Modularity Maximization

$$\Delta Q = \frac{1}{2} s^T \hat{B}[g] s = \frac{1}{2} \sum_{i=1}^{n_g} s_i \left(\sum_{j=1}^{n_g} \hat{B}[g]_{i,j} s_j \right)$$

$$s'_i = \begin{cases} s_i & i \neq k \\ -s_i & i = k \end{cases}$$

$$\frac{1}{2} s'^T \hat{B}[g] s' = \frac{1}{2} \sum_{i=1}^{n_g} s'_i \left(\sum_{j=1}^{n_g} \hat{B}[g]_{i,j} s'_j \right) = \frac{1}{2} \sum_{i=1}^{n_g} s'_i \left(\left(\sum_{j \in \{1,\ldots,n_g\} \setminus \{k\}} \hat{B}[g]_{i,j} s_j \right) - \hat{B}[g]_{i,k} s_k \right) =$$

$$= \frac{1}{2} \left(\left(\sum_{i \in \{1,\ldots,n_g\} \setminus \{k\}} s_i \left(\left(\sum_{j \in \{1,\ldots,n_g\} \setminus \{k\}} \hat{B}[g]_{i,j} s_j \right) - \hat{B}[g]_{i,k} s_k \right) \right) - s_k \left(\left(\sum_{j \in \{1,\ldots,n_g\} \setminus \{k\}} \hat{B}[g]_{k,j} s_j \right) - \hat{B}[g]_{k,k} s_k \right) \right) =$$

$$= \frac{1}{2} \left(\left(\sum_{i \in \{1,\ldots,n_g\} \setminus \{k\}} s_i \left(\left(\sum_{j=1}^{n_g} \hat{B}[g]_{i,j} s_j \right) - 2\hat{B}[g]_{i,k} s_k \right) \right) - s_k \left(\left(\sum_{j=1}^{n_g} \hat{B}[g]_{k,j} s_j \right) - 2\hat{B}[g]_{k,k} s_k \right) \right) =$$

$$= \frac{1}{2} \left(\left(\sum_{i=1}^{n_g} s_i \left(\left(\sum_{j=1}^{n_g} \hat{B}[g]_{i,j} s_j \right) - 2\hat{B}[g]_{i,k} s_k \right) \right) - 2s_k \left(\left(\sum_{j=1}^{n_g} \hat{B}[g]_{k,j} s_j \right) - 2\hat{B}[g]_{k,k} s_k \right) \right) =$$

$$= \frac{1}{2} \left(\left(\sum_{i=1}^{n_g} s_i \left(\hat{B}[g] \cdot s - 2\hat{B}[g]_{i,k} s_k \right) \right) - 2s_k \left(\left(\hat{B}[g] \cdot s \right)_k - 2\hat{B}[g]_{k,k} s_k \right) \right) =$$

$$= \frac{1}{2} \left(\sum_{i=1}^{n_g} \left(s_i \hat{B}[g] \cdot s \right) - 2 \sum_{i=1}^{n_g} \left(s_i \hat{B}[g]_{i,k} s_k \right) - 2s_k \left(\hat{B}[g] \cdot s \right)_k + 4 s_k \hat{B}[g]_{k,k} s_k \right) =$$

$$= \frac{1}{2} \left(s^T \hat{B}[g] s - 2s_k \sum_{i=1}^{n_g} \left(s_i \hat{B}[g]_{i,k} \right) - 2s_k \left(\hat{B}[g] \cdot s \right)_k + 4 s_k \hat{B}[g]_{k,k} s_k \right) =$$

$$= \frac{1}{2} \left(s^T \hat{B}[g] s - 2s_k \left(\sum_{i=1}^{n_g} \left(s_i \hat{B}[g]_{i,k} \right) + \left(\hat{B}[g] \cdot s \right)_k - 2\hat{B}[g]_{k,k} s_k \right) \right) =$$

$$= \frac{1}{2} s^T \hat{B}[g] s - s_k \left(\sum_{i=1}^{n_g} \left(s_i \hat{B}[g]_{i,k} \right) + \left(\hat{B}[g] \cdot s \right)_k - 2\hat{B}[g]_{k,k} s_k \right) =$$

$$= \Delta Q + s_k \left(2\hat{B}[g]_{k,k} s_k - \left(\hat{B}[g] \cdot s \right)_k \right) - s_k \sum_{i=1}^{n_g} \left(s_i \hat{B}[g]_{i,k} \right)$$

$$\Longrightarrow \arg\max_{1 \le k \le n_g} \left(\Delta Q \mid_{s'_k = -s_k} - \Delta Q \right) = \arg\max_{1 \le k \le n_g} \left(\Delta Q + s_k \left(2\hat{B}[g]_{k,k} s_k - \left(\hat{B}[g] \cdot s \right)_k \right) - s_k \sum_{i=1}^{n_g} \left(s_i \hat{B}[g]_{i,k} \right) \right) =$$

$$= \arg\max_{1 \le k \le n_g} \left(s_k \left(2\hat{B}[g]_{k,k} s_k - \left(\hat{B}[g] \cdot s \right)_k \right) - s_k \sum_{i=1}^{n_g} \left(s_i \hat{B}[g]_{i,k} \right) \right)$$

so we compute $\hat{B}[g] \cdot s$ once

and find $\arg\max_{1 \le k \le n_g} \left(s_k \left(2\hat{B}[g]_{k,k} s_k - \left(\hat{B}[g] \cdot s \right)_k \right) - s_k \sum_{i=1}^{n_g} \left(s_i \hat{B}[g]_{i,k} \right) \right)$ by iteraiting once over $\hat{B}[g]$

pseodo-code:

input: $\left(s, \hat{B}[g]\right)$, output: s'

$bestS \leftarrow s$

$bestM \leftarrow s^T \hat{B}[g] s$

$s' \leftarrow s$

do

  $s \leftarrow bestS$

  $M \leftarrow bestM$

  hasMoved$\leftarrow (0)_{i=1}^{n_g}$

  moved$\leftarrow 0$

  while moved$< n_g$

    $b_s \leftarrow \hat{B}[g] \cdot s$

    init $\delta \leftarrow \left(s_k \left(2\hat{B}[g]_{k,k} s_k - (b_s)_k\right)\right)_{k=1}^{n_g}$

    for $1 \leq i, j \leq n_g$

      $\delta[j] \leftarrow \delta[j] - s_j s_i \hat{B}[g]_{i,j}$

    $M \leftarrow M + \max_{1 \leq k \leq n_g \wedge \text{hasMoved}[k]=0} \delta[k]$

    $K \leftarrow \underset{1 \leq k \leq n_g \wedge \text{hasMoved}[k]=0}{\arg\max} \delta[k]$

    $s'_i \leftarrow \begin{cases} s_i & i \neq K \\ -s_i & i = K \end{cases}$

    hasMoved$[K] \leftarrow 1$

    moved $\leftarrow$ moved $+ 1$

    if $M > bestM$:

      $bestS \leftarrow s'$

      $bestM \leftarrow M$

while $bestS$ $!=$ s

return $bestS$