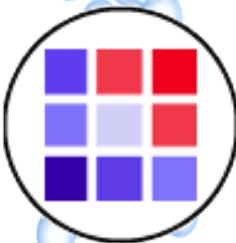


Thorin Tabor
JupyterCon 2017

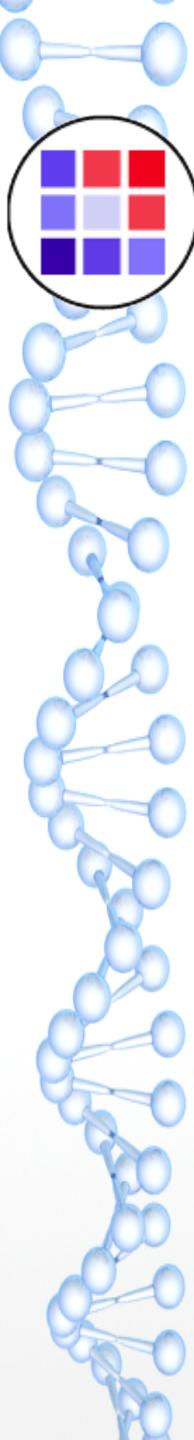
GenePattern Notebooks

Jupyter for Integrative Genomics

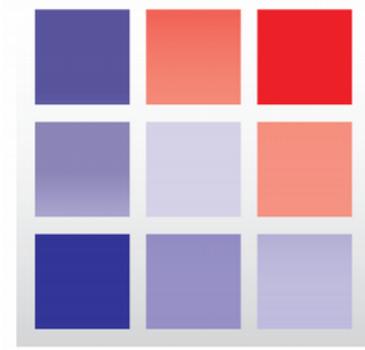
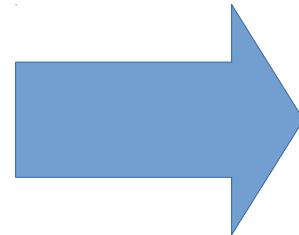


UC San Diego





From Jupyter to GenePattern





GenePattern Notebook

GenePattern Notebook Demo Notebook Last Checkpoint: 06/09/2017 (autosaved)

File Edit View Insert Cell Kernel Widgets Help

Control Panel Logout GenePatternUser Trusted Python 3.6

Experiencing a bug? Have thoughts on how to make GenePattern Notebook better? Let us know by leaving feedback.

Leave Feedback

```
In [11]: genepattern_job.get_file('parikshak2013.gene.sets.symbols.gmt.cvt.txt')
Out[11]: <gp.core.GPFile at 0x7f9edc54f6a0>
```

GenePattern FastQC Version 1

Provides quality control metrics on raw sequence data

* Required Field

Run

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

RNA-seq reads file in FASTQ (bz2 and gz compressed files are supported), SAM, or BAM format.



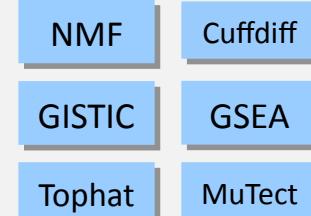
Two Open Source Projects





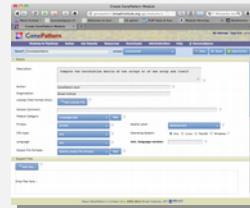
What is GenePattern?

Module Repository



Hundreds of analyses and visualizations

Module Integrator



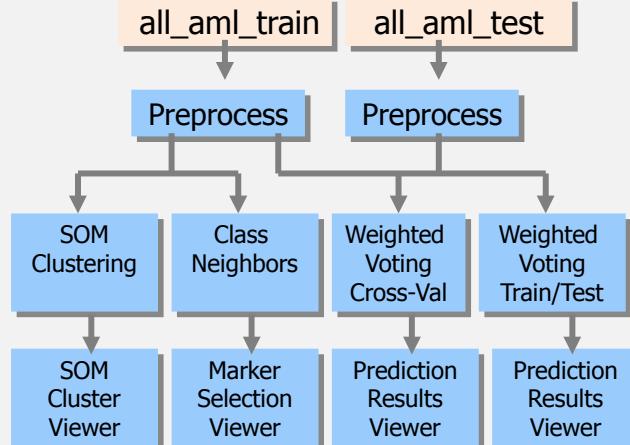
Easy addition of new tools

Community Repository

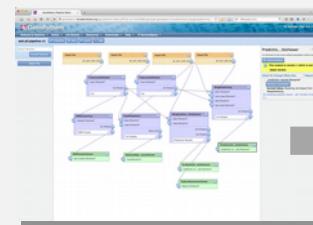


User-contributed modules

Pipeline Environment



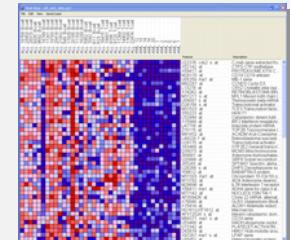
Golub and Slonim et. al 1999



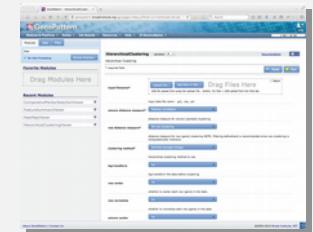
Golub.Slonim.1999.Nature.
all.aml.pipeline.zip

Support for *in silico* reproducible research

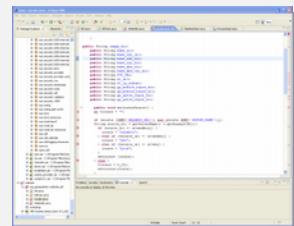
Clients



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

The screenshot shows the GenePattern homepage with a dark blue header featuring the GenePattern logo and the tagline "A Platform for Reproducible Bioinformatics". Below the header are three main navigation buttons: "Use GenePattern", "GenePattern Basics", and "Download". The main content area is titled "Features" and includes sections for "Analysis Pipelines", "Reproducible Research", and "Programming Environment". Each section contains a brief description and a list of specific features or tools.

genepattern.org

The screenshot shows the GenePattern public server interface with a light blue header. The main content area is titled "Welcome to GenePattern" and "Getting Started". It includes sections for "Public Modules", "Adding genomic data to GenePattern", and "Analyzing genomic data in GenePattern". The interface is designed for users to upload their own data and run analyses.

genepattern.broadinstitute.org

The screenshot shows the GParc website with a teal header featuring the GParc logo and the tagline "A repository and community where users can share and discuss their own GenePattern modules". Below the header is a search bar and a "Browse Modules" button. The main content area displays a list of available modules, including "Aqgh2Tab v4" and "Convert fastq files to a tab-delimited format usable by Genomics". A sidebar on the right allows users to filter modules by available tags such as "Genomics", "Bioinformatics", "Data Mining", "Machine Learning", "Classification", "Cross-validation", and "Cross-validation".

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

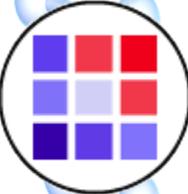
Picard Sort Sam

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

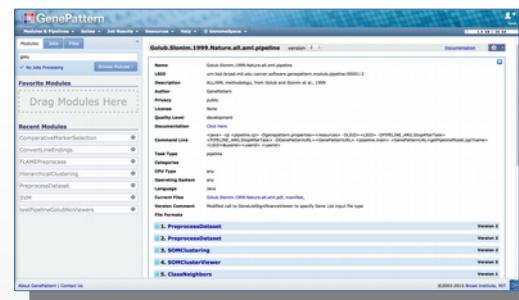
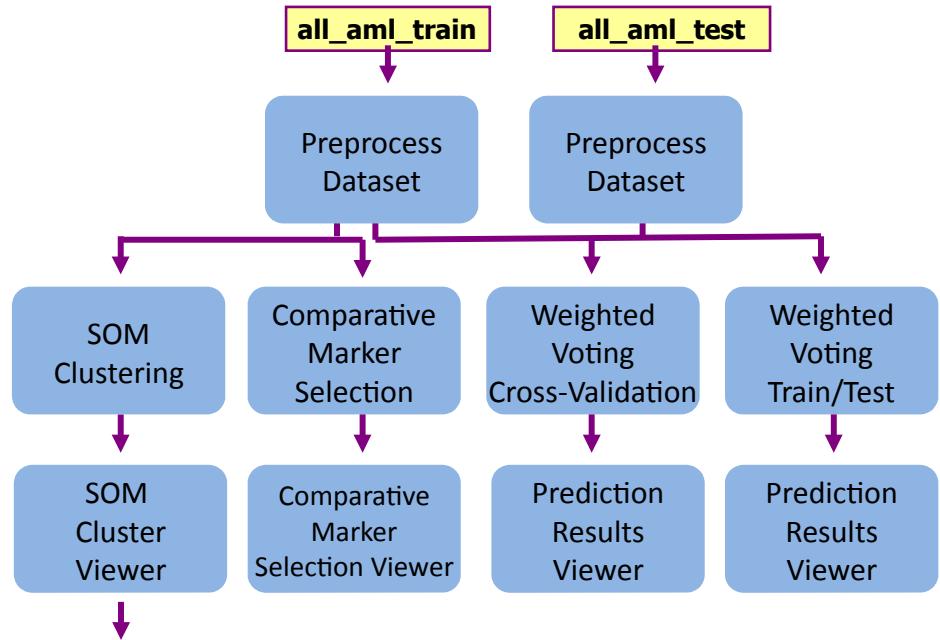
Documentation

HierarchicalClustering.pdf

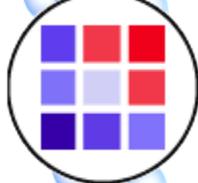
Parameter descriptions

```
-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

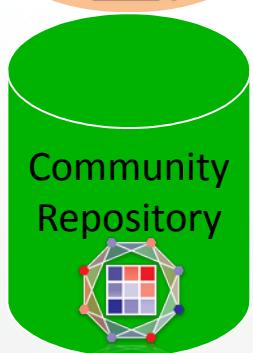
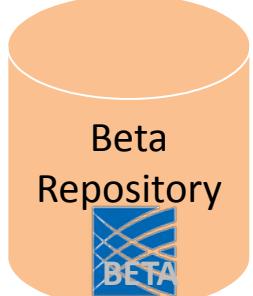
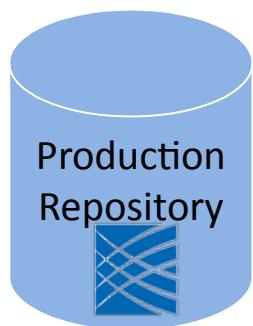


Golub.Slonim.1999.Nature.all.aml.pipeline.zip

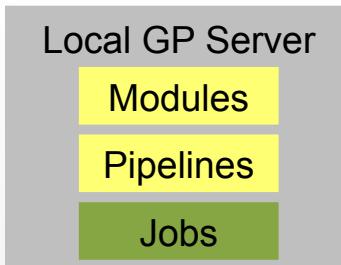
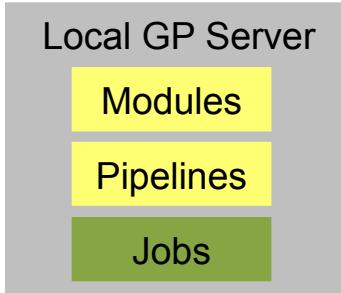
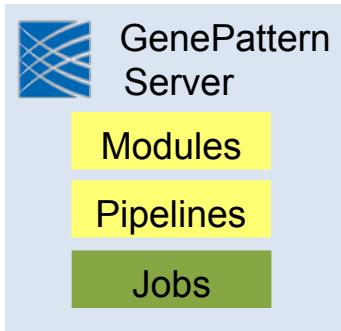


Web Server Architecture

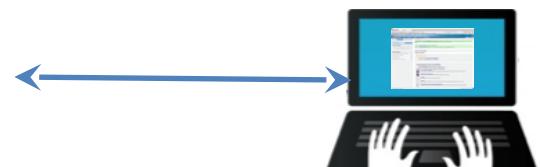
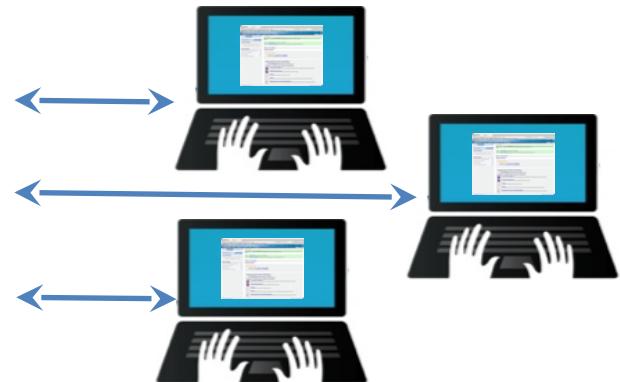
Repositories



Servers



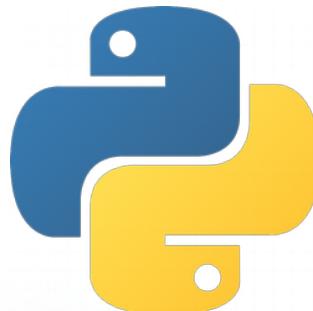
GenePattern Users





Programmatic APIs

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



REST API





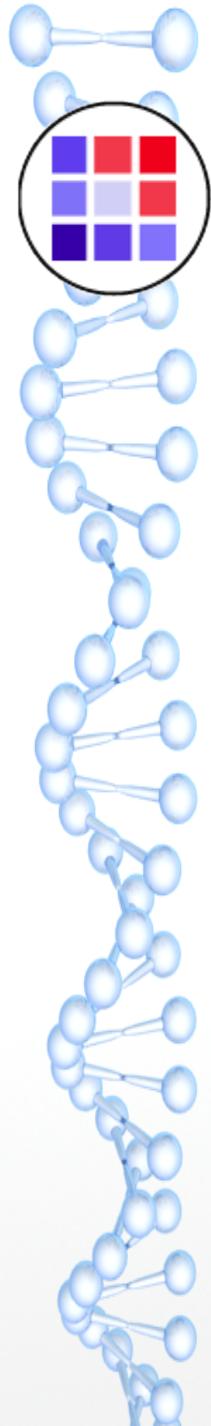
User-Friendly Interface

- Permits complex analyses without the need for a coding background

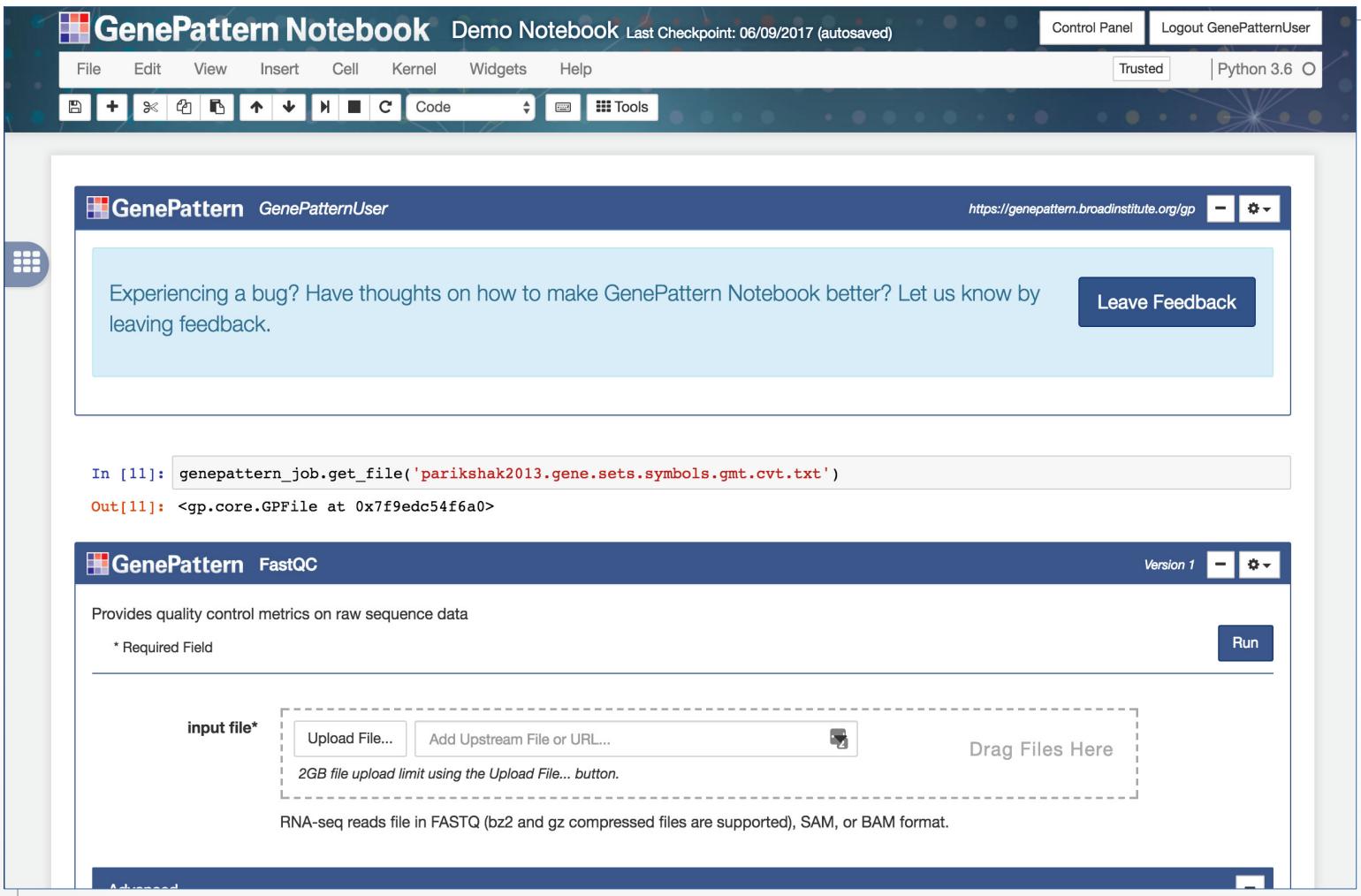
The screenshot shows the GenePattern web interface. At the top, there's a navigation bar with links for Modules & Pipelines, Suites, Job Results, Resources, Help, and GenomeSpace. A user profile icon for 'test' is also present. The main content area has several sections:

- Welcome to GenePattern**: A general welcome message.
- Getting Started**: A section with "New! Web tours" and two bullet points:
 - Click here for a tour of [what's new in GenePattern](#).
 - Click here for an [introductory tour of GenePattern](#).
- Analyzing genomic data in GenePattern**: A section with two bullet points:
 - 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:** This section lists five protocols with icons:
 - 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**: Estimate SNP copy number and loss of heterozygosity.

At the bottom, there are links for "About GenePattern" and "Contact Us". The footer includes a copyright notice: "©2003-2015 Broad Institute, MIT" and a small logo.



GenePattern Notebook Jupyter Extensions



The screenshot displays the GenePattern Notebook Jupyter Extension interface. At the top, a navigation bar includes "Control Panel" and "Logout GenePatternUser". Below it is a toolbar with icons for File, Edit, View, Insert, Cell, Kernel, Widgets, Help, and a dropdown menu set to "Code". On the right, status indicators show "Trusted" and "Python 3.6".

The main area features a feedback message: "Experiencing a bug? Have thoughts on how to make GenePattern Notebook better? Let us know by leaving feedback." with a "Leave Feedback" button. Below this is a code cell output:

```
In [11]: genepattern_job.get_file('parikshak2013.gene.sets.symbols.gmt.cvt.txt')
Out[11]: <gp.core.GPFile at 0x7f9edc54f6a0>
```

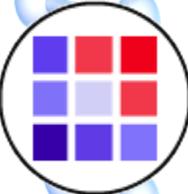
Below the code cell is the "FastQC" tool interface, titled "GenePattern FastQC". It says "Provides quality control metrics on raw sequence data". A note indicates "* Required Field". There is a "Run" button and a "Drag Files Here" area for file upload, with an "input file*" label and "Upload File..." and "Add Upstream File or URL..." buttons. A note states "2GB file upload limit using the Upload File... button." At the bottom, it specifies "RNA-seq reads file in FASTQ (bz2 and gz compressed files are supported), SAM, or BAM format." A "Advanced" button is at the bottom left.



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)

File Edit View Insert Cell Kernel Widgets Help Trusted Python 3

```
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_amr_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_amr_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

Code Tools

GenePattern SVM

Classify samples using SVM

* Required Field

train data filename

Upload File... Add Upstream File or URL... Drag Files Here
2GB file upload limit using the Upload File... button.

The training data file - .gct, .res

train cls filename

Upload File... Add Upstream File or URL... Drag Files Here
2GB file upload limit using the Upload File... button.

The training class file - .cls

test data filename

Upload File... Add Upstream File or URL... Drag Files Here
2GB file upload limit using the Upload File... button.

The test data file - .gct, .res

pred results output

<test.data.filename_basename>.pred.odf

The name of the output file for prediction results

model output file

<train.data.filename_basename>.model



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

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 tabor 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 tabor <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 maintenance 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 ? - > Run

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

* Required Field

comparative.marker.filename*

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

The results from ComparativeMarkerSelection - .odf

dataset.filename*

Upload File... Add Path or URL... 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*

<comparative.marker.selection.filename_basename>.filt

The base name for the output files

* Required Field Run

Job Cells

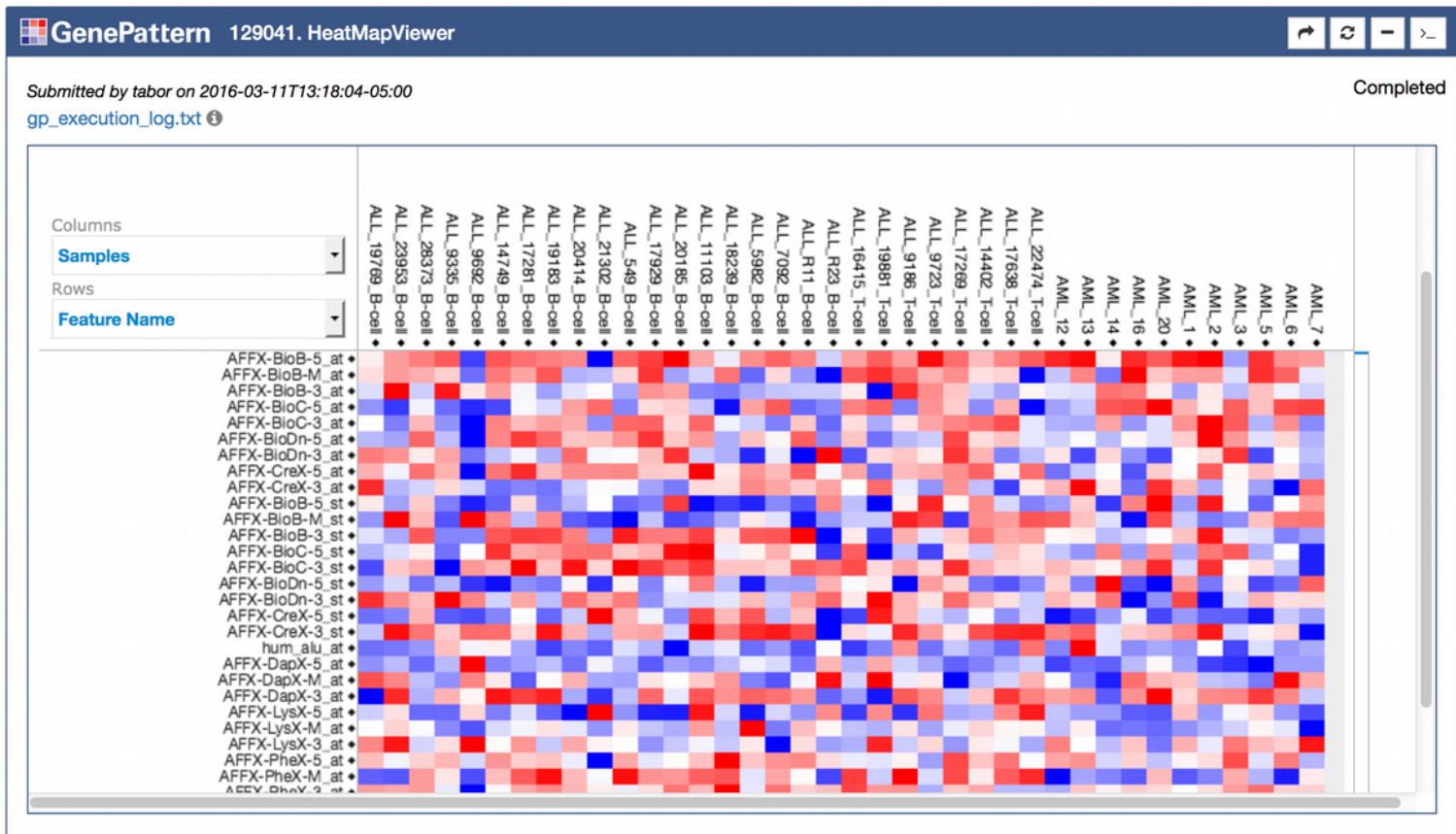


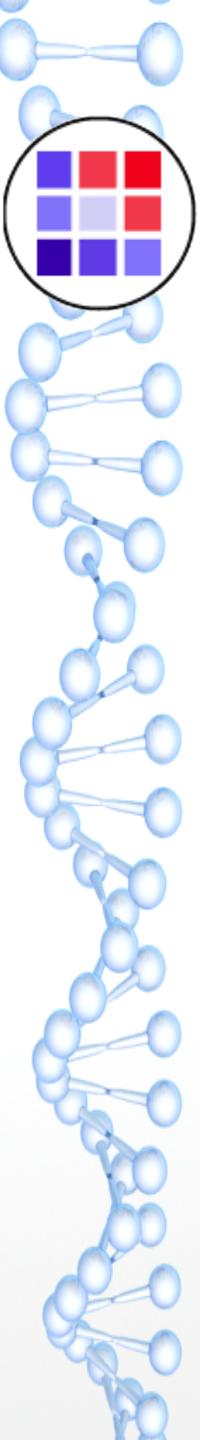
GenePattern 1251770. ConvertLineEndings

Submitted by tabor on 2016-03-03T12:09:39-05:00

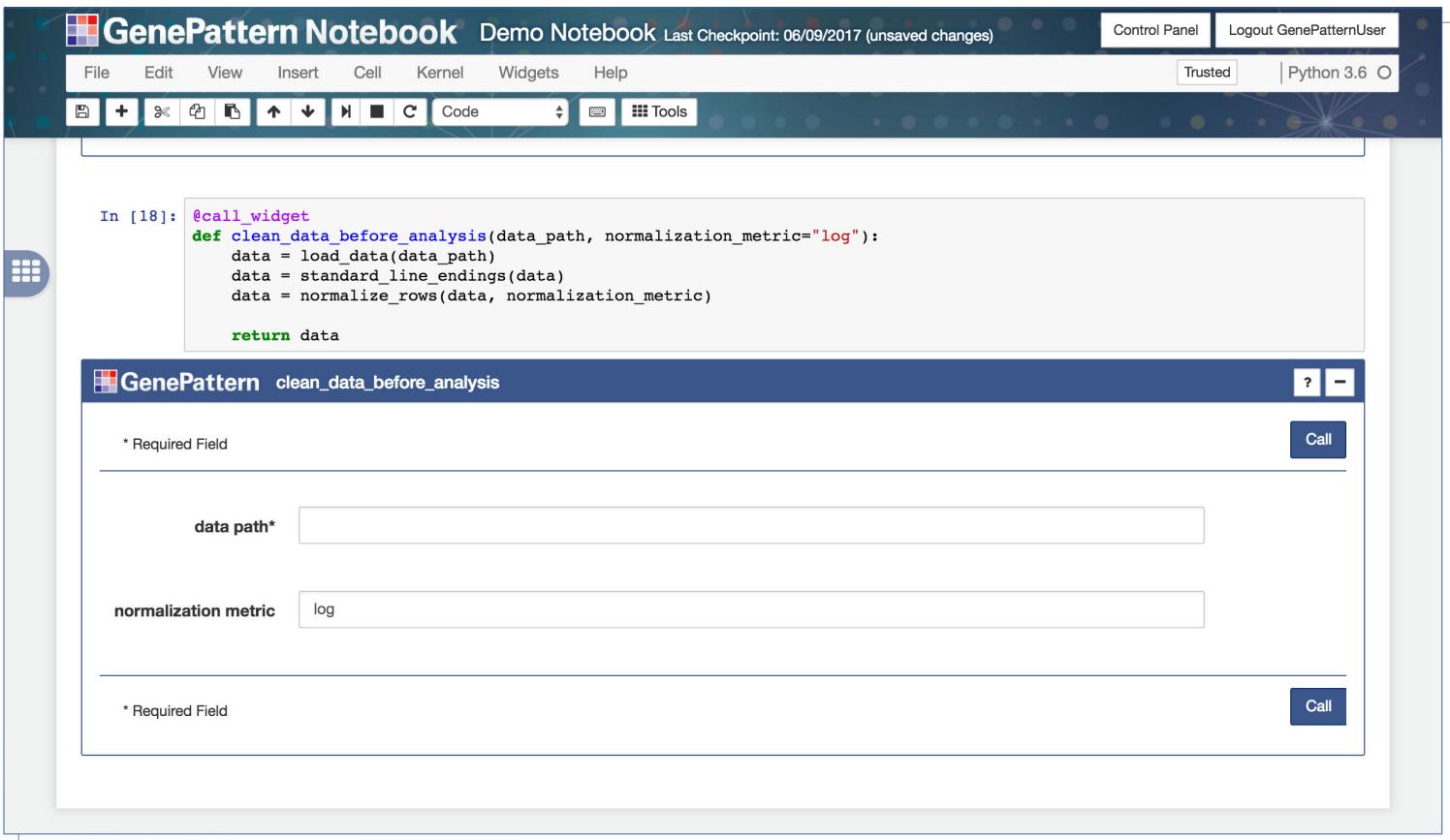
[test.cvt.txt](#) ⓘ
[gp_execution_log.txt](#) ⓘ

Completed





Python Function GUI



The screenshot shows the GenePattern Notebook interface. At the top, the title bar reads "GenePattern Notebook Demo Notebook Last Checkpoint: 06/09/2017 (unsaved changes)". The menu bar includes File, Edit, View, Insert, Cell, Kernel, Widgets, and Help. The toolbar below has icons for file operations like Open, Save, and Print, along with Code and Tools buttons. On the right, there are "Control Panel" and "Logout GenePatternUser" buttons, and a status bar indicating "Trusted" and "Python 3.6".

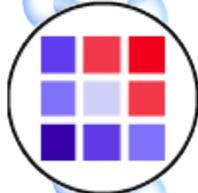
In [18]:

```
@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
```

A modal dialog box titled "GenePattern clean_data_before_analysis" is open. It contains two input fields: "data path*" and "normalization metric". The "data path" field is empty, and the "normalization metric" field contains "log". Both fields have a placeholder "* Required Field". A "Call" button is located at the bottom right of the dialog.

- Turn any Python function into an interactive user interface



Rich Text Markdown Editor

The screenshot shows the GenePattern Notebook interface. At the top, there's a navigation bar with 'GenePattern Notebook' and 'Demo Notebook'. Below it is a toolbar with various icons for file operations like opening, saving, and printing. A code cell contains Python code for data processing:

```
data = Standardize_Func_Calling(data)
data = normalize_rows(data)
```

Below the code cell is a WYSIWYG editor toolbar with buttons for styles (B, I, U, S), mathematical symbols (x_1 , x^2 , T_x), and other document tools. The main content area displays the heading 'WYSIWYG Editing in GenePattern Notebook' and a bulleted list of features:

- No markup language knowledge required
- Generates HTML / markdown
- Available as a separate extension
 - `pip install jupyter-wysiwyg`

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



Notebook Tool Manager

The screenshot shows the GenePattern Notebook interface. On the left, there are two panels: one for 'GenePattern General' showing a message about a bug and leaving feedback, and another for 'GenePattern FastQC' asking for an input file. A central 'Select Notebook Tool' dialog is open, listing various tools under the 'GenePattern' tab. The listed tools are:

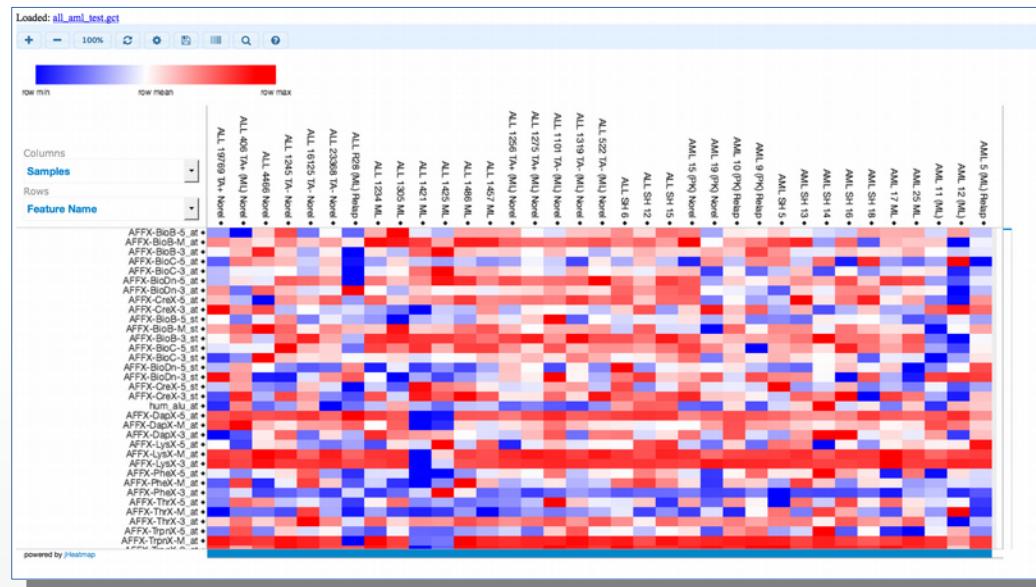
- ABSOLUTE** (GenePattern Public, v1.4)
[*Beta Release* Contact gp-help with any issues. Check stdout.txt and stderr.txt for errors] E...
SNP Analysis
- ABSOLUTE.review** (GenePattern Public, v1.2)
[*Beta Release* Contact gp-help with any issues. Check stdout.txt and stderr.txt for errors] E...
SNP Analysis
- 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 right side of the interface shows a 'Control Panel' with tabs for 'Trusted' and 'Python 3.6', and a 'Logout GenePatternUser' button. Below the control panel, there's a 'Leave Feedback' button and a 'Run' button for a selected tool.



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)
```

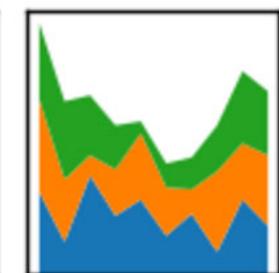
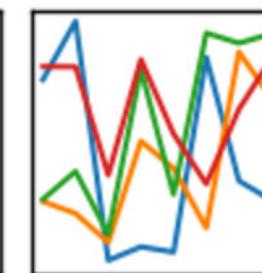
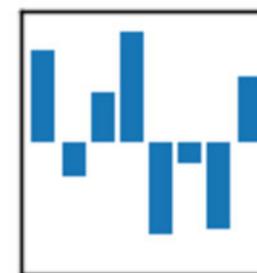


GenePattern Data Tools

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

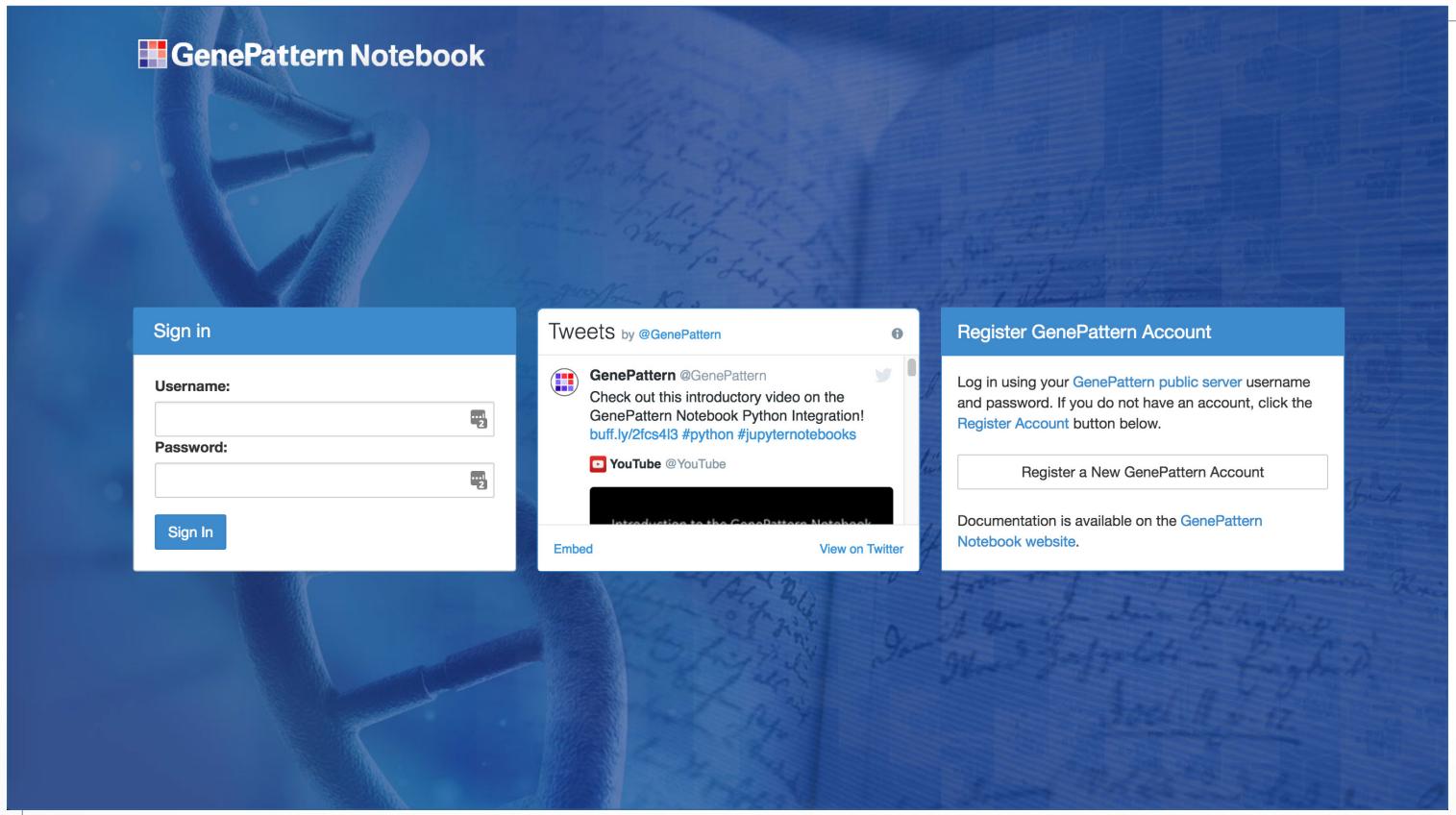
pandas

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





GenePattern Notebook Repository



The screenshot shows the GenePattern Notebook landing page. The background features a blue-tinted DNA double helix and handwritten mathematical notes. On the left, there's a "Sign in" form with fields for "Username" and "Password" and a "Sign In" button. In the center, there's a "Tweets by @GenePattern" feed with one visible tweet from GenePattern (@GenePattern) about Python integration. On the right, there's a "Register GenePattern Account" section with a "Register a New GenePattern Account" button and a link to documentation.

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/2fcs4i3 #python #jupyternotebooks

YouTube @YouTube

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.

[Register a New GenePattern Account](#)

Documentation is available on the [GenePattern Notebook website](#).

<http://genepattern-notebook.org>

Publish & Share Notebooks



GenePattern Notebook

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

Control Panel | **Logout GenePatternUser**

Upload | **New** | **Cancel** | **Publish**

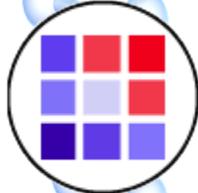
Example Notebooks

- GCT
- IGV
- Workshop
- 014_make_autism_gmt.ipynb
- After Migration.ipynb
- Classification and Prediction.ipynb** (selected)
- Classification and Prediction.ipynb
- Classification and Prediction.ipynb
- copy1_Classification and Prediction.ipynb
- cron.ipynb
- Custom.ipynb
- Demo Notebook.ipynb
- Demo.ipynb

Public Notebooks

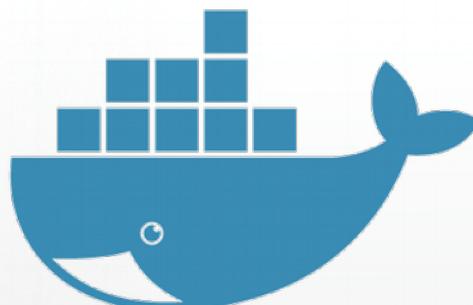
Name	Last Modified
	3 months ago
	10 days ago
	3 months ago
	10 months ago
	a year ago
	8 months ago
	5 months ago
	5 months ago
	5 months ago
	2 months ago
	9 months ago
	a year ago
Running	an hour ago
	a year ago

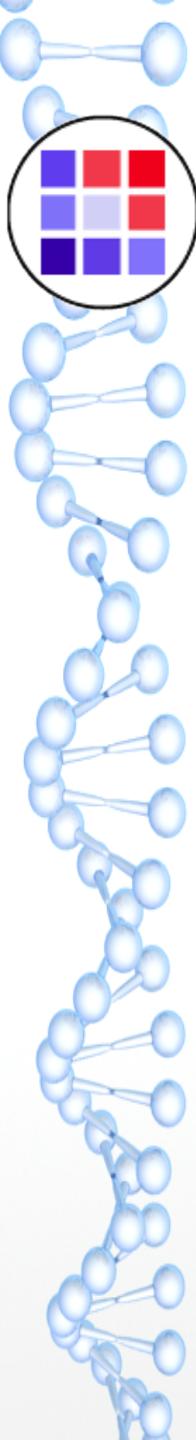
- Publish notebooks to the GenePattern Notebook Repository.
- Browse available notebooks.



Installing the Extension

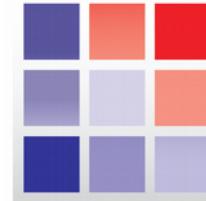
- PyPI
 - `pip install genepattern-notebook`
- Anaconda Cloud
 - `conda install -c genepattern genepattern-notebook`
- DockerHub
 - `docker pull genepattern/genepattern-notebook`





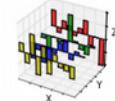
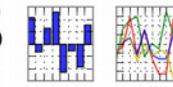
Jupyter Ecosystem

matplotlib



pandas

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



IP[y]:
IPython



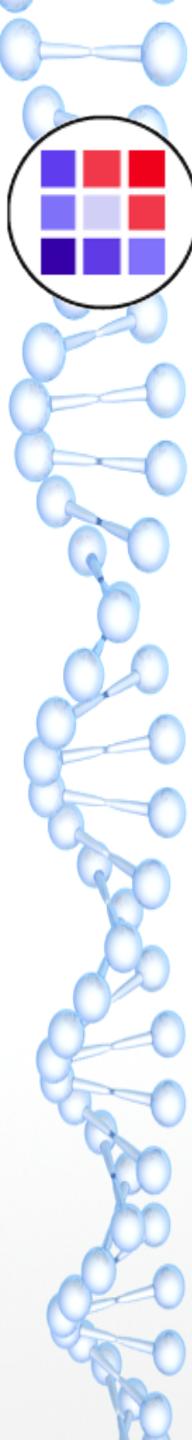

Anaconda







Acknowledgments



GenePattern Team

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GenePattern Server

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Medical Sciences





Resources

GenePattern Notebook
genepattern-notebook.org

GenePattern
genepattern.org

Public GenePattern server
genepattern.broadinstitute.org

Indiana University GenePattern server
gp.indiana.edu

GenePattern Archive (GPArc)
gparc.org

GenePattern Twitter
[@genepattern](https://twitter.com/genepattern)

GenePattern GitHub
github.com/genepattern

GenePattern DockerHub
hub.docker.com/r/genepattern