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/* ### vSDC program ###
* C language
*
*
* Argument 1 is the file containing the table
*
* The table should be formatted as follow :
*
* The line beginning by the character "#" are comment lines.
*
* The columns must be separated by space character.
*
* - First column : compounds name (limited to 50 characters)
* - Next columns : the different scores used
*
* The program accepts up to 12 scores and 1 million
compounds.
*
* Many scoring functions provide a negative score
assimilated to a binding affinity.
*
* Lower values are attributed to compounds with the most
promising affinity.
*
* For this reason, the vSDC program ranked compounds from
lower scores to higher.
*
* Attention : in the case where the score function give
positive value to the most promising
*
* compounds, the data should be pre-processed to have the
opposite value of the score.
*
* - If a score is missing for a given compound, the data must be
replaced by a string where
*
* the first character is 'N' (case sensitive)
*
*
*
* Argument 2 is the number of consensus molecules required by the user.
*
*
*/

#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <math.h>

// file with scores
FILE* fichier = NULL;
// Number of column
int i = 0;
// number of compounds
int num_compounds = 0;

char chaine[100]="";
char *mot = NULL;

double scores[1000000][12];
double sum_score[12];

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double mean[12];
double stdev[12];
double sum_deviation[12];

char compound_name[1000000][50];

int nb_score_valid[12];
double scores_valid[1000000][12];

int j;
int k;

int nb_fct_score = 0;

int main (int argc, char *argv[])
{
    fichier = fopen(argv[1], "r");

    if(fichier != NULL)
    {
        while (fgets(chaine, 1024, fichier) != NULL)
        {

            if(chaine[0]!='#')
            {
                num_compounds++;
                // printf("%d ",num_compounds);
                for(mot = strtok(chaine, " ");mot != NULL;mot = strtok(NULL, " "))
                {
                    i++;

                    // printf("%d %s",i, mot);

                    if(i==1)
                    {
                        strcpy(compound_name[num_compounds],mot);
                        // printf("%s",compound_name[num_compounds]);
                    }
                    else
                    {
                        if(mot[0]=='N')
                        {
                            scores[num_compounds][i-1]=0;
                        }
                        else
                        {
                            scores[num_compounds][i-1]=atof(mot);
                            sum_score[i-1]+=atof(mot);

                            nb_score_valid[i-1]++;
                            scores_valid[nb_score_valid[i-1]][i-1]=atof(mot);
                        }
                        // printf(" %f",scores[num_compounds][i-1]);
                    }
                }
            }
        }
    }
}

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        }

        nb_fct_score=i-1;

        i=0;
        }
//  printf(" %d\n",nb_fct_score);
    }

    else
    {
        printf("ERROR: fail to open the input file.\nArgument 1 must be the
score table and argument 2 must be the number of vSDC top-ranked compound
requested.\nSee the PDF manual for further details.\n");
        exit(0);
    }

/* Calculate means */
for(i=1; i<=nb_fct_score; i++)
{
mean[i]=sum_score[i]/nb_score_valid[i];
}

/* Calculate SD */
for(i=1; i<=nb_fct_score; i++)
{
    for(j=1;j<=nb_score_valid[i];j++)
    {
//printf("toto %d %f\n",i,scores_valid[j][i]);
        sum_deviation[i] += ( scores_valid[j][i]-mean[i] ) * (
scores_valid[j][i]-mean[i] );
    }

stdev[i] = sqrtl( sum_deviation[i] / (double)nb_score_valid[i] );

}

printf("#Prog                Mean        SD\n");

for(i=1; i<=nb_fct_score; i++)
{
printf("#%-30d %8.3f %8.3f\n",i,mean[i],stdev[i]);
}

int num_consensus_identifie = 0;

double start_sd = 3.5;

int consensus = 0;

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int table_consensus[1000000];

int numerote_cons = 0;

printf("\n### Consensus compounds ###\n\n");
printf("#1-Rank      2-vSDC      3-Compound-ID      4 to 15 =>
Scores\n");

int number_cons_asked = atoi(argv[2]);
//int number_cons_asked = 50;

while(num_consensus_identifie<number_cons_asked)
{
    for(i=1;i<=num_compounds;i++)
    {
        for(j=1;j<=nb_fct_score; j++)
        {
            if(scores[i][j]<=mean[j]-start_sd*stdev[j])
            {
                consensus++;
            }
        }
        if(consensus==nb_fct_score && table_consensus[i]!=1)
        {
            num_consensus_identifie++;
            table_consensus[i]=1;
            numerote_cons++;
            printf("%-7d   %8.3f       %s
", numerote_cons, start_sd, compound_name[i]);

            // Printf score iteratif

            for(k=1;k<=nb_fct_score;k++){
                printf(" %8.3f", scores[i][k]);
            }

            printf("\n");
            //

        }
        consensus = 0;
    }

start_sd -= 0.001;

}

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return 0;  
}
```