Automated Omega Plotter

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IIIT HYDERABAD

Automated Omega Plotter

About the Project:

RNA   molecules consist of a connected chain of nucleotide bases of four different types. Each nucleotide is associated with structure, sequential connectivity and interaction data. An in house tool defines and calculates five parameters which capture the base-pair geometry and the local strand orientation simultaneously. The parameters currently available are based on either of the factors taken one at a time. The tool built by the Centre of Computational Natural Sciences and Bioinformatics, IIITH, first detects potential base pairs within the cylinder, the height and radius of which are provided as input by the user, and thereafter calculates these parameters known as, Omega Eta, Omega Theta, Omega 1, Omega 2 (pseudo torsion angles), and omega distance (pseudo distance) for the detected base pairs. As part of the further analysis being carried out using Omega Eta and Omega Theta values, it was required that queries of different kinds (such as those based on base pair type, edge orientation type etc) be executed on all the potential base pairs and then values for these be plotted in order to analyze the base pairs behaving in a similar fashion. The GUI allows the user to detect base pairs by taking a protein data bank file (which provides the coordinates of various atoms) as input and storing these in a database. The protein data bank files (*.pdb) could be in any number (i.e. as the user wishes).

Further, it allows the user to plot the Omega Eta, Omega Theta and Omega 1, Omega 2 values for base pairs of a particular type among all those available in the database.

Technologies used:

Automated Omega Plotter

Qt3.3, C++, QSqlDatabases

QSqlDatabases were used to have greater synchronisation between the Database and the Qt Application.

Source Files :

The files which we got as the source code which were incorporated in the GUI are:

declaration.h (has basic declarations of all the classes mentioned below)

super.cpp (parent class of all the classes mentioned below)

atom.cpp

Point.cpp

Vector.cpp

Residue.cpp

model.cpp

extract_new_coord.pl

BPF_pre.pl

The perl files do the biological computation to calculate the basepairs located in the cylinder defined by the height and radius values as given by the user.

The files that make the GUI :

mainform.ui.h , mainform.ui

trialform.ui.h, trialform.ui

main.cpp

Other files necessary for running the GUI are generated automatically by the Qt compiler and the moc compiler.

Number of lines of code written :

main.cpp – 20

mainform.ui.h - 300

trialform.ui.h - 300

Automated Omega Plotter

Lines of code generated by Qt Designer - 3062

Number of functions: 10

Programmer's Manual:

Each of the supporting files (*.cpp) has around 6-8 functions necessary for some computations. All the files were given before the beginning of the project.

The mainform.ui.h has

- init() – which makes a connection to the database (RRBPF) and opens it for further use while running the program.
- BrowseFile() -necessary to upload a (*.pdb) file to the program for further execution.
- Plot_clicked() – calls another function SubmitValues() . After the execution of SubmitValues(), it builds a query based on the user specified parameters and extracts the information from the database and puts it into a new table called final_table which finally contains all the necessary points to be plotted on the graph.
- SubmitValues() – builds a database and puts the values got from the (*.pdb) files in a systematic manner into the base_pairs table.
- Plot_graph()- which is called at the end of the plot_clicked() function opens the trialform where the graph appears.

The trialfrom.ui.h has

- connectdatabase() – makes a connection between the program and the database 'RRBPF' which was updated earlier based on the user specified parameters.
- Plotgraph() – extracts the co-ordinates from the final_table and plots them onto a graph.

- Getinfo() – gets the information related to a particular selected point from the database and prints it in a particular textbox.
- Zoom_in() – allows an option to zoom in to a selected area for a much clear picture of the graph.
- Zoom_out() – allows an option to zoom out and get a more broader view of the entire graph.

Benefeciaries:

The Beneficiaries of this plotter are the pioneers in natural and biological sciences who pursue their research in the field of nucleic acids and molecules with a large number of constituent atoms.

Platform:

Linux

User Manual:

The basic prerequisites for the end-user to setup this software is that he/she should have qt-3 , mysql, qtsql, g++ compiler and other supporting packages installed on his system. Internet connection is not necessary. We are not sure whether it will be available for download in any of the public site.

Things to be done before setting up the GUI:

Before using the GUI, the user must create a database named 'RRBPF' and a table 'base_pairs' by writing the following queries on the mysql prompt

1. create database RRBPF;
2. use RRBPF;

3. In the mainform.ui.h file, modify the username and password for access to the mysql database from (username = "root" password = "root123") to the system specific username and password for mysql.

Then the code will be ready for execution. End-user doesn't require another computer for running this code.

The various buttons in the GUI are:

The Main Form GUI has:

- 'Upload File' allows the user to browse and then upload a PDB file. More than one PDB files can be uploaded.

- 'Remove File' allows the user to remove a selected file that was previously uploaded.
- 'Text box' that shows a list of all the uploaded files till then.
- 'Height' and 'Radius' fields to specify the values for the height and radius of the cylinder in which the base pair combinations are to be considered.
- 'Base1' and 'Base2' fields which provide an option among the five bases A, T, G, C, U to determine which base pair combinations are desired by the user.
- 'Edge1' and 'Edge2' fields which provide and option among the three available edges W,H,S to determine the interacting edges between which the base pair combinations are to be considered.
- 'Orientation' field that asks for a 'Cis' or a 'Trans' orientation between the base pair combinations to be plotted on the graph.
- 'Reset Values' button which resets all the parameters to their default values for another trial or run.
- 'Plot Graph' button which plots the graph on a new GUI.

- 'Cancel' button that quits the application.

The Trial Form (GUI which shows the graph) has :
- 'Graph' region which shows the graph
- 'Information Bar' which shows the information related to the selected point on the graph
- 'Get Information' button that shows different parameters related to a particular selected point on the graph in the information bar.
- 'Zoom In' button that provides an option to zoom into a particular region in the graph
- 'Zoom Out' button that provides an option to zoom out to get a broader view of the graph.
- 'Cancel' button that closes the graph window and the original application is restored.

Directory Structure:

All the files should be in the same directory for the program to run properly. The *.pdb files need not be in that directory and can be uploaded from any where. The *.pl files should be in the same directory. The other supporting files suchas atom.cpp, model.cpp,super.cpp, Vector.cpp, Point.cpp, Residue.cpp, declaration.h should also be in the same directory.

Using The GUI:

1. Alt + F2 -> type "gnome-terminal" and press <Enter> to open a terminal.
2. Go to the directory named "OmegaPlotter"
3. On the command prompt, type

    $ qmake –project

    $ qmake

Automated Omega Plotter

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$ make
$ ./OmegaPlotter
```
to run the GUI.

Contribution to the Project:

Phani Krishna K S S S – I did the basic back end part, i.e. interaction with the database and the extraction of different information from the database based on the user specified parameters and the uploaded *.pdb files. I learnt Qt 3.3 for designing the GUI and interaction with the databases .

G P Kumar – I did the basic designing of the GUI and the plotting of the graph based on the values retrieved from the databases. I learnt Qt 3.3 for designing the GUI and interaction with the databases and plotting of different graphs.