FastGCN (1.0) Manual

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July 4th, 2014

1. Introduction

FastGCN is a convenient and efficient tool for fast gene co-expression networks. First genetic entropy is exploited to filter out some genes with no or small expression change. Then Pearson Correlation Coefficients are calculated. At last these coefficients are normalized. All these calculating procedures are implemented on GPU. To save the space the coefficient matrix is compressed. To increase the convenience z-score or FDR (False Discovery Rate) is taken as the threshold for output.
We packed GPU version, multi-core CPU version, single-thread CPU version and single-thread R version in the download package.

2. Citing FastGCN

If you use FastGCN in any published work, please cite:

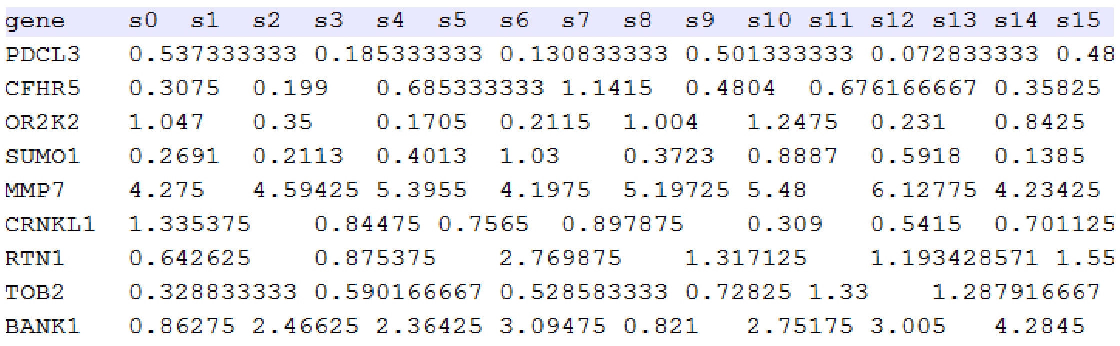
Meimei Liang, Futao Zhang, Gulei Jin and Jun Zhu* (2014) FastGCN: a GPU Accelerated Tool for Fast Gene Co-expression Networks.

3. Bugs report

If you have any questions, bug reports or comments with our software, please contact:
Dr. Liang with her email address lmm@zju.edu.cn
or
Prof. Zhu with his email address: jzhu@zju.edu.cn

4. Input Data format

The input file is a white-space (space or tab) delimited file. Currently the input files must contain the individual names in the first row and the gene names in the first column.



```
gene    s0  s1  s2  s3  s4  s5  s6  s7  s8  s9  s10 s11 s12 s13 s14 s15
PDCL3   0.537333333 0.185333333 0.130833333 0.501333333 0.072833333 0.48
CFHR5   0.3075  0.199   0.685333333 1.1415  0.4804  0.676166667 0.35825
OR2K2   1.047   0.35    0.1705  0.2115  1.004   1.2475  0.231   0.8425
SUMO1   0.2691  0.2113  0.4013  1.03    0.3723  0.8887  0.5918  0.1385
MMP7    4.275   4.59425 5.3955  4.1975  5.19725 5.48    6.12775 4.23425
CRNKL1  1.335375    0.84475 0.7565  0.897875    0.309   0.5415  0.701125
RTN1    0.642625    0.875375    2.769875    1.317125    1.193428571 1.55
TOB2    0.328833333 0.590166667 0.528583333 0.72825 1.33    1.287916667
BANK1   0.86275 2.46625 2.36425 3.09475 0.821   2.75175 3.005   4.2845
```

5. Getting started with FastGCN

5.1 Download

The source codes and binaries of FastGCN are now available for free download at http://ibi.zju.edu.cn/software/FastGCN.
The source code for GPU implementation was written with CUDA and C/C++. The source code for multi-core CPU implementation was written with C/C++ and OpenMP. The source code for single-thread CPU implementation was written with C/C++. And the single-thread R implementation is an R script.
We only offered binaries for Windows platforms and Red Hat Enterprise Linux 6.5. So for Linux/Unix users we strongly recommend downloading the source code and compiling.

5.2 Compilation

5.2.1 GPU implementation

To compile this source code, you should download and install CUDA SDK first from https://developer.nvidia.com/cuda-toolkit-archive.
For Windows System, we recommend use a C/C++ IDE such as Microsoft Visual Studio or Eclipse combined with NVIDIA NSight (http://www.nvidia.com/object/nsight.html) as the integrated compile environment.
For Linux System, we offered 2 Makefile files in the source code package, one for CUDA 5.5 and one for CUDA 6.0. Unzip the source package in the CUDA SAMPLES directory, then go to the directory where the Makefile is located and type command “make”.

5.2.2 Multi-core CPU implementation

For windows System, you need a C/C++ compiler. But make sure to keep OpenMP support open.
For Linux System, you have two options. One is to use the Makefile in the source package, another is to go to the source directory and type the command below:

```
g++ -fopenmp -m64 -o FastGCN_omp FastGCN.cpp DataBlock.cpp pear_cpu.cpp
```

5.2.3 Single-thread C implementation

For windows System, you need a C/C++ compiler. For Linux System, please use the Makefile in the source package or go to the source directory and type:

```
g++ -m64 -o FastGCN_omp FastGCN.cpp DataBlock.cpp pear_cpu.cpp
```

5.3 Run

If using GPU implementation, Multi-core CPU implementation or Single-thread C/C++ implementation, you should input 2, 3, 4, 5 or 6 arguments. For GPU implementation, CUDA driver from NVIDIA should be installed. And make sure that you system can find where the CUDA runtime dynamic link library is located. So put the library in the same directory as the executable binary file or set the "PATH" environmental variable.

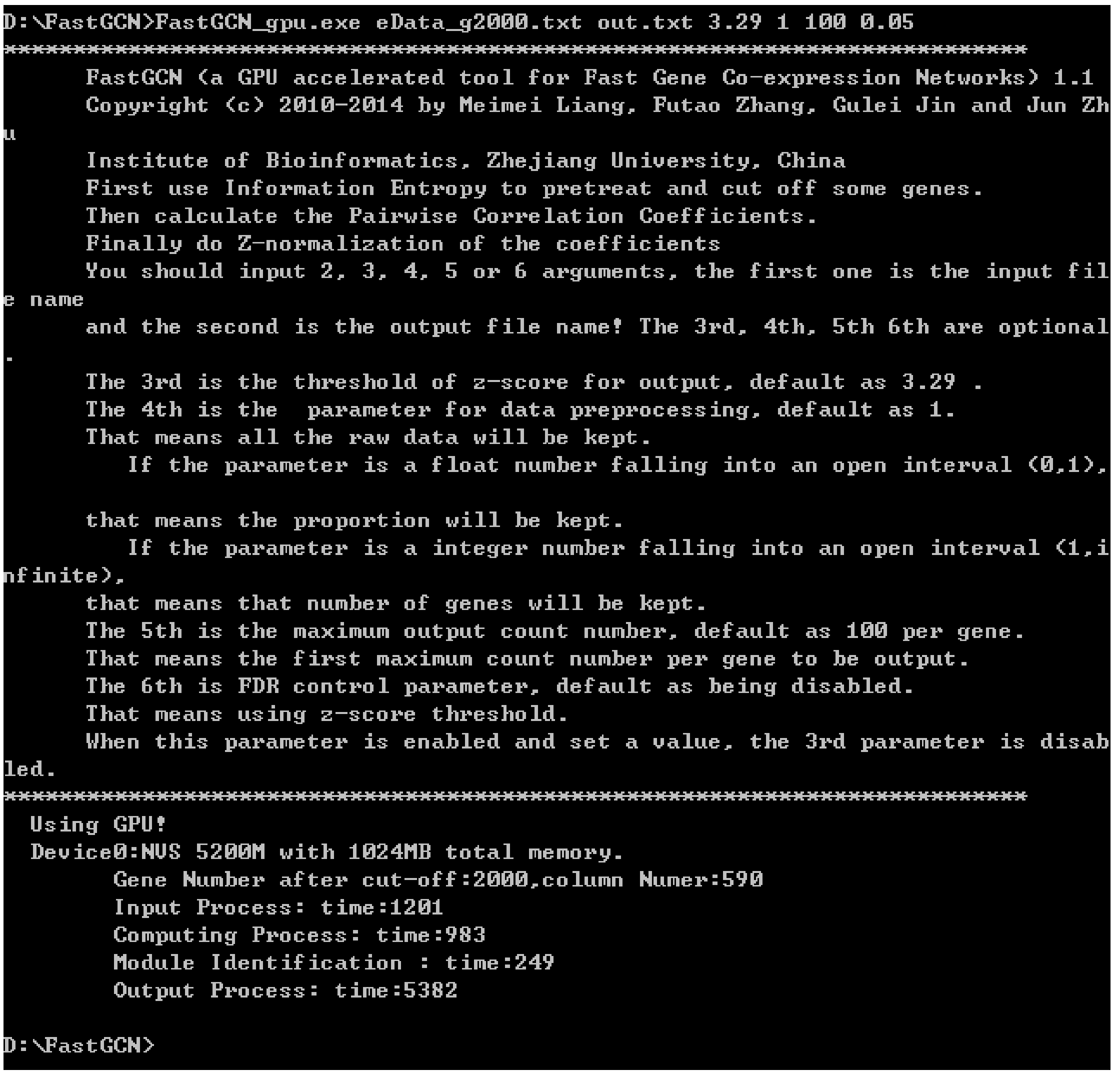
./ FastGCN_gpu para0 para1 para2 para3 para4 para5

para0: The first parameter is the input file name. This parameter is mandatory.
Para1: The second is the output file name. This parameter is mandatory.
Para2: The 3rd is the threshold of z-score for output, default as 3.29. This parameter is optional.
Para3: The 4th is the parameter for data preprocessing, default as 1. That means all the raw data will be kept. If the parameter is a float number falling into an open interval $(0,1)$, that means the proportion will be kept. If the parameter is an integer number falling into an open interval $(1, \infty)$, that means that number of genes will be kept. This parameter is optional.
Para4: The 5th is the maximum output count number, default as 100 per gene. That means the first maximum count number per gene to be output. Maybe too many co-expressions associated with one gene. For the sake of conveniences,

this tool can take maximum output count number per gene as the parameter. This parameter is optional.

Para5: The 6th is FDR control parameter, default as being disabled. That means using z-score threshold. When this parameter is enabled and set a value, the 3rd parameter is disabled. This parameter is optional.

The running example is as below:



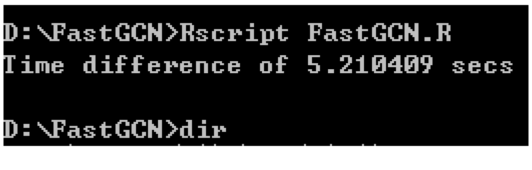
```
D:\FastGCN>FastGCN_gpu.exe eData_g2000.txt out.txt 3.29 1 100 0.05
***************************************************************************
      FastGCN (a GPU accelerated tool for Fast Gene Co-expression Networks) 1.1
      Copyright (c) 2010-2014 by Meimei Liang, Futao Zhang, Gulei Jin and Jun Zh
u
      Institute of Bioinformatics, Zhejiang University, China
      First use Information Entropy to pretreat and cut off some genes.
      Then calculate the Pairwise Correlation Coefficients.
      Finally do Z-normalization of the coefficients
      You should input 2, 3, 4, 5 or 6 arguments, the first one is the input fil
e name
      and the second is the output file name! The 3rd, 4th, 5th 6th are optional
.
      The 3rd is the threshold of z-score for output, default as 3.29 .
      The 4th is the  parameter for data preprocessing, default as 1.
      That means all the raw data will be kept.
         If the parameter is a float number falling into an open interval (0,1),

      that means the proportion will be kept.
         If the parameter is a integer number falling into an open interval (1,i
nfinite),
      that means that number of genes will be kept.
      The 5th is the maximum output count number, default as 100 per gene.
      That means the first maximum count number per gene to be output.
      The 6th is FDR control parameter, default as being disabled.
      That means using z-score threshold.
      When this parameter is enabled and set a value, the 3rd parameter is disab
led.
***************************************************************************
  Using GPU!
  Device0:NVS 5200M with 1024MB total memory.
        Gene Number after cut-off:2000,column Numer:590
        Input Process: time:1201
        Computing Process: time:983
        Module Identification : time:249
        Output Process: time:5382

D:\FastGCN>
```

Because R implementation was designed as the comparison version, currently we can’t take any parameters. If you use this implementation to analysis data, currently you should modify the R source code to set the parameters, the input file name and the output file name. After finishing this, you can run it with R GUI or Rscript.

The running example is as below:



```
D:\FastGCN>Rscript FastGCN.R
Time difference of 5.210409 secs

D:\FastGCN>dir
```

5.4 Output file

Each row of the output file is a co-expression which generally contains the first gene name, the second gene name, the coefficient, the z-score, the P-value and the Q-value. For GPU implementation, Multi-core CPU implementation or Single-thread C/C++ implementation, if you take z-score as the output threshold, P-values and Q-values would not be calculated. So the output file only contains the first gene names, the second gene names, the coefficients and the z-scores. Because of the input parameter 4, the output file may contain one significant pair two times. We call it a dual output model as showing below:

```
Gene1   Gene2   z-score coeff   p-value q-value
HIGD1B  TEK 3.736641    0.557115    0.000093    0.010112
TEK HIGD1B  3.736641    0.557115    0.000093    0.010112
```

For R implementation we output all the information including the first gene name, the second gene name, the coefficient, the z-score, the P-value and the Q-value. And output all the significant pairs within the threshold.

The output file generated by GPU implementation with test data (test_data.txt) is as below (Running Command: FastGCN_gpu.exe test_data.txt out.txt 3.29 1 100 0.05) :

```
Gene1   Gene2   z-score coeff   p-value q-value
BANK1   SELL    4.314422    0.623768    0.000008    0.002625
BANK1   CCL19   3.611350    0.542662    0.000152    0.012378
BANK1   CD160   3.289139    0.505492    0.000503    0.027222
CXCL13  SELL    4.075617    0.596220    0.000023    0.003734
HIGD1B  TEK 3.736641    0.557115    0.000093    0.010112
TEK HIGD1B  3.736641    0.557115    0.000093    0.010112
CD160   BANK1   3.289139    0.505492    0.000503    0.027222
SELL    BANK1   4.314422    0.623768    0.000008    0.002625
SELL    CXCL13  4.075617    0.596220    0.000023    0.003734
SELL    CCL19   3.117817    0.485728    0.000911    0.042300
CCL19   BANK1   3.611350    0.542662    0.000152    0.012378
CCL19   SELL    3.117817    0.485728    0.000911    0.042300
RMND5B  FSIP1   3.439584    0.522847    0.000291    0.018940
FSIP1   RMND5B  3.439584    0.522847    0.000291    0.018940
```

The output file generated by R implementation with test data (test_data.txt) is as below:

```
    gene1    gene2    coeff_pcc  z-score   p_value   q_value
1   TEK      HIGD1B    0.557115  3.736632  9.33E-05  0.010102
2   CD160    BANK1     0.505493  3.289137  0.000502  0.027217
3   SELL     BANK1     0.623767  4.314401  8.00E-06  0.002601
```

4	SELL	CXCL13	0.596219	4.075601	2.29E-05	0.003729
5	CCL19	BANK1	0.542665	3.61137	0.000152	0.012374
6	CCL19	SELL	0.485729	3.117819	0.000911	0.042295
7	FSIP1	RMND5B	0.522847	3.439577	0.000291	0.018935