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UNCONSTRAINED OPTIMIZATION MODELS FOR COMPUTING SEVERAL EXTREME EIGENPAIRS OF REAL SYMMETRIC MATRICES*

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Abstract: This paper considers the problem of computing several extreme eigenpairs of real symmetric matrices. Based on the variational principles, we put forward some new unconstrained optimization models for this classical problem and further analyze their fundamental properties. It is shown that the extreme eigenpairs of any real symmetric matrix can be recovered from the global minimizers of our unconstrained models. The alternate Barzilai-Borwein method with the adaptive nonmonotone line search is then utilized for solving the unconstrained models. The preliminary numerical results indicate that our approach is quite promising.

Key words: *extreme eigenpairs, variational principles, unconstrained optimization, alternate Barzilai-Borwein method, adaptive nonmonotone line search*

Mathematics Subject Classification: *15A18, 65F15, 65K10, 90C06*

1 Introduction

In this paper, we consider the problem of computing several extreme eigenvalues and their corresponding eigenvectors of a real symmetric matrix $A \in \mathbb{R}^{n\times n}$. This classical problem plays an important role in many fields of scientific and engineering computing and it is equivalent to some optimization problems by using the variational principles. There are two well-known principles; *i.e.,* the Rayleigh quotient minimization [1, 10, 17]

$$\min_{X\in\mathbb{R}^{n\times r}} \ \mathrm{tr}\left(X^{\mathrm{T}}AX(X^{\mathrm{T}}X)^{-1}\right),$$

and the trace minimization [12, 21, 22]

$$\min_{X\in\mathbb{R}^{n\times r}} \ \mathrm{tr}(X^{\mathrm{T}}AX), \quad \text{s.t.} \quad X^{\mathrm{T}}X = I_r, \tag{1.1}$$

where I_r means the r-by-r identity matrix. However, the above two principles involve computing the inverse or orthogonalization of a matrix, which is expensive for large dimensional eigenproblems. Thus new models with smaller computing cost are in demand.

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In 1989, Auchmuty [2] presented some new variational principles to find the extreme eigenvalue (the smallest or largest one) of a real symmetric matrix. The principles therein are to minimize some smooth functions which are the sum of a function of $\frac{1}{2}\|x\|^2$ and a function of $\frac{1}{2}x^{\mathrm{T}}Ax$. More precisely, his model is given below:

$$\min_{x\in\mathbb{R}^n} \; E(x) = \Phi\left(\frac{1}{2}\|x\|^2\right) + \Psi\left(\frac{1}{2}x^{\mathrm{T}}Ax\right), \tag{1.2}$$

where the twice continuously differentiable functions Φ and Ψ satisfy some mild assumptions. Some specific choices of Φ and Ψ were also given in [2]. Among all kinds models, the following quartic one

$$\min_{x\in\mathbb{R}^n} \; E_4(x) = \frac{1}{4}\|x\|^4 + \frac{1}{2}x^{\mathrm{T}}Ax, \tag{1.3}$$

captured the attention of some authors and was well studied in [3, 8, 18]. Note that Auchmuty [2] also considered a more general version of (1.3) as follows:

$$\min_{x\in\mathbb{R}^n} \; E_{\mu,\zeta}(x) = \frac{1}{\zeta}\|x\|_2^{\zeta} + \frac{1}{2}x^{\mathrm{T}}(A-\mu I_n)x, \;\; \zeta > 2. \tag{1.4}$$

which can compute the smallest eigenvalue smaller than μ.

However, the aforementioned variational principles (1.2) – (1.4) are only designed to compute single eigenvalue. To compute several extreme eigenpairs of a real symmetric matrix, this paper considers to extend these principles to the matrix cases. We first propose the block unconstrained β-order model

$$\min_{X\in\mathbb{R}^{n\times r}} \widehat{P}_{\mu,\beta,\theta}(X) = \frac{\theta}{\beta}\|X^{\mathrm{T}}X\|_{\mathrm{F}}^{\frac{\beta}{2}} + \frac{1}{2}\mathrm{tr}\left(X^{\mathrm{T}}(A-\mu I_n)X\right), \quad \beta > 2,\, \theta > 0, \tag{1.5}$$

where $\theta, \mu \in \mathbb{R}$ are some scaling and shifting parameters, respectively, and I_n is the n-by-n identity matrix. Model (1.5) is a natural extension of model (1.4). Setting $\beta = 4$ and $\theta = 1$ in (1.5) yields the unconstrained quartic model

$$\min_{X\in\mathbb{R}^{n\times r}} P_{\mu}(X) = \frac{1}{4}\mathrm{tr}\left(X^{\mathrm{T}}XX^{\mathrm{T}}X\right) + \frac{1}{2}\mathrm{tr}\left(X^{\mathrm{T}}(A-\mu I_n)X\right). \tag{1.6}$$

If $\mu > 0$, letting $\beta = 4$ and $\theta = \mu$, we obtain the unconstrained model below:

$$\min_{X\in\mathbb{R}^{n\times r}} \; \frac{\mu}{4}\mathrm{tr}\left(X^{\mathrm{T}}XX^{\mathrm{T}}X\right) + \frac{1}{2}\mathrm{tr}\left(X^{\mathrm{T}}(A-\mu I_n)X\right).$$

We can also extend model (1.5) to the following general model

$$\min_{X\in\mathbb{R}^{n\times r}} \; G_{\mu}(X) = \Phi\left(\frac{1}{2}\|X^{\mathrm{T}}X\|_{\mathrm{F}}\right) + \Psi\left(\frac{1}{2}\mathrm{tr}(X^{\mathrm{T}}(A-\mu I_n)X)\right), \tag{1.7}$$

where Φ and Ψ satisfy some mild conditions.

By choosing the parameter μ in (1.5) and (1.7) appropriately, we prove that their global minimizers lie in the eigenspace corresponding to the r smallest eigenvalues of A. Consequently, the desired eigenpairs can be obtained by applying the Rayleigh-Ritz procedure [20] to the global minimizers.

It should be noted here that, independently of this work, based on the Courant penalty function of (1.1), Wen *et al.* [23] proposed the trace-penalty minimization model as follows:

$$\min_{X\in\mathbb{R}^{n\times r}} f_{\mu}(X) := \frac{1}{2}\mathrm{tr}(X^{\mathrm{T}}AX) + \frac{\mu}{4}\|X^{\mathrm{T}}X - I_r\|_{\mathrm{F}}^2, \quad \mu > 0, \tag{1.8}$$

where μ is the penalty parameter. By choosing μ appropriately, they proved that model (1.8) is equivalent to the eigenvalue problem. They also gave the specific form of the nonzero stationary points and global minimizers of (1.8) and further showed that the stationary points can only be saddle points or global minimizers, provided that μ satisfies some mild condition. Besides, they developed a specialized gradient-type method for (1.8) and parallelized it by using OpenMP.

The rest of this paper is organized as follows. In §2.1, we introduce our new block unconstrained β-order model (1.5) and investigate its properties. The more general model (1.7) is then considered in §2.2. The alternate Barzilai-Borwein (BB) method with the adaptive nonmonotone line search is utilized for solving the main unconstrained models in §3.1. The preliminary numerical results in §3.2 demonstrate the usefulness of the new models. Finally, we make some conclusions and discussions in the last section.

Notations: The first r columns of $M \in \mathbb{R}^{n\times m}$ is denoted by $M_{(r)}$. The notation $\mathrm{Diag}(\gamma_1, \ldots, \gamma_n)$ denotes an n-by-n diagonal matrix whose entries are $\gamma_1, \ldots, \gamma_n$. The matrix $A \in \mathbb{R}^{n\times n}$ takes the eigenvalue decomposition of the form

$$A = Q\Lambda Q^{\mathrm{T}},$$

where $Q \in \mathbb{R}^{n\times n}$ is orthogonal, $\lambda_i(\cdot)$ designates the i-th algebraically smallest eigenvalue of a matrix, and $\Lambda = \mathrm{Diag}(\lambda_1(A), \ldots, \lambda_n(A))$. If there is no confusing, we also drop A and simply use $\lambda_1, \lambda_2, \ldots, \lambda_n$ to denote the eigenvalues of A. We assume that they are in ascending order; namely, $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$. Besides, we use $\sigma_i(\cdot)$ to denote the i-th algebraically smallest singular value of a matrix.

2 Variational Principles for Computing Extreme Eigenpairs

We propose in this section some new variational principles which can be regarded as extensions of the models in [2, 3, 18]. The block unconstrained β-order model is presented in §2.1. Our new model shares the theoretical results of the trace-penalty minimization model (1.8) in [23], but the proofs are different and the form of the nonzero stationary point is quite different. In §2.2, we illustrate a more general unconstrained optimization model. Two other specific variational principles for computing the largest eigenpairs of positive definite matrices are also given in this subsection.

2.1 Block Unconstrained β-Order Model

The unconstrained quartic model (1.3), a special case of model (1.4), works well for computing the smallest eigenvalue and its corresponding eigenvector of negative definite matrices . In this subsection, we extend model (1.4) to the block counterpart model (1.5), to compute the r smallest eigenpairs for any real symmetric matrix (not necessarily negative definite).

Throughout this paper, let $X = U\Sigma V^{\mathrm{T}} \in \mathbb{R}^{n\times r}$ be the thin singular value decomposition (SVD) of X, where $U \in \mathbb{R}^{n\times r}$ and $V \in \mathbb{R}^{r\times r}$ are matrices with orthonormal columns, and $\Sigma = \mathrm{Diag}(\sigma_1, \ldots, \sigma_r)$ with $0 \le \sigma_1 \le \cdots \le \sigma_r$. Here, for simplicity, we use σ_i to denote $\sigma_i(X)$. Denote by p the rank of X with $p \le r$. Then we know that $\sigma_1 = \cdots = \sigma_{r-p} = 0 < \sigma_{r-p+1} \le \cdots \le \sigma_r$. Further, denoting by Σ_1 the diagonal matrix $\mathrm{Diag}(\sigma_{r-p+1}, \ldots, \sigma_r)$, we have the compact SVD representation

$$X = U_1\Sigma_1 V_1^{\mathrm{T}}, \tag{2.1}$$

where U_1 and V_1 are the last p columns of U and V, respectively.

The following lemma gives the formulation of any nonzero stationary point of model (1.5). Specifically, the left singular vector of any nonzero stationary point is certain eigenvector of A, and its singular values can be computed from the eigenvalues of A.

Lemma 2.1. *Suppose $X\in\mathbb{R}^{n\times r}$ is a nonzero stationary point of (1.5). Then it takes the compact SVD form:*

$$X = Q_{p,s}\left[c_p^{\frac{4-\beta}{2}}\theta^{-1}(\mu I_p-\Lambda_p)\right]^{1/2}V_p^{\mathrm{T}}, \tag{2.2}$$

where $Q_{p,s}$ consists of the $j_1,\ldots,j_p$ columns of Q with

$$1\le j_1\le\cdots\le j_p\le s := \arg\max_{\lambda_i<\mu} i, \tag{2.3}$$

the constant c_p is defined as

$$c_p := \|X^{\mathrm{T}}X\|_{\mathrm{F}} = \theta^{-\frac{2}{\beta-2}}\left(\sum\nolimits_{i=1}^{p}(\mu-\lambda_{j_i})^2\right)^{\frac{1}{\beta-2}}, \tag{2.4}$$

$\Lambda_p=\mathrm{Diag}(\lambda_{j_1},\ldots,\lambda_{j_p})$*, and V_p is any r-by-p matrix with orthonormal columns.*

Proof. The stationary point X of (1.5) satisfies the first-order optimality condition

$$\nabla\widehat{P}_{\mu,\beta,\theta}(X) = (A-\mu I_n)X+\theta\|X^{\mathrm{T}}X\|_{\mathrm{F}}^{\frac{\beta-4}{2}}XX^{\mathrm{T}}X = 0, \tag{2.5}$$

i.e.,

$$AX = X\big(\mu I_r-\theta c_p^{\frac{\beta-4}{2}}X^{\mathrm{T}}X\big). \tag{2.6}$$

Substituting (2.1) into (2.6) and noting $U_1^{\mathrm{T}}U_1=V_1^{\mathrm{T}}V_1=I_p$, we have

$$AU_1\Sigma_1V_1^{\mathrm{T}} = U_1\big(\mu I_p-\theta c_p^{\frac{\beta-4}{2}}\Sigma_1^2\big)\Sigma_1V_1^{\mathrm{T}}.$$

By multiplying $V_1\Sigma_1^{-1}$ from the both sides of above equation, we derive

$$AU_1 = U_1(\mu I_p-\theta c_p^{\frac{\beta-4}{2}}\Sigma_1^2), \tag{2.7}$$

which means that the i-th ($i=1,\ldots,p$) column of U_1 is the eigenvector of A corresponding to the eigenvalue

$$\mu-\theta c_p^{\frac{\beta-4}{2}}\sigma_{r-p+i}^2 \triangleq \lambda_{j_i}.$$

We then have $\theta^2c_p^{\beta-4}\sum_{i=1}^{p}\sigma_{r-p+i}^4=\sum_{i=1}^{p}(\lambda_{j_i}-\mu)^2$, which with $\sum\limits_{i=1}^{p}\sigma_{r-p+i}^4=\|X^{\mathrm{T}}X\|_{\mathrm{F}}^2=c_p^2$ yields

$$c_p = \theta^{-\frac{2}{\beta-2}}\left(\sum\nolimits_{i=1}^{p}(\mu-\lambda_{j_i})^2\right)^{\frac{1}{\beta-2}}.$$

Thus X is of the form (2.2). The proof is completed. □

The following theorem shows that under a mild assumption on the parameter μ, the left singular vectors of the global minimizers X^* are exactly the extreme eigenvectors of A while the singular values of X^* can be represented by the extreme eigenvalues of A.

Theorem 2.2. *Problem (1.5) has a rank-r stationary point if and only if*

$$\mu > \lambda_r. \tag{2.8}$$

Furthermore, any global minimizer X^* of (1.5) has the thin SVD form:

$$X^* = Q_{(r)} \left[c^{\frac{4-\beta}{2}} \theta^{-1} (\mu I_r - \Lambda_r) \right]^{1/2} V_r^{\mathrm{T}}, \tag{2.9}$$

where $c := \|(X^*)^{\mathrm{T}} X^*\|_{\mathrm{F}} = \theta^{-\frac{2}{\beta-2}} \left(\sum_{i=1}^r (\mu - \lambda_i)^2 \right)^{\frac{1}{\beta-2}}$, $\Lambda_r = \mathrm{Diag}(\lambda_1, \ldots, \lambda_r)$ and V_r is any r-by-r orthogonal matrix. Additionally, the global minimum of (1.5) is

$$\widehat{P}^*_{\mu,\beta,\theta} := -\frac{\theta^{-\frac{2}{\beta-2}} (\beta - 2)}{2\beta} \left(\sum\nolimits_{i=1}^r (\mu - \lambda_i)^2 \right)^{\frac{\beta}{2(\beta-2)}}.$$

Proof. First, if problem (1.5) has a rank-r solution X, then all $\sigma_i > 0$ for $i = 1, \ldots, r$. It follows from (2.7) that $\mu - \theta c_p^{\frac{\beta-4}{2}} \sigma_r^2 \le \cdots \le \mu - \theta c_p^{\frac{\beta-4}{2}} \sigma_1^2$ are the r eigenvalues of A. Noticing that $\lambda_1 \le \cdots \le \lambda_r$ are the r smallest eigenvalues of A, we must have $\mu - \theta c_p^{\frac{\beta-4}{2}} \sigma_1^2 \ge \lambda_r$, which with $\sigma_1 > 0$ indicates $\mu > \lambda_r$.

On the other hand, if $\mu > \lambda_r$, it is easy to verify that X^* defined in (2.9) is of full column rank and satisfies the first-order optimality condition (2.5). Thus the equivalent condition (2.8) holds.

We now turn to prove the second statement. Still use X to denote any nonzero stationary point. It follows from the first-order optimality condition (2.5) and the definition (2.4) that

$$\widehat{P}_{\mu,\beta,\theta}(X) = -\frac{\theta(\beta-2)}{2\beta} \|X^{\mathrm{T}} X\|_{\mathrm{F}}^{\frac{\beta}{2}} = -\frac{\theta^{\frac{2}{\beta-2}} (\beta - 2)}{2\beta} \left(\sum\nolimits_{i=1}^p (\mu - \lambda_{j_i})^2 \right)^{\frac{\beta}{2(\beta-2)}}. \tag{2.10}$$

Noting that $\mu > \lambda_r$, we know that $s := \arg\max_{\lambda_i < \mu} \ i \ge r$, which with (2.10) implies that

$$\widehat{P}_{\mu,\beta,\theta}(X) \ge -\frac{\theta^{-\frac{2}{\beta-2}} (\beta - 2)}{2\beta} \left(\sum\nolimits_{i=1}^r (\mu - \lambda_i)^2 \right)^{\frac{\beta}{2(\beta-2)}} = \widehat{P}^*_{\mu,\beta,\theta}. \tag{2.11}$$

The equality in the above inequality holds if and only if the i-th singular value of X is $c^{\frac{4-\beta}{4}} \theta^{-\frac{1}{2}} \sqrt{\mu - \lambda_{r-i+1}}$. Since the global minimum of (1.5) is always attained at a stationary point (the function value at zero stationary point is zero), we know from (2.11) that the minimum is $\widehat{P}^*_{\mu,\beta,\theta}$ and any global minimizer X^* takes form (2.9). This completes the proof. □

Before we proceed, several remarks on Theorem 2.2 are in order. Firstly, it follows from the proof of Theorem 2.2 that model (1.5) can return the eigenvalues of A which are smaller than μ and their corresponding eigenvectors. More precisely, denoting $\hat{r} = \min\{r, \arg\max_{\lambda_i < \mu} \ i\}$, the global minimizer of (1.5) is

$$X^* = Q_{(\hat{r})} \left[\hat{c}^{\frac{4-\beta}{2}} \theta^{-1} (\mu I_r - \Lambda_{(\hat{r})}) \right]^{1/2} V_{\hat{r}}^{\mathrm{T}},$$

where $\hat{c} = \theta^{-\frac{2}{\beta-2}} \left(\sum_{i=1}^{\hat{r}} (\mu - \lambda_i)^2 \right)^{\frac{1}{\beta-2}}$, $\Lambda_{(\hat{r})} = \mathrm{Diag}(\lambda_1, \ldots, \lambda_{\hat{r}})$ and $V_{\hat{r}}$ is any r-by-$\hat{r}$ matrix with orthonormal columns. Particularly, when A is negative definite, we can easily choose $\mu = 0$. In fact, the parameter μ can be regarded as a shifting parameter of A. Secondly, if

the r largest eigenvalues are wanted, we only need to reset $A := -A$. Further, our model can be extended to compute the r smallest singular values and corresponding right (resp. left) singular vectors of a real matrix $\tilde{A}$ if we set $A := \tilde{A}^{\mathrm{T}}\tilde{A}$ (resp. $A := \tilde{A}\tilde{A}^{\mathrm{T}}$).

Let $\mathcal{L}\colon \mathbb{R}^{n\times r} \to \mathbb{R}^{n\times r}$ be a linear operator. The Fréchet derivative of $\nabla\widehat{P}_{\mu,\beta,\theta}$ at X is defined as the operator $\nabla^2\widehat{P}_{\mu,\beta,\theta}\colon \mathbb{R}^{n\times r} \to \mathcal{L}$ such that

$$\lim_{\|S\|_{\mathrm{F}}\to 0} \frac{\|\nabla\widehat{P}_{\mu,\beta,\theta}(X+S) - \nabla\widehat{P}_{\mu,\beta,\theta}(X) - \nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S)\|_{\mathrm{F}}}{\|S\|_{\mathrm{F}}} = 0.$$

We can easily derive that

$$\begin{aligned}\nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S) = (A-\mu I)S + \theta\|X^{\mathrm{T}}X\|_{\mathrm{F}}^{\frac{\beta-4}{2}}\left(SX^{\mathrm{T}}X + X(X^{\mathrm{T}}S + S^{\mathrm{T}}X)\right)\\ +\theta(\beta-4)\|X^{\mathrm{T}}X\|_{\mathrm{F}}^{\frac{\beta-8}{2}}\mathrm{tr}(S^{\mathrm{T}}XX^{\mathrm{T}}X)XX^{\mathrm{T}}X. \qquad (2.12)\end{aligned}$$

The following theorem shows that our block unconstrained β-order model enjoys the advantage that all the nonzero stationary points can only be the global minimizers or saddle points under some conditions.

Theorem 2.3. *If $\mu > \lambda_r$, any nonzero stationary point of problem (1.5) is either a saddle point or a global minimizer defined in (2.9). Furthermore, if $\lambda_r < \mu \le \lambda_{r+1}$, all the rank-$r$ stationary points are global minimizers.*

Proof. We first give a simple formulation of $\mathrm{tr}\left(S^{\mathrm{T}}\nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S)\right)$. It follows from Lemma 2.1 that any nonzero stationary point X takes the form (2.2). Without loss of generality, assume $V_p^{\mathrm{T}} = [I_p,\, 0_{p,r-p}]$ in (2.2), where $0_{p,r-p}$ is the p-by-$(r-p)$ zero matrix. Thus X can be expressed by

$$X = \left(c_p^{\frac{4-\beta}{2}}\theta^{-1}\right)^{1/2}\left[Q_p(\mu I_p - \Lambda_p)^{1/2},\ 0_{p,r-p}\right] := [X_1, X_2], \qquad (2.13)$$

where Q_p stands for the $Q_{p,s}$ in (2.2).

Let $S = [S_1, S_2]$, where $S_1 \in \mathbb{R}^{n\times p}$ and $S_2 \in \mathbb{R}^{n\times(r-p)}$ are the first p columns and last $r-p$ columns of S, respectively. Noticing that $c_p = \|X^{\mathrm{T}}X\|_{\mathrm{F}}$, with (2.12), (2.13) and the partition of S, we have

$$\begin{aligned}\mathrm{tr}\left(S^{\mathrm{T}}\nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S)\right) &= \mathrm{tr}\left(S^{\mathrm{T}}(A-\mu I_n + \theta c_p^{\frac{\beta-4}{2}}XX^{\mathrm{T}})S\right) + \theta c_p^{\frac{\beta-4}{2}}\mathrm{tr}(S^{\mathrm{T}}SX^{\mathrm{T}}X)\\ &\quad + \theta c_p^{\frac{\beta-4}{2}}\mathrm{tr}(S^{\mathrm{T}}XS^{\mathrm{T}}X) + \theta(\beta-4)c_p^{\frac{\beta-8}{2}}[\mathrm{tr}(S^{\mathrm{T}}XX^{\mathrm{T}}X)]^2\\ &= \mathrm{tr}\left(S_1^{\mathrm{T}}(A-\mu I_n + \theta c_p^{\frac{\beta-4}{2}}X_1X_1^{\mathrm{T}})S_1\right)\\ &\quad + \mathrm{tr}\left(S_2^{\mathrm{T}}(A-\mu I_n + \theta c_p^{\frac{\beta-4}{2}}X_1X_1^{\mathrm{T}})S_2\right)\\ &\quad + \theta c_p^{\frac{\beta-4}{2}}\left(\mathrm{tr}(S_1^{\mathrm{T}}S_1X_1^{\mathrm{T}}X_1) + \mathrm{tr}(S_1^{\mathrm{T}}X_1S_1^{\mathrm{T}}X_1)\right)\\ &\quad + \theta(\beta-4)c_p^{\frac{\beta-8}{2}}[\mathrm{tr}(S_1^{\mathrm{T}}X_1X_1^{\mathrm{T}}X_1)]^2, \qquad (2.14)\end{aligned}$$

where

$$X_1 = \left(c_p^{\frac{4-\beta}{2}}\theta^{-1}\right)^{1/2}Q_p(\mu I_p - \Lambda_p)^{1/2}. \qquad (2.15)$$

Let Q_{p^c} consist of the columns of Q which are not in Q_p, we have $A = Q\Lambda Q^{\mathrm{T}} = Q_p\Lambda_p Q_p^{\mathrm{T}} + Q_{p^c}\Lambda_{p^c}Q_{p^c}^{\mathrm{T}}$. Thus there holds

$$A - \mu I_n + \theta c_p^{\frac{\beta-4}{2}} X_1 X_1^{\mathrm{T}} = Q(\Lambda - \mu I_n)Q^{\mathrm{T}} + Q_p(\mu I_p - \Lambda_p)Q_p^{\mathrm{T}} = Q_{p^c}(\Lambda_{p^c} - \mu I_{n-p})Q_{p^c}^{\mathrm{T}}. \tag{2.16}$$

Substituting the above equation, (2.15) and (2.4) into (2.14), we obtain

$$\begin{aligned}
&\mathrm{tr}\left(S^{\mathrm{T}}\nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S)\right)\\
=&\,\mathrm{tr}\left(S_1^{\mathrm{T}}Q_{p^c}(\Lambda_{p^c} - \mu I_{n-p})Q_{p^c}^{\mathrm{T}}S_1\right) + \mathrm{tr}\left(S_2^{\mathrm{T}}Q_{p^c}(\Lambda_{p^c} - \mu I_{n-p})Q_{p^c}^{\mathrm{T}}S_2\right)\\
&+\mathrm{tr}\left(S_1^{\mathrm{T}}S_1(\mu I_p - \Lambda_p)\right) + \mathrm{tr}(S_1^{\mathrm{T}}Q_p(\mu I_p - \Lambda_p)^{1/2}S_1^{\mathrm{T}}Q_p(\mu I_p - \Lambda_p)^{1/2})\\
&+(\beta-4)\Big(\sum\nolimits_{i=1}^{p}(\mu - \lambda_{j_i})^2\Big)^{-1}\left[\mathrm{tr}(S_1^{\mathrm{T}}Q_p(\mu I_p - \Lambda_p)^{3/2})\right]^2.
\end{aligned} \tag{2.17}$$

We now show the first statement. Assuming $\mu > \lambda_r$, we consider three cases of Λ_p in (2.13). Firstly, if $\Lambda_p = \mathrm{Diag}(\lambda_1, \ldots, \lambda_r)$, we know from Theorem 2.2 that X is a global minimizer.

Secondly, consider the case that $\Lambda_p = \mathrm{Diag}(\lambda_1, \ldots, \lambda_p)$ but $0 < p < r$. Denote by q_i the i-th column of Q, that is the eigenvector corresponding to λ_i. Let all columns of S_1 are zeros except that its first column is q_1, and $S_2 = 0_{n,r-p}$. With (2.17), we have that

$$\begin{aligned}
\mathrm{tr}\left(S^{\mathrm{T}}\nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S)\right) = 0 \;+\; 0 + (\mu - \lambda_1) + (\mu - \lambda_1)&\\
+(\beta-4)\Big(\sum\nolimits_{i=1}^{p}(\mu - \lambda_i)^2\Big)^{-1}(\mu - \lambda_1)^3.&
\end{aligned} \tag{2.18}$$

Noticing that $\beta > 2$ and $\mu > \lambda_r \geq \lambda_1$, we have

$$\mathrm{tr}\left(S^{\mathrm{T}}\nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S)\right) > 2(\mu - \lambda_1) - 2\Big(\sum\nolimits_{i=1}^{p}(\mu - \lambda_i)^2\Big)^{-1}(\mu - \lambda_1)^3 > 0. \tag{2.19}$$

On the other hand, letting $S_1 = 0_{n,p}$ and $S_2 = \left[q_{p+1}, 0_{n,1}, \ldots, 0_{n,1}\right]$, we obtain from (2.17) that

$$\mathrm{tr}\left(S^{\mathrm{T}}\nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S)\right) = 0 + (\lambda_{p+1} - \mu) + 0 + 0 + 0 < 0, \tag{2.20}$$

where the inequality is due to the inequality $\mu > \lambda_r \geq \lambda_{p+1}$. We thus obtain from (2.19) and (2.20) that X is a saddle point.

Thirdly, consider the case that $\Lambda_p \neq \mathrm{Diag}(\lambda_1, \ldots, \lambda_p)$ and $p > 0$. Then there must exist two eigenvalues $\lambda_{t_1} > \lambda_{t_2}$, where λ_{t_1} is in Λ_p while λ_{t_2} is in Λ_{p^c}. Constructing S_1 such that all columns are zeros except that its t_1-th column is q_{t_2}, and $S_2 = 0$, we then derive from (2.17) that

$$\mathrm{tr}\left(S^{\mathrm{T}}\nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S)\right) = (\lambda_{t_2} - \mu) + 0 + (\mu - \lambda_{t_1}) + 0 + 0 < 0. \tag{2.21}$$

On the other hand, if all columns of S are zeros except its first column is q_{j_1}, similar to (2.18) and (2.19), we get by simple computations that

$$\mathrm{tr}\left(S^{\mathrm{T}}\nabla^2\widehat{P}_{\mu,\beta,\theta}(X)(S)\right) = 2(\mu - \lambda_{j_1}) + (\beta-4)\Big(\sum\nolimits_{i=1}^{p}(\mu - \lambda_{j_i})^2\Big)^{-1}(\mu - \lambda_{j_1})^3 > 0. \tag{2.22}$$

Inequalities (2.21) and (2.22) imply that X is also a saddle point in this case. Therefore, all nonzero stationary points are either saddle points or the global minimizer points. This proves the first statement.

We further show the second statement. Suppose $\lambda_r < \mu \leq \lambda_{r+1}$. Let X be any given rank-r stationary point. It is easy to see that $s = r$ in (2.3). Thus we have $j_1 = 1, \ldots, j_r = r$, which means $\Lambda_p = \mathrm{Diag}(\lambda_1, \ldots, \lambda_r)$. By Theorem 2.2, we see that X is a global minimizer of (1.5). The proof is completed. □

We now show that if the condition $\lambda_r < \mu \leq \lambda_{r+1}$ does not occur, the second statement of the above theorem may not hold. Consider the case $\lambda_r = \lambda_{r+1}$ and $\lambda_1 < \lambda_r$. From the definition, we know $s \geq r+1$. Construct the point

$$\widetilde{X} = \widetilde{Q}_{p,s} \left[\tilde{c}_p^{\frac{4-\beta}{2}} \theta^{-1} (\mu I_p - \widetilde{\Lambda}_p) \right]^{1/2},$$

where $j_1 = 2, \ldots, j_p = r+1$, $\tilde{c}_p = \theta^{-\frac{2}{\beta-2}} \left(\sum_{i=2}^{r+1} (\mu - \lambda_i)^2 \right)^{\frac{1}{\beta-2}}$ and $\widetilde{\Lambda}_p = \mathrm{Diag}(\lambda_2, \ldots, \lambda_{r+1})$. It is easy to see from Lemma 2.1 that $\widetilde{X}$ is a rank-r stationary point. On the other hand, it follows from Theorem 2.2 that $\widetilde{X}$ is not a global minimizer.

Denote by $Y(X) \in \mathbb{R}^{n \times r}$ an orthonormal basis of the range space of X. Define $R(X) := AY(X) - Y(X)\big(Y(X)^{\mathrm{T}} AY(X)\big)$. It is well known that $Y(X)$ spans the eigenspace of A if and only if $R(X) = 0$. To illustrate the relationship between $\|R(X)\|_{\mathrm{F}}$ and $\|\nabla \widehat{P}_{\mu,\beta,\theta}(X)\|_{\mathrm{F}}$, we give the following theorem.

Theorem 2.4. *Consider the model (1.5), for any rank-r matrix X, we have*

$$\|R(X)\|_{\mathrm{F}} \leq \sigma_1(X)^{-1} \|\nabla \widehat{P}_{\mu,\beta,\theta}(X)\|_{\mathrm{F}}. \tag{2.23}$$

Furthermore, given any $\epsilon > 0$ and $\delta = \frac{\epsilon}{1+\epsilon} c^{\frac{4-\beta}{4}} \theta^{-\frac{1}{2}} \sqrt{\mu - \lambda_r}$, for any X satisfying $\|X - X^*\|_{\mathrm{F}} \leq \delta$, where X^* is any global minimizer defined in (2.9), the following inequality holds

$$\|R(X)\|_{\mathrm{F}} \leq c^{\frac{\beta-4}{4}} \theta^{\frac{1}{2}} \frac{1+\epsilon}{\sqrt{\mu - \lambda_r}} \|\nabla \widehat{P}_{\mu,\beta,\theta}(X)\|_{\mathrm{F}}. \tag{2.24}$$

Proof. It follows from (2.6) that

$$AX = \nabla \widehat{P}_{\mu,\beta,\theta}(X) + X(\mu I_r - \theta \|X^{\mathrm{T}} X\|_{\mathrm{F}}^{\frac{\beta-4}{2}} X^{\mathrm{T}} X). \tag{2.25}$$

Following the definition of $Y(X)$, there must exist a nonsingular matrix K such that $X = Y(X)K$. Substituting this relation into (2.25) and multiplying K^{-1} from both sides of the relation, we obtain

$$AY(X) = \nabla \widehat{P}_{\mu,\beta,\theta}(X) K^{-1} + Y(X)(\mu I_r - \theta \|K^{\mathrm{T}} K\|_{\mathrm{F}}^{\frac{\beta-4}{2}} K^{\mathrm{T}} K).$$

Noticing that $Y(X)^{\mathrm{T}} Y(X) = I_r$ and $\big(I_n - Y(X)Y(X)^{\mathrm{T}}\big) Y(X) = 0$, we then have

$$R(X) = \big(I_n - Y(X)Y(X)^{\mathrm{T}}\big)\,(AY(X)) = \big(I_n - Y(X)Y(X)^{\mathrm{T}}\big)\, \nabla \widehat{P}_{\mu,\beta,\theta}(X) K^{-1}.$$

Therefore, there holds

$$\|R(X)\|_{\mathrm{F}} \leq \|\nabla \widehat{P}_{\mu,\beta,\theta}(X) K^{-1}\|_{\mathrm{F}} \leq \|K^{-1}\|_2 \|\nabla \widehat{P}_{\mu,\beta,\theta}(X)\|_{\mathrm{F}},$$

which with $K^{\mathrm{T}}K = X^{\mathrm{T}}X$ implies (2.23).

Now we establish the estimate (2.24). The formulation (2.9) of any global minimizer X^* indicates that $\sigma_1(X^*) = c^{\frac{4-\beta}{4}}\theta^{-\frac{1}{2}}\sqrt{\mu-\lambda_r}$. Therefore, we have that

$$\sigma_1(X) \geq \sigma_1(X^*) - \delta = \frac{c^{\frac{4-\beta}{4}}\theta^{-\frac{1}{2}}}{1+\epsilon}\sqrt{\mu-\lambda_r}. \tag{2.26}$$

This is because, for any $B_1, B_2 \in \mathbb{R}^{m\times n}$, we must have that $|\sigma_1(B_1)-\sigma_1(B_2)| \leq \|B_1-B_2\|_{\mathrm{F}}$. Combining (2.26) and (2.23) yields (2.24). We complete the proof. □

The above theorem suggests that the error of approximate eigenpairs $\|R(X)\|_{\mathrm{F}}$ can be efficiently controlled by the error $\|\nabla\widehat{P}_{\mu,\beta,\theta}(X)\|_{\mathrm{F}}$. After an approximate solution of (1.5) is obtained, we can use the Rayleigh-Ritz procedure to recover the approximate extreme eigenpairs. More exactly, we first calculate the eigenvalue decomposition $Y(X)^{\mathrm{T}}AY(X) = V\widehat{\Sigma}V^{\mathrm{T}}$ and then set the approximate eigenpairs to be $(Y(X)V, \widehat{\Sigma})$.

2.2 General Unconstrained Model

In this subsection, we investigate the more general unconstrained model (1.7), where Φ and Ψ satisfy the following assumptions which are similar to those in [2].

Assumption 2.5.

(A1) $\Phi\colon [0,+\infty) \to \mathbb{R}$ is continuous differentiable and twice continuously differentiable on $(0,+\infty)$ with $\Phi(0) = 0$ and $\Phi'(z) \neq 0$ for $z \neq 0$.

(A2) $\Psi\colon \mathbb{R} \to \mathbb{R}$ is twice continuously differentiable on $\mathbb{R}\backslash\{0\}$ with $\Psi(0) = 0$.

Further, to investigate model (1.7) easily, we make the following assumptions.

Assumption 2.6.

(A3) Φ and Ψ are monotonically increasing on their domains.

(A4) For each $z \in \mathbb{R}$, there exists a unique $w(z) \geq 0$ such that

$$\Phi'\left(\frac{1}{2}w(z)\right) - z\Psi'\left(-\frac{1}{2}z\cdot w(z)\right) = 0. \tag{2.27}$$

We first establish the formulation of any nonzero stationary point of model (1.7). Similar to Lemma 2.1, the left singular vector of the nonzero stationary point is certain eigenvector of A, and its singular values can be computed from the eigenvalues of A.

Theorem 2.7. *Suppose Φ and Ψ satisfy Assumptions 2.5 and 2.6. Let X be a nonzero stationary point of (1.7). Then it takes the compact SVD form:*

$$X = Q_{p,s}\left[\frac{w(a_p)}{a_p}\left(\mu I_p - \Lambda_p\right)\right]^{1/2} V_p^{\mathrm{T}},$$

where $Q_{p,s}$ consists of the $j_1,\ldots,j_p$ columns of Q with $1 \leq j_1 \leq \cdots \leq j_p \leq s := \arg\max_{\lambda_i<\mu} i$, the constant $a_p := \frac{\Phi'\left(\frac{1}{2}\|X^{\mathrm{T}}X\|_F\right)}{\Psi'\left(\frac{1}{2}\mathrm{tr}(X^{\mathrm{T}}(A-\mu I_n)X)\right)} = \left(\sum_{i=1}^{p}(\mu-\lambda_{j_i})^2\right)^{\frac{1}{2}}$, $w(a_p)$ is defined in (2.27), $\Lambda_p = \mathrm{Diag}(\lambda_{j_1},\ldots,\lambda_{j_p})$, and V_p is any r-by-p matrix with orthonormal columns.

Proof. Since the proof is analogous to that of Lemma 2.1, we only show some main relations. Let $X = U_1\Sigma_1 V_1^T$ be any nonzero stationary point. Using the conditions (A1) and (A4), we have

$$\mu - \lambda_{j_i} = a_p \|\Sigma_1^2\|^{-1}\sigma_i^2,\ i = 1, \ldots, p$$

and

$$\Phi'\left(\frac{1}{2}\|\Sigma_1^2\|_F\right) - a_p\Psi'\left(-\frac{1}{2}a_p\|\Sigma_1^2\|_F\right) = 0.$$

□

We now give the specific formulation of the global minimizer of (1.7) under the condition $\mu > \lambda_r$. The results are similar to those of Theorem 2.2.

Theorem 2.8. *Suppose Φ and Ψ satisfy Assumptions 2.5 and 2.6. Problem (1.7) has a rank-r stationary point if and only if*

$$\mu > \lambda_r.$$

Furthermore, the global minimizer X^* of (1.7) has the thin SVD form:

$$X^* = Q_{(r)}\left[\frac{w(a)}{a}(\mu I_r - \Lambda_r)\right]^{1/2} V_r^{\mathrm{T}}, \tag{2.28}$$

where the constant $a = \left(\sum_{i=1}^r (\mu - \lambda_i)^2\right)^{\frac{1}{2}}$, $\Lambda_r = \mathrm{Diag}(\lambda_1, \ldots, \lambda_r)$, V_r is any r-by-r orthogonal matrix, and the global minimum is

$$G_\mu^* := \Phi\left(\frac{1}{2}w(a)\right) + \Psi\left(-\frac{1}{2}a \cdot w(a)\right).$$

Proof. We only sketch the proof since it is very analogous to that of Theorem 2.2. Consider the nonzero stationary point X, we know from Theorem 2.7 that

$$G_\mu(X) = h(a_p) := \Phi\left(\frac{1}{2}w(a_p)\right) + \Psi\left(-\frac{1}{2}a_p \cdot w(a_p)\right).$$

Using Assumption 2.6, it is easy to verify that

$$h'(z) = -\frac{1}{2}\omega(z)\Psi'\left(-\frac{1}{2}z \cdot \omega(z)\right) \le 0,$$

which means that $h(z)$ is decreasing on $[0, +\infty)$. Thus the global minimum is attained when $a_p = a$, similar to the proof of Theorem 2.2, we can know that the global minimizer X^* has the form (2.28). □

We conclude this section by giving some remarks on model (1.7). Firstly, we always choose some easy Φ and Ψ since the bad ones may worsen the condition number when A is ill-conditioned. It is worth noting that model (1.5) is a special case of model (1.7) with

$$\Phi(y; \beta, \theta) = \frac{\theta}{\beta}(2y)^{\frac{\beta}{2}},\ y \ge 0 \quad \text{and} \quad \Psi(z) = z,\ z \in \mathbb{R}.$$

Here, $\beta > 2, \theta > 0$.

Secondly, considering the case when Φ is monotonically decreasing while the other conditions in Assumptions 2.5 and 2.6 are kept, we know that model (1.5) can return the largest r

eigenvalues of A and their corresponding eigenvectors under the condition $\mu < \lambda_{n-r+1}$. The proofs are similar to those for Theorems 2.7 and 2.8. We further give two specific choices of Φ and Ψ with $\mu = 0$ for the symmetric positive definite matrix. The first one is

$$\Phi(y) = y,\ y \in \mathbb{R} \ \text{ and } \ \Psi(z;\alpha) = \begin{cases} -\alpha^{-1}(2z)^{\alpha/2}, & z > 0; \\ +\infty, & z \le 0, \end{cases} \quad 1 \le \alpha < 2,$$

yielding the model

$$\min_{X \in \mathbb{R}^{n\times r}} \ \frac{1}{2}\|X^{\mathrm{T}}X\|_{\mathrm{F}} - \frac{1}{\alpha}\mathrm{tr}(X^{\mathrm{T}}AX)^{\alpha/2}, \ \ 1 \le \alpha < 2, \tag{2.29}$$

whose vector case was studied in [2]. The second one is

$$\Phi(y) = 2y,\ y \in \mathbb{R} \ \text{ and } \ \Psi(z) = \begin{cases} -\ln(2z), & z > 0; \\ +\infty, & z \le 0, \end{cases}$$

yielding the model

$$\min_{X \in \mathbb{R}^{n\times r}} \ \|X^{\mathrm{T}}X\|_{\mathrm{F}} - \ln \mathrm{tr}(X^{\mathrm{T}}AX). \tag{2.30}$$

The vector case of this model was studied in [18]. According to Theorems 2.7 and 2.8, we can employ models (2.29) and (2.30) to compute the largest eigenvalues and their corresponding eigenvectors of A.

Finally, we point out that the model (1.7) can also be extended to deal with the problem of computing the several smallest (or largest) generalized eigenvalues and corresponding eigenvectors:

$$Ax = \lambda_{A,B}Bx,$$

where $x \in \mathbb{R}^n$ and B is symmetric positive definite. The scalar $\lambda_{A,B}$ is the generalized eigenvalue of (A, B). It is clear that $\bar{A} = B^{-1/2}AB^{-1/2}$ ($B^{1/2}$ is the unique square root of B) shares the same eigenvalues with (A, B), and the eigenvector matrix X of (A, B) satisfies the condition $Z = B^{1/2}X$, where Z is the eigenvector matrix of $\bar{A}$. Notice that the unconstrained model (1.7) for $\bar{A}$ is

$$\min_{Z \in \mathbb{R}^{n\times r}} \ \widehat{G}(Z) = \Phi\left(\frac{1}{2}\|Z^{\mathrm{T}}Z\|_{\mathrm{F}}\right) + \Psi\left(\frac{1}{2}\mathrm{tr}(Z^{\mathrm{T}}(\bar{A} - \mu I_n)Z)\right).$$

Inserting $Z = B^{1/2}X$ into the above formulation, we obtain the unconstrained model for computing the extreme eigenpairs of the generalized eigenvalue problem as follows:

$$\min_{X \in \mathbb{R}^{n\times r}} \ \widehat{G}(X) = \Phi\left(\frac{1}{2}\|X^{\mathrm{T}}BX\|_{\mathrm{F}}\right) + \Psi\left(\frac{1}{2}\mathrm{tr}(X^{\mathrm{T}}(A - \mu B)X)\right).$$

3 Algorithm and Numerical Illustration

3.1 Adaptive Alternative BB Method

Since problem (1.5) is an unconstrained nonconvex minimization problem, a large number of mature unconstrained optimization algorithms can be used to solve it. For instance, Mongeau *et al.* [18] considered the steepest descent algorithm and Newton-type algorithms to solve model (1.4). By contrast, we are particularly interested in BB-like methods which

enjoy the low storage and have proved to be very efficient [4, 7, 19]. Below, we take model (1.6) (a special case of (1.5)) as an example to describe the adaptive alternate BB method.

Denote X, $P_\mu(X)$, $\nabla P_\mu(X)$ at the k-th iteration by X_k, $P_\mu(X_k)$, $\nabla P_\mu(X_k)$, respectively. Let $\mathrm{S}_{k-1} = X_k - X_{k-1}$, $\mathrm{Y}_{k-1} = \nabla P_\mu(X_k) - \nabla P_\mu(X_{k-1})$. The large and short BB stepsizes are respectively defined as follows:

$$\tau_k^{\mathrm{LBB}} = \frac{\mathrm{tr}(\mathrm{S}_{k-1}^{\mathrm{T}}\mathrm{S}_{k-1})}{|\mathrm{tr}(\mathrm{S}_{k-1}^{\mathrm{T}}\mathrm{Y}_{k-1})|} \quad \text{and} \quad \tau_k^{\mathrm{SBB}} = \frac{|\mathrm{tr}(\mathrm{S}_{k-1}^{\mathrm{T}}\mathrm{Y}_{k-1})|}{\mathrm{tr}(\mathrm{Y}_{k-1}^{\mathrm{T}}\mathrm{Y}_{k-1})}.$$

In our numerical experiments in §3.2, the following alternative BB (ABB) stepsize [4]

$$\tau_k^{\mathrm{ABB}} = \begin{cases} \tau_k^{\mathrm{SBB}}, & \text{for odd } k; \\ \tau_k^{\mathrm{LBB}}, & \text{for even } k, \end{cases} \tag{3.1}$$

is adopted since it performs better than τ_k^{LBB} or τ_k^{SBB}. The adaptive nonmonotone line search strategy proposed in [4, 5] is incorporated to ensure the global convergence. We now describe the complete ABB method with the adaptive nonmonotone line search for model (1.6).

Algorithm 3.1. (An Adaptive ABB Method)

Step 0 Give a starting point and initialize the parameters.

(i) Fix $\epsilon > 0$, $0 < \gamma, \delta < 1$, $\tau_{\min}, \tau_{\max} > 0$ and a positive integer L, set $k := 0$, $l := 0$;

(ii) Pick up X_0 with full column rank, a shifting parameter μ larger than λ_r, set $P_r = P_{\mathrm{best}} = P_c := P_0$;

(iii) Compute $\nabla P_\mu(X_0)$ and $\tau_0^{(1)}$.

Step 1 If $\|\nabla P_\mu(X_k)\|_{\mathrm{F}} \le \mathrm{tol}$, return the approximated eigenpairs via the Rayleigh-Ritz procedure and stop.

Step 2 Find the smallest nonnegative integer i_k satisfying

$$P_\mu(X_k - \gamma^{i_k}\tau_k^{(1)}\nabla P_\mu(X_k)) \le P_r - \delta\gamma^{i_k}\tau_k^{(1)}\|\nabla P_\mu(X_k)\|_{\mathrm{F}}^2,$$

and set $\tau_k = \gamma^{i_k}\tau_k^{(1)}$.

Step 3 (i) Update the new point:
$X_{k+1} = X_k - \tau_k\nabla P_\mu(X_k)$, $P_{k+1} = P_\mu(X_{k+1})$;

(ii) Update P_r, P_{best}, P_c by the following procedure:

```
if    P_{k+1} < P_best,
      P_best = P_{k+1}, P_c = P_{k+1}, l = 0,
else
      P_c = max{P_c, P_{k+1}}, l = l + 1,
      if l = L,   P_r = P_c, P_c = P_{k+1}, l = 0,   end
end
```

Step 4 Calculate τ_k^0 by (3.1) and set the first trial stepsize:

$$\tau_k^{(1)} = \max\{\tau_{\min}, \min\{\tau_k^{(0)}, \tau_{\max}\}\}.$$

Step 5 $k := k + 1$. Go to Step 1.

From Theorem 2.2, we know that any global minimizer of the quartic model (1.6) is of full rank. On the other hand, as the initial point X_0 is of full rank, we expect that the sequence $\{X_k;\ k \geq 0\}$ can retain this property. The following theorem states two sufficient conditions for X_{k+1} being rank-r if $\mathrm{rank}(X_k) = r$.

Theorem 3.2. *Consider the gradient iteration formula:*

$$X_{k+1} = X_k - \tau_k \nabla P_\mu(X_k),\ \tau_k \geq 0.$$

Suppose that X_k is of the thin SVD form:

$$X_k = U_k \Sigma_k V_k^{\mathrm{T}},$$

where $U_k \in \mathbb{R}^{n\times r}$ and $V_k \in \mathbb{R}^{r\times r}$ are matrices with orthonormal columns, and $\Sigma_k = \mathrm{Diag}\,(\sigma_1(X_k), \ldots, \sigma_r(X_k))$. If $\mathrm{rank}(X_k) = r$, then X_{k+1} is of rank-r under the condition that

$$\tau_k^{-1} \notin \{\lambda_i(U_k^{\mathrm{T}} A U_k + \Sigma_k^2) - \mu,\ i = 1 \ldots, r\}. \tag{3.2}$$

Moreover, if the stepsize satisfies

$$\tau_k < \frac{1}{\max\{\lambda_r(U_k^{\mathrm{T}} A U_k) + \sigma_r^2(X_k) - \mu, 0\}}, \tag{3.3}$$

X_{k+1} is also of rank-r. Here, $\frac{1}{0} = +\infty$.

Proof. Noticing that X_k is of full column rank, we have that

$$X_{k+1} = X_k - \tau_k \nabla P_\mu(X_k) = \left[I_n - \tau_k \nabla P_\mu(X_k)(X_k^{\mathrm{T}} X_k)^{-1} X_k^{\mathrm{T}}\right] X_k. \tag{3.4}$$

Since the matrices $\nabla P_\mu(X_k)(X_k^{\mathrm{T}} X_k)^{-1} X_k^{\mathrm{T}}$ and $X_k^{\mathrm{T}} \nabla P_\mu(X_k)(X_k^{\mathrm{T}} X_k)^{-1}$ have the same nonzero eigenvalues, the eigenvalues of the matrices in the square brackets of (3.4) are $n-r$ repeated 1, and

$$1 - \tau_k \lambda_i \left(X_k^{\mathrm{T}} \nabla P_\mu(X_k)(X_k^{\mathrm{T}} X_k)^{-1}\right),\quad i = 1, \ldots, r. \tag{3.5}$$

Using the relation $\nabla P_\mu(X_k) = X_k X_k^{\mathrm{T}} X_k + (A - \mu I_n) X_k$ and the thin SVD factorization of X_k, it is easy to verify that

$$X_k^{\mathrm{T}} \nabla P_\mu(X_k)(X_k^{\mathrm{T}} X_k)^{-1} = V_k \Sigma_k (\Sigma_k^2 + U_k^{\mathrm{T}} A U_k - \mu I_r) \Sigma_k^{-1} V_k^{\mathrm{T}},$$

which implies that

$$\lambda_i(X_k^{\mathrm{T}} \nabla P_\mu(X_k)(X_k^{\mathrm{T}} X_k)^{-1}) = \lambda_i(U_k^{\mathrm{T}} A U_k + \Sigma_k^2) - \mu,\ i = 1, \ldots, r. \tag{3.6}$$

Combing (3.6) and (3.5), we know that if (3.2) holds, the matrix in the square brackets of (3.4) must be nonsingular which with $\mathrm{rank}(X_k) = r$ implies that X_{k+1} is of rank-r.

Additionally, it is easy to see that

$$\lambda_r(U_k^{\mathrm{T}} A U_k + \Sigma_k^2) - \mu \leq \lambda_r(U_k^{\mathrm{T}} A U_k) + \sigma_r^2(X_k) - \mu.$$

Since $\tau_k \geq 0$, we only need to consider the positive elements in the set $\{\lambda_i(U_k^{\mathrm{T}} A U_k) + \sigma_r^2(X_k) - \mu,\ i = 1, \ldots, r\}$. Thus the relation (3.3) implies that (3.2) must hold, which further indicates that X_{k+1} is of full column rank. The proof is completed. □

To end this subsection, we make some remarks on Theorem 3.2. Firstly, we can see from the above theorem that X_k can always remain full rank unless the stepsize happens to be equal to one of the r values in (3.2). Also, if μ is large enough, X_k will always remain full rank. Secondly, the results of Theorem 3.2 can be extended to the β-order model easily by inserting a constant $C = \theta \|\Sigma_k^2\|_{\mathrm{F}}^{\frac{\beta-4}{2}}$ before the term Σ_k^2 in (3.2) and $\sigma_r^2(X_k)$ in (3.3), respectively.

3.2 Preliminary Numerical Results

In this subsection, we present some preliminary numerical results to illustrate the efficiency of our new models. Our code (EigUncABB) for Algorithm 3.1 was written in Matlab. All experiments were performed in Matlab R2012a under a Linux operating system on a Thinkpad T420 Laptop with an Intel® dual core CPU at 2.60GHz × 2 and 4GB of RAM.

The test matrix is constructed as the 3D negative Laplacian on a rectangular finite-difference grid. Its exact eigenpairs can be computed by the Matlab code "laplacian" [‡]. The Matlab command for generating the test matrix $A \in \mathbb{R}^{16000\times 16000}$ and its exact eigenpairs is given below,

```
[lambda,Uex,A] = laplacian([20,20,40],{'DD' 'NN' 'P'});
```

where "lambda" and "Uex" are the exact eigenvalues and corresponding eigenvectors, respectively. Note that A is symmetric positive definite and has eigenvalues with multiplicity.

We compare EigUncABB with the Matlab built-in function EIGS which interfaces with the Fortran package APPARCK [15], and a Matlab version of LOBPCG [12][§]. In order to improve the accuracy of the approximate solution, we compute additional $\bar{r} - r$ eigenpairs (called "guard vectors" [6, 11, 16]) and then truncate the r smallest eigenvalues and their corresponding eigenvectors. We choose $\bar{r} = \max(\lfloor 1.1r \rfloor, 10)$, where $\lfloor \cdot \rfloor$ returns the nearest integer less than or equal to the corresponding element. Denote by $\overline{u}_i, \overline{\lambda}_i$ the i-th approximate eigenvector and eigenvalue returned by the corresponding codes. The relative eigenvalue error and relative residual error of i-th eigenpair are respectively defined as

$$\mathrm{err}_i := \frac{|\overline{\lambda}_i - \lambda_i|}{\max(1, |\lambda_i|)} \quad \text{and} \quad \mathrm{resi}_i := \frac{|A\overline{u}_i - \overline{\lambda}_i \overline{u}_i|}{\max(1, |\overline{\lambda}_i|)}.$$

In the following tables, we use the minimal, mean and maximal of err_i and resi_i with $i = 1, \ldots, r$ to measure the solution quality of each code.

The parameters for EigUncABB are given as follows:

$$\mathrm{tol} = 10^{-3},\ \gamma = 0.5,\ \delta = 0.001,\ \tau_{\min} = 10^{-20},\ \tau_{\max} = 10^{20},\ \mathrm{L} = 4,$$

and the initial trial stepsize $\tau_0^{(1)}$ for EigUncABB is chosen to be $\|\nabla \widehat{P}_{\mu,\beta,\theta}(X_0)\|_{\mathrm{F}}^{-1}$. The initial shifting parameter μ is set to be $\mu = 1.01 \times \lambda_{\bar{r}}(X_0^{\mathrm{T}} A X_0)$. Theorem 2.3 indicates that an ideal μ should lie in $(\lambda_{\bar{r}}, \lambda_{\bar{r}+1}]$, provided that $\lambda_{\bar{r}} < \lambda_{\bar{r}+1}$, whereas the initial μ does not always satisfy this condition. Therefore, we need to update μ dynamically. From our preliminary numerical results, when μ is very close to $\lambda_{\bar{r}}$, the algorithm performs badly. Thus we will update μ at most $j_0^{\max}$ times during the iteration. Setting $j_0 = 1$ and $j_0^{\max} = 3$, the procedure for updating μ is given as follows:

```
if   ‖∇P̂_{μ,β,θ}(X_k)‖_F ≤ 0.1^{j_0} · ‖∇P̂_{μ,β,θ}(X_0)‖_F  and  j_0 ≤ j_0^max
     μ = 1.01 × λ_{r̄}(X_k^T A X_k);
     j_0 = j_0 + 1;
end
```

From the description of EIGS, we know that it stops when

$$\text{Ritz estimate residual} \le \mathrm{tol}_{\mathrm{eigs}} \cdot \|A\|_2,$$

[‡]Downloadable from
http://www.mathworks.com/matlabcentral/fileexchange/27279-laplacian-in-1d-2d-or-3d.

[§]Downloadable from http://www.mathworks.com/matlabcentral/fileexchange/48-LOBPCG-m.

where the $\|A\|_2$ is 2-norm of A. To make a fair comparison, we set $\mathrm{tol}_{\mathrm{eigs}} = \frac{10^{-3}}{\|A\|_2}$. Note that $\|A\|_2$ can be computed easily since the eigenvalues of A are available. LOBPCG stops when the residual tolerance $\|AX_{\mathrm{lobpcg}} - X_{\mathrm{lobpcg}}\Lambda_{\mathrm{lobpcg}}\|_{\mathrm{F}} \leq \mathrm{tol}_{\mathrm{lobpcg}}$, where $(X_{\mathrm{lobpcg}}, \Lambda_{\mathrm{lobpcg}})$ are approximate eigenpairs provided by LOBPCG. We first set $\mathrm{tol}_{\mathrm{lobpcg}} = 10^{-3}$. However, in this case, the quality of the eigenpairs returned by LOBPCG is worsen than that of EigUncABB. Thus, to make a fair comparison, we reset $\mathrm{tol}_{\mathrm{lobpcg}} = \omega \cdot 10^{-3}$, where $0 < \omega < 1$. The specific choices of ω are listed in Table 3.1. LOBPCG and EigUncABB use the same initial point, which is set to be some random matrix X_0 with orthonormal columns, whereas the initial point of EIGS is the first column of X_0.

We first compare EigUncABB, applied to model (1.6), with EIGS and LOBPCG to demonstrate its efficiency. Two versions of LOBPCG are considered. The first one is LOBPCG without any preconditioner (LOBPCG-0); the second one is LOBPCG with the incomplete Cholesky factorization preconditioner (LOBPCG-ichol):

```
LL = ichol(A,struct('type','ict','droptol',1e-2,'michol','off'));.
```

See [13, 14] for more possible preconditioners. Here it should be noted that EigUncABB was also implemented with the same preconditioner, but our current results showed that it performed much better than EigUncABB only for the case of small r, not for the case of large r yet. We feel that more attention is required for this issue of preconditioning.

A summary of the computational results is given in Table 3.1. In this table, "time" denotes the CPU time in seconds, "iter" represents the iteration number of LOBPCG-0 and LOBPCG-ichol, "nAx" means the cumulative number of matrix-vector multiplications in EIGS, "nfe" denotes the total number of function evaluations in EigUncABB. From the results, we can see that EigUncABB performs much better than LOBPCG-0. Comparing with LOBPCG-ichol, our EigUncABB is considerably competitive. Particularly, for the case $r \geq 300$, EigUncABB not only takes less CPU time than LOBPCG-ichol, but also finds the approximate eigenpairs with lower relative eigenvalue error and lower relative residual error. Comparing with EIGS, our EigUncABB can always find a solution with less CPU time. Note that for the case $r = 400, 500, 700, 800, 1000$, EIGS can return the solution with extremely high accuracy while for the other cases, EIGS only returns the solution with very low accuracy.

Now we consider the effect of the parameter β in model (1.5) with $\theta \equiv 1$. We test three different values: $\beta = 3$, 4, 5. According to Theorem 2.4, we stop EigUncABB when

$$\|X_k^{\mathrm{T}} X_k\|_{\mathrm{F}}^{\frac{\beta-4}{4}} \cdot \|\nabla \widehat{P}_{\mu,\beta,\theta}(X_k)\|_{\mathrm{F}} \leq \mathrm{tol}.$$

Notice that model (1.5) with $\beta = 4$ reduces to model (1.6). The corresponding results are reported in Table 3.2. The choices of β make a difference, though not great, on the performance. Overall, the 3-order model is the fast, whereas the 5-order model can return solutions with higher accuracy. It remains under study how to choose the parameter β.

4 Discussions and Conclusions

In this paper, we presented several unconstrained optimization models for computing the extreme eigenpairs of any real symmetric matrix. Our contributions are twofold. Firstly, we presented a block unconstrained β-order model. Under a mild assumption on the parameter μ, we showed that the left singular vectors of the global minimizers X^* are exactly the extreme eigenvectors. Further, we proved that the new model has no local minimizer other than global minimizers, provided that μ satisfies some more condition. Secondly, we

Table 3.1: Comparison of EIGS, LOBPCG0, LOBPCG-ichol and EigUncABB

	LOBPCG-0					EIGS			
r	ω	err (min, mean, max)	resi (min, mean, max)	iter	time	err (min, mean, max)	resi (min, mean, max)	nAx	time
20	0.50	(7e-09, 3e-08, 9e-08)	(1e-04, 2e-04, 3e-04)	124	12.2	(1e-16, 1e-02, 7e-02)	(1e-14, 6e-06, 1e-04)	456	2.3
50	0.60	(3e-09, 2e-08, 8e-08)	(8e-05, 1e-04, 3e-04)	78	19.0	(3e-16, 2e-02, 7e-02)	(1e-14, 1e-05, 3e-04)	692	6.4
100	0.40	(1e-09, 1e-08, 9e-08)	(5e-05, 1e-04, 3e-04)	85	39.3	(0e+00, 3e-03, 3e-02)	(1e-14, 3e-06, 3e-04)	1322	20.6
200	0.30	(3e-10, 3e-09, 4e-08)	(3e-05, 7e-05, 2e-04)	109	107.9	(0e+00, 5e-03, 5e-02)	(1e-14, 2e-05, 3e-03)	1772	52.7
300	0.30	(3e-10, 2e-09, 2e-08)	(3e-05, 6e-05, 1e-04)	92	192.4	(0e+00, 7e-04, 2e-02)	(1e-14, 5e-06, 1e-03)	2587	115.6
400	0.02	(7e-13, 5e-12, 2e-11)	(2e-06, 3e-06, 5e-06)	184	457.5	(0e+00, 3e-15, 1e-14)	(9e-15, 2e-14, 3e-14)	3401	207.2
500	0.05	(3e-12, 3e-11, 1e-10)	(4e-06, 8e-06, 1e-05)	503	1153.8	(0e+00, 4e-15, 2e-14)	(7e-15, 3e-14, 4e-14)	4225	326.3
600	0.05	(3e-12, 2e-11, 2e-10)	(4e-06, 7e-06, 1e-05)	343	1266.5	(0e+00, 2e-03, 4e-02)	(1e-14, 1e-05, 5e-03)	3712	312.7
700	0.04	(1e-12, 1e-11, 4e-11)	(2e-06, 5e-06, 8e-06)	138	1153.1	(0e+00, 2e-13, 1e-10)	(7e-15, 9e-09, 7e-06)	4651	486.4
800	0.04	(7e-13, 1e-11, 1e-10)	(2e-06, 5e-06, 1e-05)	125	1450.5	(0e+00, 4e-15, 2e-14)	(1e-14, 3e-14, 5e-14)	5720	694.1
900	0.07	(4e-12, 4e-11, 2e-10)	(4e-06, 9e-06, 1e-05)	217	2432.4	(0e+00, 2e-08, 1e-05)	(1e-14, 2e-06, 2e-03)	5445	727.1
1000	0.10	(7e-12, 9e-11, 5e-10)	(6e-06, 1e-05, 2e-05)	272	3739.6	(0e+00, 4e-15, 3e-14)	(1e-14, 3e-14, 5e-14)	6050	883.6
	LOBPCG-ichol					EigUncABB			
r	ω	err (min, mean, max)	resi (min, mean, max)	iter	time	err (min, mean, max)	resi (min, mean, max)	nfe	time
20	0.50	(1e-09, 1e-08, 5e-08)	(4e-05, 1e-04, 2e-04)	28	3.4	(3e-12, 1e-08, 1e-07)	(4e-06, 1e-05, 8e-05)	160	3.7
50	0.60	(1e-09, 2e-08, 2e-07)	(5e-05, 1e-04, 4e-04)	19	4.9	(4e-10, 2e-08, 4e-07)	(3e-05, 5e-05, 1e-04)	175	8.2
100	0.40	(2e-10, 7e-09, 5e-08)	(2e-05, 9e-05, 2e-04)	23	10.8	(4e-10, 2e-09, 4e-08)	(5e-05, 8e-05, 1e-04)	183	18.2
200	0.30	(6e-11, 2e-09, 2e-08)	(1e-05, 6e-05, 2e-04)	33	32.8	(5e-11, 7e-10, 6e-08)	(2e-05, 4e-05, 9e-05)	221	56.5
300	0.30	(5e-11, 2e-09, 1e-08)	(1e-05, 5e-05, 1e-04)	71	89.5	(1e-12, 8e-11, 1e-08)	(2e-06, 4e-06, 1e-04)	188	84.9
400	0.02	(7e-14, 3e-12, 4e-11)	(5e-07, 2e-06, 8e-06)	65	159.9	(0e+00, 7e-13, 1e-10)	(7e-08, 2e-07, 3e-06)	169	121.9
500	0.05	(4e-13, 2e-11, 3e-10)	(1e-06, 7e-06, 2e-05)	98	284.5	(2e-13, 7e-12, 8e-11)	(1e-06, 6e-06, 2e-05)	226	216.2
600	0.05	(5e-13, 2e-11, 2e-10)	(2e-06, 7e-06, 2e-05)	144	504.3	(0e+00, 2e-12, 2e-10)	(1e-07, 4e-07, 4e-05)	260	320.8
700	0.04	(3e-13, 1e-11, 1e-10)	(1e-06, 5e-06, 1e-05)	57	449.4	(2e-13, 5e-12, 4e-10)	(9e-07, 2e-06, 5e-05)	234	388.9
800	0.04	(2e-13, 1e-11, 9e-11)	(1e-06, 4e-06, 1e-05)	69	645.2	(0e+00, 2e-12, 2e-09)	(9e-08, 5e-07, 1e-04)	240	500.7
900	0.07	(7e-13, 3e-11, 2e-10)	(2e-06, 8e-06, 4e-05)	133	1214.4	(9e-14, 7e-12, 5e-10)	(8e-07, 4e-06, 2e-05)	194	501.3
1000	0.08	(1e-12, 7e-11, 5e-10)	(2e-06, 1e-05, 4e-05)	65	1028.6	(6e-13, 2e-11, 2e-09)	(1e-06, 8e-06, 1e-04)	211	656.7

Table 3.2: Comparison of different values of β in model (1.5) by using EigUncABB

	$\beta = 3$				$\beta = 4$				$\beta = 5$			
r	err (min, mean, max)	resi (min, mean, max)	nfe	time	err (min, mean, max)	resi (min, mean, max)	nfe	time	err (min, mean, max)	resi (min, mean, max)	nfe	time
20	(7e-10, 3e-09, 9e-09)	(4e-05, 8e-05, 1e-04)	155	3.5	(3e-12, 1e-08, 1e-07)	(4e-06, 1e-05, 8e-05)	160	3.7	(1e-11, 7e-09, 1e-07)	(1e-05, 2e-05, 1e-04)	206	4.5
50	(1e-13, 1e-08, 7e-07)	(8e-07, 5e-06, 1e-04)	171	8.8	(4e-10, 2e-08, 4e-07)	(3e-05, 5e-05, 1e-04)	175	8.2	(5e-12, 3e-08, 1e-06)	(6e-06, 3e-05, 2e-04)	197	8.9
100	(2e-11, 1e-07, 1e-05)	(1e-05, 7e-05, 8e-04)	196	19.2	(4e-10, 2e-09, 4e-08)	(5e-05, 8e-05, 1e-04)	183	18.2	(6e-12, 6e-10, 6e-08)	(7e-06, 1e-05, 5e-05)	241	24.3
200	(5e-12, 9e-10, 2e-07)	(4e-06, 8e-06, 7e-05)	240	61.1	(5e-11, 7e-10, 6e-08)	(2e-05, 4e-05, 9e-05)	221	56.5	(1e-13, 5e-11, 8e-09)	(1e-06, 2e-06, 5e-05)	243	60.1
300	(2e-13, 3e-11, 4e-09)	(1e-06, 4e-06, 2e-04)	171	79.2	(1e-12, 8e-11, 1e-08)	(2e-06, 4e-06, 1e-04)	188	84.9	(1e-12, 7e-11, 1e-08)	(3e-06, 1e-05, 3e-04)	172	78.5
400	(2e-14, 5e-11, 5e-09)	(4e-07, 3e-06, 2e-04)	166	114.5	(0e+00, 7e-13, 1e-10)	(7e-08, 2e-07, 3e-06)	169	121.9	(2e-13, 2e-12, 5e-10)	(1e-06, 2e-06, 8e-05)	190	130.7
500	(8e-14, 1e-11, 2e-09)	(7e-07, 5e-06, 1e-04)	182	175.9	(2e-13, 7e-12, 8e-11)	(1e-06, 6e-06, 2e-05)	226	216.2	(5e-13, 2e-11, 8e-11)	(2e-06, 9e-06, 2e-05)	223	210.5
600	(4e-15, 2e-13, 8e-11)	(3e-07, 7e-07, 3e-05)	214	267.8	(0e+00, 2e-12, 2e-10)	(1e-07, 4e-07, 4e-05)	260	320.8	(2e-15, 2e-13, 1e-11)	(3e-07, 5e-07, 1e-06)	242	296.0
700	(1e-13, 4e-12, 4e-10)	(8e-07, 3e-06, 6e-05)	209	353.3	(2e-13, 5e-12, 4e-10)	(9e-07, 2e-06, 5e-05)	234	388.9	(2e-14, 3e-12, 2e-09)	(3e-07, 1e-06, 1e-04)	275	450.3
800	(6e-14, 2e-12, 3e-10)	(5e-07, 3e-06, 6e-05)	207	436.4	(0e+00, 2e-12, 2e-09)	(9e-08, 5e-07, 1e-04)	240	500.7	(6e-17, 1e-14, 4e-13)	(8e-08, 1e-07, 2e-06)	235	486.2
900	(1e-12, 6e-12, 1e-10)	(3e-06, 5e-06, 3e-05)	248	621.0	(9e-14, 7e-12, 5e-10)	(8e-07, 4e-06, 2e-05)	194	501.3	(0e+00, 2e-12, 2e-09)	(7e-08, 4e-07, 2e-04)	243	619.0
1000	(7e-16, 5e-14, 2e-11)	(3e-07, 4e-07, 2e-05)	215	668.7	(6e-13, 2e-11, 2e-09)	(1e-06, 8e-06, 1e-04)	211	656.7	(0e+00, 1e-13, 1e-10)	(5e-08, 1e-07, 3e-05)	246	805.3

extended the unconstrained β-order model to a more general model which shares the similar results of the unconstrained β-order model.

We also presented some preliminary numerical results to demonstrate the efficiency of our models. In our experiments, we used the adaptive nonmonotone ABB methods. For our test problems, EigUncABB is considerably competitive with LOBPCG and EIGS.

The main work of EigUncABB per iteration is to compute the matrix multiplications $X^{\mathrm{T}}X$, $X(X^{\mathrm{T}}X)$, AX whose cost is $3nr^2+2Nr$, where N is the number of nonzero elements in A. Thus we can consider to parallelize our EigUncABB. Some other techniques such as restarting, preconditioning and polynomial filtering can also be employed to speed up and improve the solution accuracy of our EigUncABB. Besides, we do not know how to design more efficient optimization algorithms for the block unconstrained models by exploring their structures. We will investigate them in future.

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