

## 299 Appendix

### 300 5 Approximate ED Gradients with PI in Backpropagation

301 In the following two subsections, we prove that the gradients computed from the PI equals those  
302 computed from ED.

#### 303 5.1 Power Iteration Gradients

304 To compute the leading eigenvector  $\mathbf{v}$  of  $\mathbf{M}$ , PI uses the following standard formula

$$\mathbf{v}^{(k)} = \frac{\mathbf{M}\mathbf{v}^{(k-1)}}{\|\mathbf{M}\mathbf{v}^{(k-1)}\|}, \quad (15)$$

305 where  $\|\cdot\|$  denotes the  $\ell_2$  norm, and  $\mathbf{v}^{(0)}$  is usually initialized randomly with  $\|\mathbf{v}^{(0)}\|=1$ . Its gradient  
306 is [18]

$$\begin{aligned} \frac{\partial L}{\partial \mathbf{M}} &= \sum_k \frac{(\mathbf{I} - \mathbf{v}^{(k+1)}\mathbf{v}^{(k+1)\top})}{\|\mathbf{M}\mathbf{v}^{(k)}\|} \frac{\partial L}{\partial \mathbf{v}^{(k+1)}} \mathbf{v}^{(k)\top} \\ \frac{\partial L}{\partial \mathbf{v}^{(k)}} &= \mathbf{M} \frac{(\mathbf{I} - \mathbf{v}^{(k+1)}\mathbf{v}^{(k+1)\top})}{\|\mathbf{M}\mathbf{v}^{(k)}\|} \frac{\partial L}{\partial \mathbf{v}^{(k+1)}} \end{aligned} \quad (16)$$

307 Using 3 power iteration steps for demonstration, we have

$$\begin{aligned} \frac{\partial L}{\partial \mathbf{v}^{(2)}} &= \mathbf{M} \frac{(\mathbf{I} - \mathbf{v}^{(3)}\mathbf{v}^{(3)\top})}{\|\mathbf{M}\mathbf{v}^{(2)}\|} \frac{\partial L}{\partial \mathbf{v}^{(3)}} \\ \frac{\partial L}{\partial \mathbf{v}^{(1)}} &= \mathbf{M} \frac{(\mathbf{I} - \mathbf{v}^{(2)}\mathbf{v}^{(2)\top})}{\|\mathbf{M}\mathbf{v}^{(1)}\|} \frac{\partial L}{\partial \mathbf{v}^{(2)}} = \mathbf{M} \frac{(\mathbf{I} - \mathbf{v}^{(2)}\mathbf{v}^{(2)\top})}{\|\mathbf{M}\mathbf{v}^{(1)}\|} \mathbf{M} \frac{(\mathbf{I} - \mathbf{v}^{(3)}\mathbf{v}^{(3)\top})}{\|\mathbf{M}\mathbf{v}^{(2)}\|} \frac{\partial L}{\partial \mathbf{v}^{(3)}} \end{aligned} \quad (17)$$

308 Then, because we use ED's result, denoted as  $\mathbf{v}$ , as initial vector,  $\mathbf{v} = \mathbf{v}^{(0)} \approx \mathbf{v}^{(1)} \approx \mathbf{v}^{(2)} \approx \dots \approx \mathbf{v}^{(k)}$ .  
309 Therefore,  $\frac{\partial L}{\partial \mathbf{M}}$  can be re-written as

$$\begin{aligned} \frac{\partial L}{\partial \mathbf{M}} &= \frac{(\mathbf{I} - \mathbf{v}^{(3)}\mathbf{v}^{(3)\top})}{\|\mathbf{M}\mathbf{v}^{(2)}\|} \frac{\partial L}{\partial \mathbf{v}^{(3)}} \mathbf{v}^{(2)\top} + \frac{(\mathbf{I} - \mathbf{v}^{(2)}\mathbf{v}^{(2)\top})}{\|\mathbf{M}\mathbf{v}^{(1)}\|} \frac{\partial L}{\partial \mathbf{v}^{(2)}} \mathbf{v}^{(1)\top} + \frac{(\mathbf{I} - \mathbf{v}^{(1)}\mathbf{v}^{(1)\top})}{\|\mathbf{M}\mathbf{v}^{(0)}\|} \frac{\partial L}{\partial \mathbf{v}^{(1)}} \mathbf{v}^{(0)\top} \\ &= \left( \frac{(\mathbf{I} - \mathbf{v}\mathbf{v}^\top)}{\|\mathbf{M}\mathbf{v}\|} + \frac{(\mathbf{I} - \mathbf{v}\mathbf{v}^\top) \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top)}{\|\mathbf{M}\mathbf{v}\|^2} + \frac{(\mathbf{I} - \mathbf{v}\mathbf{v}^\top) \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top)}{\|\mathbf{M}\mathbf{v}\|^3} \right) \frac{\partial L}{\partial \mathbf{v}^{(3)}} \mathbf{v}^\top \end{aligned} \quad (18)$$

Since  $\mathbf{v}\mathbf{v}^\top$  and  $\mathbf{M}$  are symmetric, and  $\mathbf{M}\mathbf{v} = \lambda\mathbf{v}$ , we have

$$\mathbf{v}\mathbf{v}^\top \mathbf{M} = (\mathbf{M}^\top \mathbf{v}\mathbf{v}^\top)^\top = (\mathbf{M}\mathbf{v}\mathbf{v}^\top)^\top = (\lambda\mathbf{v}\mathbf{v}^\top)^\top = \lambda\mathbf{v}\mathbf{v}^\top = \mathbf{M}\mathbf{v}\mathbf{v}^\top.$$

310 Introducing the equation above into the numerator of the second term of Eq. [18] yields

$$\begin{aligned} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) &= (\mathbf{M} - \mathbf{v}\mathbf{v}^\top \mathbf{M}) (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) = (\mathbf{M} - \mathbf{M}\mathbf{v}\mathbf{v}^\top) (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) \\ &= \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) = \mathbf{M} (\mathbf{I} - 2\mathbf{v}\mathbf{v}^\top + \cancel{\mathbf{v}(\mathbf{v}^\top \mathbf{v})\mathbf{v}^\top}) = \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top). \end{aligned} \quad (19)$$

311 Similarly, for the numerator in the third term in Eq. [18] we have

$$(\mathbf{I} - \mathbf{v}\mathbf{v}^\top) \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) = \mathbf{M} \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top). \quad (20)$$

312 Introducing Eq. [19] and Eq. [20] into Eq. [18] we obtain

$$\frac{\partial L}{\partial \mathbf{M}} = \left( \frac{(\mathbf{I} - \mathbf{v}\mathbf{v}^\top)}{\|\mathbf{M}\mathbf{v}\|} + \frac{\mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top)}{\|\mathbf{M}\mathbf{v}\|^2} + \frac{\mathbf{M} \mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top)}{\|\mathbf{M}\mathbf{v}\|^3} \right) \frac{\partial L}{\partial \mathbf{v}^{(3)}} \mathbf{v}^\top \quad (21)$$

313 When extending the iteration number from 3 to  $k$ , Eq. [18] becomes

$$\frac{\partial L}{\partial \mathbf{M}} = \left( \frac{(\mathbf{I} - \mathbf{v}\mathbf{v}^\top)}{\|\mathbf{M}\mathbf{v}\|} + \frac{\mathbf{M} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top)}{\|\mathbf{M}\mathbf{v}\|^2} + \dots + \frac{\mathbf{M}^{k-1} (\mathbf{I} - \mathbf{v}\mathbf{v}^\top)}{\|\mathbf{M}\mathbf{v}\|^k} \right) \frac{\partial L}{\partial \mathbf{v}^{(k)}} \mathbf{v}^\top \quad (22)$$

314 Eq. [22] is the form we adopt to compute the gradients of ED.

## 315 5.2 Analytic ED Gradients

316 The analytic solution of the ED gradients is [4].

$$\frac{\partial L}{\partial \mathbf{M}} = V \left\{ \left( \tilde{K}^\top \circ \left( V^\top \frac{\partial L}{\partial V} \right) \right) + \left( \frac{\partial L}{\partial \Sigma} \right)_{diag} \right\} V^\top \quad (23)$$

$$\tilde{K}_{ij} = \begin{cases} \frac{1}{\lambda_i - \lambda_j}, & i \neq j \\ 0, & i = j \end{cases} \quad (24)$$

$$\tilde{K} = \begin{bmatrix} 0 & \frac{1}{\lambda_1 - \lambda_2} & \frac{1}{\lambda_1 - \lambda_3} & \cdots & \frac{1}{\lambda_1 - \lambda_n} \\ \frac{1}{\lambda_2 - \lambda_1} & 0 & \frac{1}{\lambda_2 - \lambda_3} & \cdots & \frac{1}{\lambda_2 - \lambda_n} \\ \frac{1}{\lambda_3 - \lambda_1} & \frac{1}{\lambda_3 - \lambda_2} & 0 & \cdots & \frac{1}{\lambda_3 - \lambda_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\lambda_n - \lambda_1} & \frac{1}{\lambda_n - \lambda_2} & \frac{1}{\lambda_n - \lambda_3} & \cdots & 0 \end{bmatrix} \quad (25)$$

317 where  $\lambda_i$  is an eigenvalue, and

$$V = [\mathbf{v}_1 \quad \mathbf{v}_2 \quad \mathbf{v}_3 \quad \cdots \quad \mathbf{v}_n] \quad (26)$$

318 where  $\mathbf{v}_i$  is an eigenvector. Then,

$$\frac{\partial L}{\partial V} = \begin{bmatrix} \frac{\partial L}{\partial \mathbf{v}_1} & \frac{\partial L}{\partial \mathbf{v}_2} & \frac{\partial L}{\partial \mathbf{v}_3} & \cdots & \frac{\partial L}{\partial \mathbf{v}_n} \end{bmatrix} \quad (27)$$

$$V^\top \frac{\partial L}{\partial V} = \begin{bmatrix} \mathbf{v}_1^\top \frac{\partial L}{\partial \mathbf{v}_1} & \mathbf{v}_1^\top \frac{\partial L}{\partial \mathbf{v}_2} & \mathbf{v}_1^\top \frac{\partial L}{\partial \mathbf{v}_3} & \cdots & \mathbf{v}_1^\top \frac{\partial L}{\partial \mathbf{v}_n} \\ \mathbf{v}_2^\top \frac{\partial L}{\partial \mathbf{v}_1} & \mathbf{v}_2^\top \frac{\partial L}{\partial \mathbf{v}_2} & \mathbf{v}_2^\top \frac{\partial L}{\partial \mathbf{v}_3} & \cdots & \mathbf{v}_2^\top \frac{\partial L}{\partial \mathbf{v}_n} \\ \mathbf{v}_3^\top \frac{\partial L}{\partial \mathbf{v}_1} & \mathbf{v}_3^\top \frac{\partial L}{\partial \mathbf{v}_2} & \mathbf{v}_3^\top \frac{\partial L}{\partial \mathbf{v}_3} & \cdots & \mathbf{v}_3^\top \frac{\partial L}{\partial \mathbf{v}_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{v}_n^\top \frac{\partial L}{\partial \mathbf{v}_1} & \mathbf{v}_n^\top \frac{\partial L}{\partial \mathbf{v}_2} & \mathbf{v}_n^\top \frac{\partial L}{\partial \mathbf{v}_3} & \cdots & \mathbf{v}_n^\top \frac{\partial L}{\partial \mathbf{v}_n} \end{bmatrix} \quad (28)$$

$$\tilde{K} \circ V^\top \frac{\partial L}{\partial V} = \begin{bmatrix} 0 & \frac{1}{\lambda_2 - \lambda_1} \mathbf{v}_1^\top \frac{\partial L}{\partial \mathbf{v}_2} & \frac{1}{\lambda_3 - \lambda_1} \mathbf{v}_1^\top \frac{\partial L}{\partial \mathbf{v}_3} & \cdots & \frac{1}{\lambda_n - \lambda_1} \mathbf{v}_1^\top \frac{\partial L}{\partial \mathbf{v}_n} \\ \frac{1}{\lambda_1 - \lambda_2} \mathbf{v}_2^\top \frac{\partial L}{\partial \mathbf{v}_1} & 0 & \frac{1}{\lambda_3 - \lambda_2} \mathbf{v}_2^\top \frac{\partial L}{\partial \mathbf{v}_3} & \cdots & \frac{1}{\lambda_n - \lambda_2} \mathbf{v}_2^\top \frac{\partial L}{\partial \mathbf{v}_n} \\ \frac{1}{\lambda_1 - \lambda_3} \mathbf{v}_3^\top \frac{\partial L}{\partial \mathbf{v}_1} & \frac{1}{\lambda_2 - \lambda_3} \mathbf{v}_3^\top \frac{\partial L}{\partial \mathbf{v}_2} & 0 & \cdots & \frac{1}{\lambda_n - \lambda_3} \mathbf{v}_3^\top \frac{\partial L}{\partial \mathbf{v}_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\lambda_1 - \lambda_n} \mathbf{v}_n^\top \frac{\partial L}{\partial \mathbf{v}_1} & \frac{1}{\lambda_2 - \lambda_n} \mathbf{v}_n^\top \frac{\partial L}{\partial \mathbf{v}_2} & \frac{1}{\lambda_3 - \lambda_n} \mathbf{v}_n^\top \frac{\partial L}{\partial \mathbf{v}_3} & \cdots & 0 \end{bmatrix} \quad (29)$$

$$V \tilde{K} \circ V^\top \frac{\partial L}{\partial V} = \left[ \sum_{i \neq 1}^n \frac{1}{\lambda_1 - \lambda_i} \mathbf{v}_i \mathbf{v}_i^\top \frac{\partial L}{\partial \mathbf{v}_1}, \quad \cdots, \quad \sum_{i \neq n}^n \frac{1}{\lambda_n - \lambda_i} \mathbf{v}_i \mathbf{v}_i^\top \frac{\partial L}{\partial \mathbf{v}_n} \right] \quad (30)$$

$$V \tilde{K} \circ V^\top \frac{\partial L}{\partial V} V^\top = \sum_{i \neq 1}^n \frac{1}{\lambda_1 - \lambda_i} \mathbf{v}_i \mathbf{v}_i^\top \frac{\partial L}{\partial \mathbf{v}_1} \mathbf{v}_1 + \cdots + \sum_{i \neq n}^n \frac{1}{\lambda_n - \lambda_i} \mathbf{v}_i \mathbf{v}_i^\top \frac{\partial L}{\partial \mathbf{v}_n} \mathbf{v}_n \quad (31)$$

$$V \left( \frac{\partial L}{\partial \Sigma} \right)_{diag} V^\top = \sum_{i=1}^n \frac{\partial L}{\partial \lambda_i} \mathbf{v}_i \mathbf{v}_i^\top \quad (32)$$

319 Let us now consider the partial derivative w.r.t. the dominant eigenvector  $\mathbf{v}_1$  and ignore the remaining  
320  $\frac{\partial L}{\partial \mathbf{v}_i}, i \neq 1$ . Then  $\frac{\partial L}{\partial \mathbf{M}}$  becomes

$$\frac{\partial L}{\partial M} = \sum_{i=2}^n \frac{1}{\lambda_1 - \lambda_i} \mathbf{v}_i \mathbf{v}_i^\top \frac{\partial L}{\partial \mathbf{v}_1} \mathbf{v}_1^\top + \frac{\partial L}{\partial \lambda_1} \mathbf{v}_1 \mathbf{v}_1^\top. \quad (33)$$