
MoML example style

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Abstract

Abstracts should be a single paragraph, ideally between 4–6 sentences long.

1 Submission Guidelines

We welcome papers related to machine learning for molecules, from small drug-like molecules to proteins and organic crystals. Papers can be submitted on the MoML website, where you have to provide a two-page .pdf file explaining your work together with a poster of your work to present at the conference.

To ensure that the reference information in the bottom of the first page is rendered appropriately and concisely, please specify an abbreviated author list by shortening the first name of the first author in initials followed by “et al.”: `\author[Y. Zhu et al.]{Yanqiao Zhu \and Yuanqi Du}`.

With the provided style file, the author information can be set in various styles. If all authors are from the same institution, authors can use:

```
\author[F. Last et al.]
{First Last 1, First Last 2, ... \and First Last n \
 \institute{Institute \ Address line}\
 \email{first.last@example.com}}
```

For authors from different institutions, please use the `\And` command:

```
\author[F. Last et al.]
{First Last 1 \
 \institute{Institute 1\ Address line} \
 \email{first.last.1@example.com}\And
 First Last 2 \
 \institute{Institute 2\ Address line} \
 \email{first.last.2@example.com}}
```

If author names do not fit in one line, use the `\AND` command to start a separate row of authors:

```
\author[F. Last et al.]
{First Last 1, ..., \and First Last n \
 \institute{Institute 1\ Address line} \
 \email{first.last.1@example.com}\AND
 First Last n+1 \
 \institute{Institute 2\ Address line} \
 \email{first.last.n.1@example.com}}
```

1.1 Figures

All included artwork must be neat, legible, and separated from the text. The figure number and caption always appear below the figure. The figure label should be in boldface and numbered consecutively. The caption should be set in 9-point type, in sentence case, and centered unless it runs more than one lines, in which case it should be flush left. See Figure 1 for an example.

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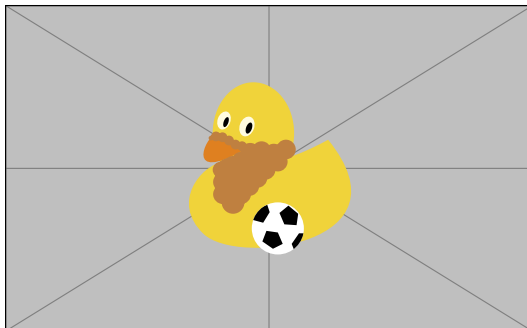


Figure 1: A sample figure.

Table 1: A sample table.

Method	Data 1		Data 2	
	X	Y	X	Y
A	0.8817	0.9572	0.1893	0.1725
B	0.7126	0.2615	0.9173	0.1286
C	0.2716	0.1826	0.2836	0.1836

1.2 Tables

Like figures, tables should be legible and numbered consecutively. However, the table number and caption should always appear above the table. See Table 1 for an example.

Note that publication-quality tables *do not contain vertical rules and double rules*. We strongly suggest the use of the `booktabs` package which provides the commands `\toprule`, `\midrule`, and `\bottomrule` to enhance the quality of tables.

1.3 Paragraphs

Paragraphs are separated by 1/2 line space (5.5 points). Do not indent the first line of a given paragraph.

1.4 Equations

The provided style file loads the `amsmath` package automatically. Unnumbered single-lined equations should be displayed using `\[` and `\]`. For example:

$$\mathbf{X}' = \sigma(\tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} \mathbf{X} \mathbf{W}).$$

Numbered single-line equations should be displayed using the `equation` environment. For example:

$$\mathbf{X}' = \sigma(\tilde{\mathbf{D}}^{-1} \tilde{\mathbf{A}} \mathbf{X} \mathbf{W}). \quad (1)$$

1.5 Bibliographies

Use an unnumbered first-level heading for the references. For a citation, use `\cite`, e.g., [1]. For a textual citation, use `\citet`, e.g., Veličković et al. [2]. *Any choice* of citation style is allowed as long as it is used consistently throughout the whole paper. Additionally, both `natbib` and `bibLaTeX` packages are supported. It is also possible to reduce the font size to `\small` (9-point font) when listing the references.

Author Contributions

Authors of accepted papers are *encouraged* to include a statement that declares the individual contribution of every author, especially when there are co-authors that made equal contributions to

the research. You may adopt the [Contributor Roles Taxonomy \(CRediT\)](#) methodology for attributing contributions. Do not include this section in the version for blind review. This section does not count towards the page limit.

Acknowledgements

The L^AT_EX template is heavily borrowed from LoG 2022.

The acknowledgements do not count towards the page limit.

References

- [1] Thomas N. Kipf and Max Welling. Semi-Supervised Classification with Graph Convolutional Networks. In *ICLR*, 2017. 2
- [2] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. Graph Attention Networks. In *ICLR*, 2018. 2

A Appendix

Any possible appendices should be placed after bibliographies. If your paper has appendices, please submit the appendices together with the main body of the paper. There will be no separate supplementary material submission. The main text should be self-contained; reviewers are not obliged to look at the appendices when writing their review comments.