Implementation of Prize-Collecting Steiner Trees in Signaling Hypergraphs

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A Thesis
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()

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I want to thank a few people.

Preface

This is an example of a thesis setup to use the reed thesis document class.

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Abstract

The preface pretty much says it all.

Dedication

You can have a dedication here if you wish.

Introduction

Cell signaling networks are comprised of numerous complex interactions between many different proteins and protein complexes, and together comprise a cell's interactome. Many of these interactions have been studied in great detail, and are illustrated by numerous manually-created images of cell signaling networks. Recently, many of these figures have been converted into graphs, in which each node represents a unique protein, and each edge represents a known pairwise interaction between two proteins. These graphs have made it possible for researchers to implement the multitude of known graph algorithms to try and find new areas of research that may yield novel or interesting results. Unfortunately, the limited ways in which graphs allow protein-protein interactions to be represented lack biological realism, and struggle to represent complex interactions such as phosphorylation, negative regulation, and the existence of protein complexes.

0.1 Traditional Representations of Cell Signaling

0.2 Graphs of Cell Signaling Networks

Chapter 1

Hypergraphs & Hyperpaths

While standard graphs are useful for many applications, they are severely limited in their ability to represent cell-signaling interactions. Since they can only show pairwise interactions between nodes, whenever there is an interaction that requires more than two connections, the visualization of the graph becomes confusing, and biologically meaningless. Furthermore, interactions involving multiple molecules require an enormous amount of different edges to represent all of the sub-interactions that take place. Determining whether two edges are part of the same biological event is a non-trivial problem, and requires manual curation to solve, at this time.

One area of cell-signaling that becomes particularly problematic in standard graphs is the formation, interaction, and destruction of protein complexes. The only way that complexes can be represented in standard graphs is by creating a complete subgraph of all of the elements of the protein complex. On their own, these complete subgraphs can yield useful information about the make-up of a protein complex, but once they begin interacting with other elements of the graph, the graph becomes much more complex, as all of the proteins in the complex must be represented independently. In the case of interactions between multiple large complexes, it becomes the case that the standard graph representation of this interaction is a large complete subgraph that contains nodes for all of the proteins involved in either complex. It is then computationally impossible to distinguish whether the entity being described by the subgraph is the interaction between multiple protein complexes, or simply one large complex that contains all of the components of both complexes. Furthermore, since the complete subgraphs which represent complexes are undirected, it is not possible *(is this the case?)* to tell what the inputs or outputs of a biochemical reaction may be.

Another shortcoming of standard graphs in representing complex biological interactions is that there is no way in which to represent positive or negative regulation of interactions. Since there is a standardized way in which edges interact with nodes, there is no way to differentiate types of interactions between nodes. This poses a challenge when there are regulators or catalysts present that are necessary for a reaction, but are not part of the inputs or outputs of the reaction. If regulators are to be included in a standard graph representation of a cell-signaling network, they become indistinguishable from any other types of interactions that are taking place.

This lack of specificity is problematic, as it treats all interactions as equal, and hides potentially useful information from the graph.

To resolve the issues presented by standard graphs, we instead use a generalization called a *hypergraph* that allows for the addition of more detail and specificity within the data structure than standard graphs allow for. In particular, hypergraphs allow for both the representation of protein complexes in the form of *hypernodes*, which we think of simply as a set of one or more nodes, and for the representation of complex, directed interactions that can have multiple inputs and outputs. We represent these interactions with the use of *hyperedges*, which define a set of one or more hypernodes. Since a hyperedge may include more than two hypernodes, we gain the ability to represent both multi-protein interactions, as well as to define the notions of regulation on reactions.

1.1 Hypergraph Definitions

Where a directed graph represents directed, pairwise interactions between only two vertices, we can use *directed hypergraph* to represent directed interactions between sets of vertices (nodes). We formally define a directed hypergraph, $\mathcal{H}$, as a pair (V, E), where V is a finite set of vertices and $E \subseteq 2^V \times 2^V$ is a finite set of *directed hyperedges* connecting members of V such that, for every $e = (T(e), H(e)) \in E$, $T(e) \cap H(e) = \emptyset$, and $T(e)$, $H(e) \neq \emptyset$. We refer to $T(e)$ as the *tail* of the hyperedge, and to $H(e)$ as the *head* of the hyperedge.

Furthermore, we can define sets of two or more nodes as a hypernode, which are members of the power set of V. These can be incorporated into a directed hypergraph to form a *complexed directed hypergraph*. We define a *complexed directed hypergraph*, $\mathcal{H}$, as the triple (V, U, E) in which V is a finite set of vertices, $U \subseteq 2^V$ is a finite set of hypernodes, and $E \subseteq 2^U \times 2^U$ is a finite set of hyperedges such that, for every $e = (T(e), H(e)) \in E$, $T(e) \cap H(e) = \emptyset$ and $T(e)$, $H(e) \neq \emptyset$.

It is important to note that a standard directed graph is a special case of a directed hypergraph. This is the case if every hypernode in the graph contains only one element, and if each edge has exactly one head element, and one tail element. This has two important implications for algorithms that run on directed hypergraphs. First, this means that there is no loss in functionality caused by using a hypergraph representation of a cell network, since anything that could be computed on a standard directed graph can be recreated exactly using the special case of the hypergraph. Secondly, this is important, because it means that anything that can be computed on a standard graph will be at least as computationally difficult to compute when generalized to a hypergraph. In fact, we find that many tasks that are computationally easy on standard graphs become very difficult when generalized to hypergraphs *(cite Anna's paper on K shortest hyperpaths).*

1.2 Hyperpath Definitions

In order to find the shortest route between two vertices, in a directed hypergraph, we define the notion of a *hyperpath*, P, on the directed hypergraph $\mathcal{H}$. We think of P as the list of vertices and hyperedges that one must pass through in order to traverse through the directed hypergraph from vertex s to get to t.

1.2.1 Finding Hyperpaths

1.2.2 Hyperpath Algorithms

1.3 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.

1.3.1 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.

1.3.2 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

1.3.3 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.

1.4 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`), *bibtexstyles* (about how to find and use the bibliography style that best suits your needs, at `/latex/bibtexstyles.html`) and *bibman* (which covers how to make and maintain a bibliography by hand, without BibTeX, at at `/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.

1.4.1 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.

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 citation[3] option. The best way to do this is to use the phdthesis type of citation, and use the optional "type" field to enter "Reed

[1] footnote text
[2] Reed College (2007)
[3] Noble (2002)

thesis" or "Undergraduate thesis". Here's a test of Chicago, showing the second cite in a row[4] being different. Also the second time not in a row[5] should be different. Of course in other styles they'll all look the same.

1.5 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 LaTeX for their theses, and are happy to help.

[4]Noble (2002)
[5]Reed College (2007)

Chapter 2

Mathematics and Science

2.1 Math

TEX is the best way to typeset mathematics. Donald Knuth designed TEX 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.)

$$\sum_{j=1}^{n}(\delta\theta_j)^2 \leq \frac{\beta_i^2}{\delta_i^2+\rho_i^2}\left[2\rho_i^2+\frac{\delta_i^2\beta_i^2}{\delta_i^2+\rho_i^2}\right] \equiv \omega_i^2$$

From Informational Dynamics, we have the following (Dave Braden):
After n such encounters the posterior density for θ is

$$\pi(\theta|X_1 < y_1, \ldots, X_n < y_n) \propto \pi(\theta)\prod_{i=1}^{n}\int_{-\infty}^{y_i}\exp\left(-\frac{(x-\theta)^2}{2\sigma^2}\right)\,dx$$

Another equation:

$$\det\begin{vmatrix} c_0 & c_1 & c_2 & \cdots & c_n \\ c_1 & c_2 & c_3 & \cdots & c_{n+1} \\ c_2 & c_3 & c_4 & \cdots & c_{n+2} \\ \vdots & \vdots & \vdots & & \vdots \\ c_n & c_{n+1} & c_{n+2} & \cdots & c_{2n} \end{vmatrix} > 0$$

Lapidus and Pindar, Numerical Solution of Partial Differential Equations in Science and Engineering. Page 54

$$\int_t\left\{\sum_{j=1}^{3}T_j\left(\frac{d\phi_j}{dt}+k\phi_j\right)-kT_e\right\}w_i(t)\,dt=0, \qquad i=1,2,3.$$

L&P Galerkin method weighting functions. Page 55

$$\sum_{j=1}^{3} T_j \int_0^1 \left\{ \frac{d\phi_j}{dt} + k\phi_j \right\} \phi_i \; dt = \int_0^1 k\, T_e \phi_i dt, \qquad i = 1, 2, 3$$

Another L&P (p145)

$$\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} f(\xi,\eta,\zeta) = \sum_{k=1}^{n}\sum_{j=1}^{n}\sum_{i=1}^{n} w_i w_j w_k f(\xi,\eta,\zeta).$$

Another L&P (p126)

$$\int_{A_e} (\,\cdot\,) dx dy = \int_{-1}^{1}\int_{-1}^{1} (\,\cdot\,) \det[J] d\xi d\eta.$$

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, $Fe_2^{2+}Cr_2O_4$ is written `$\mathrm{Fe_2^{2+}Cr_2O_4}$`
Exponent or Superscript: O^-
Subscript: CH_4

To stack numbers or letters as in Fe_2^{2+}, the subscript is defined first, and then the superscript is defined.
Angstrom: Å
Bullet: $CuCl \bullet 7H_2O$
Double Dagger: ‡
Delta: Δ
Reaction Arrows: $\longrightarrow$ or $\xrightarrow{solution}$
Resonance Arrows: $\leftrightarrow$
Reversible Reaction Arrows: $\rightleftharpoons$ or $\xrightleftharpoons{solution}$ (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:

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

Figure 2.1: Combustion of glucose

2.2.2 Other examples of reactions

$NH_4Cl_{(s)} \rightleftharpoons NH_{3(g)} + HCl_{(g)}$
$MeCH_2Br + Mg \xrightarrow[below]{above} MeCH_2 \bullet Mg \bullet Br$

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 LaTeX 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 1.3.2.

2.4 Biology

You will probably find the resources at `http://www.lecb.ncifcrf.gov/~toms/latex.html` helpful, particularly the links to bsts 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 bsts 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, LaTeX 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:

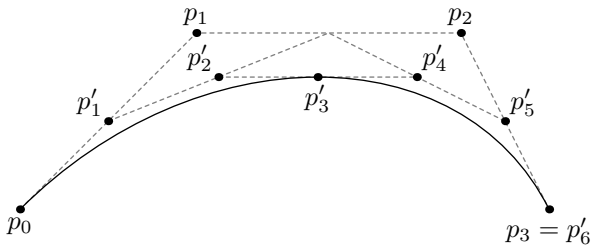

Figure 3.1: A Figure

3.3 More Figure Stuff

You can also scale and rotate figures.

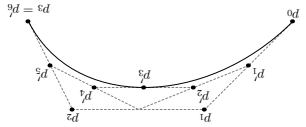

Figure 3.2: A Smaller Figure, Flipped Upside Down

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.

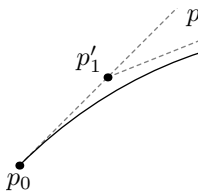

Figure 3.3: A Cropped Figure

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`.

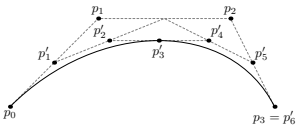

Figure 0.8: Interaction bar plot showing the degree of specialization for each flower type.

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 LaTeX 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 LaTeX 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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