

Sequential Model-Based Optimization of Expensive Blackbox Functions

A Thesis
Presented to
The Division of Mathematics and Natural Sciences
Reed College

In Partial Fulfillment
of the Requirements for the Degree
Bachelor of Arts

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(Mathematics)

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Abstract

The preface pretty much says it all.

Dedication

You can have a dedication here if you wish.

Introduction

Welcome to the \LaTeX thesis template. If you've never used \TeX or \LaTeX before, you'll have an initial learning period to go through, but the results of a nicely formatted thesis are worth it for more than the aesthetic benefit: markup like \LaTeX is more consistent than the output of a word processor, much less prone to corruption or crashing and the resulting file is smaller than a Word file. While you may have never had problems using Word in the past, your thesis is going to be about twice as large and complex as anything you've written before, taxing Word's capabilities. If you're still on the fence about using \LaTeX , read the Introduction to LaTeX on the CUS site as well as skim the following template and give it a few weeks. Pretty soon all the markup gibberish will become second nature.

0.1 Why use it?

\LaTeX does a great job of formatting tables and paragraphs. Its line-breaking algorithm was the subject of a PhD. thesis. It does a fine job of automatically inserting ligatures, and to top it all off it is the only way to typeset good-looking mathematics.

0.2 Who should use it?

Anyone who needs to use math, tables, a lot of figures, complex cross-references, IPA or who just cares about the final appearance of their document should use \LaTeX . At Reed, math majors are required to use it, most physics majors will want to use it, and many other science majors may want it also.

Chapter 1

The First

This is the first page of the first chapter. You may delete the contents of this chapter so you can add your own text; it's just here to show you some examples.

1.1 References, Labels, Custom Commands and Footnotes

It is easy to refer to anything within your document using the `label` and `ref` tags. Labels must be unique and shouldn't use any odd characters; generally sticking to letters and numbers (no spaces) should be fine. Put the label on whatever you want to refer to, and put the reference where you want the reference. \LaTeX will keep track of the chapter, section, and figure or table numbers for you.

1.1.1 References and Labels

Sometimes you'd like to refer to a table or figure, e.g. you can see in Figure 3.2 that you can rotate figures. Start by labeling your figure or table with the `label` command (`\label{labelvariable}`) below the caption (see the chapter on graphics and tables for examples). Then when you would like to refer to the table or figure, use the `ref` command (`\ref{labelvariable}`). Make sure your label variables are unique; you can't have two elements named "default." Also, since the reference command only puts the figure or table number, you will have to put "Table" or "Figure" as appropriate, as seen in the following examples:

As I showed in Table 3.1 many factors can be assumed to follow from inheritance. Also see the Figure 3.1 for an illustration.

1.1.2 Custom Commands

Are you sick of writing the same complex equation or phrase over and over?

The custom commands should be placed in the preamble, or at least prior to the first usage of the command. The structure of the `\newcommand` consists of the name of the new command in curly braces, the number of arguments to be made in square

brackets and then, inside a new set of curly braces, the command(s) that make up the new command. The whole thing is sandwiched inside a larger set of curly braces.

In other words, if you want to make a shorthand for H_2SO_4 , which doesn't include an argument, you would write: `\newcommand{\hydro}{H$_2$SO$_4$}` and then when you needed to use the command you would type `\hydro`. (sans verb and the equals sign brackets, if you're looking at the .tex version). For example: H_2SO_4

1.1.3 Footnotes and Endnotes

You might want to footnote something.¹ Be sure to leave no spaces between the word immediately preceding the footnote command and the command itself. The footnote will be in a smaller font and placed appropriately. Endnotes work in much the same way. More information can be found about both on the CUS site.

1.2 Bibliographies

Of course you will need to cite things, and you will probably accumulate an armful of sources. This is why BibTeX was created. For more information about BibTeX and bibliographies, see our CUS site (web.reed.edu/cis/help/latex/index.html)². There are three pages on this topic: *bibtex* (which talks about using BibTeX, at [/latex/bibtex.html](http://latex/bibtex.html)), *bibtexstyles* (about how to find and use the bibliography style that best suits your needs, at [/latex/bibtexstyles.html](http://latex/bibtexstyles.html)) and *bibman* (which covers how to make and maintain a bibliography by hand, without BibTeX, at [/latex/bibman.html](http://latex/bibman.html)). The last page will not be useful unless you have only a few sources. There used to be APA stuff here, but we don't need it since I've fixed this with my `apa-good natbib` style file.

1.2.1 Tips for Bibliographies

1. Like with thesis formatting, the sooner you start compiling your bibliography for something as large as thesis, the better. Typing in source after source is mind-numbing enough; do you really want to do it for hours on end in late April? Think of it as procrastination.
2. The cite key (a citation's label) needs to be unique from the other entries.
3. When you have more than one author or editor, you need to separate each author's name by the word "and" e.g.
`Author = {Noble, Sam and Youngberg, Jessica},.`
4. Bibliographies made using BibTeX (whether manually or using a manager) accept LaTeX markup, so you can italicize and add symbols as necessary.

¹footnote text

²Reed College (2007)

5. To force capitalization in an article title or where all lowercase is generally used, bracket the capital letter in curly braces.
6. You can add a Reed Thesis citation³ option. The best way to do this is to use the phdthesis type of citation, and use the optional “type” field to enter “Reed thesis” or “Undergraduate thesis”. Here’s a test of Chicago, showing the second cite in a row⁴ being different. Also the second time not in a row⁵ should be different. Of course in other styles they’ll all look the same.

1.3 Anything else?

If you’d like to see examples of other things in this template, please contact CUS (email cus@reed.edu) with your suggestions. We love to see people using L^AT_EX for their theses, and are happy to help.

³Noble (2002)

⁴Noble (2002)

⁵Reed College (2007)

Chapter 2

Mathematics and Science

2.1 Math

T_EX is the best way to typeset mathematics. Donald Knuth designed T_EX when he got frustrated at how long it was taking the typesetters to finish his book, which contained a lot of mathematics.

If you are doing a thesis that will involve lots of math, you will want to read the following section which has been commented out. If you're not going to use math, skip over this next big red section. (It's red in the .tex file but does not show up in the .pdf.)

2.2 Chemistry 101: Symbols

Chemical formulas will look best if they are not italicized. Get around math mode's automatic italicizing by using the argument `$\mathrm{formula here}$` , with your formula inside the curly brackets.

So, Fe₂²⁺Cr₂O₄ is written `$\mathrm{Fe_2^{2+}Cr_{20_4}}$`

Exponent or Superscript: O⁻

Subscript: CH₄

To stack numbers or letters as in Fe₂²⁺, the subscript is defined first, and then the superscript is defined.

Angstrom: Å

Bullet: CuCl • 7H₂O

Double Dagger: ‡

Delta: Δ

Reaction Arrows: → or $\xrightarrow{\text{solution}}$

Resonance Arrows: ↔

Reversible Reaction Arrows: ⇌ or $\xrightleftharpoons{\text{solution}}$ (the latter requires the chemarr package)

2.2.1 Typesetting reactions

You may wish to put your reaction in a figure environment, which means that LaTeX will place the reaction where it fits and you can have a figure legend if desired:

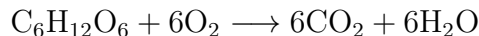
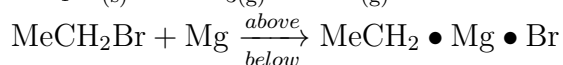


Figure 2.1: Combustion of glucose

2.2.2 Other examples of reactions



2.3 Physics

Many of the symbols you will need can be found on the math page (<http://web.reed.edu/cis/help/latex/math.html>) and the Comprehensive L^AT_EX Symbol Guide (enclosed in this template download). You may wish to create custom commands for commonly used symbols, phrases or equations, as described in Chapter 1.1.2.

2.4 Biology

You will probably find the resources at <http://www.lecb.ncifcrf.gov/~toms/latex.html> helpful, particularly the links to bst's for various journals. You may also be interested in TeXShade for nucleotide typesetting (<http://homepages.uni-tuebingen.de/beitz/txe.html>). Be sure to read the proceeding chapter on graphics and tables, and remember that the thesis template has versions of Ecology and Science bst's which support webpage citation formats.

Chapter 3

Tables and Graphics

3.1 Tables

The following section contains examples of tables, most of which have been commented out for brevity. (They will show up in the .tex document in red, but not at all in the .pdf). For more help in constructing a table (or anything else in this document), please see the LaTeX pages on the CUS site.

Table 3.1: A Basic Table: Correlation of Factors between Parents and Child, Showing Inheritance

Factors	Correlation between Parents & Child	Inherited
Education	-0.49	Yes
Socio-Economic Status	0.28	Slight
Income	0.08	No
Family Size	0.19	Slight
Occupational Prestige	0.21	Slight

If you want to make a table that is longer than a page, you will want to use the longtable environment. Uncomment the table below to see an example, or see our online documentation.

Table 3.2: An example of a long table, with headers that repeat on each subsequent page: Results from the summers of 1998 and 1999 work at Reed College done by Grace Brannigan, Robert Holiday and Lien Ngo in 1998 and Kate Brown and Christina Inman in 1999.

Chromium Hexacarbonyl			
State	Laser wavelength	Buffer gas	Ratio of $\frac{\text{Intensity at vapor pressure}}{\text{Intensity at 240 Torr}}$
$z^7P_4^\circ$	266 nm	Argon	1.5
$z^7P_2^\circ$	355 nm	Argon	0.57
$y^7P_3^\circ$	266 nm	Argon	1
$y^7P_3^\circ$	355 nm	Argon	0.14
$y^7P_2^\circ$	355 nm	Argon	0.14
$z^5P_3^\circ$	266 nm	Argon	1.2
$z^5P_3^\circ$	355 nm	Argon	0.04
$z^5P_3^\circ$	355 nm	Helium	0.02
$z^5P_2^\circ$	355 nm	Argon	0.07
$z^5P_1^\circ$	355 nm	Argon	0.05
$y^5P_3^\circ$	355 nm	Argon	0.05, 0.4
$y^5P_3^\circ$	355 nm	Helium	0.25
$z^5F_4^\circ$	266 nm	Argon	1.4
$z^5F_4^\circ$	355 nm	Argon	0.29
$z^5F_4^\circ$	355 nm	Helium	1.02
$z^5D_4^\circ$	355 nm	Argon	0.3
$z^5D_4^\circ$	355 nm	Helium	0.65
$y^5H_7^\circ$	266 nm	Argon	0.17
$y^5H_7^\circ$	355 nm	Argon	0.13
$y^5H_7^\circ$	355 nm	Helium	0.11
a^5D_3	266 nm	Argon	0.71
a^5D_2	266 nm	Argon	0.77
a^5D_2	355 nm	Argon	0.63
a^3D_3	355 nm	Argon	0.05
a^5S_2	266 nm	Argon	2
a^5S_2	355 nm	Argon	1.5
a^5G_6	355 nm	Argon	0.91
a^3G_4	355 nm	Argon	0.08
e^7D_5	355 nm	Helium	3.5
e^7D_3	355 nm	Helium	3
f^7D_5	355 nm	Helium	0.25
f^7D_5	355 nm	Argon	0.25

State	Laser wavelength	Buffer gas	Ratio of $\frac{\text{Intensity at vapor pressure}}{\text{Intensity at 240 Torr}}$
f^7D_4	355 nm	Argon	0.2
f^7D_4	355 nm	Helium	0.3
Propyl-ACT			
$z^7P_4^\circ$	355 nm	Argon	1.5
$z^7P_3^\circ$	355 nm	Argon	1.5
$z^7P_2^\circ$	355 nm	Argon	1.25
$z^7F_5^\circ$	355 nm	Argon	2.85
$y^7P_4^\circ$	355 nm	Argon	0.07
$y^7P_3^\circ$	355 nm	Argon	0.06
$z^5P_3^\circ$	355 nm	Argon	0.12
$z^5P_2^\circ$	355 nm	Argon	0.13
$z^5P_1^\circ$	355 nm	Argon	0.14
Methyl-ACT			
$z^7P_4^\circ$	355 nm	Argon	1.6, 2.5
$z^7P_4^\circ$	355 nm	Helium	3
$z^7P_4^\circ$	266 nm	Argon	1.33
$z^7P_3^\circ$	355 nm	Argon	1.5
$z^7P_2^\circ$	355 nm	Argon	1.25, 1.3
$z^7F_5^\circ$	355 nm	Argon	3
$y^7P_4^\circ$	355 nm	Argon	0.07, 0.08
$y^7P_4^\circ$	355 nm	Helium	0.2
$y^7P_3^\circ$	266 nm	Argon	1.22
$y^7P_3^\circ$	355 nm	Argon	0.08
$y^7P_2^\circ$	355 nm	Argon	0.1
$z^5P_3^\circ$	266 nm	Argon	0.67
$z^5P_3^\circ$	355 nm	Argon	0.08, 0.17
$z^5P_3^\circ$	355 nm	Helium	0.12
$z^5P_2^\circ$	355 nm	Argon	0.13
$z^5P_1^\circ$	355 nm	Argon	0.09
$y^5H_7^\circ$	355 nm	Argon	0.06, 0.05
a^5D_3	266 nm	Argon	2.5
a^5D_2	266 nm	Argon	1.9
a^5D_2	355 nm	Argon	1.17
a^5S_2	266 nm	Argon	2.3
a^5S_2	355 nm	Argon	1.11
a^5G_6	355 nm	Argon	1.6
e^7D_5	355 nm	Argon	1

3.2 Figures

If your thesis has a lot of figures, L^AT_EX might behave better for you than that other word processor. One thing that may be annoying is the way it handles “floats” like

tables and figures. \LaTeX will try to find the best place to put your object based on the text around it and until you're really, truly done writing you should just leave it where it lies. There are some optional arguments to the figure and table environments to specify where you want it to appear; see the comments in the first figure.

If you need a graphic or tabular material to be part of the text, you can just put it inline. If you need it to appear in the list of figures or tables, it should be placed in the floating environment.

To get a figure from StatView, JMP, SPSS or other statistics program into a figure, you can print to pdf or save the image as a jpg or png. Precisely how you will do this depends on the program: you may need to copy-paste figures into Photoshop or other graphic program, then save in the appropriate format.

Below we have put a few examples of figures. For more help using graphics and the float environment, see our online documentation.

And this is how you add a figure with a graphic:

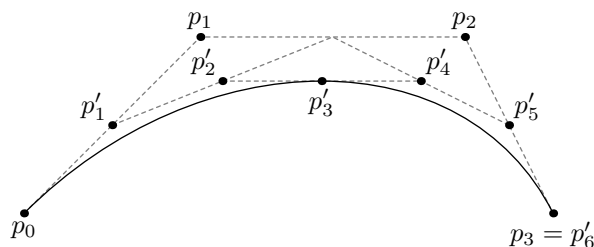


Figure 3.1: A Figure

3.3 More Figure Stuff

You can also scale and rotate figures.

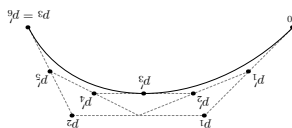


Figure 3.2: A Smaller Figure, Flipped Upside Down

3.4 Even More Figure Stuff

With some clever work you can crop a figure, which is handy if (for instance) your EPS or PDF is a little graphic on a whole sheet of paper. The viewport arguments are the lower-left and upper-right coordinates for the area you want to crop.

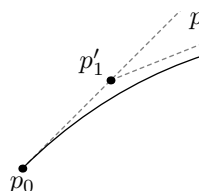


Figure 3.3: A Cropped Figure

3.4.1 Common Modifications

The following figure features the more popular changes thesis students want to their figures. This information is also on the web at web.reed.edu/cis/help/latex/graphics.html.

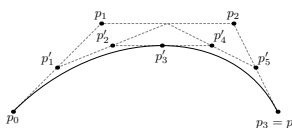


Figure 0.8: Interaction bar plot showing the degree of specialization for each flower type.

Conclusion

Here's a conclusion, demonstrating the use of all that manual incrementing and table of contents adding that has to happen if you use the starred form of the chapter command. The deal is, the chapter command in L^AT_EX does a lot of things: it increments the chapter counter, it resets the section counter to zero, it puts the name of the chapter into the table of contents and the running headers, and probably some other stuff.

So, if you remove all that stuff because you don't like it to say "Chapter 4: Conclusion", then you have to manually add all the things L^AT_EX would normally do for you. Maybe someday we'll write a new chapter macro that doesn't add "Chapter X" to the beginning of every chapter title.

4.1 More info

And here's some other random info: the first paragraph after a chapter title or section head *shouldn't be* indented, because indents are to tell the reader that you're starting a new paragraph. Since that's obvious after a chapter or section title, proper typesetting doesn't add an indent there.

Appendix A

The First Appendix

Appendix B

The Second Appendix, for Fun

References

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