

Thorin Tabor
JupyterCon 2017

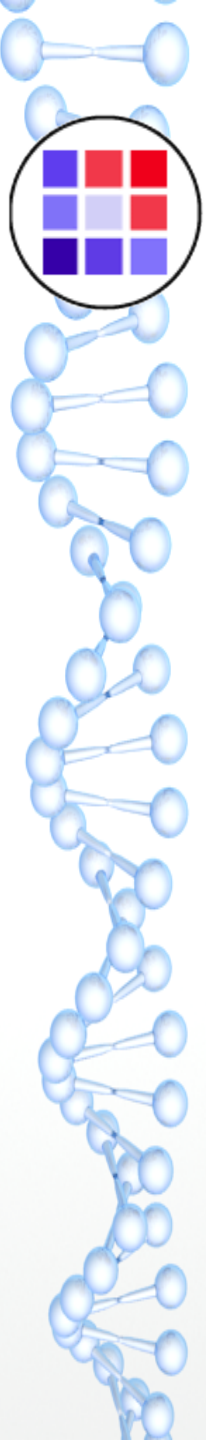


GenePattern Notebooks

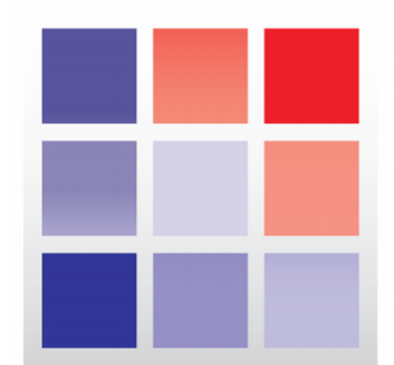
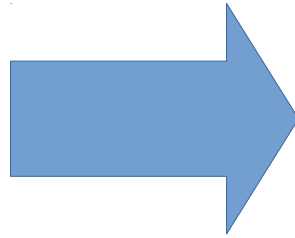
Jupyter for Integrative Genomics

UC San Diego

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INSTITUTE



From Jupyter to GenePattern





GenePattern Notebook

The screenshot displays the GenePattern Notebook interface. At the top, the title bar reads "GenePattern Notebook Demo Notebook" with a "Last Checkpoint: 06/09/2017 (autosaved)" and a "Control Panel" button. The user is logged in as "GenePatternUser". Below the title bar is a menu bar with options: File, Edit, View, Insert, Cell, Kernel, Widgets, Help. A "Trusted" status indicator and "Python 3.6" version are also visible. The main workspace contains a code cell with the following content:

```
In [11]: genepattern_job.get_file('parikshak2013.gene.sets.symbols.gmt.cvt.txt')
```

The output of the cell is:

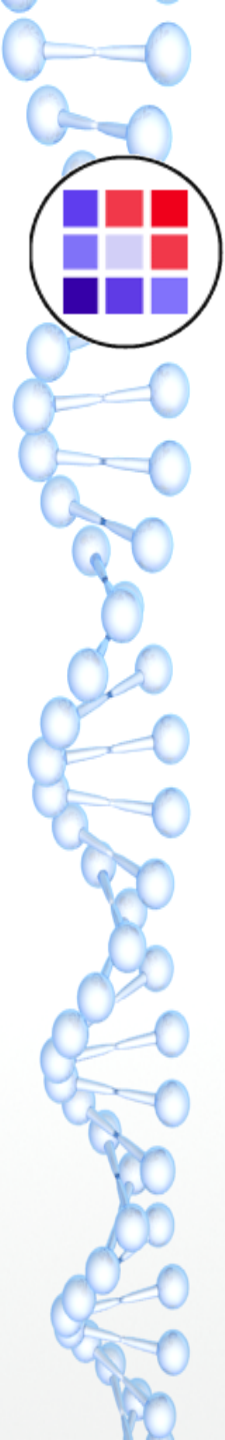
```
Out[11]: <gp.core.GPFile at 0x7f9edc54f6a0>
```

Below the code cell is a widget titled "GenePattern FastQC". The widget description is "Provides quality control metrics on raw sequence data". It includes a "Run" button and a section for "input file*" with an "Upload File..." button, an "Add Upstream File or URL..." input field, and a "Drag Files Here" area. A note states: "2GB file upload limit using the Upload File... button." Below the input area, it specifies: "RNA-seq reads file in FASTQ (bz2 and gz compressed files are supported), SAM, or BAM format."



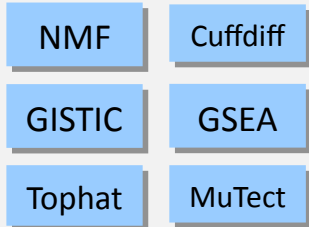
Two Open Source Projects





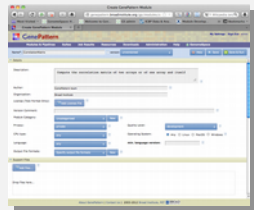
What is GenePattern?

Module Repository



Hundreds of analyses and visualizations

Module Integrator



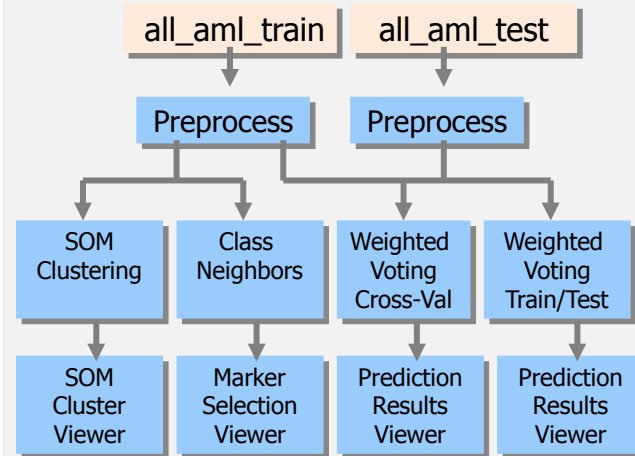
Easy addition of new tools

Community Repository

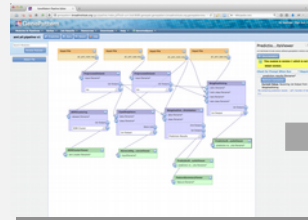



User-contributed modules

Pipeline Environment



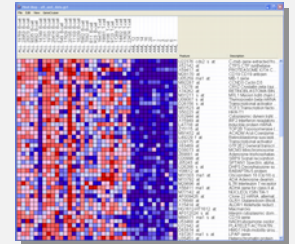
Golub and Slonim et. al 1999



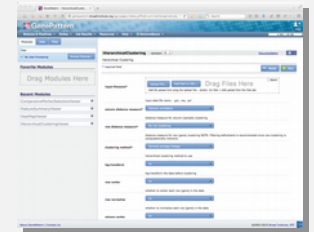
 Golub, Slonim, 1999, Nature, all_aml_pipeline.zip

Support for *in silico* reproducible research

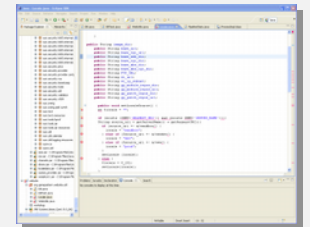
Clients



Visualizer

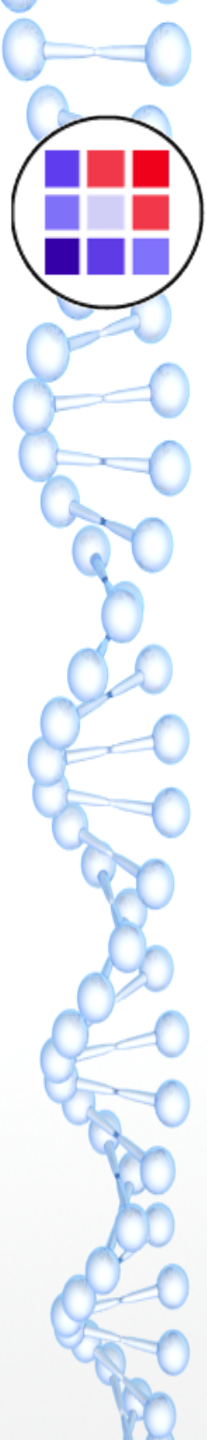


Web



Programming

Access for all levels of user



Platform for Reproducible Bioinformatic Research

- First public release in 2004 (similar footing to IPython)
- Open Source
- ~50,000 registered users
- Public server runs ~4,000 analyses per week
- Community-contributed methods
 - CRISPR analysis
 - Bisulfite sequencing
 - Flow cytometry
 - RNAi screens



genepattern.org



genepattern.broadinstitute.org



gparc.org



Analysis Tool Repository

Copy Number
Divide
by Normals

GSEA

Variation
Filter

Cuffdiff

GISTIC

CBS

k-Nearest
Neighbors

MutSigCV

Classification
and
Regression Trees

Support
Vector
Machines

Hierarchical
Clustering

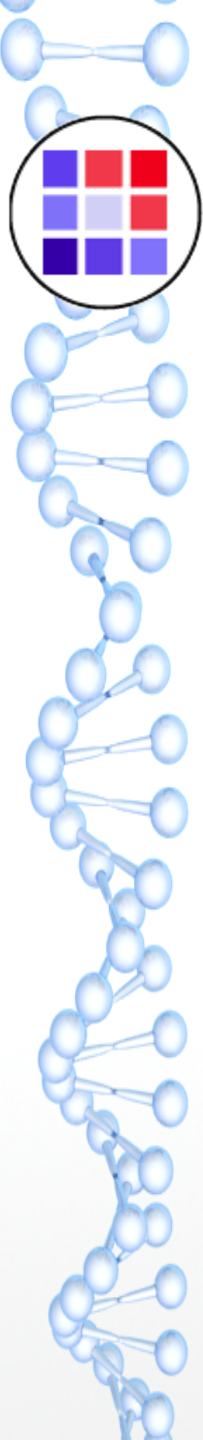
Picard Sort Sam

TopHat

Expression
File
Creator

Metagene
Projection

RNASEQC



Custom Modules & Pipelines

Modules

Hierarchical Clustering

Files

HCL.jar
cluster.sh
ant.jar
gp-modules.jar
Jama-1.0.2.jar

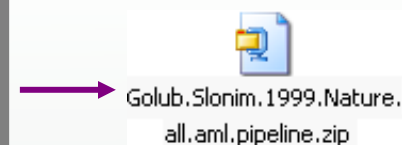
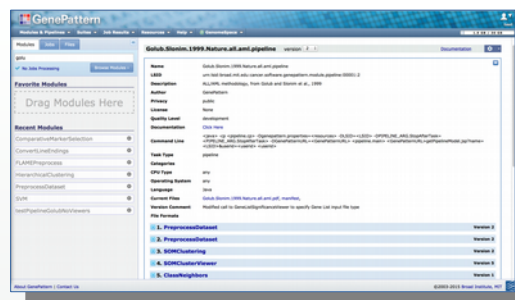
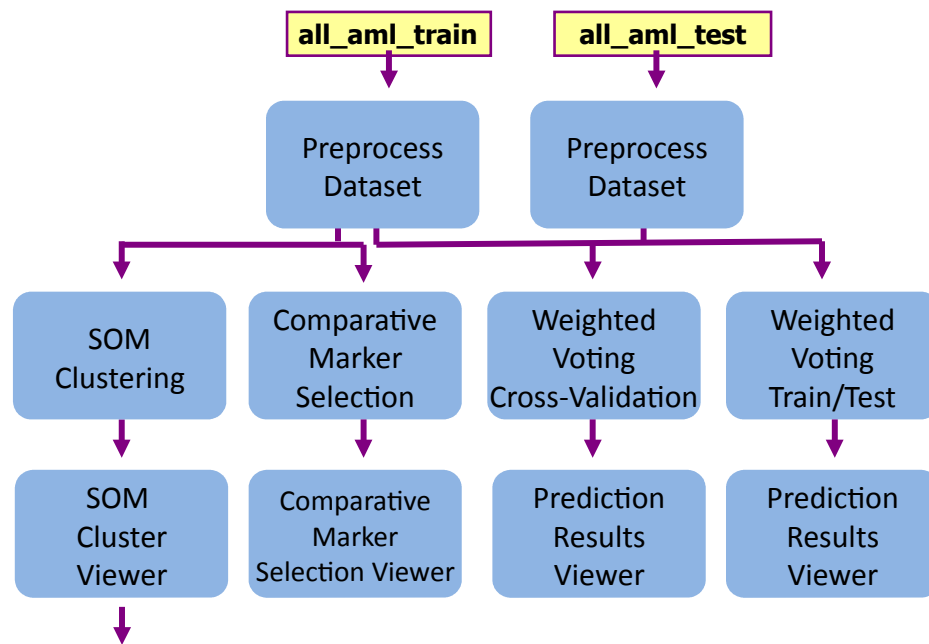
Documentation

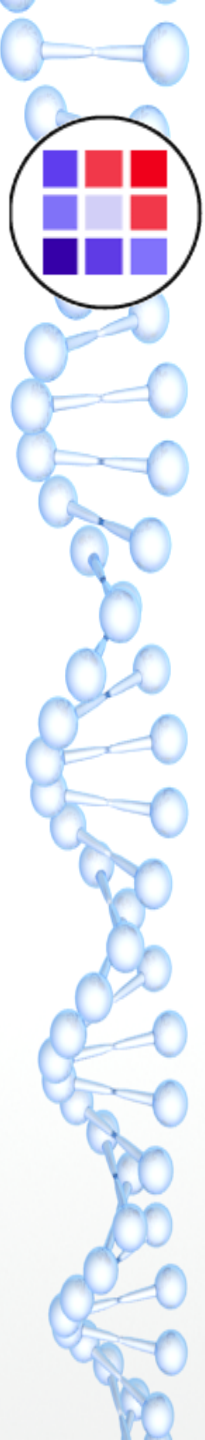
HierarchicalClustering.pdf

Parameter descriptions

-f <input.filename>
<log.transform>
<row.center>
<row.normalize>
<column.center>
<column.normalize>
-u <output.base.name>
-e <column.distance.measure>
-g <row.distance.measure>
-m <clustering.method>

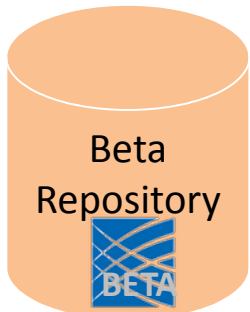
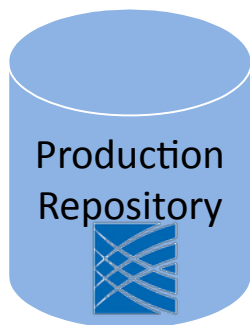
Pipelines



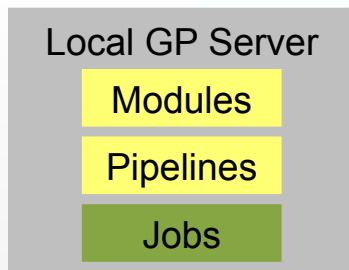
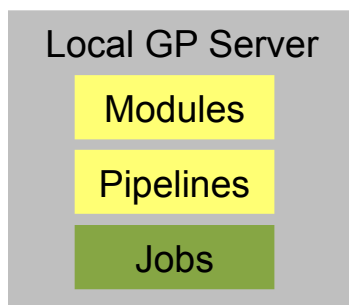
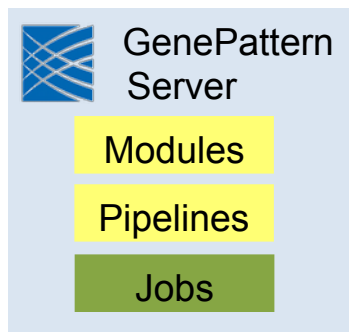


Web Server Architecture

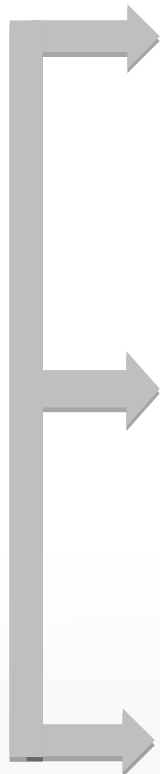
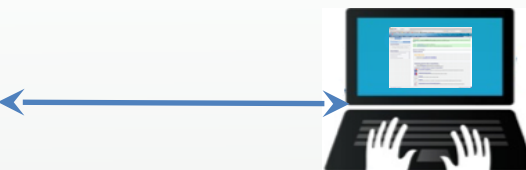
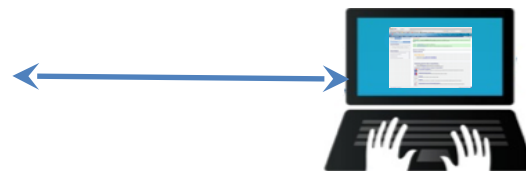
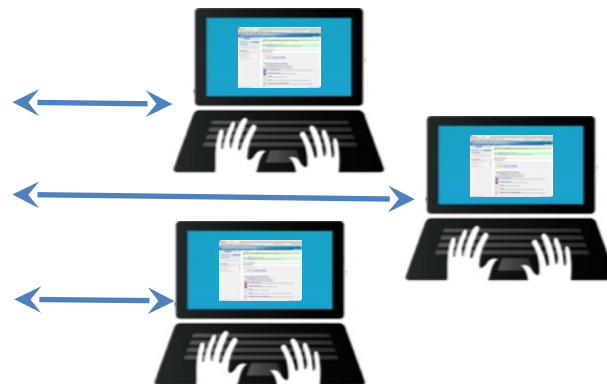
Repositories



Servers



GenePattern Users



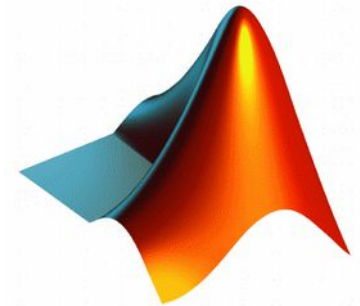


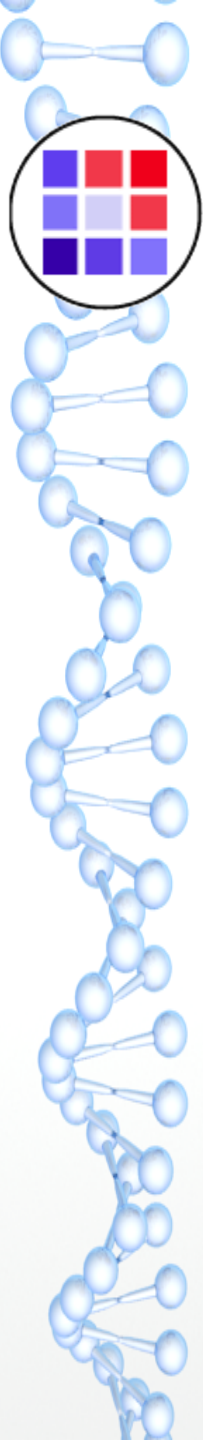
Programmatic APIs

- Libraries for Python, R, MATLAB & Java
- REST API
- Used to back portals and other web applications



REST API





User-Friendly Interface

- Permits complex analyses without the need for a coding background

GenePattern

Modules & Pipelines ▾ Suites ▾ Job Results ▾ Resources ▾ Help ▾ GenomeSpace ▾ 1.9 GB / 30 GB test

Modules Jobs Files

Search Modules & Pipelines

✓ No Jobs Processing Browse Modules >

Favorite Modules

Drag Modules Here

Recent Modules

- ComparativeMarkerSelection ⚙
- ConvertLineEndings ⚙
- FLAMEPreprocess ⚙
- HierarchicalClustering ⚙
- PreprocessDataset ⚙
- SVM ⚙
- testPipelineGolubNoViewers ⚙

Welcome to GenePattern

Getting Started






New! Web tours

- Click here for a tour of **what's new in GenePattern**.
- Click here for an **introductory tour of GenePattern**.

Analyzing genomic data in GenePattern

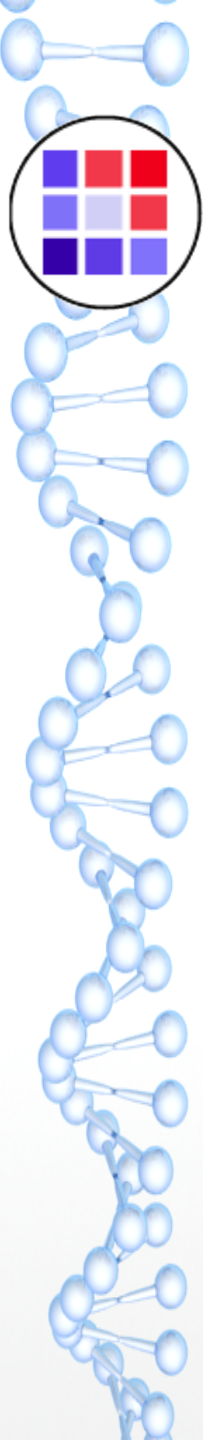
- Select a **protocol** below for a step by step guide to run an analysis.
- Click here for a **Quick Start** tutorial on how to run any module in GenePattern.

Protocols for running common analyses in GenePattern:

-  **Run an Analysis in GenePattern**
Learn how to run an analysis in GenePattern by preprocessing gene expression data and visualizing the resulting data as a heat map.
-  **Differential Expression Analysis**
Find genes that are significantly differentially expressed between classes of samples.
-  **Clustering**
Group genes and/or samples by similar expression profiles.
-  **Prediction**
Create a model, also referred to as a classifier or class predictor, that correctly classifies unlabeled samples into known classes.
-  **SNP Copy Number and Loss of Heterozygosity Estimation**

About GenePattern | Contact Us

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GenePattern Notebook Jupyter Extensions

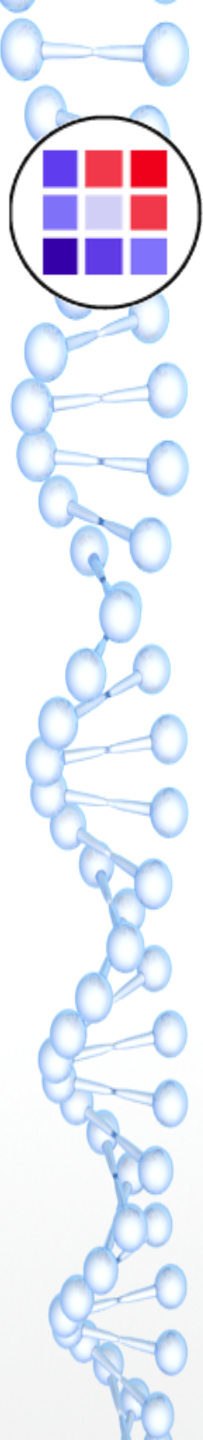
The screenshot displays the GenePattern Notebook interface. At the top, the title bar reads "GenePattern Notebook Demo Notebook" with a "Last Checkpoint: 06/09/2017 (autosaved)" and a "Control Panel" button. The user is logged in as "GenePatternUser". The menu bar includes "File", "Edit", "View", "Insert", "Cell", "Kernel", "Widgets", and "Help". The status bar shows "Trusted" and "Python 3.6".

The main workspace contains a Jupyter Notebook cell with the following code and output:

```
In [11]: genepattern_job.get_file('parikshak2013.gene.sets.symbols.gmt.cvt.txt')
```

```
Out[11]: <gp.core.GPFile at 0x7f9edc54f6a0>
```

Below the code cell is a "GenePattern FastQC" widget. It provides quality control metrics on raw sequence data. The widget includes a "Run" button and a form for inputting a file. The form has a label "input file*" and a "Required Field" indicator. The input area contains an "Upload File..." button, an "Add Upstream File or URL..." field, and a "Drag Files Here" area. A note below the input area states: "2GB file upload limit using the Upload File... button." At the bottom of the widget, it specifies: "RNA-seq reads file in FASTQ (bz2 and gz compressed files are supported), SAM, or BAM format."



Complete Research Narrative

- Leverage the best of Jupyter and GenePattern
- Interleave text, visualizations, graphics and analytical aspects





SVM Example #1

```
jupyter SVM Analysis Last Checkpoint: 18 minutes ago (unsaved changes) Python 3 O
File Edit View Insert Cell Kernel Widgets Help Trusted Python 3 O
In [ ]: %matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
from sklearn import svm

In [ ]: # Load the training data
train_data = None
with open('/home/thorin/datasets/all_aml_train.gct', 'r') as td:
    raw_txt = td.read()
    train_data = np.genfromtxt(fname=raw_txt, delimiter='\t', dtype=None, comments=None)

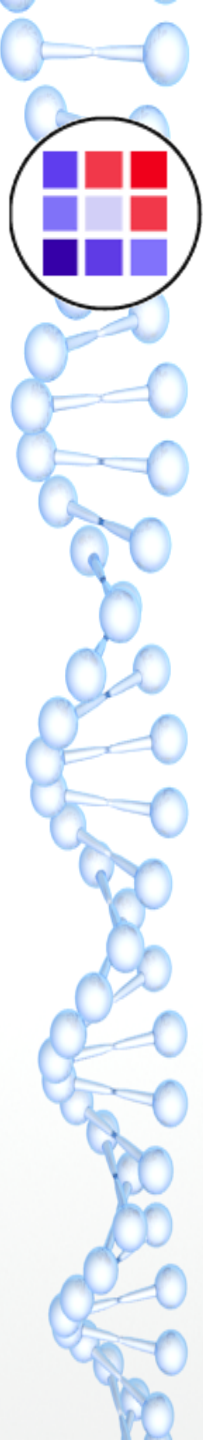
In [ ]: # Load the training classes
train_classes = None
with open('/home/thorin/datasets/all_aml_train.cls', 'r') as tc:
    raw_txt = tc.read()
    train_classes = np.genfromtxt(fname=raw_txt, delimiter=' ', dtype=None, comments=None)

In [ ]: # Slice the data for SVM fitting
X = train_data.data[:, :2]
y = train_classes

In [ ]: # Create an instance of SVM and fit out data. Do not scale the data.
C = 1.0 # SVM regularization parameter
svc = svm.SVC(kernel='linear', C=1, gamma='auto').fit(X, y)

In [ ]: # Create a mesh to plot in
x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1
h = (x_max - x_min) / 100
xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                    np.arange(y_min, y_max, h))

In [ ]: plt.subplot(1, 1, 1)
```



SVM Example #2

GenePattern Notebook SVM Last Checkpoint: 19 hours ago (autosaved) Control Panel Logout tabor@broadinstitute.org

File Edit View Insert Cell Kernel Widgets Help Trusted | Python 3.6

Code Tools

GenePattern SVM Version 4

Classify samples using SVM Run

* Required Field

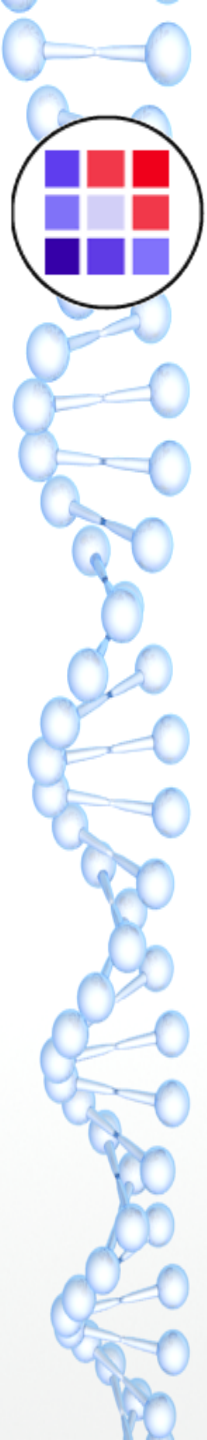
train data filename Drag Files Here
2GB file upload limit using the Upload File... button.
The training data file - .gct, .res

train cls filename Drag Files Here
2GB file upload limit using the Upload File... button.
The training class file - .cls

test data filename Drag Files Here
2GB file upload limit using the Upload File... button.
The test data file - .gct, .res

pred results output
The name of the output file for prediction results

model output file



GenePattern Cells

Auth
Cell

GenePattern Login

GenePattern Server
Broad Institute

GenePattern Username
Username

GenePattern Password
Password

Log into GenePattern Register an Account

Analysis
Cell

GenePattern ConvertLineEndings Version 2

Converts line endings to the host operating system's format.

* Required Field Run

input.filename* Upload File... Add Path or URL... Drag Files Here
2GB file upload limit using the Upload File... button.

The input file (any non-binary file format)

output.file* <input.filename_basename>.cvt.<input.filename_extension>

The output file

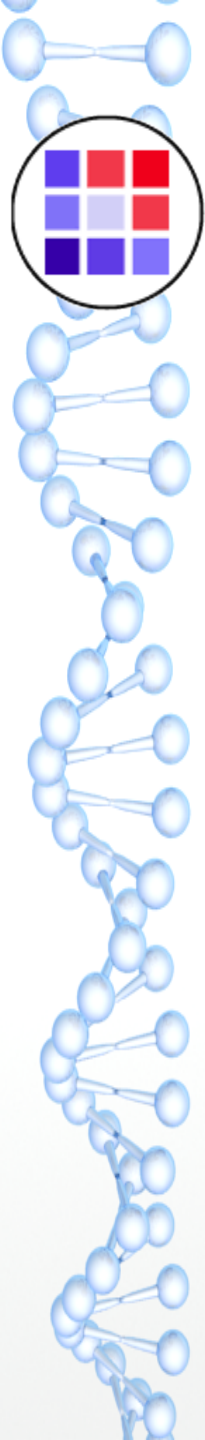
* Required Field Run

Job
Cell

GenePattern 1251770. ConvertLineEndings

Submitted by labor on 2016-03-03T12:09:39-05:00
test.cvt.txt
gp_execution_log.txt

Completed



Authentication Cells

GenePattern *Login*

GenePattern Server
Broad Institute

GenePattern Username
Username

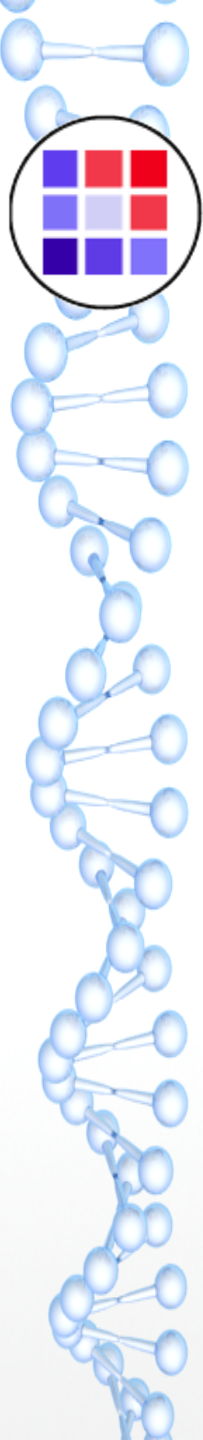
GenePattern Password
Password

[Log into GenePattern](#) [Register an Account](#)

GenePattern *tab* <http://genepattern.broadinstitute.org/gp>

-- Sun 5:00 pm -- Update: The job queue is back online and accepting new jobs. For best results you should cancel any jobs which you had started before today at 5:00 pm. We can not make any guarantees about results obtained for jobs that had not yet completed before the start of the maintenace window. Thanks,The GenePattern Team -- Sat 5:00 pm -- Update: The job queue is not yet ready to accept new jobs. Please refrain from starting new jobs until further notice. We expect it to be ready during the day Sunday.Thanks,The GenePattern Team Important message: The GenePattern Server will go offline for quarterly maintenance just before 8:00 am, Saturday March 5. We expect the maintenance to last the majority of the day.Thanks,The GenePattern Team -- March 7 -- New Blog Post: Older Java Applet Visualizers Blocked by Default in Updated FirefoxOlder Java Applet visualizers are no longer supported in Chrome. Please read our blog post for more information.

Experiencing a bug? Have thoughts on how to make GenePattern Notebook better? Let us know by leaving feedback. [Leave Feedback](#)



Analysis Cells

GenePattern ExtractComparativeMarkerResults Version 4 ? - >

Creates a derived dataset and feature list file from the results of ComparativeMarkerSelection

* Required Field Run

comparative.marker.filename* **Drag Files Here**
2GB file upload limit using the Upload File... button.

The results from ComparativeMarkerSelection - .odf

dataset.filename* **Drag Files Here**
2GB file upload limit using the Upload File... button.

The dataset file used to select markers - .gct, .res, Dataset

statistic ▼
The statistic to filter features on

min ▲▼
Select features with statistic \geq min

max ▲▼
Select features with statistic \leq max

number.of.neighbors ▲▼
Number of neighbors to select by score in each direction

base.output.name*
The base name for the output files

* Required Field Run



Python Function GUI

The screenshot displays the GenePattern Notebook interface. At the top, the title bar reads "GenePattern Notebook Demo Notebook" with a "Last Checkpoint: 06/09/2017 (unsaved changes)" and a "Logout GenePatternUser" button. Below the title bar is a menu bar with "File", "Edit", "View", "Insert", "Cell", "Kernel", "Widgets", and "Help". A toolbar contains icons for file operations and a "Code" dropdown menu. The main area shows a Python code cell with the following code:

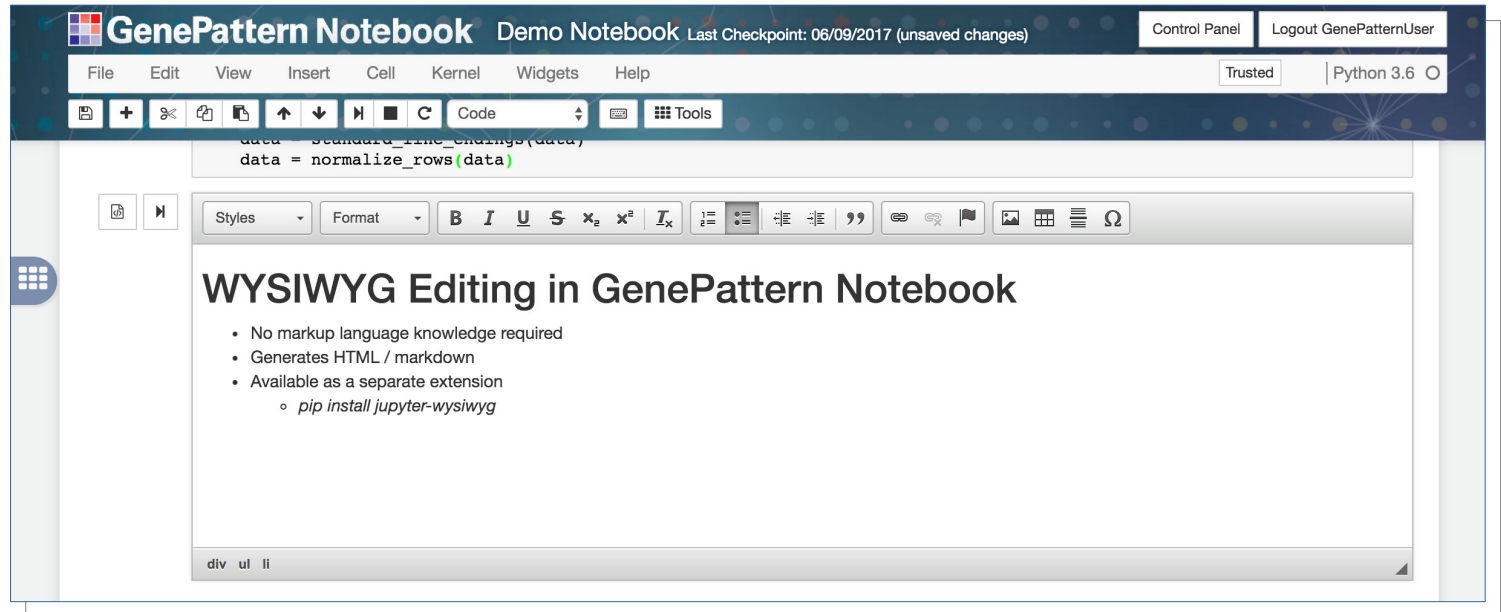
```
In [18]: @call_widget
def clean_data_before_analysis(data_path, normalization_metric="log"):
    data = load_data(data_path)
    data = standard_line_endings(data)
    data = normalize_rows(data, normalization_metric)
    return data
```

Below the code cell, a GUI window titled "GenePattern clean_data_before_analysis" is shown. It features a "Call" button in the top right corner. The form contains two input fields: "data path*" and "normalization metric" (with "log" entered). The "data path*" field is marked as a required field. A second "Call" button is located at the bottom right of the form.

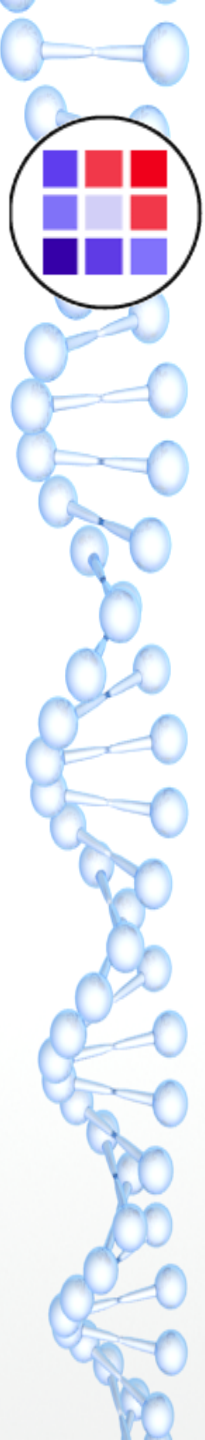
- Turn any Python function into an interactive user interface



Rich Text Markdown Editor



- No markup knowledge required
- Generates HTML / markdown
- Available as a separate extension

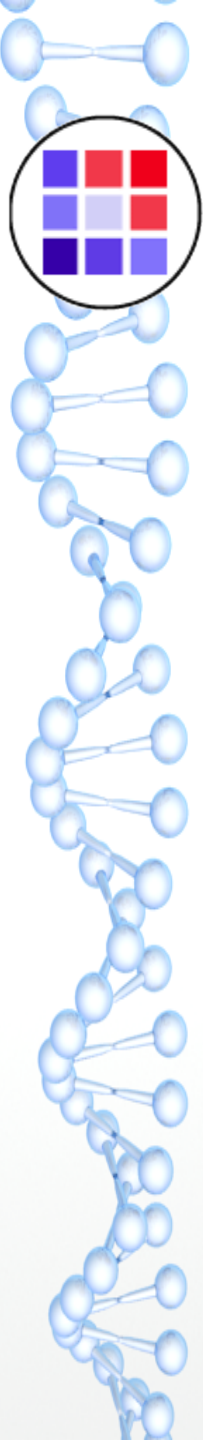


Notebook Tool Manager

The screenshot shows the GenePattern Notebook interface with a 'Select Notebook Tool' dialog box open. The dialog has a search bar labeled 'Type to Filter' and a tab labeled 'GenePattern'. Below the tab, there is a list of tools:

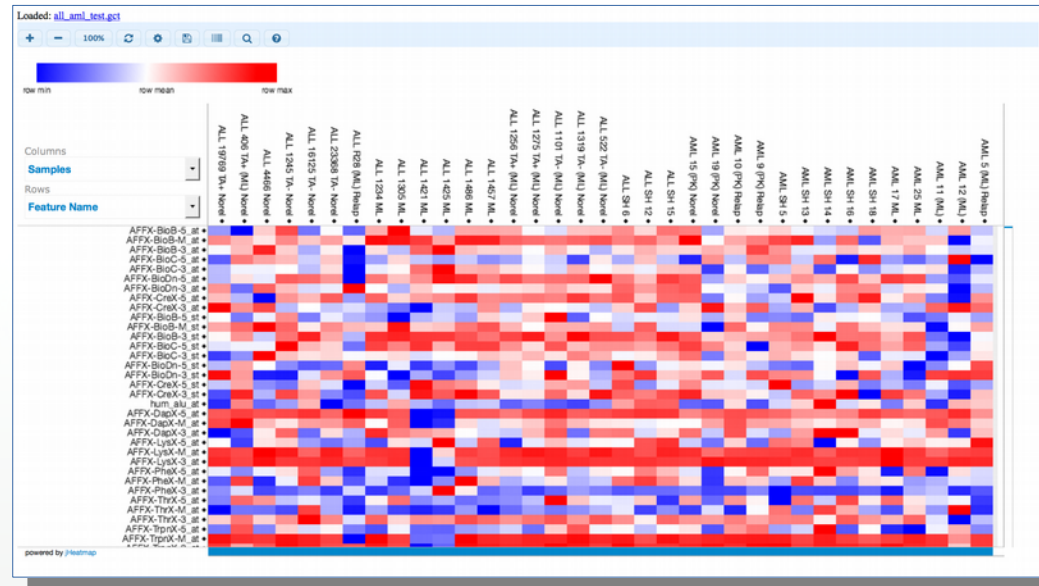
- ABSOLUTE** (GenePattern Public, v1.4)
[**Beta Release** Contact gp-help with any issues. Check stdout.txt and stderr.txt for errors] E...
SNP Analysis
- ABSOLUTE.review** (GenePattern Public, v1.2)
[**Beta Release** Contact gp-help with any issues. Check stdout.txt and stderr.txt for errors] E...
SNP Analysis
- ABSOLUTE.summarize** (GenePattern Public, v1.2)
[**Beta Release** Contact gp-help with any issues. Check stdout.txt and stderr.txt for errors] ...
SNP Analysis
- Acgh2Tab** (GenePattern Public, v4)
Converts acgh files to a tab-delimited format usable by Genomica
Data Format Conversion
- AddFCSEventIndex** (GenePattern Public, v2)
Adds indexes to events in a Flow Cytometry Standard (FCS) data file.

The background interface shows the GenePattern Notebook title bar, a menu bar (File, Edit, View, Insert), and a toolbar. The main content area displays a notebook cell with the text 'Experiencing a bug? leaving feedback.' and a code cell with the output '<gp.core.GPFile'.



Behind the Scenes

- Interactive widgets use the Jupyter widget framework (ipywidgets, traitlets)
- Can use Python variables as input
- Not limited by GenePattern analyses





GenePattern Python Library

- Complete programmatic access
- Automatic integration with GenePattern cell data

```
import gp

# Create a GenePattern server proxy instance
gpserver = gp.GPServer('http://localhost:8080/gp','myusername', 'mypassword')

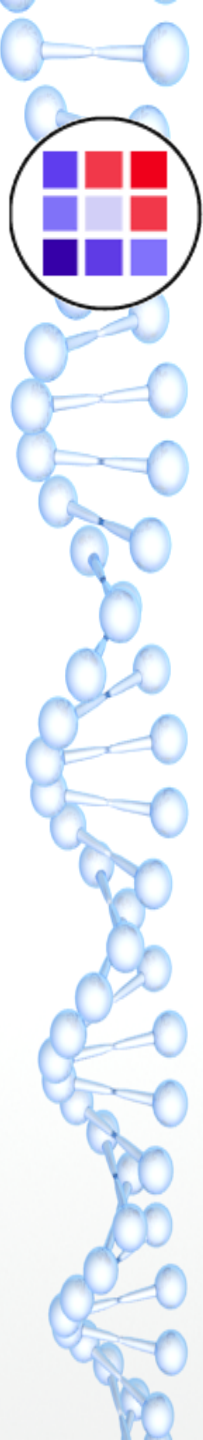
# Obtain GPTask by module name
module = gp.GPTask(gpserver, "PreprocessDataset")

# Load module parameter data
module.param_load()

# Create a job specification
job_spec = module.make_job_spec()

# Upload a file to the server
uploaded_file = gpserver.upload_file("file_name", "/path/to/the/file/file_name")
job_spec.set_parameter("input.filename", uploaded_file.get_url())

# Submit the job to the GenePattern server
job = gpserver.run_job(job_spec)
```

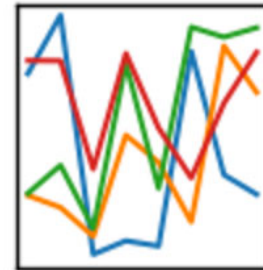



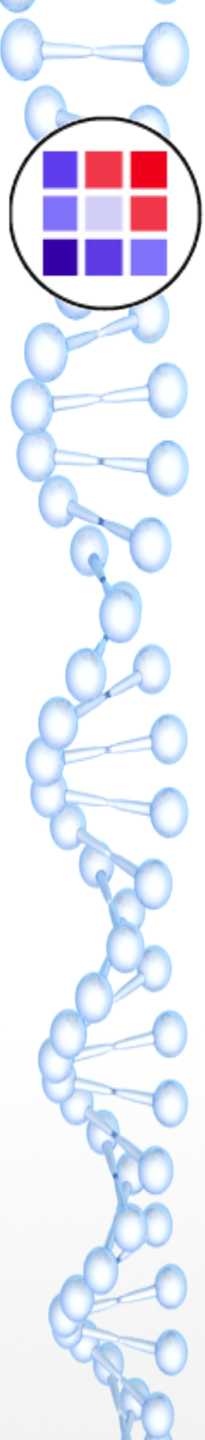
GenePattern Data Tools

- Easily import common bioinformatic data formats as pandas DataFrames
- Work with GenePattern files using popular Python libraries

pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$





GenePattern Notebook Repository

GenePattern Notebook

Sign in

Username:

Password:

[Sign In](#)

Tweets by @GenePattern

GenePattern @GenePattern
Check out this introductory video on the GenePattern Notebook Python Integration! buff.ly/2fcs413 #python #jupyternotebooks

YouTube @YouTube
[Introduction to the GenePattern Notebook](#)

[Embed](#) [View on Twitter](#)

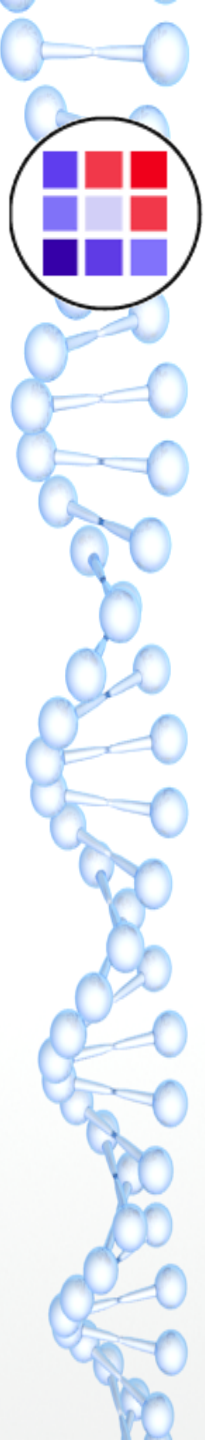
Register GenePattern Account

Log in using your [GenePattern public server](#) username and password. If you do not have an account, click the [Register Account](#) button below.

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<http://genepattern-notebook.org>



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- IGV
- Workshop
- 014_make_autism_gmt
- After Migration.ipynb
- Classification and Pred
- Classification and Pred
- Classification and Pred
- copy1_Classification ar
- cron.ipynb
- Custom.ipynb
- Demo Notebook.ipynb
- Demo.ipynb

Publish Notebook to Repository

This will make a copy of the notebook available to anyone. A published notebook does not update automatically when you save it again in the future. To update the published copy you will have to click publish again after making any changes and saving.

Notebook Name

Classification and Prediction - RNAseq

Description

Use RNA-seq data with k-Nearest Neighbors (kNN) to build a predictor, use it to classify leukemia subtypes, an

Authors

GenePattern Team

Quality

Release

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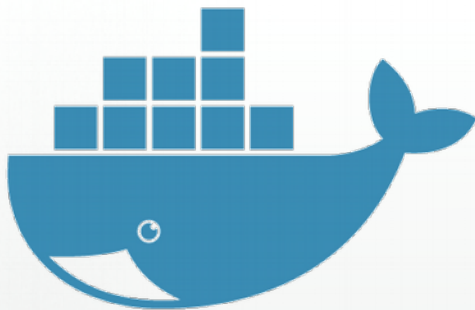
Name	Last Modified
	3 months ago
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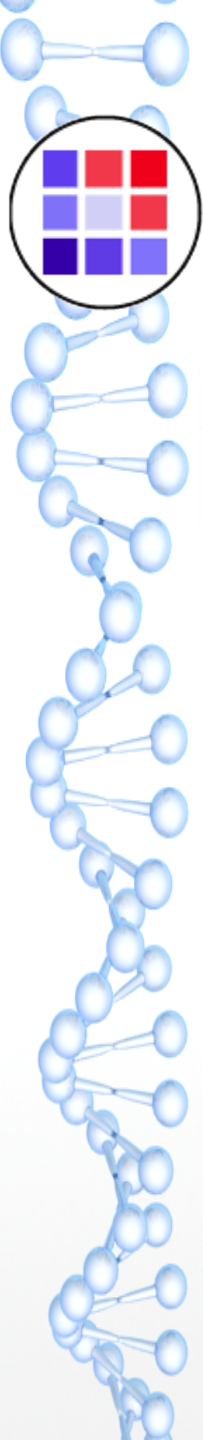
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- Browse available notebooks.



Installing the Extension

- **PyPI**
 - `pip install genepattern-notebook`
- **Anaconda Cloud**
 - `conda install -c genepattern genepattern-notebook`
- **DockerHub**
 - `docker pull genepattern/genepattern-notebook`



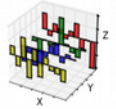


Jupyter Ecosystem

matplotlib



pandas
 $y_{it} = \beta x_{it} + \mu_i + \epsilon_{it}$



IP[y]:
IPython

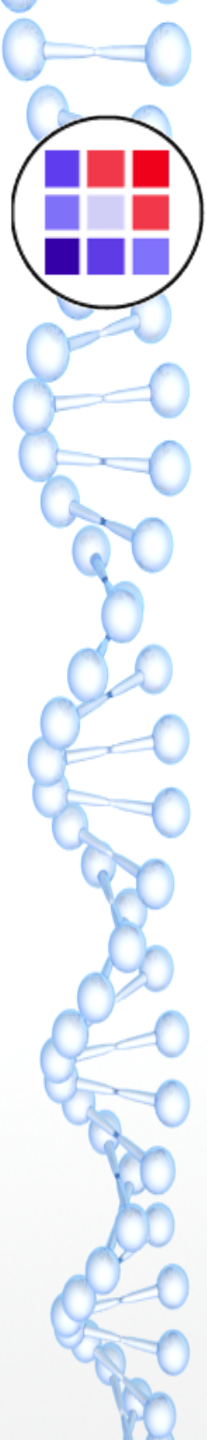
jupyter



Anaconda



jupyterhub



Acknowledgments

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PI

Jill Mesirov

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Medical Sciences





Resources

GenePattern Notebook

genepattern-notebook.org

GenePattern GitHub

github.com/genepattern

GenePattern

genepattern.org

GenePattern DockerHub

hub.docker.com/r/genepattern

Public GenePattern server

genepattern.broadinstitute.org

Indiana University GenePattern server

gp.indiana.edu

GenePattern Archive (GPArC)

gparc.org

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