Algorithm convergence

THEOREM 1. Given matrix $H$ and vector $d$, the algorithm converges. The number of iteration depends on parameters $\alpha$ and $\varepsilon$.

PROOF. The convergence of the algorithm depends on Equation (6). Equation (6) converges if and only if $\rho(aH) < 1$, where $\rho(aH)$ is the spectral radius of matrix $aH$.

Since $h(i, j) \geq 0$ and for each row $i$ of matrix $H$, either $\sum_{j \in \text{Ne}(i)} h(i, j) = 1$ or $\sum_{j \in \text{Ne}(i)} h(i, j) = 0$.

$$\rho(H) = \|H\|_1 = 1.$$ It is easy to see that $\rho(aH) = a\rho(H) < 1$ for $0 \leq \alpha < 1$.

Therefore, Equation (6) converges and so does the algorithm. Furthermore, according to Equation (6),

$$pr'^t = (1 - \alpha)d + aH \ast pr'^{t-1}$$

$$pr^{t-1} = (1 - \alpha)d + aH \ast pr'^{t-2}$$

And thus, we have

$$pr' - pr'^{t-1} = aH(pr'^{t-1} - pr'^{t-2}) = \cdots = (aH)^{t-1}(pr^1 - pr^0) = (aH)^{t-1}[\alpha(H - I)d]$$

Therefore

$$\|pr' - pr'^{t-1}\| = \|(aH)^{t-1}(pr^1 - pr^0)\| = \|(aH)^{t-1}[\alpha(H - I)d]\| \leq \alpha^t\|(H - I)d\| \leq \varepsilon,$$

and

$$t \geq \log[\varepsilon / \|(H - I)d\|] / \log \alpha$$

Clearly, given matrix $H$ and vector $d$, the iteration times $t$ depends on parameter $\alpha$ and $\varepsilon$.

To investigate the influence of the parameter $\alpha$ and $\varepsilon$ on the number of iterations which are needed to converge, firstly, taking $\varepsilon = 10^{-8}$ we compare the number of iterations required to converge by setting different values of $\alpha$, ranging from 0.5 to 0.999. The results are tabulated in Table 1. As shown in Table 1, for $\alpha = 0.5$, the
algorithm needs only 28 iterations to converge to a tolerance of $10^{-8}$. For $\alpha = 0.8$, the number of iterations increases to 80. For $\alpha = 0.999$, the number of iterations rise sharply up to 1615, which is about 58 times larger than for $\alpha = 0.5$. So parameter $\alpha$ can indeed control the convergence rate of the algorithm.

To investigate the influence of the parameter $\varepsilon$ on the convergence, we compare the iterations by setting $\varepsilon$ different values ranging from $10^{-2}$ to $10^{-13}$ for $\alpha = 0.5, 0.7, 0.8, 0.9$, respectively. Figure 1 shows that no matter what the value of $\alpha$ is, with the decrease of $\varepsilon$ the number of iterations increases slowly. When the value of $\varepsilon$ is $10^{-13}$, which is $10^{-11}$ times smaller than $10^{-2}$, the number of iterations required for convergence only increases about 4 times. Compared with $\alpha$, the effect of $\varepsilon$ on the iteration is smaller. In fact, $\varepsilon$ controls the precision of $pr$ values. The smaller the $\varepsilon$ value is, the more precise the $pr$ values are. In order to distinguish the ranking scores of proteins, a suitable value of $\varepsilon$ should be set. However, the exact values of the $pr$ vector are not as important as the correct ordering of the values in the vector.

Moreover, the algorithm needs more time to converge, if the value of $\varepsilon$ is too small. Compromising the convergence of the algorithm and the precision of $pr$ values, the parameter $\varepsilon$ is set as $10^{-8}$ in this study.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>0.5</th>
<th>0.6</th>
<th>0.7</th>
<th>0.8</th>
<th>0.9</th>
<th>0.99</th>
<th>0.999</th>
</tr>
</thead>
<tbody>
<tr>
<td>number of iterations</td>
<td>28</td>
<td>37</td>
<td>52</td>
<td>80</td>
<td>160</td>
<td>900</td>
<td>1615</td>
</tr>
</tbody>
</table>

The table shows the relationship between the values of parameter $\alpha$ and the number of iterations required to converge.

Table 1 - Effect of parameter $\alpha$ on the number of iterations
Figure 1 - Number of iterations needed for ION convergence with different parameter $\varepsilon$. 

X-axis represents the values of parameter $\varepsilon$. Y-axis represents the number of iterations needed for ION convergence.