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[Supplementary Material] Disease gene prioritization by integrating tissue-specific molecular networks using a robust multi-network model

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Summary

In this supplementary material, we provide the matrix form of J_{CR}, the optimization solution to J_{CR}, the algorithm and the theoretical analysis of CR.

Algorithm CR

Algorithm 1: CR

Input: (1) a disease similarity network $\mathbf{A}$; (2) the tissue-specific molecular networks $\{\mathbf{G}_i\}$; (3) the seed vectors $\{\mathbf{e}_i\}$; and (4) the parameters β and c
Output: the ranking vectors $\mathbf{r}_1, ..., \mathbf{r}_h$

Offline-computation: Construct $\tilde{\mathbf{G}}$ and $\tilde{\mathbf{Y}}$ from $\mathbf{A}$ and $\{\mathbf{G}_i\}$;
Online-ranking:
Construct the aggregated seed vector $\mathbf{e} = (\mathbf{e}_1^T, ..., \mathbf{e}_h^T)^T$;
Initialize the aggregated ranking vector $\mathbf{r} = \mathbf{e}$;
while *not convergence* **do**
  Update: $\mathbf{r} \leftarrow (\frac{c}{1+2\beta}\tilde{\mathbf{G}} + \frac{2\beta}{1+2\beta}\tilde{\mathbf{Y}})\mathbf{r} + \frac{1-c}{1+2\beta}\mathbf{e}$;
end
return the ranking vectors $\mathbf{r}_1, ..., \mathbf{r}_h$ based on $\mathbf{r}$

Complexity Analysis of CR

Let n_i be the number of nodes in $\mathbf{G}_i$ and $n = \sum_{i=1}^{h} n_i$. Let m_i be the number of edges in $\mathbf{G}_i$ and $m = \sum_{i=1}^{h} m_i$. There are $O(m + hn)$ nonzero entries in $\tilde{\mathbf{G}}$ and $\tilde{\mathbf{Y}}$ in total. Thus the offline-computation and online-ranking time complexities of Algorithm 1 are $O(m+hn)$ and $O(T^*(m+hn))$, respectively, where T^* is the total number of iterations. Since we need to store $\tilde{\mathbf{G}}$ and $\tilde{\mathbf{Y}}$, thus the space complexity is $O(m + hn)$.

Generally, h is much smaller than n and can be regarded as constants. Hence we can regard the time and space complexities of Algorithm 1 as $O(T^*(m + n))$ and $O(m + n)$, respectively.

Matrix Form of J_{CR}

The objective function J_{CR} is jointly convex in $\mathbf{r}_1, ..., \mathbf{r}_h$. This can be shown by first deriving its matrix form.

Let $\mathbf{r} = (\mathbf{r}_1^T, ..., \mathbf{r}_h^T)^T$, $\mathbf{e} = (\mathbf{e}_1^T, ..., \mathbf{e}_h^T)^T$, i.e., we concatenate all ranking and seed vectors. Let $\tilde{\mathbf{G}} = \text{diag}(\tilde{\mathbf{G}}_1, ..., \tilde{\mathbf{G}}_h)$ be a diagonal block matrix. Then we have

$$c\mathbf{r}^T(\mathbf{I}_n - \tilde{\mathbf{G}})\mathbf{r} + (1-c)\|\mathbf{r} - \mathbf{e}\|_F^2 = \sum_{i=1}^{h} \Theta_{\text{within}}(\mathbf{r}_i) \tag{1}$$

where $\mathbf{I}_n$ is an $n \times n$ identity matrix and $n = \sum_{i=1}^{h} n_i$.

Define a common gene mapping matrix $\mathbf{O}_{ij} \in \{0,1\}^{n_i \times n_j}$ where $\mathbf{O}_{ij}(x,y) = 1$ if node x in $\mathbf{G}_i$ and node y in $\mathbf{G}_j$ represent the same gene; $\mathbf{O}_{ij} = 0$ otherwise. Then $\mathbf{Y}$ is a block matrix whose $(i,j)^{\text{th}}$ block is $\mathbf{A}(i,j)\mathbf{O}_{ij}$. Note that $\mathbf{A}(i,i) = 0$. Further, let $\mathbf{D}_{\mathbf{V}} = \text{diag}(d_{\mathbf{A}}(1)\mathbf{I}_{n_1}, ..., d_{\mathbf{A}}(h)\mathbf{I}_{n_h})$ be a diagonal matrix, where $d_{\mathbf{A}}(i) = \sum_{j=1}^{h} \mathbf{A}(i,j)$. We define $\mathbf{X} = \mathbf{D}_{\mathbf{V}}^{-\frac{1}{2}}(\mathbf{D}_{\mathbf{V}} - \mathbf{Y})\mathbf{D}_{\mathbf{V}}^{-\frac{1}{2}} = \mathbf{I}_n - \tilde{\mathbf{Y}}$, where $\tilde{\mathbf{Y}} = \mathbf{D}_{\mathbf{V}}^{-\frac{1}{2}}\mathbf{Y}\mathbf{D}_{\mathbf{V}}^{-\frac{1}{2}}$. We have

$$\mathbf{r}^T\mathbf{X}\mathbf{r} = \frac{1}{2}\sum_{i,j=1}^{h} \Theta_{\text{cross}}(\mathbf{r}_i, \mathbf{r}_j) \tag{2}$$

According to Eq. (1) and Eq. (2), we have the following theorem.

Theorem 1 ***Matrix Form of J_{CR}.*** *J_{CR} has the following matrix form*

$$\min_{\mathbf{r} \geq 0} J_{CR} = c\mathbf{r}^T(\mathbf{I}_n - \tilde{\mathbf{G}})\mathbf{r} + (1-c)\|\mathbf{r} - \mathbf{e}\|_F^2 + 2\beta\mathbf{r}^T\mathbf{X}\mathbf{r} \tag{3}$$

Proof The proof of Theorem 1 includes two equivalence validations:

(1) $c\mathbf{r}^T(\mathbf{I}_n - \tilde{\mathbf{G}})\mathbf{r} + (1-c)\|\mathbf{r} - \mathbf{e}\|_F^2 = \sum_{i=1}^{h} \Theta_{\text{within}}(\mathbf{r}_i)$

(2) $\mathbf{r}^T\mathbf{X}\mathbf{r} = \frac{1}{2}\sum_{i,j=1}^{h} \Theta_{\text{cross}}(\mathbf{r}_i, \mathbf{r}_j)$

Since the equivalence (1) is obvious, we only need to prove the equivalence (2).

According to the definition of $\mathbf{X}$ and $\mathbf{r}$, we have

$$\mathbf{r}^T\mathbf{X}\mathbf{r} = \mathbf{r}^T\mathbf{I}_n\mathbf{r} - \mathbf{r}^T\tilde{\mathbf{Y}}\mathbf{r} = \sum_{i=1}^{h} \mathbf{r}_i^T\mathbf{I}_{n_i}\mathbf{r}_i - \sum_{i,j=1}^{h} \mathbf{r}_i^T\tilde{\mathbf{Y}}_{ij}\mathbf{r}_j \tag{4}$$

where $\tilde{\mathbf{Y}}_{ij} \in \mathbb{R}_+^{n_i \times n_j}$ is the $(i,j)^{\text{th}}$ block of $\tilde{\mathbf{Y}}$. Note $\tilde{\mathbf{Y}}_{ii} = \mathbf{0}$ $(1 \leq i \leq h)$. Then let $(\mathbf{D}_{\mathbf{V}})_i$ be the i^{th} diagonal block of $\mathbf{D}_{\mathbf{V}}$ and $\mathbf{Y}_{ij}$ be the $(i,j)^{\text{th}}$ block of $\mathbf{Y}$. Recall $\mathbf{Y}_{ij} = \mathbf{A}(i,j)\mathbf{O}_{ij}$. We have

$$\mathbf{r}^T\mathbf{X}\mathbf{r} = \frac{1}{2}\Big(\sum_{i=1}^{h} \frac{\mathbf{r}_i^T}{\sqrt{d_{\mathbf{A}}(i)}}(\mathbf{D}_{\mathbf{V}})_i\frac{\mathbf{r}_i}{\sqrt{d_{\mathbf{A}}(i)}} - 2\sum_{i,j=1}^{h} \frac{\mathbf{r}_i^T}{\sqrt{d_{\mathbf{A}}(i)}}\mathbf{Y}_{ij}\frac{\mathbf{r}_j}{\sqrt{d_{\mathbf{A}}(j)}} + \sum_{j=1}^{h} \frac{\mathbf{r}_j^T}{\sqrt{d_{\mathbf{A}}(j)}}(\mathbf{D}_{\mathbf{V}})_j\frac{\mathbf{r}_j}{\sqrt{d_{\mathbf{A}}(j)}}\Big)$$

Let $\mathbf{D}_{\mathbf{Y}}$ be the degree matrix of $\mathbf{Y}$ and $(\mathbf{D}_{\mathbf{Y}})_i$ be the i^{th} diagonal block of $\mathbf{D}_{\mathbf{Y}}$. Define $\mathbf{D}_{\mathbf{Y}_{ij}}$ to be the degree matrix of $\mathbf{Y}_{ij}$ (note the nonzero diagonal values of $\mathbf{D}_{\mathbf{Y}_{ij}}$ are $\mathbf{A}(i,j)$). Then $(\mathbf{D}_{\mathbf{Y}})_i = \sum_{j=1}^{h} \mathbf{D}_{\mathbf{Y}_{ij}}$. Define $\bar{\mathbf{D}}_{\mathbf{Y}_{ij}}$ to be an $n_i \times n_i$ diagonal matrix s.t. $\mathbf{D}_{\mathbf{Y}_{ij}} + \bar{\mathbf{D}}_{\mathbf{Y}_{ij}} = \mathbf{A}(i,j)\mathbf{I}_{n_i}$. Then let $(\bar{\mathbf{D}}_{\mathbf{Y}})_i = \sum_{j=1}^{h} \bar{\mathbf{D}}_{\mathbf{Y}_{ij}}$, we have $(\mathbf{D_V})_i = (\mathbf{D_Y} + \bar{\mathbf{D}}_\mathbf{Y})_i$. Thus

$$\begin{aligned}
\mathbf{r}^T\mathbf{X}\mathbf{r} &= \frac{1}{2}\Big(\sum_{i=1}^{h} \frac{\mathbf{r}_i^T}{\sqrt{d_\mathbf{A}(i)}}(\mathbf{D_Y}+\bar{\mathbf{D}}_\mathbf{Y})_i \frac{\mathbf{r}_i}{\sqrt{d_\mathbf{A}(i)}} - 2\sum_{i,j=1}^{h}\frac{\mathbf{r}_i^T}{\sqrt{d_\mathbf{A}(i)}}\mathbf{Y}_{ij}\frac{\mathbf{r}_j}{\sqrt{d_\mathbf{A}(j)}} \\
&+ \sum_{j=1}^{h}\frac{\mathbf{r}_j^T}{\sqrt{d_\mathbf{A}(j)}}(\mathbf{D_Y}+\bar{\mathbf{D}}_\mathbf{Y})_j\frac{\mathbf{r}_j}{\sqrt{d_\mathbf{A}(j)}}\Big) \\
&= \frac{1}{2}\Big(\sum_{i,j=1}^{h}\frac{\mathbf{r}_i^T}{\sqrt{d_\mathbf{A}(i)}}\mathbf{D}_{\mathbf{Y}_{ij}}\frac{\mathbf{r}_i}{\sqrt{d_\mathbf{A}(i)}} - 2\sum_{i,j=1}^{h}\frac{\mathbf{r}_i^T}{\sqrt{d_\mathbf{A}(i)}}\mathbf{Y}_{ij}\frac{\mathbf{r}_j}{\sqrt{d_\mathbf{A}(j)}} \\
&+ \sum_{j,i=1}^{h}\frac{\mathbf{r}_j^T}{\sqrt{d_\mathbf{A}(j)}}\mathbf{D}_{\mathbf{Y}_{ji}}\frac{\mathbf{r}_j}{\sqrt{d_\mathbf{A}(j)}} + \sum_{i,j=1}^{h}\frac{\mathbf{r}_i^T}{\sqrt{d_\mathbf{A}(i)}}\bar{\mathbf{D}}_{\mathbf{Y}_{ij}}\frac{\mathbf{r}_i}{\sqrt{d_\mathbf{A}(i)}} + \sum_{j,i=1}^{h}\frac{\mathbf{r}_j^T}{\sqrt{d_\mathbf{A}(j)}}\bar{\mathbf{D}}_{\mathbf{Y}_{ji}}\frac{\mathbf{r}_j}{\sqrt{d_\mathbf{A}(j)}}\Big) \\
&= \frac{1}{2}\sum_{i,j=1}^{h}\mathbf{A}(i,j)\Big(\frac{\mathbf{r}_i^T(\mathcal{I}_{ij})}{\sqrt{d_\mathbf{A}(i)}}\frac{\mathbf{r}_i(\mathcal{I}_{ij})}{\sqrt{d_\mathbf{A}(i)}} - 2\frac{\mathbf{r}_i^T(\mathcal{I}_{ij})}{\sqrt{d_\mathbf{A}(i)}}\frac{\mathbf{r}_j(\mathcal{I}_{ij})}{\sqrt{d_\mathbf{A}(j)}} + \frac{\mathbf{r}_j^T(\mathcal{I}_{ij})}{\sqrt{d_\mathbf{A}(j)}}\frac{\mathbf{r}_j(\mathcal{I}_{ij})}{\sqrt{d_\mathbf{A}(j)}} \\
&+ \frac{\mathbf{r}_i^T(\bar{\mathcal{I}}_{ij})}{\sqrt{d_\mathbf{A}(i)}}\frac{\mathbf{r}_i(\bar{\mathcal{I}}_{ij})}{\sqrt{d_\mathbf{A}(i)}} + \frac{\mathbf{r}_j^T(\bar{\mathcal{I}}_{ji})}{\sqrt{d_\mathbf{A}(j)}}\frac{\mathbf{r}_j(\bar{\mathcal{I}}_{ji})}{\sqrt{d_\mathbf{A}(j)}}\Big) \\
&= \frac{1}{2}\sum_{i,j=1}^{h}\mathbf{A}(i,j)\Big(\|\frac{\mathbf{r}_i(\mathcal{I}_{ij})}{\sqrt{d_\mathbf{A}(i)}} - \frac{\mathbf{r}_j(\mathcal{I}_{ij})}{\sqrt{d_\mathbf{A}(j)}}\|_F^2 + \|\frac{\mathbf{r}_i(\bar{\mathcal{I}}_{ij})}{\sqrt{d_\mathbf{A}(i)}}\|_F^2 + \|\frac{\mathbf{r}_j(\bar{\mathcal{I}}_{ji})}{\sqrt{d_\mathbf{A}(j)}}\|_F^2\Big) \\
&= \frac{1}{2}\sum_{i,j=1}^{h}\Theta_{\text{cross}}(\mathbf{r}_i,\mathbf{r}_j)
\end{aligned}$$

This completes the proof. □

Optimization Solution to $\mathrm{J_{CR}}$

From Theorem 1, $\mathrm{J_{CR}}$ is a quadratic function of $\mathbf{r}$. We can derive a power method to minimize $\mathrm{J_{CR}}$ as follows.

$$\frac{\partial \mathrm{J_{CR}}}{\partial \mathbf{r}} = 2\Big((1+2\beta)\mathbf{I}_n - (c\tilde{\mathbf{G}} + 2\beta\tilde{\mathbf{Y}})\Big)\mathbf{r} - 2(1-c)\mathbf{e}$$

Using gradient descent, if we set $\mathbf{r} \leftarrow \mathbf{r} - \eta\frac{\partial \mathrm{J_{CR}}}{\partial \mathbf{r}}$, where $\eta = \frac{1}{2(1+2\beta)}$, we have

$$\mathbf{r} \leftarrow \Big(\frac{c}{1+2\beta}\tilde{\mathbf{G}} + \frac{2\beta}{1+2\beta}\tilde{\mathbf{Y}}\Big)\mathbf{r} + \frac{1-c}{1+2\beta}\mathbf{e} \tag{5}$$

Eq. (5) is a fixed-point approach to compute $\mathbf{r}$ that converges to the global optimal solution of $\mathrm{J_{CR}}$. Algorithm 1 summarizes our approach according to the optimization solution.

Theoretical Analysis of CR

In this section, we show that Algorithm 1 converges to the global minimum of $\mathrm{J_{CR}}$ by Theorem 2 and Theorem 3.

Theorem 2 ***Convergence of* CR.** *Algorithm 1 converges to the closed-form solution*

$$\mathbf{r} = (\mathbf{I}_n - \frac{c}{1+2\beta}\tilde{\mathbf{G}} - \frac{2\beta}{1+2\beta}\tilde{\mathbf{Y}})^{-1}\frac{1-c}{1+2\beta}\mathbf{e}$$

Proof First, the closed-form solution can be obtained by solving $\frac{\partial \mathrm{J_{CR}}}{\partial \mathbf{r}} = 0$. Then let $\mathbf{M} = \frac{c}{1+2\beta}\tilde{\mathbf{G}} + \frac{2\beta}{1+2\beta}\tilde{\mathbf{Y}}$, the CR updating rule in Eq. (5) becomes $\mathbf{r} = \mathbf{M}\mathbf{r} + \frac{1-c}{1+2\beta}\mathbf{e}$. Next, we show that the eigenvalues of $\mathbf{M}$ are in the range of $(-1, 1)$.

Let $\mathbf{G} = \mathrm{diag}(\mathbf{G}_1, ..., \mathbf{G}_h)$ and $\mathbf{D_G}$ be its degree matrix, then $\tilde{\mathbf{G}} = \mathbf{D}_{\mathbf{G}}^{-\frac{1}{2}}\mathbf{G}\mathbf{D}_{\mathbf{G}}^{-\frac{1}{2}}$. Since $\tilde{\mathbf{G}}$ is similar to the stochastic matrix $\mathbf{G}\mathbf{D}_{\mathbf{G}}^{-1} = \mathbf{D}_{\mathbf{G}}^{\frac{1}{2}}\tilde{\mathbf{G}}\mathbf{D}_{\mathbf{G}}^{-\frac{1}{2}}$, it has eigenvalues within $[-1, 1]$. Also, $\tilde{\mathbf{Y}}$ is similar to the matrix $\mathbf{Y}\mathbf{D}_{\mathbf{V}}^{-1} = \mathbf{D}_{\mathbf{V}}^{\frac{1}{2}}\tilde{\mathbf{Y}}\mathbf{D}_{\mathbf{V}}^{-\frac{1}{2}}$ where each column sum of $\mathbf{Y}\mathbf{D}_{\mathbf{V}}^{-1}$ is no greater than 1.

The Gershgorin Circle Theorem [1] states that for a complex $n \times n$ matrix $\mathbf{B}$, every eigenvalue λ of $\mathbf{B}$ lies within at least one of the Gershgorin discs $\{\lambda : |\lambda - b_{ii}| \leq \sum_{j=1, j\neq i}^{n} |b_{ji}|\}$ $(i = 1, ..., n)$, where b_{ii} is the i^{th} diagonal value of $\mathbf{B}$ and b_{ji} is the $(j, i)^{\mathrm{th}}$ entry of $\mathbf{B}$. Since $\mathbf{A}(i, i) = 0$ for $i = 1, ..., h$, the diagonal values of $\mathbf{Y}$ are zero. Therefore, the eigenvalues of $\mathbf{Y}\mathbf{D}_{\mathbf{V}}^{-1}$ satisfy $|\lambda| \leq 1$, which implies the eigenvalues of $\tilde{\mathbf{Y}}$ are within $[-1, 1]$.

One result of the Weyl's Inequality Theorem [2] states that for matrices $\hat{\mathbf{H}}, \mathbf{H}, \mathbf{P} \in \mathcal{H}_n$, where $\mathcal{H}_n$ is the set of $n \times n$ Hermitian matrices, if $\hat{\mathbf{H}} = \mathbf{H} + \mathbf{P}$ and their eigenvalues are arranged in non-increasing orders, i.e., $\lambda_1(\hat{\mathbf{H}}) \geq ... \geq \lambda_n(\hat{\mathbf{H}})$, $\lambda_1(\mathbf{H}) \geq ... \geq \lambda_n(\mathbf{H})$, $\lambda_1(\mathbf{P}) \geq ... \geq \lambda_n(\mathbf{P})$, then the following inequalities hold:

$$\lambda_n(\mathbf{P}) \leq \lambda_i(\hat{\mathbf{H}}) - \lambda_i(\mathbf{H}) \leq \lambda_1(\mathbf{P}), \forall i = 1, ..., n$$

Since $\tilde{\mathbf{G}}, \tilde{\mathbf{Y}}, \mathbf{M} \in \mathcal{H}_n$ and $\mathbf{M} = \frac{c}{1+2\beta}\tilde{\mathbf{G}} + \frac{2\beta}{1+2\beta}\tilde{\mathbf{Y}}$, we have

$$\lambda_1(\mathbf{M}) \leq \frac{c}{1+2\beta}\lambda_1(\tilde{\mathbf{G}}) + \frac{2\beta}{1+2\beta}\lambda_1(\tilde{\mathbf{Y}})$$
$$\lambda_n(\mathbf{M}) \geq \frac{c}{1+2\beta}\lambda_n(\tilde{\mathbf{G}}) + \frac{2\beta}{1+2\beta}\lambda_n(\tilde{\mathbf{Y}})$$

which means the eigenvalues of $\mathbf{M}$ are in the range of $[-\frac{c+2\beta}{1+2\beta}, \frac{c+2\beta}{1+2\beta}]$. Since $0 < c < 1$, the eigenvalues of $\mathbf{M}$ are in the range of $(-1, 1)$.

Based on this property, we can show the convergence of the fixed-point approach. Without loss of generality, let $\mathbf{r}^{(0)} = \mathbf{e}$, and t be the iteration index $(t \geq 1)$. According to the CR updating rule in Eq. (5), we have

$$\mathbf{r}^{(t)} = \mathbf{M}^t\mathbf{e} + \sum_{i=0}^{t-1} \mathbf{M}^i \frac{1-c}{1+2\beta}\mathbf{e}$$

Since the eigenvalues of $\mathbf{M}$ are all in $(-1, 1)$, we have

$$\lim_{t\to\infty} \mathbf{M}^t = 0, \text{ and } \lim_{t\to\infty} \sum_{i=0}^{t-1} \mathbf{M}^i = (\mathbf{I}_n - \mathbf{M})^{-1}$$

Therefore

$$\mathbf{r} = \lim_{t\to\infty} \mathbf{r}^{(t)} = (\mathbf{I}_n - \mathbf{M})^{-1}\frac{1-c}{1+2\beta}\mathbf{e} = (\mathbf{I}_n - \frac{c}{1+2\beta}\tilde{\mathbf{G}} - \frac{2\beta}{1+2\beta}\tilde{\mathbf{Y}})^{-1}\frac{1-c}{1+2\beta}\mathbf{e}$$

which is the closed-form solution. □

Theorem 3 ***Optimality of* CR.** *At convergence, Algorithm 1 gives the global minimum of J_{CR} defined in Eq.* (3).

Proof This can be proved by showing that the function in Eq. (3) is convex. The Hessian matrix of Eq. (3) is $\bigtriangledown^2 \mathrm{J}_{\mathrm{CR}} = 2((1+2\beta)\mathbf{I}_n - (c\tilde{\mathbf{G}} + 2\beta\tilde{\mathbf{Y}}))$. Following the similar idea as in the proof of Theorem 2, we have that the eigenvalues of $\bigtriangledown^2 \mathrm{J}_{\mathrm{CR}}$ are no less than $2(1-c)$. Since $0 < c < 1$, $\bigtriangledown^2 \mathrm{J}_{\mathrm{CR}}$ is positive-definite. Therefore, Eq. (3) is convex. □

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