

Supplementary Material for Identifying Multiple Causal Anomalies by Modeling Local Propagations

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1. GRADIENT DEFINITIONS

First, from Sec. 3.3, $\mathcal{J}_{CR}(\mathbf{U})$ and $\mathcal{J}_{CR}(\mathbf{s})$ can be written as following

$$\begin{aligned}\mathcal{J}_{CR}(\mathbf{U}) &= -\sum_{xy} \mathbf{A}_{xy} \log \hat{\mathbf{A}}_{xy} - (\alpha - 1) \sum_{xi} \log \mathbf{U}_{xi} \\ &\quad - \beta \sum_{xy} \mathbf{B}_{xy} \log \left(\sum_i \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i \right) + \beta \sum_{xy} \mathbf{W}_{xy} \sum_i \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i \\ \mathcal{J}_{CR}(\mathbf{s}) &= -\beta \sum_{xy} \mathbf{B}_{xy} \log \left(\sum_i \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i \right) + \beta \sum_{xyi} \mathbf{W}_{xy} \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i\end{aligned}$$

where $\hat{\mathbf{A}}$ is defined in Eq. (2)¹.

Then the positive and non-positive parts of the gradients of $\mathcal{J}_{CR}(\mathbf{U})$ w.r.t. \mathbf{U} and those of $\mathcal{J}_{CR}(\mathbf{s})$ w.r.t. \mathbf{s} are given as following

$$\begin{aligned}(\nabla_U)_{xi}^+ &= 2(\mathbf{ZU})_{xi} \mathbf{h}_i^{-1} + \alpha \mathbf{U}_{xi}^{-1} + 2\beta(\mathbf{YU})_{xi} \mathbf{s}_i \\ (\nabla_U)_{xi}^- &= (\mathbf{U}^T \mathbf{ZU})_{ii} \mathbf{h}_i^{-2} + \mathbf{U}_{xi}^{-1} + 2\beta(\mathbf{WU})_{xi} \mathbf{s}_i \\ (\nabla_s)_i^+ &= \beta(\mathbf{U}^T \mathbf{WU})_{ii} + \mathbf{s}_i^{-1} \\ (\nabla_s)_i^- &= \beta(\mathbf{U}^T \mathbf{YU})_{ii} + \gamma \mathbf{s}_i^{-1}\end{aligned}$$

where

$$\begin{aligned}\mathbf{Z}_{xy} &= \mathbf{A}_{xy} \left(\sum_i \frac{\mathbf{U}_{xi} \mathbf{U}_{yi}}{\sum_z \mathbf{U}_{zi}} \right)^{-1}, \quad \mathbf{h}_i = \sum_z \mathbf{U}_{zi} \\ \mathbf{Y}_{xy} &= \mathbf{B}_{xy} \left(\sum_i \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i \right)^{-1}\end{aligned}$$

2. PROOF OF THEOREM 3.1

PROOF. First, the Lagrangian multipliers λ can be derived by using the equality constraints in Eq. (8). The gradient of \mathcal{L}_U w.r.t. \mathbf{U}_{xi} can be written as

$$\frac{\partial \mathcal{L}_U}{\partial \mathbf{U}_{xi}} = (\nabla_U)_{xi}^+ - (\nabla_U)_{xi}^- + \lambda_x \quad (25)$$

The Karush-Kuhn-Tucker (KKT) completeness slackness condition [1] on the non-negative constraint of \mathbf{U} suggests a fixed-point updating rule for \mathbf{U}_{xi} as

$$\mathbf{U}_{xi}^{\text{new}} = \mathbf{U}_{xi} \frac{(\nabla_U)_{xi}^- - \lambda_x}{(\nabla_U)_{xi}^+} \quad (26)$$

By imposing $\sum_{i=1}^k (\mathbf{U}_{xi})^{\text{new}} = 1$, we can derive

$$\lambda_x = (b_x - 1)/a_x \quad (27)$$

¹The equation numbers in this supplementary material are consistent with those in the original paper.

where

$$a_x = \sum_{i=1}^k \frac{\mathbf{U}_{xi}}{(\nabla_U)_{xi}^+}, \quad b_x = \sum_{i=1}^k \mathbf{U}_{xi} \frac{(\nabla_U)_{xi}^-}{(\nabla_U)_{xi}^+}$$

Such inferred λ will adjust \mathbf{U} toward the equality constraint. With the use of it, we prove Theorem 3.1. The proof follows a Majorization-Minimization approach [4], which is similar to the auxiliary function approach [2]. In the following, we use \mathbf{U} to denote variable and $\tilde{\mathbf{U}}$ to denote current estimate (i.e., a constant). Let $\mathcal{L}_U(\mathbf{U})$ be the function in Eq. (14) w.r.t. \mathbf{U} when fix λ as the constant in Eq. (27). Next, we derive a tight upper bound for $\mathcal{L}_U(\mathbf{U})$, which can be written by

$$\begin{aligned}\mathcal{L}_U(\mathbf{U}) &= -\sum_{xy} \mathbf{A}_{xy} \log \hat{\mathbf{A}}_{xy} - (\alpha - 1) \sum_{xi} \log \mathbf{U}_{xi} \\ &\quad - \beta \sum_{xy} \mathbf{B}_{xy} \log \left(\sum_i \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i \right) + \beta \sum_{xy} \mathbf{W}_{xy} \sum_i \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i \\ &\quad + \sum_x \lambda_x \left(\sum_i \mathbf{U}_{xi} - 1 \right)\end{aligned}$$

Let $\phi_{xyi} = \frac{\tilde{\mathbf{U}}_{xi} \tilde{\mathbf{U}}_{yi}}{\sum_z \tilde{\mathbf{U}}_{zi}} \left(\sum_j \frac{\tilde{\mathbf{U}}_{xj} \tilde{\mathbf{U}}_{yj}}{\sum_z \tilde{\mathbf{U}}_{zj}} \right)^{-1}$, $\theta_{xyi} = \frac{\tilde{\mathbf{U}}_{xi} \tilde{\mathbf{U}}_{yi} \mathbf{s}_i}{\sum_j \tilde{\mathbf{U}}_{xj} \tilde{\mathbf{U}}_{yj} \mathbf{s}_j}$, using the convexity of $\log(\cdot)$, we have

$$\begin{aligned}\mathcal{L}_U(\mathbf{U}) &\leq -\sum_{xyi} \mathbf{A}_{xy} \phi_{xyi} (\log \mathbf{U}_{xi} + \log \mathbf{U}_{yi} - \log \sum_z \mathbf{U}_{zi}) \\ &\quad - (\alpha - 1) \sum_{xi} \log \mathbf{U}_{xi} - \beta \sum_{xyi} \mathbf{B}_{xy} \theta_{xyi} (\log \mathbf{U}_{xi} + \log \mathbf{U}_{yi}) \quad (28) \\ &\quad + \beta \sum_{xyi} \mathbf{W}_{xy} \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i + \sum_{xi} \lambda_x \mathbf{U}_{xi} + C_1\end{aligned}$$

where C_1 is a constant. Using the fact that $d \geq 1 + \log d$ for any $d > 0$, we have

$$\log \sum_z \mathbf{U}_{zi} \leq \frac{\sum_z \mathbf{U}_{zi}}{\sum_z \tilde{\mathbf{U}}_{zi}} - 1 + \log \sum_z \tilde{\mathbf{U}}_{zi}$$

We can further upper bound the first term in Eq. (28) by

$$-\sum_{xyi} \mathbf{A}_{xy} \phi_{xyi} (\log \mathbf{U}_{xi} + \log \mathbf{U}_{yi} - \frac{\sum_z \mathbf{U}_{zi}}{\sum_z \tilde{\mathbf{U}}_{zi}}) + C_2$$

where C_2 is another constant. Therefore, we define the fol-

lowing function as an upper bound of $\mathcal{L}_U(\mathbf{U})$.

$$\begin{aligned}\mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}}) &= -\sum_{xyi} \mathbf{A}_{xy} \phi_{xyi} (\log \mathbf{U}_{xi} + \log \mathbf{U}_{yi} - \frac{\sum_z \mathbf{U}_{zi}}{\sum_z \tilde{\mathbf{U}}_{zi}}) \\ &\quad - (\alpha - 1) \sum_{xi} \log \mathbf{U}_{xi} - \beta \sum_{xyi} \mathbf{B}_{xy} \theta_{xyi} (\log \mathbf{U}_{xi} + \log \mathbf{U}_{yi}) \\ &\quad + \beta \sum_{xyi} \mathbf{W}_{xy} \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i + \sum_{xi} \lambda_x \mathbf{U}_{xi} \\ &\quad + \sum_{xi} (\frac{1}{a_x} + \frac{1}{\tilde{\mathbf{U}}_{xi}}) \tilde{\mathbf{U}}_{xi} (\frac{\mathbf{U}_{xi}}{\tilde{\mathbf{U}}_{xi}} - \log \frac{\mathbf{U}_{xi}}{\tilde{\mathbf{U}}_{xi}} - 1) + C_3\end{aligned}$$

where $C_3 = C_1 + C_2$ is a constant. The term before C_3 is non-negative and is added to guarantee the non-negativity of the multiplicative updating rule. It is known as the “moving term” technique in existing work [3].

Note $\mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}})$ is a tight upper bound of $\mathcal{L}_U(\mathbf{U})$. That is, $\mathcal{Z}_U(\mathbf{U}, \mathbf{U}) = \mathcal{L}_U(\mathbf{U})$ (Some terms are hidden in C_3). According to Definition 3.5, $\mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}})$ is also an *auxiliary function* of $\mathcal{L}_U(\mathbf{U})$ [2].

Next, we derive the minimal solution to $\mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}})$. The gradient of $\mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}})$ w.r.t. \mathbf{U}_{xi} is

$$\begin{aligned}\frac{\partial \mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}})}{\partial \mathbf{U}_{xi}} &= -2 \sum_y \mathbf{A}_{xy} \phi_{xyi} \frac{1}{\mathbf{U}_{xi}} + \sum_y \mathbf{A}_{xy} \phi_{xyi} \frac{1}{\sum_z \tilde{\mathbf{U}}_{zi}} \\ &\quad - (\alpha - 1) \frac{1}{\mathbf{U}_{xi}} - 2\beta \sum_y \mathbf{B}_{xy} \theta_{xyi} \frac{1}{\mathbf{U}_{xi}} \\ &\quad + 2\beta \sum_y \mathbf{W}_{xy} \mathbf{U}_{yi} \mathbf{s}_i + \lambda_x + (\frac{1}{a_x} + \frac{1}{\tilde{\mathbf{U}}_{xi}}) \tilde{\mathbf{U}}_{xi} (\frac{1}{\tilde{\mathbf{U}}_{xi}} - \frac{1}{\mathbf{U}_{xi}})\end{aligned}$$

Equivalently,

$$\begin{aligned}\frac{\partial \mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}})}{\partial \mathbf{U}_{xi}} &= ((\nabla_U)_{xi}^+ - \frac{1}{\tilde{\mathbf{U}}_{xi}}) - \frac{\tilde{\mathbf{U}}_{xi}}{\mathbf{U}_{xi}} ((\nabla_U)_{xi}^- - \frac{1}{\tilde{\mathbf{U}}_{xi}}) \\ &\quad + \frac{b_x - 1}{a_x} + \frac{1}{a_x} + \frac{1}{\tilde{\mathbf{U}}_{xi}} - \frac{\tilde{\mathbf{U}}_{xi}}{a_x \mathbf{U}_{xi}} - \frac{1}{\mathbf{U}_{xi}} \\ &= -\frac{\tilde{\mathbf{U}}_{xi}}{\mathbf{U}_{xi}} ((\nabla_U)_{xi}^- + \frac{1}{a_x}) + ((\nabla_U)_{xi}^+ + \frac{b_x}{a_x})\end{aligned}$$

Therefore, the global minimum of $\mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}})$ can be obtained by solving $\frac{\partial \mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}})}{\partial \mathbf{U}_{xi}} = 0$. This gives the solution

$$\mathbf{U}_{xi} = \tilde{\mathbf{U}}_{xi} \frac{a_x (\nabla_U)_{xi}^- + 1}{a_x (\nabla_U)_{xi}^+ + b_x}$$

which is consistent with the updating rule in Eq. (16). According to the following tight upper bound properties

$$(1) \mathcal{Z}_U(\mathbf{U}, \tilde{\mathbf{U}}) \geq \mathcal{L}_U(\mathbf{U}), (2) \mathcal{Z}_U(\mathbf{U}, \mathbf{U}) = \mathcal{L}_U(\mathbf{U})$$

At any iteration $\kappa \geq 1$ during updating \mathbf{U} by Eq. (16), we have

$$\begin{aligned}\mathcal{L}_U(\mathbf{U}^{(\kappa)}, \boldsymbol{\lambda}) &= \mathcal{Z}_U(\mathbf{U}^{(\kappa)}, \mathbf{U}^{(\kappa)}) \\ &\geq \mathcal{Z}_U(\mathbf{U}^{(\kappa+1)}, \mathbf{U}^{(\kappa)}) \geq \mathcal{L}_U(\mathbf{U}^{(\kappa+1)}, \boldsymbol{\lambda})\end{aligned}$$

which completes the proof of Theorem 3.1. \square

3. PROOF OF THEOREM 3.2

PROOF. In the following, we use \mathbf{s} to denote variable and $\tilde{\mathbf{s}}$ to denote current estimate (i.e., a constant). First, let

$\mathcal{J}_{CR}(\mathbf{s})$ be the objective function in Eq. (8) w.r.t. \mathbf{s} , which can be written by

$$\mathcal{J}_{CR}(\mathbf{s}) = -\beta \sum_{xy} \mathbf{B}_{xy} \log (\sum_i \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i) + \beta \sum_{xyi} \mathbf{W}_{xy} \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i$$

Let $\pi_{xyi} = \frac{\mathbf{U}_{xi} \mathbf{U}_{yi} \tilde{\mathbf{s}}_i}{\sum_j \tilde{\mathbf{U}}_{xj} \tilde{\mathbf{U}}_{yj} \tilde{\mathbf{s}}_j}$, using the convexity of $\log(\cdot)$, we have

$$\begin{aligned}\mathcal{J}_{CR}(\mathbf{s}) &\leq -\beta \sum_{xyi} \mathbf{B}_{xy} \pi_{xyi} \log \mathbf{s}_i + \beta \sum_{xyi} \mathbf{W}_{xy} \mathbf{U}_{xi} \mathbf{U}_{yi} \mathbf{s}_i \\ &\quad + \sum_i (\frac{\mathbf{s}_i}{\tilde{\mathbf{s}}_i} - \log \frac{\mathbf{s}_i}{\tilde{\mathbf{s}}_i} - 1) + C_4\end{aligned}$$

where C_4 is a constant, the term before C_4 is non-negative and is added to guarantee the non-negativity of the multiplicative updating rule.

Let function $\mathcal{Z}_s(\mathbf{s}, \tilde{\mathbf{s}})$ be the above upper bound, it is a tight upper bound of $\mathcal{J}_{CR}(\mathbf{s})$, i.e., we have $\mathcal{Z}_s(\mathbf{s}, \mathbf{s}) = \mathcal{J}_{CR}(\mathbf{s})$ (some terms are hidden in C_4).

Next, we enforce the inequality constraint $\mathbf{s}_i \leq 1$ of Eq. (8) and solve the following optimization problem, which will give us a solution that decreases the objective value in Eq. (8) and satisfies the constraints in Eq. (8).

$$\min_{\mathbf{s}} \mathcal{Z}_s(\mathbf{s}, \tilde{\mathbf{s}}), \quad \text{s.t. } 0 \leq \mathbf{s}_i \leq 1, \quad \forall 1 \leq i \leq k \quad (29)$$

Let \mathcal{L}_s be the Lagrangian function of the above optimization problem, which can be represented by

$$\mathcal{L}_s(\mathbf{s}) = \mathcal{Z}_s(\mathbf{s}, \tilde{\mathbf{s}}) + \sum_{i=1}^k \mu_i (\mathbf{s}_i - 1)$$

where μ_i ($1 \leq i \leq k$) is the Lagrangian multiplier.

Then the gradient of $\mathcal{L}_s(\mathbf{s})$ w.r.t. \mathbf{s}_i is

$$\frac{\partial \mathcal{L}_s(\mathbf{s})}{\partial \mathbf{s}_i} = -\beta \sum_{xy} \mathbf{B}_{xy} \pi_{xyi} \frac{1}{\mathbf{s}_i} + \beta \sum_{xy} \mathbf{W}_{xy} \mathbf{U}_{xi} \mathbf{U}_{yi} + \frac{1}{\tilde{\mathbf{s}}_i} - \frac{1}{\mathbf{s}_i} + \mu_i$$

Equivalently,

$$\begin{aligned}\frac{\partial \mathcal{L}_s(\mathbf{s})}{\partial \mathbf{s}_i} &= ((\nabla_s)_i^+ - \frac{1}{\tilde{\mathbf{s}}_i}) - \frac{\tilde{\mathbf{s}}_i}{\mathbf{s}_i} ((\nabla_s)_i^- - \frac{1}{\tilde{\mathbf{s}}_i}) + \frac{1}{\tilde{\mathbf{s}}_i} - \frac{1}{\mathbf{s}_i} + \mu_i \\ &= -\frac{\tilde{\mathbf{s}}_i}{\mathbf{s}_i} (\nabla_s)_i^- + (\nabla_s)_i^+ + \mu_i\end{aligned}$$

According to the Karush-Kuhn-Tucker (KKT) conditions [1], for $1 \leq i \leq k$, we have

- Gradient: $\mu_i = \frac{\tilde{\mathbf{s}}_i}{\mathbf{s}_i} ((\nabla_s)_i^- - (\nabla_s)_i^+)$
- Non-negativity: $\mu_i \geq 0$
- Feasibility: $\mathbf{s}_i \leq 1$
- Complementary slackness: $\mu_i (\mathbf{s}_i - 1) = 0$

The gradient and complementary slackness conditions suggest the optimal solution \mathbf{s}_i^* can be either $\tilde{\mathbf{s}}_i [(\nabla_s)_i^- / (\nabla_s)_i^+]$ or 1. The non-negativity and feasibility conditions suggest $\mathbf{s}_i^* \leq \tilde{\mathbf{s}}_i [(\nabla_s)_i^- / (\nabla_s)_i^+]$ and $\mathbf{s}_i^* \leq 1$.

Therefore, we obtain the global minimal \mathbf{s}_i^* to Eq. (29) as

$$\mathbf{s}_i^* = \min (\tilde{\mathbf{s}}_i [(\nabla_s)_i^- / (\nabla_s)_i^+], 1)$$

which is consistent with the updating rule in Eq. (17). According to the following tight upper bound properties

$$(1) \mathcal{Z}_s(\mathbf{s}, \tilde{\mathbf{s}}) \geq \mathcal{J}_{CR}(\mathbf{s}), (2) \mathcal{Z}_s(\mathbf{s}, \mathbf{s}) = \mathcal{J}_{CR}(\mathbf{s})$$

At any iteration $\kappa \geq 1$ when we update \mathbf{s} by Eq. (17), we have

$$\mathcal{J}_{CR}(\mathbf{s}^{(\kappa)}) = \mathcal{Z}_s(\mathbf{s}^{(\kappa)}, \mathbf{s}^{(\kappa)}) \geq \mathcal{Z}_s(\mathbf{s}^{(\kappa+1)}, \mathbf{s}^{(\kappa)}) \geq \mathcal{J}_{CR}(\mathbf{s}^{(\kappa+1)})$$

which completes the proof of Theorem 3.2. \square

4. PROOF OF THEOREM 3.4

PROOF. First, we can rewrite the objective function in Eq. (13) as (after removing some constants)

$$\mathcal{J}_H(\mathbf{E}) = -2\text{tr}(\mathbf{Q}(\mathbf{U} \circ \mathbf{E})(\mathbf{U} \circ \mathbf{E})) + \text{tr}(\mathbf{R}\mathbf{R}) + \tau \sum_{xi} \mathbf{E}_{xi}$$

where

$$\begin{aligned} \mathbf{Q} &= \mathbf{H}^T(\mathbf{B} \circ \mathbf{C})^T \mathbf{H} \\ \mathbf{R} &= \mathbf{C} \circ [\mathbf{H}(\mathbf{U} \circ \mathbf{E})(\mathbf{U} \circ \mathbf{E})^T \mathbf{H}^T] \end{aligned}$$

We then derive upper bounds for the above three terms. Let $\tilde{\mathbf{E}}$ be current estimate (i.e., a constant). Using the general inequality $d \geq 1 + \log d$ for any $d > 0$, we have

$$\frac{\mathbf{E}_{xi}\mathbf{E}_{yi}}{\tilde{\mathbf{E}}_{xi}\tilde{\mathbf{E}}_{yi}} \geq 1 + \log \frac{\mathbf{E}_{xi}\mathbf{E}_{yi}}{\tilde{\mathbf{E}}_{xi}\tilde{\mathbf{E}}_{yi}}$$

Then we can write an upper bound for the first term

$$\begin{aligned} -\text{tr}(\mathbf{Q}(\mathbf{U} \circ \mathbf{E})(\mathbf{U} \circ \mathbf{E})) &= -\sum_{xyi} \mathbf{Q}_{xy} \mathbf{U}_{xi} \mathbf{E}_{xi} \mathbf{U}_{yi} \mathbf{E}_{yi} \\ &\leq -\sum_{xyi} \mathbf{Q}_{xy} \mathbf{U}_{xi} \mathbf{U}_{yi} \tilde{\mathbf{E}}_{xi} \tilde{\mathbf{E}}_{yi} (1 + \log \frac{\mathbf{E}_{xi}\mathbf{E}_{yi}}{\tilde{\mathbf{E}}_{xi}\tilde{\mathbf{E}}_{yi}}) \end{aligned} \quad (30)$$

For the second term, using the following property of Hadamard product (i.e., entry-wise product) [5]

$$\begin{aligned} \text{tr}((\mathbf{P} \circ \mathbf{V})^T (\mathbf{P} \circ \mathbf{M})) &= \text{tr}((\mathbf{P} \circ \mathbf{V})^T \mathbf{M}) \\ \forall \mathbf{P} \in \{0, 1\}^{n \times n}, \mathbf{V} \in \mathbb{R}_+^{n \times n}, \mathbf{M} \in \mathbb{R}_+^{n \times n} \end{aligned}$$

We can write

$$\begin{aligned} \text{tr}(\mathbf{R}\mathbf{R}) &= \text{tr}(\mathbf{R}[\mathbf{H}(\mathbf{U} \circ \mathbf{E})(\mathbf{U} \circ \mathbf{E})^T \mathbf{H}^T]) \\ &= \sum_{xyzirpjq} \mathbf{C}_{xy} \mathbf{H}_{xz} \mathbf{U}_{zi} \mathbf{E}_{zi} \mathbf{U}_{ri} \mathbf{E}_{ri} \mathbf{H}_{yr} \mathbf{H}_{xp} \mathbf{U}_{pj} \mathbf{E}_{pj} \mathbf{U}_{qj} \mathbf{E}_{qj} \mathbf{H}_{yq} \end{aligned} \quad (31)$$

Let $\mathcal{F}(\mathbf{E}_{zi}, \mathbf{E}_{ri}, \mathbf{E}_{pj}, \mathbf{E}_{qj})$ be a function w.r.t. \mathbf{E}_{zi} , \mathbf{E}_{ri} , \mathbf{E}_{pj} and \mathbf{E}_{qj} as defined by

$$\begin{aligned} \mathcal{F}(\mathbf{E}_{zi}, \mathbf{E}_{ri}, \mathbf{E}_{pj}, \mathbf{E}_{qj}) &= \mathbf{C}_{xy} \mathbf{H}_{xz} \mathbf{U}_{zi} \mathbf{E}_{zi} \mathbf{U}_{ri} \mathbf{E}_{ri} \mathbf{H}_{yr} \mathbf{H}_{xp} \mathbf{U}_{pj} \mathbf{E}_{pj} \mathbf{U}_{qj} \mathbf{E}_{qj} \mathbf{H}_{yq} \end{aligned}$$

Also, let $\mathbf{E}_{zi} = \tilde{\mathbf{E}}_{zi} v_{zi}$, $\mathbf{E}_{ri} = \tilde{\mathbf{E}}_{ri} v_{ri}$, $\mathbf{E}_{pj} = \tilde{\mathbf{E}}_{pj} v_{pj}$ and $\mathbf{E}_{qj} = \tilde{\mathbf{E}}_{qj} v_{qj}$ for non-negative values v_{zi} , v_{ri} , v_{pj} and v_{qj} , we can rewrite Eq. (31) by

$$\begin{aligned} \text{tr}(\mathbf{R}\mathbf{R}) &= \sum_{xyzirpjq} \mathcal{F}(\tilde{\mathbf{E}}_{zi}, \tilde{\mathbf{E}}_{ri}, \tilde{\mathbf{E}}_{pj}, \tilde{\mathbf{E}}_{qj}) v_{zi} v_{ri} v_{pj} v_{qj} \\ &\leq \sum_{xyzirpjq} \mathcal{F}(\tilde{\mathbf{E}}_{zi}, \tilde{\mathbf{E}}_{ri}, \tilde{\mathbf{E}}_{pj}, \tilde{\mathbf{E}}_{qj}) \frac{v_{zi}^4 + v_{ri}^4 + v_{pj}^4 + v_{qj}^4}{4} \\ &= \frac{1}{4} \left(\sum_{zi} (\tilde{\mathbf{E}} \circ \mathbf{U})_{zi} \frac{\mathbf{E}_{zi}^4}{\tilde{\mathbf{E}}_{zi}^3} + \sum_{ri} (\tilde{\mathbf{E}} \circ \mathbf{U})_{ri} \frac{\mathbf{E}_{ri}^4}{\tilde{\mathbf{E}}_{ri}^3} \right. \\ &\quad \left. + \sum_{pj} (\tilde{\mathbf{E}} \circ \mathbf{U})_{pj} \frac{\mathbf{E}_{pj}^4}{\tilde{\mathbf{E}}_{pj}^3} + \sum_{qj} (\tilde{\mathbf{E}} \circ \mathbf{U})_{qj} \frac{\mathbf{E}_{qj}^4}{\tilde{\mathbf{E}}_{qj}^3} \right) \\ &= \sum_{xi} (\tilde{\mathbf{E}} \circ \mathbf{U})_{xi} \frac{\mathbf{E}_{xi}^4}{\tilde{\mathbf{E}}_{xi}^3} \end{aligned} \quad (32)$$

where $\tilde{\mathbf{E}} = \mathbf{H}^T \{ \mathbf{C} \circ [\mathbf{H}(\mathbf{U} \circ \tilde{\mathbf{E}})(\mathbf{U} \circ \tilde{\mathbf{E}})^T \mathbf{H}^T] \} \mathbf{H}(\mathbf{U} \circ \tilde{\mathbf{E}})$. The last equation is obtained by switching indexes.

For the third term, using the fact that $2ab \leq a^2 + b^2$, we have

$$\tau \sum_{xi} \mathbf{E}_{xi} \leq \frac{\tau}{2} \sum_{xi} \frac{\mathbf{E}_{xi}^2 + \tilde{\mathbf{E}}_{xi}^2}{\tilde{\mathbf{E}}_{xi}} \leq \frac{\tau}{4} \sum_{xi} \frac{\mathbf{E}_{xi}^4 + 3\tilde{\mathbf{E}}_{xi}^4}{\tilde{\mathbf{E}}_{xi}^3} \quad (33)$$

Therefore, by collecting Eq. (30), Eq. (32) and Eq. (33), we obtain an auxiliary function for $\mathcal{J}_H(\mathbf{E})$ as

$$\begin{aligned} \mathcal{Z}_E(\mathbf{E}, \tilde{\mathbf{E}}) &= -2 \sum_{xyi} \mathbf{Q}_{xy} \mathbf{U}_{xi} \mathbf{U}_{yi} \tilde{\mathbf{E}}_{xi} \tilde{\mathbf{E}}_{yi} (1 + \log \frac{\mathbf{E}_{xi}\mathbf{E}_{yi}}{\tilde{\mathbf{E}}_{xi}\tilde{\mathbf{E}}_{yi}}) \\ &\quad + \sum_{xi} (\tilde{\mathbf{E}} \circ \mathbf{U})_{xi} \frac{\mathbf{E}_{xi}^4}{\tilde{\mathbf{E}}_{xi}^3} + \frac{\tau}{4} \sum_{xi} \frac{\mathbf{E}_{xi}^4 + 3\tilde{\mathbf{E}}_{xi}^4}{\tilde{\mathbf{E}}_{xi}^3} \end{aligned}$$

which is a tight upper bound satisfies $\mathcal{Z}_E(\mathbf{E}, \tilde{\mathbf{E}}) = \mathcal{J}_H(\mathbf{E})$. Then the derivative

$$\begin{aligned} \frac{\partial \mathcal{Z}_E(\mathbf{E}_{xi}, \tilde{\mathbf{E}}_{xi})}{\partial \mathbf{E}_{xi}} &= -4 \{ [\mathbf{Q}(\mathbf{U} \circ \tilde{\mathbf{E}})] \circ \mathbf{U} \}_{xi} \frac{\tilde{\mathbf{E}}_{xi}}{\mathbf{E}_{xi}} \\ &\quad + 4(\tilde{\mathbf{E}} \circ \mathbf{U})_{xi} \frac{\mathbf{E}_{xi}^3}{\tilde{\mathbf{E}}_{xi}^3} + \tau \frac{\mathbf{E}_{xi}^3}{\tilde{\mathbf{E}}_{xi}^3} \end{aligned}$$

By setting $\frac{\partial \mathcal{Z}_E(\mathbf{E}_{xi}, \tilde{\mathbf{E}}_{xi})}{\partial \mathbf{E}_{xi}} = 0$, we obtain the optimal solution

$$\mathbf{E}_{xi} = \tilde{\mathbf{E}}_{xi} \left(\frac{4(\tilde{\mathbf{E}} \circ \mathbf{U})_{xi}}{4(\tilde{\mathbf{E}} \circ \mathbf{U})_{xi} + \tau} \right)^{\frac{1}{4}} \quad (34)$$

where $\tilde{\mathbf{E}} = \mathbf{H}^T \{ \mathbf{C} \circ [\mathbf{H}(\mathbf{U} \circ \tilde{\mathbf{E}})(\mathbf{U} \circ \tilde{\mathbf{E}})^T \mathbf{H}^T] \} \mathbf{H}(\mathbf{U} \circ \tilde{\mathbf{E}})$ and $\tilde{\mathbf{E}} = \mathbf{H}^T(\mathbf{B} \circ \mathbf{C})\mathbf{H}(\mathbf{U} \circ \tilde{\mathbf{E}})$.

Note Eq. (34) is consistent with the updating rule of Eq. (19) in Theorem 3.4. Because of the properties of the auxiliary function [2], i.e.,

$$(1) \mathcal{Z}_E(\mathbf{E}, \tilde{\mathbf{E}}) \geq \mathcal{J}_H(\mathbf{E}), \quad (2) \mathcal{Z}_E(\mathbf{E}, \mathbf{E}) = \mathcal{J}_H(\mathbf{E})$$

We have

$$\mathcal{J}_H(\mathbf{E}^{(t)}) = \mathcal{Z}_E(\mathbf{E}^{(t)}, \mathbf{E}^{(t)}) \geq \mathcal{Z}_E(\mathbf{E}^{(t+1)}, \mathbf{E}^{(t)}) \geq \mathcal{J}_H(\mathbf{E}^{(t+1)})$$

which completes the proof of Theorem 3.4. \square

5. REFERENCES

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