

Description of the algorithms:

N is the total number of genes (or interchangeably probes) on the microarray platform used.
An index from 0 to N-1 uniquely specifies one of the N genes.

R is a reference gene expression profile

It is represented by a 1D integer array of length N

The array index specifies the gene, while the integer value gives the signed rank of the gene

T is a refset, ie, a set of n individual reference profiles; n is also referred to as setSize

s is a query gene signature of length m

where m is the number of genes included in the gene signature

A gene signature is represented by two integer arrays of length m.

One array contains integers from 0 to N-1, indicating which genes are included in this gene signature

The other array contains +1 or -1, indicating the up- or down- regulation status of the corresponding genes.

N_rdmSIGs is the total number of random signatures for each p value estimation, which is usually set as 10,000 or 100,000.

The following pseudo code describes the key process in sscMap

```
For (each refset T) {
  For (each query signature s){

    observed_score = connection score between T and s according to Eq(6) in Zhang&Gant2008

    // allocate a real-valued array to hold N_rdmsigs random scores
    float randomscores[N_rdmsigs]

    //////////////////////////////////////
    For(i in 1:N_rdmsigs){

      generate a random gene signature si, represented by two integer arrays of length m,
      One array contains random indexes from 0 to N-1, to indicate
      which genes have been selected into this random gene signature.
      The other array contain +1 or -1, randomly selected to indicate the up- or
      down- status of the corresponding gene.

      randomscores[i]= the connection score between T and si according to Eq(6)Zhang&Gant2008

    }
    //////////////////////////////////////

    compare observed_score against randomscores to get the p value

  }// end of For (each query signature s) loop
}// end of For (each refset T)
```

As can be seen from the pseudo code above, the generation of N_rdmsigs random gene signatures and the calculation of the connection score between each random signature and the refset are carried out sequentially in sscMap. As N_rdmsigs is a very large number (100K normally), this is the most time consuming part of the sscMap program.

In cudaMap, this part of the task (**highlighted in red fonts above**) is parallelised using a GPU device.

In cudaMap we create one random gene signature with m random real numbers U[0,1) (uniformly distributed between 0 and 1) using an algorithm essentially the same as the following.

X[m] is an array of random real numbers uniformly distributed U[0,1)

Status[m] is an array of integers +1 or -1, indicating the up- or down- regulation status of m genes

Indexes[m] is an array of integers specifying the indexes from 0 to N-1

```
For(k in 1:m){
    If(X[k]<0.5) Status[k]=1 // this gene is up-regulated
    Else Status[k]=-1 // otherwise it is down-regulated
    // X[k] is also used to select a gene from N
    X[k]=X[k]*2.0
    If(X[k]>=1.0) X[k]=X[k]-1.0
    Indexes[k]= integer (N*X[k])
}
```

To generate N_rdmsigs random gene signatures of length m, a total m*N_rdmsigs uniformly distributed real numbers are required.

The following pseudo code describes the algorithm for the key task

```
// allocate memory space on cuda device to hold a total m*N_rdmsigs random number U[0,1)
// allocate memory space on cuda device to hold N_rdmsigs random connection scores

float *device_randomValues, *device_randomScores;
CUDA_CHECK_RETURN(cudaMalloc((void **) &device_randomValues, sizeof(float) * m*N_rdmsigs));
CUDA_CHECK_RETURN(cudaMalloc((void **) &device_randomScores, sizeof(float) * N_rdmsigs));

// Create an array of uniformly distributed random numbers between 0 and 1,
// curandGenerator_t gen;
```

```

// gen is a cuda random number generator, which had been defined and initialized

CUDA_CHECK_STATUS(curandGenerateUniform(gen, device_randomValues, m*N_rdmsigs));
// now device_randomValues holds an array of m*N_rdmsigs random U[0,1) real numbers.

////////////////////////////////////
// Compute the connection scores of the N_rdmsigs random gene signatures with the Refset T
// The array device_refRanks stores the (summed) Ranks for the Refset T, which
// had been copied to the CUDA device

int blocksPerGrid = (int)ceil((float)N / (float)threadsPerBlock);
// const int threadsPerBlock = 128 had been defined elsewhere

computeRandomConnectionScores <<< blocksPerGrid, threadsPerBlock >>>(device_randomValues,
    device_refRanks , device_randomScores);

// see the pseudo codes below for more detailed steps within the function above
////////////////////////////////////

CUDA_CHECK_RETURN(cudaThreadSynchronize());
// the N_rdmsigs random scores are now stored in the array device_randomScores

// copy these random scores from device memory to main memory
float randomScores[N_rdmsigs];
CUDA_CHECK_RETURN(cudaMemcpy(randomScores, device_randomScores,
    N_rdmsigs * sizeof(float), cudaMemcpyDeviceToHost));

// Then Compute the p-value
pValue = compare_observed_score_against_the_distribution_of_randomScores

```

The following pseudo code gives more details on the computing of random scores on the GPU

```
float temp = 0.0;
int idx = blockIdx.x * blockDim.x + threadIdx.x;
if (idx < N_rdmsigs) {
    int M=m* N_rdmsigs;
    for(int col = idx; col < M; col += N_rdmsigs) {
        float random = device_randomValues[col];
        float regulationStatus = 1.0;
        if (random >= 0.5) {
            regulationStatus = -regulationStatus;
            random = random - 0.5;
        }
        // now random is a real number in [0,0.5)
        // Scale up random to become an integer index < N
        int rangeInArray = __float2int_rd(random * N * 2);

        // Add the contribution to the connection strength
        temp += device_refRanks[rangeInArray] * regulationStatus;
    }

    // Normalizing by appropriate factors UCmax and setSize
    // UCmax is defined by Eq.(3) in Zhang&Gant2008; setSize refers to the n in Eq.(6).
    device_randomScores[idx] = temp / UCmax /setSize;
} //end of if (idx < N_rdmsigs)
```