

Using *MLFlow* to monitor an *end-to-end* machine learning pipeline

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Machine Learning performs very well in labotory settings but doesn't seem transpose well into real world setting. Following this, the objective of this project was to use the tool *MLFlow* to monitor and improve an existing machine learning model (Bayesian Netowrk) for the application Meditrinae. However, because of the immense number of parameters to track, it was impossible to use such a tool to imprpove the model's accuracy when tested with real world data.

Introduction

Machinee Learning has been a *hot topic* in the last decade as we've seen its performance on specific tasks get better and better to a point of surpassing human capabilities, amoungs other, for image recognition.

In this file, we present some tips and sample mark-up to assure your \LaTeX file of the smoothest possible journey from review manuscript to published *Science* paper. We focus here

particularly on issues related to style files, citation, and math, tables, and figures, as those tend to be the biggest sticking points. Please use the source file for this document, `scifile.tex`, as a template for your manuscript, cutting and pasting your content into the file at the appropriate places.

Science's publication workflow relies on Microsoft Word. To translate \LaTeX files into Word, we use an intermediate MS-DOS routine (?) that converts the \TeX source into HTML. The routine is generally robust, but it works best if the source document is clean \LaTeX without a significant freight of local macros or `.sty` files. Use of the source file `scifile.tex` as a template, and calling *only* the `.sty` and `.bst` files specifically mentioned here, will generate a manuscript that should be eminently reviewable, and yet will allow your paper to proceed quickly into our production flow upon acceptance (?).

Formatting Citations

Citations can be handled in one of three ways. The most straightforward (albeit labor-intensive) would be to hardwire your citations into your \LaTeX source, as you would if you were using an ordinary word processor. Thus, your code might look something like this:

```
However, this record of the solar nebula may have been  
partly erased by the complex history of the meteorite  
parent bodies, which includes collision-induced shock,  
thermal metamorphism, and aqueous alteration  
(\it 1, 2, 5--7\}).
```

Compiled, the last two lines of the code above, of course, would give notecalls in *Science* style:

```
... thermal metamorphism, and aqueous alteration (1, 2, 5--7).
```

Under the same logic, the author could set up his or her reference list as a simple enumeration,

```
{\bf References and Notes}

\begin{enumerate}
\item G. Gamow, {\it The Constitution of Atomic Nuclei
and Radioactivity\} (Oxford Univ. Press, New York, 1931).
\item W. Heisenberg and W. Pauli, {\it Zeitschr.\ f.\
Physik\} {\bf 56}, 1 (1929).
\end{enumerate}
```

yielding

References and Notes

1. G. Gamow, *The Constitution of Atomic Nuclei and Radioactivity* (Oxford Univ. Press, New York, 1931).
2. W. Heisenberg and W. Pauli, *Zeitschr. f. Physik* **56**, 1 (1929).

That's not a solution that's likely to appeal to everyone, however — especially not to users of BIB_TE_X (?). If you are a BIB_TE_X user, we suggest that you use the `Science.bst` bibliography style file and the `scicite.sty` package, both of which we are downloadable from our author help site (http://www.sciencemag.org/about/authors/prep/TeX_help/). You can also generate your reference lists by using the list environment `{thebibliography}` at the end of your source document; here again, you may find the `scicite.sty` file useful.

Whether you use BIB_TE_X or `{thebibliography}`, be very careful about how you set up your in-text reference calls and notecalls. In particular, observe the following requirements:

1. Please follow the style for references outlined at our author help site and embodied in recent issues of *Science*. Each citation number should refer to a single reference; please do not concatenate several references under a single number.
2. Please cite your references and notes in text *only* using the standard \LaTeX `\cite` command, not another command driven by outside macros.
3. Please separate multiple citations within a single `\cite` command using commas only; there should be *no space* between reference keynames. That is, if you are citing two papers whose bibliography keys are `keyname1` and `keyname2`, the in-text cite should read `\cite{keyname1, keyname2}`, *not* `\cite{keyname1, keyname2}`.

Failure to follow these guidelines could lead to the omission of the references in an accepted paper when the source file is translated to Word via HTML.

Handling Math, Tables, and Figures

Following are a few things to keep in mind in coding equations, tables, and figures for submission to *Science*.

In-line math. The utility that we use for converting from \LaTeX to HTML handles in-line math relatively well. It is best to avoid using built-up fractions in in-line equations, and going for the more boring “slash” presentation whenever possible — that is, for $\$a/b\$$ (which comes out as a/b) rather than $\$\frac{a}{b}\$$ (which compiles as $\frac{a}{b}$). Likewise, HTML isn’t tooled to handle certain overaccented special characters in-line; for $\hat{\alpha}$ (coded $\$\hat{\alpha}\$$), for example, the HTML translation code will return $^{\wedge}(\alpha)$. Don’t drive yourself crazy — but if it’s possible to avoid such constructs, please do so. Please do not code arrays or matrices as in-line

math; display them instead. And please keep your coding as \TeX -y as possible — avoid using specialized math macro packages like `amstex.sty`.

Displayed math. Our HTML converter sets up \TeX displayed equations using nested HTML tables. That works well for an HTML presentation, but Word chokes when it comes across a nested table in an HTML file. We surmount that problem by simply cutting the displayed equations out of the HTML before it's imported into Word, and then replacing them in the Word document using either images or equations generated by a Word equation editor. Strictly speaking, this procedure doesn't bear on how you should prepare your manuscript — although, for reasons best consigned to a note (?), we'd prefer that you use native \TeX commands within displayed-math environments, rather than \LaTeX sub-environments.

Tables. The HTML converter that we use seems to handle reasonably well simple tables generated using the \LaTeX `{tabular}` environment. For very complicated tables, you may want to consider generating them in a word processing program and including them as a separate file.

Figures. Figure callouts within the text should not be in the form of \LaTeX references, but should simply be typed in — that is, (Fig. 1) rather than `\ref{fig1}`. For the figures themselves, treatment can differ depending on whether the manuscript is an initial submission or a final revision for acceptance and publication. For an initial submission and review copy, you can use the \LaTeX `{figure}` environment and the `\includegraphics` command to include your PostScript figures at the end of the compiled PostScript file. For the final revision, however, the `{figure}` environment should *not* be used; instead, the figure captions themselves should be typed in as regular text at the end of the source file (an example is included here), and the figures should be uploaded separately according to the Art Department's instructions.

What to Send In

What you should send to *Science* will depend on the stage your manuscript is in:

- **Important:** If you're sending in the initial submission of your manuscript (that is, the copy for evaluation and peer review), please send in *only* a PostScript or PDF version of the compiled file (including figures). Please do not send in the \TeX source, `.sty`, `.bbl`, or other associated files with your initial submission. (For more information, please see the instructions at our Web submission site, <http://www.submit2science.org/>.)
- When the time comes for you to send in your revised final manuscript (i.e., after peer review), we require that you include all source files and generated files in your upload. Thus, if the name of your main source document is `ltxfile.tex`, you need to include:
 - `ltxfile.tex`.
 - `ltxfile.aux`, the auxilliary file generated by the compilation.
 - A PostScript file (compiled using `dvips` or some other driver) of the `.dvi` file generated from `ltxfile.tex`, or a PDF file distilled from that PostScript. You do not need to include the actual `.dvi` file in your upload.
 - From \BIBTeX users, your bibliography (`.bib`) file, *and* the generated file `ltxfile.bbl` created when you run \BIBTeX .
 - Any additional `.sty` and `.bst` files called by the source code (though, for reasons noted earlier, we *strongly* discourage the use of such files beyond those mentioned in this document).
- 1. We've included in the template file `scifile.tex` a new environment, `{scilastnote}`, that generates a numbered final citation without a corresponding signal in the text. This en-

vironment can be used to generate a final numbered reference containing acknowledgments, sources of funding, and the like, per *Science* style.

Fig. 1. Please do not use figure environments to set up your figures in the final (post-peer-review) draft, do not include graphics in your source code, and do not cite figures in the text using \LaTeX `\ref` commands. Instead, simply refer to the figure numbers in the text per *Science* style, and include the list of captions at the end of the document, coded as ordinary paragraphs as shown in the `scifile.tex` template file. Your actual figure files should be submitted separately.