

HemI Manual

Heatmap Illustrator

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Contact: Dr. Yu Xue, <u>xueyu@hust.edu.cn</u>; Wankun Deng, dengwankun@hust.edu.cn The CUCKOO Workgroup The latest version of HemI is available from <u>http://hemi.biocuckoo.org/down.php</u> Copyright © The CUCKOO Workgroup.

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Statement

1. **Implementation**. The softwares of the CUCKOO Workgroup are implemented in JAVA (J2SE). Usually, both of online service and local stand-alone packages will be provided.

2. **Availability**. Our softwares are freely available for academic researches. For non-profit users, you can copy, distribute and use the softwares for your scientific studies. Our softwares are not free for commercial usage.

3. **GPS**. Previously, we used the GPS to denote our Group-based Phosphorylation Scoring algorithm. Currently, we are developing an integrated computational platform for post-translational modifications (PTMs) of proteins. We re-denote the GPS as Group-based Prediction Systems. This software is an indispensable part of GPS.

4. **Usage**. Our softwares are designed in an easy-to-use manner. Also, we invite you to read the manual before using the softwares.

5. **Updation**. Our softwares will be updated routinely based on users' suggestions and advices. Thus, your feedback is greatly important for our future updation. Please do not hesitate to contact with us if you have any concerns.

6. **Citation**. Usually, the latest published articles will be shown on the software websites. We wish you could cite the article if the software has been helpful for your work.

7. **Acknowledgements**. The work of CUCKOO Workgroup is supported by grants from Chinese 973 project (2002CB713700, 2006CBOF0503, and 2006CB933300), Chinese Academy of Sciences (KSCX1-YW-R65, KSCX2-YW-21, and KJCX2-YW-M02), Chinese Natural Science Foundation (39925018, 30270293, 90508002, 30700138) and National Institutes of Health (DK56292).

Introduction

File Option Help		
Canvas		High
Pulling Pullin		Customized Default
		DEMO
		REFRESH
Carvas (Pixel) Space (Pixel) Note Clustering Width 5000 Left 200 Top 20 X- Axis Top V Font Column	Rotate X- Axis (*) 90 🌧 Graph (*) 0 💌	

Figure 1, HemI 1.0 User Interface

Download & Installation

The HemmI 1.0 was implemented in JAVA (J2SE) and SWT was used to implement the user interface, and could support three major Operating Systems (OS), including Windows, Linux/Unix or Mac OS X systems. Local stand-alone packages is available from: <u>http://hemi.biocuckoo.org/down.php</u>. We recommend that users could download the latest release.

Please choose the proper package to download. After downloading, please double-click on the software package to begin installation, following the user prompts through the installation. And snapshots of the setup program under windows 7 are shown below:



Figure 2



Figure 3

🚳 Setup - Heml 1.0_alpha_win32_x86 📃 💷 📧
Select Start Menu Folder Where should Setup place the program's shortcuts?
Select the Start Menu folder in which you would like Setup to create the program's shortcuts, then click Next.
HemI
360 皂污樹窠 ^ 7-Zip
Accessories Acronis Administrative Tools
Adobe Client-end Software of ICBC Internet Backing
✓ Create shortcuts for all users
Don't create a Start Menu folder
install4j
< Back Next > Cancel





Figure 5



Figure 6

Finally, please click on the **Finish** button to complete the setup program.

Usage of HemI

1. A fast guide for using Heml

Before we start:



Figure 7

A: notes of column

B: notes of row

C: cluster of row

D: cluster of column

E: bar

F: canvas size (pixel)

G: height of A (Top)/D (Bottom) and width of B (Left)/C (Right), (pixel)

H: note setting, include position and font.

I: whether you want column or row cluster

J: rotate setting, X-axis: rotate angel of words of notes of columns (A), Y-axis: rotate angel of words of rows of notes of rows (B), Graph: angel of this graph (transform X axis to Y axis e.g.).

K: colors of this heatmap

L: commands, whatever change you made, it will take effect after you click "UPDATE".

(1) Firstly, please hit button "LOAD" to select a data file to load to HemI, 4 kinds of file are supported: Microsoft Excel workbook (97-2003,*.xls), comma split file (*.csv), tab split file (*.txt, this file format is not recommended) and HemI project file (*.xml). In these four kinds of file, HemI project contains all information needed to draw a heatmap and will draw a heatmap after loaded, this kind of file can be generated by HemI. Usually, users do not have a project file. We use an Excel workbook file as an example.

Hemill.0 - Heatmap Illustrator File Option Help	
	Color
Search Example	High
Organize ▼ New folder III @	
Documents Name Date modified Type	
Findarce Findarce	
■ Videos Nomegroup ■ Computer ■ Vin64 (C:) ■ Ubuntu64 (D:) ■ PROGRAMS (E:) ■ DATA (F:) ● BD-ROM Drive (■ DOWNLOAD (E:) ■ Compute (■ DOWNLOAD (E:)	Low Customized Default Command
File name: Example.xls	DEMO
Canvas (Pixel) Note Clustering Rotate	REFRESH
Width 1600 Left 120 Top 120 X- Axis Top Font Image: Column Action X- Axis (*) 90 # Graph (*) 0 Image: Column Action Y- Axis (*) 90 # Graph (*) 0 Image: Column Action Y- Axis Image: Column Action Y- Axis (*) 0 Image: Column Action	CANCEL

Figure 8

(2) After selected Excel workbook, you need to choose a sheet as data source from list, in this example, we select "sheet 1", then click "OK".

Hemil1.0 - Heatmap Illustrator	
Carvas	Color High LOW Customized Default Command DEMO LOAD
Carvas (Pixel) Space (Pixel) Note Clustering Rotate Width 1600 Left 120 Top 120 Y- Axis Top • Font Image: Column value X- Axis (*) 90 m/s Graph (*) 0 Image: Column value Height 1200 Right 120 Bottom 120 Y- Axis Left • Font Image: Column value Y- Axis (*) 0 Image: Column value	CANCEL

Figure 9

(3) Then data loader popped out, in this dialog follow "Tip" above to select data which need to present in your heatmap, or click "Auto select" to let the program decide for you.



Figure 10

(5) Hit button "Finish", and right click on canvas and select "Export Image" or choose "File"-"Export Image" to export image in certain format and resolution.



Figure 11

If you choose 72dpi, export format can be JPEG, PNG and TIFF, if you choose 300dpi or 600dpi, file format can only be TIFF.

2. More feature of Heml

1. Pop-out menu of canvas



Figure 12

A:

Export Image: To export image to certain destination, resolution and format.

View data: View data used to draw this heatmap.

Export data: Export data used to draw this heatmap to Excel file, Comma-split file or text file.

B:

1. Set up bar: define your own style bar (Figure 7, E)

	Note	Bar						
P	osition F	Right 👻	Length (Pix.)	400	Width (Pix) 40	Note width (Pix	.) <mark>60</mark>
🔲 Gra	idient bar							
Bar if	tem num	ber <mark>5</mark>	Deci	mal places	2 N	lin	Step	Auto fill
	Value 1		Value	2		'alue 3		
	Value 4		Value	5				
	tem num	ber 15	Deci	mal places	0			
	Value 1	0	Sele	ct	Value 2	1	Select	
	Value 1 Value 3	0 2	Sele Sele		Value 2 Value 4	1 3	Select	
				ct				
	Value 3	2	Sele	ct ct	Value 4	3	Select	
	Value 3 Value 5	2	Sele	ct ct ct	Value 4 Value 6	3 5 7	Select	
	Value 3 Value 5 Value 7 Value 9 Value 11	2 4 6 8 10	Sele	d d d d d	Value 4 Value 6 Value 8 Value 10 Value 12	3 5 7 9 11	Select Select Select	
	Value 3 Value 5 Value 7 Value 9 Value 11 Value 13	2 4 6 8 10 12	Sele Sele Sele	ct c	Value 4 Value 6 Value 8 Value 10	3 5 7 9 11	Select Select Select Select	
	Value 3 Value 5 Value 7 Value 9 Value 11	2 4 6 8 10 12	Sele Sele Sele Sele Sele	ct c	Value 4 Value 6 Value 8 Value 10 Value 12	3 5 7 9 11	Select Select Select Select Select	

Figure 13

1) Position: position of bar, it can be left, right, top and bottom.

Length: length of bar (pixel, length in y-axis when position=left or right, and length in x-axis when position=top or bottom).

- 2) Width: width of bar (pixel).
- 3) Bar note width: width of note of bar.
- 4) Gradient bar: set bar to gradient, color of each value of your data will be scaled to a specific interval on number line, and color for this value will be determined according its value and color you selected for this map. Below is an example of gradient bar.



Figure 14

5) Discrete bar: In this mode, you can define color for a serial of number, these number must goes from small to large, and set color for each number, color of values in your data set will be color of largest value in values smaller than it in this number serial, below is an example of discrete bar.



Figure 15

2. Set up note: define color of note of x-axis and y-axis. (Figure 7, A, B)

🚳 Option				-	
Statistics Note	Bar				
Row notes					Â
	Row 1	Select	Row 2	Select	
	Row 3	Select	Row 4	Select	
	Row 5	Select	Row 6	Select	
	Row 7	Select	Row 8	Select	
	Row 9	Select	Row 10	Select	
	Row 11	Select	Row 12	Select	=
	Row 13	Select	Row 14	Select	
	Row 15	Select	Row 16	Select	
	Row 17	Select	Row 18	Select	
	Row 19	Select	Row 20	Select	
	Row 21	Select	Row 22	Select	
	Row 23	Select	Row 24	Select	
	Row 25	Select	Row 26	Select	
	Row 27	Select	Row 28	Select	
	Row 29	Select	Row 30	Select	
	Row 31	Select			
Colum notes					
	Colum 1	Select	Colum 2	Select	Ŧ
	(Cancel		ок	

Figure 16

3. Set up statistic: set up some statistic properties of heatmap.

@ Option	- • •
Statistics Note Bar	
Normalization	Logarithmic Base 2 -
Cluster	
Distance between sets	
Euclidean distance (default)	Pearson distance
$ a - b _2 = \sqrt{\sum_i (a_i - b_i)^2}$	$1 \cdot \frac{n \sum x_i y_i - \sum x_i \sum y_i}{\sqrt{n \sum x_i^2 - (\sum x_i)^2} \sqrt{n \sum y_i^2 - (\sum y_i)^2}} \equiv$
Squared euclidean distance	🗐 Spearman distance
$ a - b _2^2 = \sum_i (a_i - b_i)^2$	$1 - \frac{6\sum d_i^2}{n(n^2 - 1)}.$
🕅 Manhattan distance	🕅 Kendall's tau distance
$\ a-b\ _1 = \sum_i a_i - b_i $	$1 - \frac{number \ of \ discordant \ pairs}{n \times (n-1)}$
Maximum distance	
$ a - b _{\infty} = \max_{i} a_i - b_i $	
Distance between clusters	
Cancel	ок

Figure 17

 Normalization: Usually, you should select Liner, but if range of your data is very large, for example, read number of NGS result, you should choose Logarithmic, base of log can be chose or define it yourself.

- 4. Cluster: If you need to do hierarchical clustering analysis to your data, you should select a strategy to calculate distance between two data sets. We use an two step strategy to calculate this distance: First, calculate distance of correspond data in two data set, second calculate distance between two cluster, Figure 18 shows how we calculate distance when distance between sets= "Euclidean Distance" and distance between clusters= "Average Linkage Clustering".
 - Distance calculation
 - Distance between set a and set b:

$$d_{ab} = \frac{\sum |ai-bi|}{i}$$

 Distance between two cluster m and n (sets number in m is e and in n is f):



Figure 18

- 5. Set up empty color: If your data set contains empty values, you need to assign a color for them, default color is black.
- 6. Set up line size: if you want to customize line size of hierarchical clustering, select it.

C.

1. Add frame around each data unit: add a white frame around every cell. Figure 19 is a comparison of this effect, (left, not added; right, added)





2. About this picture: Some information about this picture: title, journal and date of paper which using this map, it can be null.

2. Menu

A:

File:

File Opti	on He	lp	
Load		Ctrl+L	
Save		Ctrl+S	
Save	as	Ctrl+Shift+S	
Expo	t Image	Ctrl+E	
Exit		Alt+F4	

Figure 20

- 1. Load: load HemI project file or Excel/CSV/TEXT file.
- 2. Save: save current project.
- 3. Save as: save current project to another file.
- 4. Export Image: export current heatmap to local file.
- 5. Exit: exit HemI

Option:



Figure 21

- 1. Statistic: same as "set up statistic" in pop-out menu.
- 2. Note: same as "set up note" in pop-out menu.
- 3. Bar: same as "set up bar" in pop-out menu.

Help:

File Option	Help
Canvas	Acknowledgement
	Citation
	Contact Us
	Check for Update
	About

Figure 22

- 1. Acknowledgement: Acknowledgement of help from other group for products of THE CUCKOO WORKGROUP.
- 2. Citation: If you used HemI for your publications, please cite this paper.
- 3. Contact Us: If you have any suggestion or problem, please contact us.
- 4. Check for Update: check if there is any updating of HemI.
- 5. About: Other tools of THE CUCKOO WORKGROUP and their link.