular groups of spectrum features corresponding to consistently appearing chemical substructures, using labeled latent Dirichlet Allocation (LLDA) and a new document generation process. We compare our approach an existing alternative and find that our approach yields similar performance, more interpretability, and more compatibility with substructure label sets. We then adapt the RankFromSets model to this problem and see qualitative improvement. RankFromSets is a recently developed recommender system which has been shown to have optimal recall.

1 GENERAL FORMATTING INSTRUCTIONS

The camera-ready versions of the accepted papers are 8 pages, plus any additional pages needed for references.

Papers are in 2 columns with the overall line width of 6.75 inches (41 picas). Each column is 3.25 inches wide (19.5 picas). The space between the columns is .25 inches wide (1.5 picas). The left margin is

0.88 inches (5.28 picas). Use 10 point type with a vertical spacing of 11 points. Please use US Letter size paper instead of A4.

Paper title is 16 point, caps/lc, bold, centered between 2 horizontal rules. Top rule is 4 points thick and bottom rule is 1 point thick. Allow 1/4 inch space above and below title to rules.

Author descriptions are center-justified, initial caps. The lead author is to be listed first (left-most), and the Co-authors are set to follow. If up to three authors, use a single row of author descriptions, each one center-justified, and all set side by side; with more authors or unusually long names or institutions, use more rows.

Use one-half line space between paragraphs, with no indent.

2 FIRST LEVEL HEADINGS

First level headings are all caps, flush left, bold, and in point size 12. Use one line space before the first level heading and one-half line space after the first level heading.

2.1 Second Level Heading

Second level headings are initial caps, flush left, bold, and in point size 10. Use one line space before the second level heading and one-half line space after the second level heading.

2.1.1 Third Level Heading

Third level headings are flush left, initial caps, bold, and in point size 10. Use one line space before the third level heading and one-half line space after the third level heading.

Fourth Level Heading Fourth level headings must be flush left, initial caps, bold, and Roman type. Use one line space before the fourth level heading, and place the section text immediately after the heading with no line break, but an 11 point horizontal space.

2.2 Citations, Figure, References

2.2.1 Citations in Text

Citations within the text should include the author’s last name and year, e.g., (Cheesman, 1985). Be sure that the sentence reads correctly if the citation is deleted: e.g., instead of “As described by (Cheesman, 1985), we first frobulate the widgets,” write “As described by Cheesman (1985), we first frobulate the widgets.”

The references listed at the end of the paper can follow any style as long as it is used consistently.

2.2.2 Footnotes

Indicate footnotes with a number¹ in the text. Use 8 point type for footnotes. Place the footnotes at the bottom of the column in which their markers appear, continuing to the next column if required. Precede the footnote section of a column with a 0.5 point horizontal rule 1 inch (6 picas) long.²

2.2.3 Figures

All artwork must be centered, neat, clean, and legible. All lines should be very dark for purposes of reproduction, and art work should not be hand-drawn. Figures may appear at the top of a column, at the top of a page spanning multiple columns, inline within a column, or with text wrapped around them, but the figure number and caption always appear immediately below the figure. Leave 2 line spaces between the figure and the caption. The figure caption is initial caps and each figure should be numbered consecutively.

Make sure that the figure caption does not get separated from the figure. Leave extra white space at the bottom of the page rather than splitting the figure and figure caption.

This figure intentionally left non-blank

Figure 1: Sample Figure Caption

2.2.4 Tables

All tables must be centered, neat, clean, and legible. Do not use hand-drawn tables. Table number and title always appear above the table. See Table 1.

¹Sample of the first footnote.

²Sample of the second footnote.

Use 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 initial caps and each table numbered consecutively.

Table 1: Sample Table Title

PART	DESCRIPTION
Dendrite	Input terminal
Axon	Output terminal
Soma	Cell body (contains cell nucleus)

3 SUPPLEMENTARY MATERIAL

If you need to include additional appendices during submission, you can include them in the supplementary material file. You can submit a single file of additional supplementary material which may be either a pdf file (such as proof details) or a zip file for other formats/more files (such as code or videos). Note that reviewers are under no obligation to examine your supplementary material. If you have only one supplementary pdf file, please upload it as is; otherwise gather everything to the single zip file.

You must use `aistats2021.sty` as a style file for your supplementary pdf file and follow the same formatting instructions as in the main paper. The only difference is that it must be in a *single-column* format. You can use `supplement.tex` in our starter pack as a starting point. Alternatively, you may append the supplementary content to the main paper and split the final PDF into two separate files.

4 SUBMISSION INSTRUCTIONS

To submit your paper to AISTATS 2021, please follow these instructions.

1. Download `aistats2021.sty`, `fancyhdr.sty`, and `sample_paper.tex` provided in our starter pack. Please, do not modify the style files as this might result in a formatting violation.
2. Use `sample_paper.tex` as a starting point.
3. Begin your document with

```
\documentclass[twoside]{article}
\usepackage{aistats2021}
```

The `twoside` option for the class `article` allows the package `fancyhdr.sty` to include headings for even and odd numbered pages.

4. When you are ready to submit the manuscript, compile the latex file to obtain the pdf file.
5. Check that the content of your submission, *excluding* references, is limited to **8 pages**. The number of pages containing references alone is not limited.
6. Upload the PDF file along with other supplementary material files to the CMT website.

4.1 Camera-ready Papers

If your papers are accepted, you will need to submit the camera-ready version. Please make sure that you follow these instructions:

1. Change the beginning of your document to

```
\documentclass[twoside]{article}
\usepackage[accepted]{aistats2021}
```

The option `accepted` for the package `aistats2021.sty` will write a copyright notice at the end of the first column of the first page. This option will also print headings for the paper. For the *even* pages, the title of the paper will be used as heading and for *odd* pages the author names will be used as heading. If the title of the paper is too long or the number of authors is too large, the style will print a warning message as heading. If this happens additional commands can be used to place as headings shorter versions of the title and the author names. This is explained in the next point.

2. If you get warning messages as described above, then immediately after `\begin{document}`, write

```
\runningtitle{Provide here an alternative
shorter version of the title of your
paper}
\runningauthor{Provide here the surnames
of the authors of your paper, all
separated by commas}
```

Note that the text that appears as argument in `\runningtitle` will be printed as a heading in the *even* pages. The text that appears as argument in `\runningauthor` will be printed as a heading in the *odd* pages. If even the author surnames do not fit, it is acceptable to give a subset of author names followed by “et al.”

3. The camera-ready versions of the accepted papers are 8 pages, plus any additional pages needed for references.

4. If you need to include additional appendices, you can include them in the supplementary material file.
5. Please, do not change the layout given by the above instructions and by the style file.

Acknowledgements

All acknowledgments go at the end of the paper, including thanks to reviewers who gave useful comments, to colleagues who contributed to the ideas, and to funding agencies and corporate sponsors that provided financial support. To preserve the anonymity, please include acknowledgments *only* in the camera-ready papers.

References

References follow the acknowledgements. Use an unnumbered third level heading for the references section. Please use the same font size for references as for the body of the paper—remember that references do not count against your page length total.

References

- J. Alspector, B. Gupta, and R. B. Allen (1989). Performance of a stochastic learning microchip. In D. S. Touretzky (ed.), *Advances in Neural Information Processing Systems 1*, 748–760. San Mateo, Calif.: Morgan Kaufmann.
- F. Rosenblatt (1962). *Principles of Neurodynamics*. Washington, D.C.: Spartan Books.
- G. Tesauro (1989). Neurogammon wins computer Olympiad. *Neural Computation* **1**(3):321–323.