The ω-Condition Number for Optimal Preconditioning and Low Rank Generalized Jacobian Updating [*†]

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Abstract

Preconditioning is essential in iterative methods for solving linear systems. It is also the implicit objective in updating approximations of Jacobians in optimization methods, e.g., in quasi-Newton methods. Motivated by the latter, we study a nonclassic matrix condition number, the ω-condition number. We do this in the context of optimal conditioning for: (i) our application to low rank updating of generalized Jacobians; (ii) iterative methods for linear systems: (iia) clustering of eigenvalues and (iib) convergence rates.

For a positive definite matrix, the ω-condition measure is the ratio of the arithmetic and geometric means of the eigenvalues. In particular, our applications concentrate on linear systems with low rank updates of ill-conditioned positive definite matrices. These systems arise in the context of nonsmooth Newton methods using generalized Jacobians. We are able to use optimality conditions and derive *explicit* formulae for ω-optimal preconditioners and preconditioned updates. Connections to partial Cholesky sparse preconditioners are made.

Evaluating or estimating the classical condition number κ can be expensive. We show that the ω-condition number can be evaluated explicitly following a Cholesky or LU factorization. Moreover, the simplicity of ω allows for the derivation of formulae for optimal preconditioning in various scenarios, i.e., this avoids the need for expensive algorithmic calculations. And, our empirics show that ω estimates the actual condition of a linear system significantly better. Moreover, our empirical results show a significant decrease in the number of iterations required for a requested accuracy in the residual during an iterative method, i.e., these results confirm the efficacy of using the ω-condition number compared to the classical condition number.

1 Introduction

Preconditioning is essential in iterative and direct solutions of linear systems e.g., [4]. It is also the implicit objective in low rank updating of approximate Jacobians in optimization, e.g., in quasi-Newton methods [9]. In this paper we study the ω-condition number, a nonclassic matrix condition number that, for a positive definite matrix, is the ratio of the arithmetic and geometric means of the eigenvalues. In particular, our original motivation is to find ω-optimal low rank updates of the positive definite generalized Jacobian that arises in nonsmooth Newton methods e.g., [3]. In addition, we use the optimality conditions to find *explicit formulae* for the ω-optimal diagonal and sparse upper triangular preconditioners.

This relates to a sparse incomplete Cholesky factorization. We illustrate both the efficiency and effectiveness of using this condition number compared to the classic κ-condition number when solving positive definite linear systems. In particular, our empirics show that it is more effective in promoting the clustering of eigenvalues. In addition, we show that the ω-condition number can be evaluated exactly following a Cholesky or LU factorization; and that it is a better indication of the conditioning of a problem when compared to the standard κ-condition number.

In numerical analysis, a condition number of a matrix A is the main tool in the study of error propagation in the problem of solving the linear equation $Ax = b$. The classical condition number of A, denoted $\kappa(A)$, is defined as the ratio of the largest and smallest singular values of A. The linear system $Ax = b$ is said to be well-conditioned when A has a low condition number. In particular, $\kappa(A)$ attempts to measure how much a solution x, the output, will change with respect to changes in the right-hand side b, the input: $\boxed{\frac{\Delta x/x}{\Delta b/b}}$ e.g., [31, Sect. 1.3]. In general, iterative algorithms used to solve the system $Ax = b$ require a large number of iterations to achieve a solution with high accuracy if the problem is not well-conditioned, i.e., is ill-conditioned. In this paper, we restrict ourselves to A positive definite and so $\kappa = \lambda_1(A)/\lambda_n(A)$, the ratio of largest and smallest eigenvalues.

In order to improve the conditioning of a problem, preconditioners are employed for obtaining equivalent systems with better condition number. For example, in [7] a preconditioner that minimizes the classical condition number κ is obtained in the Broyden family of rank-two updates. Also, for applications to inexact Newton methods see [1,2], where it is emphasized that the goal is to improve the *clustering of eigenvalues* around 1. The ω-condition number in particular uses *all* the eigenvalues, rather than just the largest and smallest as in the classical κ. A recent survey on preconditioning is given in [27]. We emphasize that though many heuristics are given, the main measure of conditioning in [27] is κ.

The standard measure for improving the conditioning is the κ-condition number. The nonstandard condition number ω was proposed in [9]. Interestingly enough, the authors show that the inverse-sized BFGS and sized DFP [26] are obtained as optimal quasi-Newton updates with respect to this measure. The *ω-condition number* is defined as the ratio of the arithmetic and geometric means of the eigenvalues of a positive definite matrix A:

$$\omega(A) := \frac{\operatorname{tr}(A)/n}{\det(A)^{\frac{1}{n}}} = \frac{\frac{1}{n}\sum_{i=1}^{n}\lambda_i(A)}{\left(\prod_{i=1}^{n}\lambda_i(A)\right)^{\frac{1}{n}}}. \tag{1.1}$$

In addition, we illustrate that the ω-condition number presents advantages with respect to the classic condition number κ. Both are pseudoconvex over the open convex cone of positive definite matrices, $\mathbb{S}^n_{++}$; thus a local minimum is a global minimum. But, κ is differentiable if, and only if, both largest and smallest eigenvalues are singletons, while ω is differentiable on all of $\mathbb{S}^n_{++}$. This facilitates obtaining explicit formulae for optimal preconditioners and

avoids expensive calculations, see e.g., [9] and Section 2.1, below.[1] Moreover, it is expensive to evaluate the classic condition number [18] as it uses both $\|A\|, \|A^{-1}\|$. For large scale, one often uses the ℓ_1 approximation in [18]. We show that we can find the exact value of the ω-condition number when a Cholesky or LU factorization is done. Finally, we show that the ω-condition number provides a significantly better estimate for the true conditioning of a linear system.

1.1 Outline

Preliminaries are presented in Section 1.2. Then Section 2.1 introduces basic and new properties of the ω-condition number. We derive ω-optimal triangular preconditioners that include ones that preserve sparsity and connect these to partial Cholesky preconditioners. In particular, in Section 2.2 we empirically motivate the use of the ω-condition number as a better indicator of the conditioning of the problem compared to the κ-condition number. This includes empirical results for better clustering of eigenvalues, Figure 2.1, an important indicator of improved convergence. In Section 3, we derive ω-optimal conditioning for low rank updates of positive definite matrices. These updates often arise in the construction of generalized Jacobians. In Section 4, we use the linear equations that involve positive definite matrices as well as the generalized Jacobians for our original motivation. We empirically illustrate that reducing the ω-condition number improves the performance of iterative methods for solving these linear systems. Conclusions are provided in Section 5.

1.2 Preliminaries and Notation

We denote: $\mathbb{R}^n$ as the real Euclidean space of dimension n; $\mathbb{R}^{m\times n}$ as the space of $m \times n$ matrices; $\mathbb{S}^n$ as the space of $n \times n$ symmetric matrices; $\mathbb{S}^n_+$ and $\mathbb{S}^n_{++}$ for the cone of positive semidefinite and positive definite $n \times n$ symmetric matrices, respectively; and $A \succeq 0$ (resp., $\succ 0$) to denote A is in $\mathbb{S}^n_+$ (respectively, $\mathbb{S}^n_{++}$).

We use $\mathrm{Diag} : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ to denote the linear operator that maps a vector v into the diagonal matrix $\mathrm{Diag}(v)$ whose diagonal is v. Its adjoint operator is denoted by $\mathrm{diag} = \mathrm{Diag}^*$.

For integers $t \geqslant s$, we let $[s, t] = \{s, s + 1, \ldots, t\}$. For a positive integer k, let $[k] = [1, k]$ and denote $t(k) = k(k + 1)/2$, *triangular number*.

For a differentiable function $f : \mathbb{R}^n \to \mathbb{R}$, we use ∇f for the gradient. If the dimension $n = 1$, we just write f' for the derivative of f. Given a nonempty open set $\Omega \subseteq \mathbb{R}^n$, a function $f : \Omega \to \mathbb{R}$ is said to be *pseudoconvex* on Ω if it is differentiable and

$$\nabla f(x)^T(y - x) \geqslant 0 \Longrightarrow f(y) \geqslant f(x), \quad \forall x, y \in \Omega.$$

This implies that for an open convex set Ω and a *pseudoconvex function* $f : \Omega \to \mathbb{R}$, we have:

[1] Since the original version of this paper was submitted, the recent report [12] (and many references therein) discusses numerical scalable algorithms for κ-optimal diagonal preconditioning. We have added relationships to this paper in this revised version. In particular, we present an alternative algorithm as well as illustrate that using the ω-optimal formula has relatively no cost in evaluation, and is a better preconditioner.

$\nabla f(x) = 0$ is a necessary and sufficient condition for x to be a global minimizer of f in Ω, see, e.g., [24].

2 Properties and Numerical Evaluation of ω

We now introduce basic and new properties of the ω-condition number, and we study its efficient numerical evaluation. In addition, we empirically compare its effectiveness with the κ-condition number for preconditioning, clustering of eigenvalues, and in estimating the actual conditioning of positive definite linear systems.

We derive and test empirically the following explicitly found optimal ω-preconditioners (scalings):
(i) optimal diagonal (2.1);
(ii) optimal block diagonal (2.2);
(iii) lower triangular two diagonal scaling (2.16);
(iv) upper triangular D_{+k} diagonal (2.19);
(v) incomplete upper triangular (2.5).

2.1 Basic Properties and ω-Optimal Preconditioning

For iterative solutions of linear systems a preconditioner S is often essential, i.e., we solve $(AS)y = b$, $x = Sy$, see e.g., [4, 14]. Moreover, it is known that the simple scaling diagonal preconditioner using the norms of the columns of A is the optimal diagonal preconditioner with respect to the ω-condition number and is efficient in practice, see [9, 28]. Various preconditioners based on (partial) factorizations of A, are compared in [14]. One is the QR-factorization. We note that scaling columns is an essential part of a QR-factorization. We see below that our ω-optimal preconditioners are related to a modified QR-factorization (Cholesky for positive definite systems). Moreover, convergence rates of iterative methods are correlated to clustering of eigenvalues of A^TA, see e.g., [15]. We see below that the ω-optimal preconditioners promote this property better than those for κ.

The optimal diagonal preconditioner is extended to the block diagonal case in [10]. We now summarize these and other basic properties of the ω-condition number in the following Proposition 2.1. We include a proof of Proposition 2.1, Item 2, that is different than that provided in [9] so as to emphasize the extension to new formulae for ω-optimal preconditioners in Sections 2.1.1 to 2.1.3.

Proposition 2.1 ([9, 10]). *The following statements are true.*

1 *The measure ω is pseudoconvex on the set of symmetric positive definite matrices, and thus any stationary point is a global minimizer of ω.*

2 *Let A be a full rank $m \times n$ matrix, $n \leqslant m$. Then the optimal column scaling that minimizes the measure ω, i.e.,*

$$\min \ \omega((A\mathrm{Diag}(d))^T(A\mathrm{Diag}(d))), \tag{2.1}$$

over $d \in \mathbb{R}^n_{++}$, *is given by*

$$d_i = \frac{1}{\|A_{:,i}\|}, \quad i = 1, ..., n,$$

where $A_{:,i}$ *is the* i*-th column of* A.

3 Let A *be a full rank* $m \times n$ *matrix,* $n \leqslant m$ *with block structure* $A = \begin{bmatrix} A_1 & A_2 & \dots & A_k \end{bmatrix}$, $A_i \in \mathbb{R}^{m \times n_i}$. *Then* an *optimal corresponding block diagonal scaling*

$$D = \begin{bmatrix} D_1 & 0 & 0 & \dots & 0 \\ 0 & D_2 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & D_k \end{bmatrix}, \quad D_i \in \mathbb{R}^{n_i \times n_i},$$

that minimizes the measure ω, *i.e.,*

$$\min \ \omega((AD)^T(AD)), \tag{2.2}$$

over D *block diagonal, is given by the factorization*

$$D_i D_i^T = \{A_i^T \, A_i\}^{-1}, \quad i = 1, ..., k.$$

Proof. The results are proved in [9, 10]. We provide a new proof of Item 2 as it leads to the extensions in Theorem 2.5 below. Let $d := \text{diag}(D), W := A^T A, w = \text{diag}(W)$ and note that

$$\begin{aligned} \omega(d) := \omega((A\text{Diag}(d))^T(A\text{Diag}(d))) &= \frac{1}{n \det(A^T A)^{1/n}} \frac{\langle w, d \circ d \rangle}{\det(D)^{2/n}} \\ &=: K \frac{\sum_{i=1}^n w_i d_i^2}{\prod_{i=1}^n d_i^{2/n}} \\ &=: K \frac{f_w(d)}{g(d)}, \end{aligned}$$

thus defining the constant $K > 0$ and functions $f_w, g : \mathbb{R}^n_{++} \to \mathbb{R}_{++}$. The reason for including this proof is to emphasize that A only appears in the numerator f_w of the function to be minimized as the denominator involves only d.

We now differentiate this pseudoconvex function with respect to d_i :

$$\begin{aligned} \frac{\partial \omega(d)}{\partial d_i} &= \frac{K}{g(d)^2} \left(g(d) 2 w_i d_i - f_w(d) \frac{2}{n} g(d) \frac{1}{d_i} \right) \\ &= \frac{2K}{g(d)} \left(w_i d_i - \frac{1}{n} f_w(d) \frac{1}{d_i} \right) \\ &= \frac{2K}{g(d)} \left(\frac{1}{d_i} - \frac{1}{n} f_w(d) \frac{1}{d_i} \right) \\ &= 0, \end{aligned}$$

since $w_i = \|A_{:,i}\|^2 = 1/d_i^2 \implies f_w(d) = n$.

■

We now include the gradients of the condition numbers for use in the definitions below. For simplicity and to avoid subgradients of κ, we assume that the largest and smallest eigenvalues are singletons.

Lemma 2.2. *Let $A \in \mathbb{S}^n_{++}$ with eigenvalues $\lambda_1 > \lambda_2 \geqslant \ldots \geqslant \lambda_{n-1} > \lambda_n$, with corresponding orthonormal eigenvectors $v_1, \ldots, v_n$. Then:*

1

$$\begin{aligned} \nabla\omega(A) &= \tfrac{1}{n\det(A)^{1/n}}\left(I - \tfrac{\operatorname{tr} A}{n}A^{-1}\right) \quad \textit{is indefinite,} \\ &\qquad \|\nabla\omega(A)\| = \tfrac{1}{n\det(A)^{1/n}}\max\left\{1 - \tfrac{\operatorname{tr} A}{n\lambda_1}, \tfrac{\operatorname{tr} A}{n\lambda_n} - 1\right\}. \end{aligned}$$

2

$$\nabla\kappa(A) = \frac{1}{\lambda_n}\left(v_1v_1^T - \kappa(A)v_nv_n^T\right), \quad \textit{is indefinite,} \quad \|\nabla\kappa(A)\| = \max\left\{\frac{1}{\lambda_n}, \frac{\kappa(A)}{\lambda_n}\right\}.$$

Proof. 1 The gradient is

$$\begin{aligned} \nabla\omega(A) &= \tfrac{1}{n\det(A)^{2/n}}\left(\tfrac{\det(A)^{1/n}}{n}I - \tfrac{\operatorname{tr} A}{n}\tfrac{1}{n}\det A^{\frac{1}{n}-1}\operatorname{adj} A\right) \succ 0; \\ &= \tfrac{1}{n\det(A)^{2/n}}\left(\det(A)^{1/n}I - \tfrac{\operatorname{tr} A}{n}\det A^{\frac{1}{n}-1}\operatorname{adj} A\right) \succ 0; \\ &= \tfrac{1}{n\det(A)^{1/n}}\left(I - \tfrac{\operatorname{tr} A}{n}A^{-1}\right), \end{aligned}$$

where $\operatorname{adj} A$ is the adjunct, the matrix of cofactors. The last expression follows from $A^{-1} = \frac{1}{\det(A)}\operatorname{adj} A$. The positive definiteness and norm follow from:

$$\begin{aligned} \lambda_{\max}(I - \tfrac{\operatorname{tr} A}{n}A^{-1}) &= \max_{\|x\|=1} x^T(I - \tfrac{\operatorname{tr} A}{n}A^{-1})x \\ &= 1 - \tfrac{\operatorname{tr} A}{n}\min_{\|x\|=1} x^TA^{-1}x \\ &= 1 - \tfrac{\operatorname{tr} A}{n\lambda_1}, && \text{with attainment at } x = v_1, \\ &> 0; \end{aligned}$$

$$\begin{aligned} \lambda_{\min}(I - \tfrac{\operatorname{tr} A}{n}A^{-1}) &= \min_{\|x\|=1} x^T(I - \tfrac{\operatorname{tr} A}{n}A^{-1})x \\ &= 1 + \tfrac{\operatorname{tr} A}{n}\min_{\|x\|=1}(-x^TA^{-1}x) \\ &= 1 - \tfrac{\operatorname{tr} A}{n}\max_{\|x\|=1} x^TA^{-1}x \\ &= 1 - \tfrac{\operatorname{tr} A}{n\lambda_n}, && \text{with attainement at } x = v_n, \\ &< 0; \end{aligned}$$

2 Since the eigenvalues are singletons, they are differentiable with gradients $v_1v_1^T, v_nv_n^T$, respectively. The result follows from the definitions of the gradient of the fractional function κ and the norm.

■

2.1.1 ω-Optimal Incomplete Upper Triangular Predonditioner

Approximations of the inverse of the Cholesky decomposition are widely used as preconditioners for linear systems. It is easy to check that the inverse of the Cholesky coincides with the minimization of the ω-condition number. Indeed, let $W = R^T R$ be the Cholesky decomposition of W. Then $\omega(R^{-T} W R^{-1}) = \omega(I) = 1$. However, it is well-known that sparsity can be lost when finding R. Therefore, permutations techniques are used when finding an incomplete Cholesky decomposition, e.g., [14].

In this section we aim to obtain an ω-optimal *incomplete upper triangular preconditioner*. (We start with a triangular structure but this technique can be modified to choose positions so as to preserve sparsity.) Specifically, given an integer $2 \leqslant k \leqslant n$, let $\alpha = (\alpha_{1,2}, \alpha_{1,3}, \alpha_{2,3}, \ldots, \alpha_{1,k}, \ldots, \alpha_{k-1,k}) \in \mathbb{R}^{t(k-1)}$ and $d \in \mathbb{R}^n$. We consider a preconditioner in the form of

$$\begin{aligned} \mathrm{D}_{+\mathrm{tk}}(d, \alpha) &= \mathrm{Diag}(d) + \mathrm{Trir_k}(\alpha) \\ &= \begin{pmatrix} d_1 & \alpha_{1,2} & \alpha_{1,3} & \ldots & \alpha_{1,k} & 0 & \ldots & 0 \\ 0 & d_2 & \alpha_{2,3} & \ldots & \alpha_{2,k} & 0 & \ldots & 0 \\ 0 & 0 & d_3 & \ddots & \alpha_{3,k} & 0 & \ldots & 0 \\ 0 & \ldots & \ldots & \ddots & \alpha_{k-1,k} & 0 & \ldots & 0 \\ \vdots & \ldots & \ldots & \ldots & d_k & 0 & \ldots & 0 \\ 0 & \ldots & \ldots & \ldots & 0 & d_{k+1} & \ldots & 0 \\ 0 & \ldots & \ldots & \ldots & \ldots & 0 & \ddots & 0 \\ 0 & \ldots & \ldots & \ldots & \ldots & 0 & \ldots & d_n \end{pmatrix}, \end{aligned} \tag{2.3}$$

where the linear mapping $\mathrm{Trir_k} : \mathbb{R}^{t(k-1)} \to \mathbb{R}^{n \times n}$ is defined accordingly. Its adjoint operator is $\mathrm{Trir_k}^* = \mathrm{trir_k} : \mathbb{R}^{n \times n} \to \mathbb{R}^{t(k-1)}$, $M \mapsto (M_{1,2}, M_{1,3}, M_{2,3}, \ldots, M_{1,k}, \ldots, M_{k-1,k})$.

Observe that if $k = n$ then $\mathrm{D}_{+\mathrm{tk}}(d, \alpha)$ returns a complete upper triangular. In that case it trivially follows that the ω-optimal preconditioner will be given by the Cholesky decomposition. In any case, even when $k < n$, the ω-optimal incomplete upper triangular preconditioner will be related to the Cholesky factorization. Therefore, we recall the following recursive formula for computing the latter.

Remark 2.3 (Recursive formula for the Cholesky decomposition)**.** *Let $W \in \mathbb{S}^k$ be a positive definite matrix and let $W = RR^T$ be the Cholesky decomposition of W. We recall that the upper triangular Cholesky factor R admits the following recursive construction:*

$$\begin{aligned} R_{j,j} &= \sqrt{W_{j,j} - \sum_{t=1}^{j-1} R_{t,j}^2}, \\ R_{i,j} &= \frac{1}{R_{i,i}} \left(W_{i,j} - \sum_{t=1}^{i-1} R_{t,j} \, R_{t,i} \right), \qquad \text{for } j > i. \end{aligned} \tag{2.4}$$

Theorem 2.4. *Let $W \in \mathbb{S}^n_{++}$. The ω-optimal incomplete upper triangular preconditioner in the form of (2.3) for W, i.e.,*

$$(\bar{d}, \bar{\alpha}) := \operatorname*{argmin}_{(d,\alpha)\in\mathbb{R}^n_{++}\times\mathbb{R}^{t(k-1)}} \omega\left(\mathrm{D}_{+\mathrm{tk}}(d,\alpha)^T W\, \mathrm{D}_{+\mathrm{tk}}(d,\alpha)\right), \tag{2.5}$$

is given by

$$\begin{aligned} \bar{d}_j &= R^{-1}_{j,j}, && \text{for } j = 1,\dots,k;\\ \bar{d}_j &= W^{-1/2}_{j,j}, && \text{for } j = k+1,\dots,n;\\ \bar{\alpha}_{i,j} &= -\frac{1}{R_{i,i}}\left(\sum_{s=i+1}^{j-1} R_{i,s}\bar{\alpha}_{s,j} + R_{i,j}\bar{d}_j\right), && \text{for } k \geqslant j > i \geqslant 1, \end{aligned} \tag{2.6}$$

where $R \in \mathbb{R}^{k\times k}$ stands for the Cholesky decomposition of $W_{1:k,1:k} = R^T R$.

Proof. We divide the proof into three claims.

Claim 1: The ω-optimal $\mathrm{D}_{+\mathrm{tk}}$ preconditioner is obtained by $(\bar{d}, \bar{\alpha})$ solving the nonlinear system

$$\begin{bmatrix} \operatorname{diag} W\left(\operatorname{Diag}(\bar{d}) + \operatorname{Trir_k}(\bar{\alpha})\right)\\ \operatorname{trir_k} W\left(\operatorname{Diag}(\bar{d}) + \operatorname{Trir_k}(\bar{\alpha})\right)\end{bmatrix} = \begin{pmatrix}\bar{d}^{-1}\\ 0\end{pmatrix}, \tag{2.7}$$

where $\bar{d}^{-1} = (\bar{d}_1^{-1},\dots,\bar{d}_n^{-1})^T$.

In order to prove this, and to ease the notation, fix W and consider the ω-condition number, f and g as functions of a pair $(d,\alpha) \in \mathbb{R}^n_{++}\times\mathbb{R}^{t(k-1)}$. Namely, we set

$$\omega_{+tk}(d,\alpha) = \frac{f_{+tk}(d,\alpha)}{g_{+tk}(d,\alpha)} := \frac{\operatorname{tr}\left(\mathrm{D}_{+\mathrm{tk}}(d,\alpha)^T W\, \mathrm{D}_{+\mathrm{tk}}(d,\alpha)\right)/n}{\det\left(\mathrm{D}_{+\mathrm{tk}}(d,\alpha)^T W\, \mathrm{D}_{+\mathrm{tk}}(d,\alpha)\right)^{1/n}}.$$

Alternatively, we can rewrite f_{+tk} as

$$\begin{aligned} f_{+tk}(d,\alpha) &= \frac{1}{n}\operatorname{tr}\left(\mathrm{D}_{+\mathrm{tk}}(d,\alpha)^T W\, \mathrm{D}_{+\mathrm{tk}}(d,\alpha)\right)\\ &= \frac{1}{n}\left\langle \mathrm{D}_{+\mathrm{tk}}{}^{*}\, W\, \mathrm{D}_{+\mathrm{tk}}(d,\alpha), \begin{pmatrix} d\\ \alpha\end{pmatrix}\right\rangle. \end{aligned} \tag{2.8}$$

Hence,

$$\begin{aligned} \nabla f_{+tk}(d,\alpha) &= \frac{2}{n}\,\mathrm{D}_{+\mathrm{tk}}{}^{*}\, W\, \mathrm{D}_{+\mathrm{tk}}(d,\alpha)\\ &= \frac{2}{n}\begin{bmatrix}\operatorname{diag} W\left(\operatorname{Diag}(d) + \operatorname{Trir_k}(\alpha)\right)\\ \operatorname{trir_k} W\left(\operatorname{Diag}(d) + \operatorname{Trir_k}(\alpha)\right)\end{bmatrix}. \end{aligned} \tag{2.9}$$

On the other hand, we have that

$$g_{+tk}(d,\alpha) = \det(W)\left(\prod_{i=1}^n d_i\right)^{\frac{2}{n}} \quad \text{and} \quad \nabla g_{+tk}(d,\alpha) = \frac{2}{n} g_{+tk}(d,\alpha)\begin{pmatrix} d^{-1}\\ 0\end{pmatrix},$$

where $d^{-1} = (d_1^{-1}, \dots, d_n^{-1})^T \in \mathbb{R}^n_{++}$.

Therefore, the optimality condition for the pseudoconvex function ω_{+t} is given by

$$\nabla \omega_{+tk}(d, \alpha) = K \left(\mathrm{D_{+tk}}^* W \, \mathrm{D_{+tk}}(d, \alpha) - f_{+tk}(d, \alpha) \begin{pmatrix} d^{-1} \\ 0 \end{pmatrix} \right) = 0, \tag{2.10}$$

with $K := 2/(n\, g_{+tk}(d, \alpha)) > 0$. Finally, observe that it suffices to obtain $(\bar{d}, \bar{\alpha}) \in \mathbb{R}^n_{++} \times \mathbb{R}^{t(k-1)}$ such that

$$\mathrm{D_{+tk}}^* W \, \mathrm{D_{+tk}}(\bar{d}, \bar{\alpha}) - \begin{pmatrix} \bar{d}^{-1} \\ 0 \end{pmatrix} = 0,$$

as by (2.8) this immediately implies

$$f_{+tk}(\bar{d}, \bar{\alpha}) = \frac{1}{n} \left\langle \begin{pmatrix} \bar{d}^{-1} \\ 0 \end{pmatrix}, \begin{pmatrix} \bar{d} \\ \bar{\alpha} \end{pmatrix} \right\rangle = 1,$$

which in turn would yield (2.10). Thus, (2.10) together with (2.9) concludes this part of the proof.

Claim 2: A solution $(\bar{d}, \bar{\alpha})$ to (2.7) is given by $\bar{d}_i = W_{i,i}^{-1/2}$, for $i = k+1, \dots, n$, and with

$$Q := \mathrm{Diag}(\bar{d}_{1:k}) + \mathrm{Triu}(\bar{\alpha}) \tag{2.11}$$

being the inverse of the Cholesky decomposition of the matrix $W_{1:k,1:k}$.

We start by fixing notation. Let $\widehat{W} := W_{1:k,1:k}$ and $\widetilde{W} := W_{k+1:n,k+1:n}$. Recall the definition of the operator Triu which applied to a vector $\alpha = (\alpha_{1,2}, \alpha_{1,3}, \alpha_{2,3}, \dots, \alpha_{1,k}, \dots, \alpha_{k-1,k}) \in \mathbb{R}^{t(k-1)}$ returns the upper triangular matrix $\mathrm{Triu}(\alpha) = T \in \mathbb{R}^{k \times k}$ such that $T_{i,j} = \alpha_{i,j}$ if $1 \leqslant i < j \leqslant n$, and $T_{i,j} = 0$ otherwise. The adjoint of Triu is denoted as triu. Then the system (2.7) can be split into the two equations

$$\mathrm{diag}\, W \left(\mathrm{Diag}(\bar{d}) + \mathrm{Trir_k}(\bar{\alpha}) \right) = \begin{bmatrix} \mathrm{diag}\, \widehat{W} \left(\mathrm{Diag}(\bar{d}_{1:k}) + \mathrm{Triu}(\bar{\alpha}) \right) \\ \mathrm{diag}\, \widetilde{W}\, \mathrm{Diag}(\bar{d}_{k+1:n}) \end{bmatrix} = \bar{d}^{-1} \tag{2.12}$$

and

$$\mathrm{trir_k}\, W \left(\mathrm{Diag}(\bar{d}) + \mathrm{Trir_k}(\bar{\alpha}) \right) = \mathrm{triu}\, \widehat{W} \left(\mathrm{Diag}(\bar{d}_{1:k}) + \mathrm{Triu}(\bar{\alpha}) \right) = 0. \tag{2.13}$$

Observe that the variables $\bar{d}_{k+1}, \dots, \bar{d}_n$ only appear in the lower block of (2.12), that can be directly solved to obtain $\bar{d}_i = W_{i,i}^{-1/2}$ for all $i = k+1, \dots, n$.

On the other hand, the variables $\bar{d}_1, \dots, \bar{d}_k$ and $\bar{\alpha}$ are present in (2.13) and the upper block of (2.12). Nonetheless, by taking into account that if $n = k$ then $\mathrm{Triu} = \mathrm{Trir_k}$, it is easy to check that these equations define the ω-optimal triangular preconditioner of the matrix $\widehat{W} \in \mathbb{S}^k_{++}$. Therefore we conclude that Q coincides with the inverse of the Cholesky factorization of $\widehat{W}$.

Claim 3: Let $Q := \mathrm{Diag}(\bar{d}_{1:k}) + \mathrm{Triu}(\bar{\alpha})$ be the inverse of the Cholesky decomposition of $\widehat{W}$. Then $(\bar{d}_{1:k}, \bar{\alpha})$ is given as in (2.6).

Let $\widehat{W} = R^T R$ be the Cholesky decomposition of $\widehat{W}$, where

$$R = \begin{pmatrix} R_{1,1} & R_{1,2} & R_{1,3} & \dots & R_{1,k} \\ 0 & R_{2,2} & R_{2,3} & \dots & R_{2,k} \\ \vdots & \dots & \dots & \dots & \vdots \\ 0 & \dots & \dots & 0 & R_{k,k} \end{pmatrix},$$

and the entries are given as in (2.4). Let $Q = R^{-1}$ be the matrix defined in (2.11). We now use the equation $RQ = \mathrm{Id}$ to obtain an expression of Q in terms of R. We have:

$$\mathrm{Id} = \begin{pmatrix} R_{1,1} & R_{1,2} & R_{1,3} & \dots & R_{1,k} \\ 0 & R_{2,2} & R_{2,3} & \dots & R_{2,k} \\ \vdots & \dots & \ddots & \dots & \vdots \\ \vdots & \dots & \dots & R_{k-1,k-1} & R_{k-1,k} \\ 0 & \dots & \dots & 0 & R_{k,k} \end{pmatrix} \begin{pmatrix} \bar{d}_1 & \bar{\alpha}_{1,2} & \bar{\alpha}_{1,3} & \dots & \bar{\alpha}_{1,k-1} & \bar{\alpha}_{1,k} \\ 0 & \bar{d}_2 & \bar{\alpha}_{2,3} & \dots & \dots & \bar{\alpha}_{2,k} \\ \vdots & \dots & \dots & \dots & \dots & \vdots \\ \vdots & \dots & \dots & \dots & \bar{d}_{k-1} & \bar{\alpha}_{k-1,k} \\ 0 & \dots & \dots & \dots & 0 & \bar{d}_k \end{pmatrix}.$$

For each column $j \in \{1, \dots, k\}$ of Q, this leads to the following linear system of j equations:

$$1 = R_{j,j}\, \bar{d}_j, \tag{2.14a}$$
$$0 = R_{j-1,j-1}\, \bar{\alpha}_{j-1,j} + R_{j-1,j}\, \bar{d}_j, \tag{2.14b}$$
$$\vdots$$
$$0 = R_{j-\ell+1,j-\ell+1}\, \bar{\alpha}_{j-\ell+1,j} + \sum_{s=j-\ell+2}^{j-1} R_{j-\ell+1,s}\, \bar{\alpha}_{s,j} + R_{j-\ell+1,j}\, \bar{d}_j, \tag{2.14c}$$
$$\vdots$$
$$0 = R_{1,1}\, \bar{\alpha}_{1,j} + \sum_{s=2}^{j-1} R_{1,s}\, \bar{\alpha}_{s,j} + R_{1,j}\, \bar{d}_j. \tag{2.14d}$$

Equation (2.14a) readily implies that $\bar{d}_j = R_{j,j}^{-1}$ for all $j \in \{1, \dots, k\}$. Moreover, for any $\ell \in \{2, \dots, j\}$, we can solve (2.14c) for getting an expression for $\bar{\alpha}_{j-\ell+1,j}$ in terms of $\bar{d}_j, \bar{\alpha}_{j-1,j}, \dots, \bar{\alpha}_{j-\ell+2,j}$. This yields

$$\bar{\alpha}_{j-\ell+1,j} = -\frac{1}{R_{j-\ell+1,j-\ell+1}} \left(\sum_{s=j-\ell+2}^{j-1} R_{j-\ell+1,s}\, \bar{\alpha}_{s,j} + R_{j-\ell+1,j}\, \bar{d}_j \right), \tag{2.15}$$

which concludes Claim 3 and the proof.

■

We conclude this section with a simple MATLAB's code for an efficient computation of the ω-optimal incomplete upper triangular preconditioner.

```
%%% Function for computing the $\omega$-optimal incomplete
   upper triangular preconditioner
%
% Input:
%        - W <- pos. def. matrix
%        - k <- size of the triangular block
%
% Output:
%        - D <-  optimal preconditioner minimizing omega(D'*W*D)

function D = i_upper_tri_preconditioner(W,k)

    n = length(W);

    tempW = W(1:k,1:k);
    R = chol(tempW);

    tempW = W(k+1:n,k+1:n);
    tempD = diag(diag(tempW).^(-1/2));

    D = blkdiag(inv(R),tempD);

end
```

In the following sections we derive expressions for ω-optimal preconditioner matrices in different forms. The first one of them is a lower triangular two diagonal preconditioner. The second is a diagonal + upper triangular preconditioner. The proofs of both results proceed similarly to Claim 1 in Theorem 2.4. Therefore, we will not reproduce the complete proofs and limit ourselves to highlight the main steps.

2.1.2 Lower Triangular, Two Diagonal Preconditioning

In this section, we extend the ω-optimal diagonal scaling to an ω-optimal *lower triangular two diagonal scaling*. We define Diags_2 and $\mathrm{diags}_2 = \mathrm{Diags}_2{}^*$ in obvious ways to construct the lower triangular two diagonal matrix from a vector and its adjoint. Specifically, for a

matrix $L = (L_{ij})_{i,j=1}^n \in \mathbb{R}^{n\times n}$, we get that

$$\operatorname{diags}_2(L) = \begin{pmatrix} L_{1,1} \\ L_{2,2} \\ \dots \\ L_{n,n} \\ L_{2,1} \\ L_{3,2} \\ L_{4,3} \\ \dots \\ L_{n,n-1} \end{pmatrix} =: \begin{pmatrix} \bar{l} \\ \hat{l} \end{pmatrix} \in \mathbb{R}^{n+(n-1)},$$

while, given vectors $\bar{d} = (\bar{d}_1, \dots, \bar{d}_n)^T \in \mathbb{R}^n$ and $\hat{d} = (\hat{d}_1, \dots, \hat{d}_{n-1}) \in \mathbb{R}^{n-1}$, we have

$$\operatorname{Diags}_2(\bar{d}, \hat{d}) = \begin{bmatrix} \bar{d}_1 & 0 & \dots & \dots & \dots & 0 \\ \hat{d}_1 & \bar{d}_2 & 0 & \dots & \dots & 0 \\ 0 & \hat{d}_2 & \bar{d}_3 & \vdots & \vdots & 0 \\ \vdots & \dots & \ddots & \ddots & \vdots & \vdots \\ 0 & \dots & \dots & \hat{d}_{n-1} & \bar{d}_{n-1} & 0 \\ 0 & 0 & \dots & 0 & \hat{d}_{n-1} & \bar{d}_n \end{bmatrix}.$$

Note that $\operatorname{Diags}_2 : \mathbb{R}^{2n-1} \to \mathbb{R}^{n\times n}$ and $\langle \operatorname{Diags}_2(\bar{d}, \hat{d}), L\rangle = \left\langle \begin{pmatrix} \bar{d} \\ \hat{d} \end{pmatrix}, \operatorname{diags}_2(L) \right\rangle$, for any squared matrix $L \in \mathbb{R}^{n\times n}$.

Theorem 2.5. *Let $W \in \mathbb{S}^n_{++}$ and set*

$$\bar{d}_i^* = \begin{cases} \left(W_{i,i} - \frac{W_{i,i+1}^2}{W_{i+1,i+1}}\right)^{-1/2} = \left(\frac{W_{i,i}W_{i+1,i+1} - W_{i,i+1}^2}{W_{i+1,i+1}}\right)^{-1/2}, & \text{if } i = 1, \dots, n-1; \\ W_{n,n}^{-1/2}, & \text{if } i = n \end{cases}$$

and

$$\hat{d}_i^* = -\frac{W_{i,i+1}}{W_{i+1,i+1}} \bar{d}_i^*, \quad i = 1, \dots, n-1.$$

Then the ω-optimal lower triangular two diagonal scaling of W is given by

$$(\bar{d}^*, \hat{d}^*) = \operatorname*{argmin}_{(\bar{d},\hat{d})\in\mathbb{R}^n_{++}\times\mathbb{R}^{n-1}} \omega(\bar{d}, \hat{d}), \tag{2.16}$$

where $\omega(\bar{d}, \hat{d}) := \omega\left(\operatorname{Diags}_2(\bar{d}, \hat{d})^T W \operatorname{Diags}_2(\bar{d}, \hat{d})\right)$.

Proof. First we note, since the 2×2 principal minors for $W \succ 0$ are all positive, the definitions of the optimal d^* are well defined. Let $\bar{d} \in \mathbb{R}^n_{++}$ and $\hat{d} \in \mathbb{R}^{n-1}$. Define the ω-condition number, f and g as functions of a pair $(\bar{d}, \hat{d}) \in \mathbb{R}^n_{++} \times \mathbb{R}^{n-1}$. This is

$$\omega(\bar{d}, \hat{d}) = \frac{f(\bar{d}, \hat{d})}{g(d, \hat{d})} := \frac{\operatorname{tr}\big(\operatorname{Diags}_2(\bar{d}, \hat{d})^T W \operatorname{Diags}_2(\bar{d}, \hat{d})\big)/n}{\det(W)^{1/n} \prod_{i=1}^n (\bar{d}_i)^{2/n}}.$$

Differentiating the pseudoconvex ω and equating to 0, we get the optimality condition

$$(\text{diags}_2\, W\, \text{Diags}_2)\,(\bar{d}, \hat{d}) = \begin{pmatrix} \bar{d}^{-1} \\ 0_{n-1} \end{pmatrix} \tag{2.17}$$

Solving (2.17) for $(\bar{d}, \hat{d})$, results in

$$\bar{d}_i = \begin{cases} \left(W_{i,i} - \frac{W_{i,i+1}^2}{W_{i+1,i+1}}\right)^{-1/2} = \left(\frac{W_{i,i}W_{i+1,i+1} - W_{i,i+1}^2}{W_{i+1,i+1}}\right)^{-1/2}, & \text{if } i = 1, \ldots, n-1; \\ W_{n,n}^{-1/2}, & \text{if } i = n; \end{cases}$$

and

$$\hat{d}_i = -\frac{W_{i,i+1}}{W_{i+1,i+1}}\bar{d}_i, \quad i = 1, \ldots, n-1.$$

■

2.1.3 Upper Triangular D_{+k} Diagonal Preconditioning; QR-Decomposition

We note that the ω-optimal lower triangular two diagonal preconditioner in Theorem 2.5 is sparse but its inverse though still lower triangular is not necessarily as sparse, i.e., the two diagonal structure can be lost completely, sparsity can be lost. We now consider the diagonal with upper triangular elements that maintain the same structure in the inverse, i.e., maintain sparsity for the inverse. Recall that the triangular number $t(k) = k(k+1)/2$ and define the transformation $D_{+k} : \mathbb{R}^{n+t(k)} \to \mathbb{R}^{n\times n}$:

$$\begin{aligned} D_{+k}(d, \alpha) &= \text{Diag}(d) + \left[\begin{bmatrix} 0_{n\times n-k} \end{bmatrix} \;\middle|\; \begin{bmatrix} \begin{bmatrix} \text{Triu}(\alpha) \end{bmatrix} \\ \begin{bmatrix} 0_{n-k\times k} \end{bmatrix} \end{bmatrix}\right] \\ &= \text{Diag}(d) + \text{Triu}_{\text{k}}(\alpha) = \begin{bmatrix} \text{Diag} & \text{Triu}_{\text{k}} \end{bmatrix} \begin{pmatrix} d \\ \alpha \end{pmatrix} \\ &= \begin{pmatrix} d_1 & 0 & \ldots & 0 & \ldots & \alpha_{1,n-k+1} & \alpha_{1,n-k+2} & \ldots & \alpha_{1,n} \\ 0 & d_2 & \ldots & 0 & \ldots & 0 & \alpha_{2,n-k+2} & \ldots & \alpha_{2,n} \\ \vdots & \vdots & \ddots & \vdots & \ldots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & d_k & \ldots & 0 & 0 & 0 & \alpha_{k,n} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & \ldots & d_{n-k+1} & 0 & 0 & 0 \\ 0 & 0 & \ldots & 0 & \ldots & 0 & d_{n-k+2} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ldots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 0 & \ldots & 0 & 0 & 0 & d_n \end{pmatrix} \end{aligned} \tag{2.18}$$

where $d \in \mathbb{R}^n$ and $\alpha := (\alpha_{1,n-k+1}, \alpha_{1,n-k+2}, \alpha_{2,n-k+2}, \ldots, \alpha_{1,n}, \ldots, \alpha_{k,n})^T \in \mathbb{R}^{t(k)}$. Then the optimal upper triangular $D_{+k}(d, \alpha)$ diagonal preconditioner is given by solving the following

optimization problem:

$$(\bar{d},\bar{\alpha}) := \operatorname*{argmin}_{(d,\alpha)\in\mathbb{R}^n_{++}\times\mathbb{R}^{t(k)}} \omega\big(D_{+k}(d,\alpha)^T W D_{+k}(d,\alpha)\big). \tag{2.19}$$

Theorem 2.6. *Let $W \in \mathbb{S}^n_{++}$ be given and let $(\bar{d},\bar{\alpha}) \in \mathbb{R}^{n+t(k)}$ such that*

$$\bar{d}_i = W_{i,i}^{-1/2}, \quad \forall i = 1,\dots,n-k \tag{2.20}$$

and the following hold for each $i = n-k+1,\dots,n$:

$$\begin{array}{rcll} W_{i,i}\bar{d}_i + \sum_{\ell=1}^{i-n+k} \bar{\alpha}_{\ell,i} W_{\ell,i} & = & 1/\bar{d}_i, & \\ W_{i,j}\bar{d}_i + \sum_{\ell=1}^{i-n+k} \bar{\alpha}_{\ell,i} W_{\ell,j} & = & 0, & j = 1,\dots,i-n+k. \end{array} \tag{2.21}$$

Then, $(\bar{d},\bar{\alpha})$ is the optimal solution of (2.19).

Proof. The proof follows simlarly to the finding of the optimal preconditioners in the sections above. We include it in Appendix B, below. ∎

The following Example 2.7 and Example 2.8 solve (2.21) for $k = 1$ and $k = 2$.

Example 2.7 ($k = 1$)**.** *Let $W \in \mathbb{S}^n_{++}$ be given. Set*

$$\bar{d}_i = \begin{cases} W_{i,i}^{-1/2}, & \text{if } i = 1,\dots,n-1 \\ \left(\frac{W_{1,1}W_{n,n}-W_{1,n}^2}{W_{1,1}}\right)^{-1/2}, & \text{if } i = n. \end{cases}$$

and

$$\bar{\alpha} = -\frac{W_{1n}}{W_{11}}\bar{d}_n.$$

Then the optimal D_{+1}-diagonal upper triangular scaling is given by

$$(\bar{d},\bar{\alpha}) = \operatorname*{argmin}_{d\in\mathbb{R}^n_{++},\alpha\in\mathbb{R}} \omega\big(D_{+1}(d,\alpha)^T W D_{+1}(d,\alpha)\big).$$

Example 2.8 ($k = 2$)**.** *Let $W \in \mathbb{S}^n_{++}$ be given. Set*

$$\bar{d}_i = \begin{cases} W_{i,i}^{-1/2}, & \text{if } i = 1,\dots,n-2 \\ \left(\frac{W_{1,1}W_{n-1,n-1}-W_{1,n-1}^2}{W_{1,1}}\right)^{-1/2}, & \text{if } i = n-1 \\ \left(W_{n,n} + \frac{W_{1,n}^2W_{2,2}-2W_{1,n}W_{2,n}W_{1,2}+W_{2,n}^2W_{1,1}}{W_{1,2}^2-W_{1,1}W_{2,2}}\right)^{-1/2}, & \text{if } i = n. \end{cases}$$

$$\begin{array}{rcl} \bar{\alpha}_{1,n} & = & \left(\frac{W_{1,n}W_{2,2}-W_{1,2}W_{2,n}}{W_{1,2}^2-W_{1,1}W_{2,2}}\right)\bar{d}_n, \\ \bar{\alpha}_{1,n-1} & = & -\frac{W_{1,n-1}}{W_{1,1}}\bar{d}_{n-1}, \\ \bar{\alpha}_{2,n} & = & \left(\frac{W_{1,1}W_{2,n}-W_{1,2}W_{1,n}}{W_{1,2}^2-W_{1,1}W_{2,2}}\right)\bar{d}_n. \end{array}$$

Then the optimal D_{+2}-diagonal upper triangular scaling is given by

$$(\bar{d},\bar{\alpha}) = \operatorname*{argmin}_{d\in\mathbb{R}^n_{++},\alpha\in\mathbb{R}^3} \omega\big(D_{+2}(d,\alpha)^T W D_{+2}(d,\alpha)\big).$$

2.2 The ω Condition Number in Iterative Methods and Error Analysis

Consider the linear system $Ax = b$ with $A \in \mathbb{S}^n_{++}$ and $b \in \mathbb{R}^n$ given.

2.2.1 Iterative Methods

As stated above, preconditioning is essential for iterative methods for solving linear systems. And, many of the convergence analysis results depend on clustering of eigenvalues. A typical comparison for the eigenvalues of $A \succ 0$ after preconditioning with the optimal κ, ω diagonal preconditioners is given in Figure 2.1 (The corresponding MATLAB code is available online in https://github.com/DavidTBelen/omega-condition-number). We clearly see the improved clustering of eigenvalues. The effect on iterations for solving the system is given in Section 4, below.

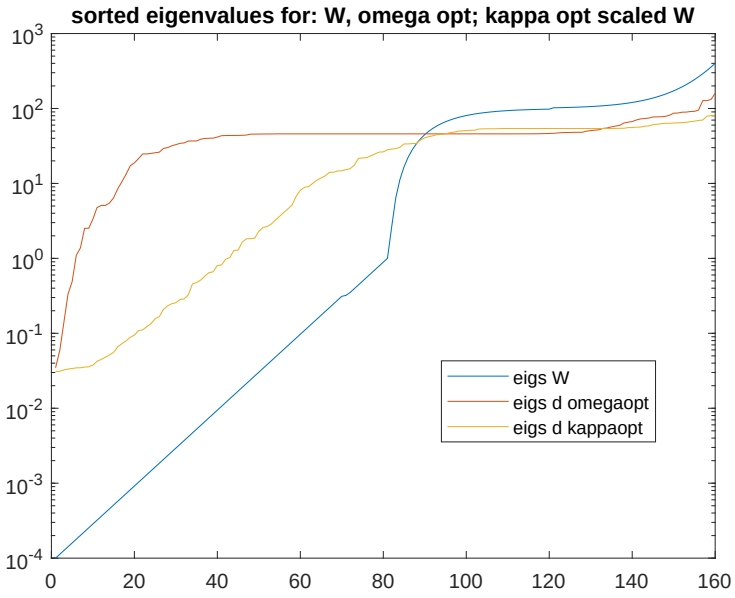

Figure 2.1: Comparison for clustering of eigenvalues pre-post preconditioning

2.2.2 Error Analysis

We are intereseted in understanding how small changes in the data affect the solution of the system $x = A^{-1}b$. Let $x + \Delta x$ be a solution of the perturbed system

$$A(x + \Delta x) = b + \Delta b, \tag{2.22}$$

where $\Delta x, \Delta b \in \mathbb{R}^n$. The *condition number* aims to be a measure on how strongly a relative error in the data affects the relative error in the solution [31]. Therefore, it can be estimated as the ratio

$$\text{cond} :\approx \frac{\|\Delta x\|\|b\|}{\|x\|\|\Delta b\|} \quad \text{(rel. error output/rel. error input)}. \tag{2.23}$$

Note that the above ratio depends on the choice of the perturbation Δb. In practice, $\kappa(A) := \lambda_{\max}(A)/\lambda_{\min}(A)$ is taken as an estimator of the condition number cond as the inequality

$$\frac{\|\Delta x\|}{\|x\|} \leqslant \kappa(A)\frac{\|\Delta b\|}{\|b\|},$$

holds for all $\Delta b \in \mathbb{R}^n$, see, e.g., [18] or [32, Chapter 7] for further details.

Remark 2.9. *Moreover, if we consider b as the input to a function G with output x, then a Taylor type argument gives to first order condition number as in (2.23)*

$$\text{cond}(G) = \frac{\|b\|}{\|G(b)\|}\frac{\|\Delta G\|}{\|\Delta b\|} \cong \|\nabla G(b)\|\frac{\|b\|}{\|G(b)\|}, \tag{2.24}$$

a first order approximation for the condition number of G. Therefore, if G is one of κ, ω, we get the condition number of the condition number, see e.g., [19] and the related result that for κ, the condition number of the condition number is the condition number, see Lemma 2.2. We have observed empirically that the condition number of ω is significantly smaller than the condition number of κ.

If $\kappa(A)$ is *large* we say that the system is *ill-conditioned*, and *well-conditioned* otherwise.[2] We proceed to measure the difference in the condition numbers:

1 we use 200 instances $i = 1, \dots 200$ consisting of random positive definite matrices $\{A_i\}$ of size 200×200 with eigenvalues randomly uniformly distributed in $(0, 1)$;

2 for each i:

   (a) we choose x_i sampled from the standard normal distribution and set $b_i = A_i x_i$;

   (b) we generate random perturbed linear systems $j = 1, \dots, 1000$ of the form of (2.22), where Δb is random with norm 10^{-6} and we denote $\Delta x = A_i^{-1}\Delta b$;

   (c) we compute the relative residual ratio of the perturbed system in (2.23) for all j and consider the mean of the 1000 ratios as an estimation of the condition number of the system i, denoted as $\text{cond}(A_i)$.

3 We then check the resulting correlation between the vectors $(\kappa(A_i))_{i=1}^{200}$, $(\omega(A_i))_{i=1}^{200}$ and $(\text{cond}(A_i))_{i=1}^{200}$, repectively, by comparing the corresponding linear regression models. Figure 2.2, page 19, reveals a significant linear correlation between cond and ω, with a correlation coefficient of 0.9062; whereas in contrast, cond and κ are not linearly correlated as the correlation coefficient is 0.4530.

[2] $\kappa(A)$ is also used to measure error that arises from perturbations in A: $\frac{\|\Delta x\|}{\|x+\Delta x\|} \leqslant \kappa(A)\frac{\|\Delta A\|}{\|A\|}$. The results are essentially equivalent.

The same experiment was conducted for the case where the eigenvalues of the matrices $\{A_i\}_{i=1}^{200}$ are generated from the normal standard distribution. The results are displayed in Figure 2.3, page 19. In this case, we cannot conclude the existence of a linear relation between κ and cond nor between ω and cond. However ω still provides a better estimate for cond as the correlation coefficients are: 0.4847 with ω and 0.0295 with κ.

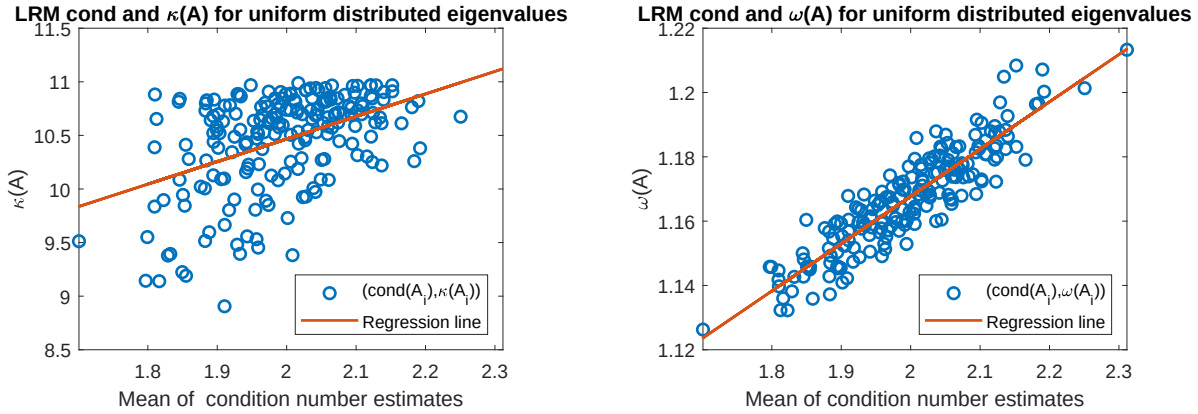

Figure 2.2: Linear regression models between cond and κ, and cond and ω for matrices with uniformly distributed eigenvalues.

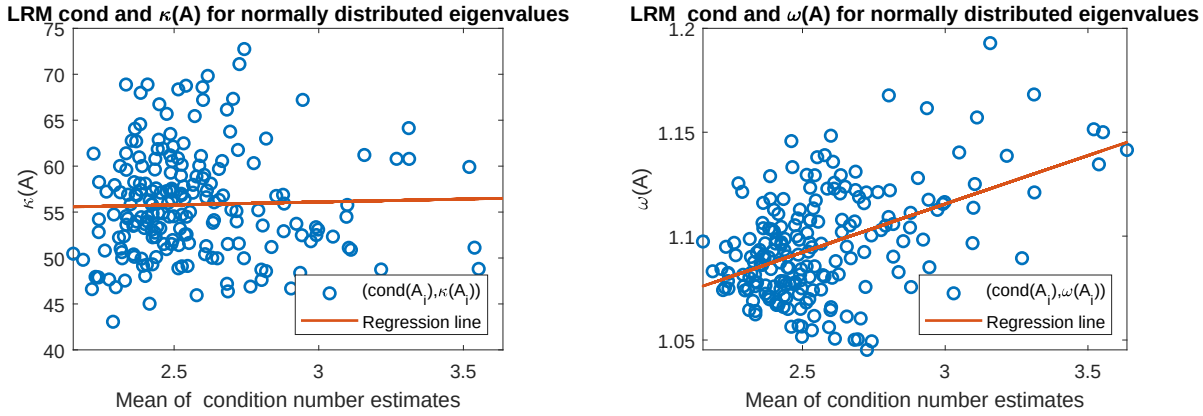

Figure 2.3: Linear regression models between cond and κ, and cond and ω for matrices with normally distributed eigenvalues.

2.3 Efficiency and Accuracy of Evaluation of $\omega(A)$

Since eigenvalue decompositions can be expensive, one issue with $\kappa(A)$ is how to estimate it efficiently when the size of matrix A is large. A survey of estimates and, in particular, estimates using the ℓ_1-norm, is given in [18, 20]. Extensions to sparse matrices and block-oriented generalizations are given in [17, 21]. Results from these papers form the basis of the *condest* command in MATLAB. More recently [12] deals with scalable methods for finding the κ-optimal diagonal preconditioner. This illustrates the difficulty in accurately estimating $\kappa(A)$.

On the other hand, the measure $\omega(A)$ can be calculated using the trace and determinant function which do not require eigenvalue decompositions.[3] However, for large n, the determinant is also numerically difficult to compute as it could easily result in an overflow $+\infty$ or 0 due to the limits of finite precision arithmetic, e.g., if the order of A is $n = 50$ and the eigenvalues $\lambda_i = .5, \forall i$, then the determinant $.5^n$ is zero to machine precision. A similar problem arises for e.g., $\lambda_i = 2, \forall i$ with overflow. In order to overcome this problem, we take the n-th root first and then the product, i.e., we define the value obtained from the spectral factorization as

$$\omega_{\text{eig}}(A) = \frac{\sum_{i=1}^n \lambda_i(A)/n}{\prod_{i=1}^n (\lambda_i(A)^{1/n})}.$$

We now let $A = R^T R = LUP$ denote the Cholesky and LU factorizations, respectively, with appropriate permutation matrix P. We assume that L is unit lower triangular. Therefore,

$$\det(A)^{1/n} = \det\left(R^T R\right)^{1/n} = \det(R)^{2/n} = \prod_{i=1}^n \left(R_{ii}^{2/n}\right). \tag{2.25}$$

Similarly,

$$\det(A)^{1/n} = \det(LUP)^{1/n} = \prod_{i=1}^n \left(|U_{ii}|^{1/n}\right). \tag{2.26}$$

Therefore, we find $\omega(A)$ with numerator $\text{tr}(A)/n$ and denominator given in (2.25) and (2.26), respectively:

$$\omega_R(A) = \frac{\text{tr}(A)/n}{\prod_{i=1}^n \left(R_{ii}^{2/n}\right)}, \quad \omega_{LU}(A) = \frac{\text{tr}(A)/n}{\prod_{i=1}^n \left(|U_{ii}|^{1/n}\right)}.$$

Tables 2.1 and 2.2 provide comparisons on the time and precision from the three different factorization methods. Each column presents different order of κ-condition number, while each row corresponds to different decompositions with different size n of the problem. We form the random matrix using $A = QDQ^T$ for random orthogonal Q and positive definite diagonal D. We then symmetrize $A \leftarrow (A + A^T)/2$ to avoid roundoff error in the multiplications. Therefore, we consider the evaluation using D as the *exact value* of $\omega(A)$,

[3] Since the first version of this paper we have been made aware of the new CVX MATLAB function *det_rootn* that calculates $\det(A)^{1/n}$, the denominator of ω, using the Cholesky decomposition.

i.e.,

$$\omega(A) = \frac{\sum_{i=1}^{n} (D_{ii})/n}{\prod_{i=1}^{n} \left(D_{ii}^{1/n}\right)}.$$

Table 2.2 shows the absolute value of the difference between the exact ω-condition number and the ω-condition numbers obtained by making use of each factorization, namely, ω_{eig}, ω_R and ω_{LU}. Surprisingly, we see that both the Cholesky and LU decompositions give better results than the eigenvalue decomposition.

n	Fact.	order κ 1e2	order κ 1e3	order κ 1e4	order κ 1e5	order κ 1e6	order κ 1e7	order κ 1e8	order κ 1e9
500	eig	5.5267e-02	5.7766e-02	5.2747e-02	5.9256e-02	6.0856e-02	6.2197e-02	5.5592e-02	5.7626e-02
	R	1.1218e-02	8.0907e-03	7.5172e-03	8.4705e-03	9.2774e-03	8.5553e-03	8.1462e-03	7.9027e-03
	LU	2.2893e-02	1.8159e-02	1.8910e-02	2.0902e-02	2.0057e-02	2.0308e-02	1.9060e-02	1.8879e-02
1000	eig	3.0664e-01	2.8968e-01	2.6095e-01	2.7796e-01	5.7083e-01	5.9007e-01	5.8351e-01	5.9630e-01
	R	2.9328e-02	2.8339e-02	2.7869e-02	3.1909e-02	5.8628e-02	6.0873e-02	6.2429e-02	6.1074e-02
	LU	7.5011e-02	7.2666e-02	7.0497e-02	7.6778e-02	1.6313e-01	1.7313e-01	1.7666e-01	1.7326e-01
2000	eig	3.4794e+00	3.4804e+00	3.1916e+00	3.4386e+00	3.4235e+00	3.4766e+00	3.2327e+00	3.3704e+00
	R	3.5644e-01	3.5989e-01	2.9556e-01	3.6375e-01	3.5847e-01	3.5972e-01	3.2629e-01	3.4227e-01
	LU	9.0136e-01	9.0537e-01	7.1161e-01	8.7445e-01	8.6420e-01	8.8027e-01	8.1990e-01	8.1383e-01

Table 2.1: CPU sec. for evaluating $\omega(A)$, averaged over the same 10 random instances; eig, R, LU are eigenvalue, Cholesky, LU decompositions, respectively.

n	Fact.	order κ 1e2	order κ 1e3	order κ 1e4	order κ 1e5	order κ 1e6	order κ 1e7	order κ 1e8	order κ 1e9
500	eig	1.5632e-13	2.7853e-12	2.2618e-10	1.2695e-08	8.9169e-07	5.4109e-05	2.2610e-03	1.7349e-01
	R	1.7053e-13	2.5580e-12	1.0039e-10	1.1339e-08	4.9818e-07	2.6470e-05	1.3173e-03	1.6217e-01
	LU	1.5987e-13	2.4585e-12	1.0652e-10	1.1987e-08	5.1592e-07	2.1372e-05	1.3641e-03	1.4268e-01
1000	eig	2.1316e-13	2.1032e-12	8.7653e-11	4.6271e-09	3.1477e-07	1.9602e-05	9.9290e-04	7.6469e-02
	R	4.2633e-13	1.5632e-12	4.2235e-11	3.9297e-09	2.9562e-07	1.1498e-05	9.1506e-04	5.3287e-02
	LU	4.4054e-13	1.4850e-12	3.7858e-11	3.8287e-09	2.7390e-07	1.3820e-05	6.0492e-04	4.8568e-02
2000	eig	2.4336e-13	4.1780e-12	4.2019e-10	2.0080e-08	7.7358e-07	6.4819e-05	5.5339e-03	3.7527e-01
	R	4.3698e-13	2.0819e-12	5.0704e-11	2.3442e-09	1.8376e-07	8.9575e-06	5.5255e-04	4.8842e-02
	LU	4.3165e-13	2.2595e-12	2.3249e-11	2.5057e-09	1.5020e-07	6.0479e-06	5.4228e-04	4.4205e-02

Table 2.2: Precision of evaluation of $\omega(A)$ averaged over the same 10 random instances. eig, R, LU are eigenvalue, Cholesky, LU decompositions, respectively.

3 Optimal Conditioning for Generalized Jacobians

We now consider the problem of improving conditioning for low rank updates of very ill-conditioned (close to singular) positive definite matrices.

3.1 Preliminaries

More precisely, given a positive definite matrix $A \in \mathbb{S}^n_{++}$ and a matrix $U \in \mathbb{R}^{n\times t}$ with $t << n$, we aim to find $\gamma \in \mathbb{R}^t$ so as to minimize the condition number of the low rank update

$$A + U\,\mathrm{Diag}(\gamma)U^T. \tag{3.1}$$

This kind of updating arises when finding generalized Jacobians in nonsmooth optimization. We provide insight on the problem in the following Example 3.1.

Example 3.1 (Generalized Jacobians)**.** *In many nonsmooth and semismooth Newton methods one aims to find a root of a function $F : \mathbb{R}^n \to \mathbb{R}^n$ of the form*

$$F(y) := B(v + B^T y)_+ - c,$$

where $B \in \mathbb{R}^{n\times m}$, $v \in \mathbb{R}^m$, $c \in \mathbb{R}^n$ and $(\cdot)_+$ denotes the projection onto the nonnegative orthant, e.g., [3, 22, 29]. At every iteration of these algorithms a generalized Jacobian of F is computed of the form

$$J := \sum_{i\in\mathcal{I}_+} B_i B_i^T + \sum_{j\in\mathcal{I}_0} \gamma_j B_j B_j^T, \text{ with } \gamma_j \in [0, 1]$$

and where B_i and B_j denote columns of B over the set of indices $\mathcal{I}_+ := \{i \in \{1, \dots, m\} : (v + B^T y)_i > 0\}$ and

$$\mathcal{I}_0 := \{j \in \{1, \dots, m\} : (v + B^T y)_j = 0 \text{ and } (B_j)_{j\in\mathcal{I}_0} \text{ is a maximal linearly independent subset}\}.$$

The generalized Jacobian J, which is usually singular, is then used to obtain a Newton direction $d \in \mathbb{R}^n$ by solving a least-square problem for the system $(J + \epsilon I)\, d = -F(y)$, where ϵI, with $\epsilon > 0$, is analogous to the regularization term of the well-known Levenberg–Marquardt method*. Thus, this linear system is very ill-conditioned. This makes preconditioning by optimal updating appropriate.*

The optimal preconditioned update can be done in our framework as we start with

$$A := \sum_{i\in\mathcal{I}_+} B_i B_i^T + \epsilon I, \quad U = [B_j]_{j\in\mathcal{I}_0},$$

and then find an optimal low rank update as in (3.1); done with additional box constraints on γ, namely, $\gamma \in [0, 1]^t$.

Similar conditioning questions also appear in the normal equations matrix, ADA^T, in interior point methods, e.g., modifying the weights in D appropriately to avoid ill-conditioning [6, 13]. For other related work on minimizing condition numbers for low rank updates see, e.g., [5, 16].

Here, we propose obtaining an optimal conditioning of the update (3.1) by using the ω-condition number of [9], instead of the classic κ-condition number. The ω-condition number presents some advantages with respect to the classic condition number, since it is differentiable and pseudoconvex in the interior of the positive semidefinite cone, which facilitates addressing minimization problems involving it. Our empirical results show a significant decrease in the number of iterations required for a requested accuracy in the residual.

3.2 Optimal Conditioning for Rank One Updates

We first consider the special case where the update is rank one. Related eigenvalue results for rank one updates are well known in the quasi-Newton literature, e.g., [8,30]. We include this special rank one case as it yields interesting results. The general rank-t update is studied in Section 3.3, below.

Theorem 3.2. *Suppose we have a given $A \in \mathbb{S}^n_{++}$ and $u \in \mathbb{R}^n$. Let $A = QDQ^T$ be the (orthogonal) spectral decomposition of A. Let $U = uu^T$ and define the rank one update*

$$A(\gamma) = A + \gamma U,\ \gamma \in \mathbb{R}.$$

Set

$$w = D^{-1/2}Q^T u, \tag{3.2}$$

and

$$\gamma^* = \frac{\operatorname{tr}(A)\|w\|^2 - n\|u\|^2}{(n-1)\|u\|^2\|w\|^2}. \tag{3.3}$$

Then, $\gamma^* \in \left]-\|w\|^{-2}, +\infty\right[$ provides the optimal ω-conditioning, i.e.,

$$\gamma^* = \operatorname*{argmin}_{A(\gamma)\succ 0} \omega(\gamma). \tag{3.4}$$

Proof. Let

$$f(\gamma) := \operatorname{tr}(A(\gamma))/n \quad \text{and} \quad g(\gamma) := \det(A(\gamma))^{1/n}.$$

We want to find the optimal γ to minimize the condition number

$$\omega(\gamma) = f(\gamma)/g(\gamma)$$

subject to $A(\gamma)$ being positive definite. By Proposition 2.1 1, $\omega : \mathbb{R} \to \mathbb{R};\ \gamma \to \omega(\gamma)$ is pseudoconvex as long as $A(\gamma) \succ 0$. We prove that the later is true for γ belonging to an open interval in the real line. Indeed, let $A = QDQ^T$ be the spectral decomposition of A and define

$$w = D^{-1/2}Q^T u \quad \text{and} \quad W = ww^T = D^{-1/2}Q^T uu^T QD^{-1/2}. \tag{3.5}$$

Then we can rewrite

$$A(\gamma) = QD^{1/2}(I + \gamma W)D^{1/2}Q^T, \tag{3.6}$$

which is positive definite if and only if the rank one update of I, $I + \gamma W$, belongs to the cone of positive definite matrices. Now, note that the eigenvalues of this term are $\lambda_1 = 1$, with multiplicity $n-1$, and $\lambda_2 = 1 + \gamma\|w\|^2$ with multiplicity 1. We then conclude that

$$A(\gamma) \in \mathbb{S}^n_{++} \iff \gamma \in \left]-\frac{1}{\|w\|^2}, +\infty\right[,$$

in which case $\lambda_2 > 0$. Here $]a, b[$ denotes the open interval in $\mathbb{R}$ formed by a, b. Moreover, $\omega(\gamma)$ tends to ∞ as γ approaches the extreme of the above interval. Therefore ω possesses a

minimizer in the open interval, $\gamma^* \in]-\|w\|^{-2}, +\infty[$, that satisfies $\omega'(\gamma^*) = 0$. Note that since ω is pseudoconvex the fact that its derivative is equal to zero is also a sufficient condition for global optimality (see Fact 3.7 below).

In the following we obtain an explicit expression for the (unique) minimizer of (3.4), γ^*, by studying the zeros of ω'. Using the notation introduced in (3.5), f and its derivative are expressed as

$$f(\gamma) = \left(\operatorname{tr}(A) + \gamma\|u\|^2\right)/n \quad \text{and} \quad f'(\gamma) = \|u\|^2/n,$$

respectively. By making use of (3.6), g becomes

$$g(\gamma) := \left(\det(A)\det(I + \gamma W)\right)^{1/n},$$

since $\det(D) = \det(A)$. As explained above the eigenvalues of $I + \gamma W$, are $\lambda_1 = 1 + \gamma\|w\|^2$, and the others are all 1, which yields that

$$g(\gamma) = \left(\det(A)(1 + \gamma\|w\|^2)\right)^{1/n} = \det(A)^{1/n}(1 + \gamma\|w\|^2)^{1/n}.$$

We get

$$g'(\gamma) = \frac{1}{n}\det(A)^{1/n}\|w\|^2(1 + \gamma\|w\|^2)^{(1-n)/n}.$$

The derivative of ω is then obtained as follows

$$\begin{aligned}
\omega'(\gamma) &= \frac{f'(\gamma)g(\gamma) - f(\gamma)g'(\gamma)}{g(\gamma)^2} \\
&= \frac{1}{g(\gamma)^2}\left[\frac{\|u\|^2}{n}\det(A)^{1/n}\left(1 + \gamma\|w\|^2\right)^{1/n}\right. \\
&\quad \left. -\frac{\|w\|^2}{n^2}\left(\operatorname{tr}(A) + \gamma\|u\|^2\right)\det(A)^{1/n}\left(1 + \gamma\|w\|^2\right)^{(1-n)/n}\right] \\
&= \frac{\det(A)^{1/n}}{g(\gamma)^2 n^2}\left(1 + \gamma\|w\|^2\right)^{(1-n)/n}\left[n\|u\|^2 + (n-1)\gamma\|u\|^2\|w\|^2 - \operatorname{tr}(A)\|w\|^2\right].
\end{aligned} \tag{3.7}$$

A simple computation shows that this derivative is 0 only when γ attains the value

$$\gamma^* = \frac{\operatorname{tr}(A)\|w\|^2 - n\|u\|^2}{(n-1)\|u\|^2\|w\|^2}, \tag{3.8}$$

which then has to be in the interval $]-\|w\|^{-2}, +\infty[$. Since ω is pseudoconvex, we conclude that γ^* is the optimal preconditioner which solves (3.4).

■

Equivalently, we can deduce an expression for the optimal ω-conditioning by making use of the Cholesky decomposition of A instead of the spectral decomposition. This is gathered in our next corollary. The proof follows from the same calculations than Theorem 3.2 and thus is omitted.

Corollary 3.3. *Given A and U as in Theorem 3.2. Let $A = LL^T$ be the Cholesky decomposition of A. Then, the formula for the optimal ω-conditioning γ^* in (3.3) holds with the replacement*

$$w \leftarrow L^{-1}u.$$

As shown in Example 3.1, in some applications the preconditioner multiplier γ is required to take values in the interval $[0, 1]$. In the following, we analize the optimal ω-preconditioner for the rank 1 update subject to this interval constraint.

Corollary 3.4. *Let the assumptions of Theorem 3.2 hold and let $\bar{\gamma}$ be the optimal ω-preconditioner in the interval $[0, 1]$, i.e.,*

$$\bar{\gamma} = \arg \min_{\substack{0 \leqslant \gamma \leqslant 1 \\ A(\gamma) > 0}} \omega(\gamma).$$

Then, if $\gamma^* \in \,]-\|w\|^2, +\infty[$ is the optimal "unconstrained" ω-preconditioner obtained in Theorem 3.2, the following hold:

(i) If $\gamma^* \in [0, 1] \implies \bar{\gamma} = \gamma^*$;

(ii) If $\gamma^* < 0 \implies \bar{\gamma} = 0$;

(iii) If $\gamma^* > 1 \implies \bar{\gamma} = 1$.

Proof. (i) In this case, since γ^* is the global optimum of ω in $]-\|w\|^2, +\infty[$, it would also be so in the interval $[0, 1]$.

For (ii) and (iii), it suffices to observe that, by (3.7) and (3.8), when $\gamma^* < 0$ (respectively, $\gamma^* > 1$) the derivative of ω is monotonically increasing (respectively, decreasing) in the interval $[0, 1]$.

■

3.3 Optimal Conditioning with a Low Rank Update

We now consider the case where the update is low rank. We need the following notations. For a matrix $Z \in \mathbb{R}^{n\times t}$, we use MATLAB notation and define the function $\text{norms}(Z) : \mathbb{R}^{n\times t} \to \mathbb{R}^t$ as the (column) vector of column 2-norms of Z. We let $\text{norms}^\alpha(Z)$ denote the vector of column norms with each norm to the power α.

Theorem 3.5 (Rank t-update)**.** *Let $A \in \mathbb{S}^n_{++}$, $U = [u_1, \ldots, u_t] \in \mathbb{R}^{n\times t}$, be given with $n > t \geqslant 2$, and $\text{norms}(U) > 0$. Set*

$$A(\gamma) = A + U\,\text{Diag}(\gamma)U^T, \text{ for } \gamma \in \mathbb{R}^t.$$

Let the spectral decomposition of A be given by $A = QDQ^T$, define $w_i = D^{-1/2}Q^T u_i, i \in \{1, \ldots, t\}$, as in (3.2), with $W = \begin{bmatrix} w_1 \ldots w_t \end{bmatrix}$. Let

$$\begin{array}{rcl} K(U) & = & \left[n \operatorname{Diag}\left(\operatorname{norms}^2(U)\right) - e \operatorname{norms}^2(U)^T \right], \\ b(U) & = & \left(\operatorname{tr}(A) e - n \operatorname{Diag}\left(\operatorname{norms}^2(W)\right)^{-1} \operatorname{norms}^2(U) \right), \end{array} \tag{3.9}$$

where e denotes the vector of all ones. Then, the optimal ω-preconditioner,

$$\gamma^* = \underset{A(\gamma) \succ 0}{\operatorname{argmin}}\, \omega(\gamma), \tag{3.10}$$

is given component-wise by

$$\begin{aligned} (\gamma^*)_i &= (K(U)^{-1} b(U))_i \\ &= \frac{\operatorname{tr}(A)\|w_i\|^2 - (n-t+1)\|u_i\|^2}{(n-t)\|u_i\|^2\|w_i\|^2} - \frac{1}{(n-t)\|u_i\|^2} \sum_{j=1, j\neq i}^{t} \frac{\|u_j\|^2}{\|w_j\|^2}, \end{aligned} \tag{3.11}$$

for $i = 1, \ldots, t$.

Proof. Let $A \succ 0$ and

$$U = \begin{bmatrix} u_1 & \ldots & u_t \end{bmatrix} \in \mathbb{R}^{n \times t}, \qquad \text{with } n > t \geqslant 2.$$

We consider the update of the form

$$A(\gamma) = A + U \operatorname{Diag}(\gamma) U^T = A + \sum_{i=1}^{t} \gamma_i u_i u_i^t, \quad \gamma \in \mathbb{R}^t.$$

Same than in Theorem 3.2, we start characterizing an open subset of $\mathbb{R}^t$ where $A(\gamma)$ is positive definite. In order to do this, we again transform the problem using the spectral decomposition of A, $A = QDQ^T$, and setting

$$w_i = D^{-1/2} Q^T u_i \quad \text{and} \quad W_i = w_i w_i^T \quad \text{for } i = 1, \ldots, t.$$

Then, we can express $A(\gamma)$ as

$$\begin{array}{rcl} A(\gamma) & = & A + U \operatorname{Diag}(\gamma) U^T \\ & = & QD^{1/2} \left(I + D^{-1/2} Q^T U \operatorname{Diag}(\gamma) U^T Q D^{-1/2} \right) D^{1/2} Q^T \\ & = & QD^{1/2} \left(I + \sum_{i=1}^{t} \gamma_i (D^{-1/2} Q^T u_i)(u_i^T Q D^{-1/2}) \right) D^{1/2} Q^T \\ & = & QD^{1/2} \left(I + \sum_{i=1}^{t} \gamma_i W_i \right) D^{1/2} Q^T. \end{array}$$

By repeatedly making use of the formula for the determinant of the sum of an invertible matrix and a rank one matrix (see, e.g., [25, Example 4]), we obtain the following expression for the determinant of $A(\gamma)$

$$\det(A(\gamma)) = \det(A)\left(\prod_{i=1}^{t}(1+\gamma_i\|w_i\|^2)\right). \tag{3.12}$$

Consequently, $A(\gamma)$ is nonsingular and, by continuity of the eigenvalues, positive definite for γ belonging to the set

$$\Omega := \left]-\frac{1}{\|w_1\|^2},+\infty\right[\times \left]-\frac{1}{\|w_2\|^2},+\infty\right[\times \ \ldots \ \times \left]-\frac{1}{\|w_t\|^2},+\infty\right[. \tag{3.13}$$

Now, note that the constraint $A(\gamma) \succ 0$ is a positive definite constraint, so it is convex. Therefore, if there exists some γ outside of Ω such that $A(\gamma) \succ 0$, we would loose the convexity of the feasible set, since $A(\gamma)$ is singular on the boundary of Ω. This implies that

$$A(\gamma) \succ 0 \Longleftrightarrow \gamma \in \Omega.$$

Moreover, since $\omega(\gamma) \to +\infty$ as γ tends to the border of Ω or to $+\infty$, we can ensure that γ has a minimizer in Ω. Since the function is pseudoconvex on this open set, the global minimum is attained at a point γ^* such that $\nabla\omega(\gamma^*) = 0$. Next, we prove that γ^* is given by (3.11).

For this, note that $f(\gamma)$ can be expressed as

$$f(\gamma) = \frac{1}{n}\operatorname{tr}(A + U\operatorname{Diag}(\gamma)U^T) = \frac{1}{n}\left(\operatorname{tr}(A) + \sum_{i=1}^{t}\gamma_i\|u_i\|^2\right) = \frac{1}{n}\left(\operatorname{tr}(A) + \gamma^T \operatorname{norms}^2(U)\right),$$

and its gradient is $\nabla f(\gamma) = \frac{1}{n}\operatorname{norms}^2(U)$. On the other hand, by (3.12) $g(\gamma)$ can be expressed as

$$g(\gamma) = \det(A)^{1/n}\left(\prod_{i=1}^{t}(1+\gamma_i\|w_i\|^2)\right)^{1/n}.$$

The gradient of $g(\gamma)$ is then given component-wise by

$$\frac{\partial g(\gamma)}{\partial \gamma_j} = \frac{1}{n}\det(A)^{1/n}\left(\prod_{i=1}^{t}(1+\gamma_i\|w_i\|^2)\right)^{(1-n)/n}\left(\prod_{i=1,i\neq j}^{t}(1+\gamma_i\|w_i\|^2)\right)\|w_j\|^2,\ j=1,\ldots,t.$$

We make use of these expressions in order to compute the partial derivatives of ω. For every

$j = 1, \ldots, t$, we have

$$\begin{aligned}\frac{\partial \omega(\gamma)}{\partial \gamma_j} &= \frac{\frac{\partial f(\gamma)}{\partial \gamma_j} g(\gamma) - f(\gamma) \frac{\partial g(\gamma)}{\partial \gamma_j}}{g(\gamma)^2} \\ &= \frac{1}{g(\gamma)^2} \det(A)^{1/n} \left[\frac{\|u_j\|^2}{n} \left(\prod_{i=1}^{t} (1 + \gamma_i \|w_i\|^2) \right)^{1/n} \right. \\ &\quad \left. - \frac{\|w_j\|^2}{n^2} \left(\operatorname{tr}(A) + \gamma^T \operatorname{norms}^2(U) \right) \left(\prod_{i=1}^{t} (1 + \gamma_i \|w_i\|^2) \right)^{(1-n)/n} \left(\prod_{i=1, i \neq j}^{t} (1 + \gamma_i \|w_i\|^2) \right) \right].\end{aligned}$$

By defining the positive function $C(\gamma) : \mathbb{R}^t \to \mathbb{R}_{++}$ as

$$C(\gamma) = \frac{\det(A)^{1/n}}{g(\gamma)^2 n^2} \left(\prod_{i=1}^{t} (1 + \gamma_i \|w_i\|^2) \right)^{(1-n)/n} \left(\prod_{i=1, i \neq j}^{t} (1 + \gamma_i \|w_i\|^2) \right),$$

we finally get that

$$\frac{\partial \omega(\gamma)}{\partial \gamma_j} = C(\gamma) \left[n \|u_j\|^2 (1 + \gamma_j \|w_j\|^2) - \left(\operatorname{tr}(A) + \gamma^T \operatorname{norms}^2(U) \right) \|w_j\|^2 \right], \tag{3.14}$$

for all $j = 1, \ldots, t$. After setting the derivative (gradient) of ω to zero, and ignoring the positive factor given by C, we get that the minimum of the pseudoconvex function is obtained as the solution of the linear system defined by the t equations

$$(n-1)\|u_k\|^2 \gamma_k - \sum_{i=1, i \neq k}^{t} \|u_i\|^2 \gamma_i = \operatorname{tr}(A) - n \frac{\|u_k\|^2}{\|w_k\|^2}, \quad k = 1, \ldots, t.$$

Equivalently,

$$\begin{bmatrix} (n-1)\|u_1\|^2 & -\|u_2\|^2 & \ldots & & -\|u_t\|^2 \\ -\|u_1\|^2 & (n-1)\|u_2\|^2 & -\|u_3\|^2 & \ldots & -\|u_t\|^2 \\ \ldots & & & & \\ -\|u_1\|^2 & \ldots & \ldots & -\|u_{t-1}\|^2 & (n-1)\|u_t\|^2 \end{bmatrix} \gamma = \begin{pmatrix} \operatorname{tr}(A) - n\|u_1\|^2/\|w_1\|^2 \\ \ldots \\ \operatorname{tr}(A) - n\|u_t\|^2/\|w_t\|^2 \end{pmatrix}.$$

This is further equivalent to

$$\left[n \operatorname{Diag}(\operatorname{norms}^2(U)) - e \operatorname{norms}^2(U)^T \right] \gamma = \left(\operatorname{tr}(A) e - n \operatorname{Diag}\left(\operatorname{norms}^2(W) \right)^{-1} \operatorname{norms}^2(U) \right),$$

which is the system $K(U)\gamma = b(U)$ using the notation in (3.9).

Now we derive an explicit expression for the optimal γ. In order to do this, note that $K(U)$ is given as the sum of an invertible matrix, $n \operatorname{Diag}(\operatorname{norms}^2(U))$, and an outer product of vectors, $-e \operatorname{norms}^2(U)^T$. By the *Sherman-Morrison formula*, this sum is invertible if and only if

$$1 - \frac{1}{n} \operatorname{norms}^2(U)^T \operatorname{Diag}(\operatorname{norms}^2(U))^{-1} e \neq 0.$$

This is always true for $t < n$. Indeed, we have

$$1 - \frac{1}{n}\operatorname{norms}^2(U)^T \operatorname{Diag}(\operatorname{norms}^2(U))^{-1} e = 1 - \frac{1}{n} e^T e = 1 - \frac{t}{n} > 0.$$

Moreover, we obtain the following expression for the inverse

$$\begin{aligned}
&(n \operatorname{Diag}(\operatorname{norms}^2(U)) - e \operatorname{norms}^2(U)^T)^{-1} \\
&\quad = \frac{1}{n} \operatorname{Diag}(\operatorname{norms}^2(U))^{-1} + \frac{1}{\left(1 - \frac{t}{n}\right) n^2} \operatorname{Diag}(\operatorname{norms}^2(U))^{-1} e \operatorname{norms}^2(U)^T \operatorname{Diag}(\operatorname{norms}^2(U))^{-1} \\
&\quad = \frac{1}{n} \operatorname{Diag}(\operatorname{norms}^{-2}(U)) + \frac{1}{(n-t)n} \operatorname{Diag}(\operatorname{norms}^{-2}(U)) e e^T.
\end{aligned}$$

Therefore, the inverse of $K(U)$ in matrix form is given by

$$K(U)^{-1} = \frac{1}{n} \begin{bmatrix} \frac{1}{\|u_1\|^2} & 0 & \dots & 0 \\ 0 & \frac{1}{\|u_2\|^2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{\|u_t\|^2} \end{bmatrix} + \frac{1}{(n-t)n} \begin{bmatrix} \frac{1}{\|u_1\|^2} & \frac{1}{\|u_1\|^2} & \dots & \frac{1}{\|u_1\|^2} \\ \frac{1}{\|u_2\|^2} & \frac{1}{\|u_2\|^2} & \dots & \frac{1}{\|u_2\|^2} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{1}{\|u_t\|^2} & \frac{1}{\|u_t\|^2} & \dots & \frac{1}{\|u_t\|^2} \end{bmatrix}.$$

Finally, we obtain γ^* by calculating the product $\gamma^* = K(U)^{-1} b(U)$ which yields

$$\gamma_i^* = \frac{\operatorname{tr}(A)\|w_i\|^2 - (n-t+1)\|u_i\|^2}{(n-t)\|u_i\|^2\|w_i\|^2} - \frac{1}{(n-t)\|u_i\|^2} \sum_{j=1, j\neq i}^{t} \frac{\|u_j\|^2}{\|w_j\|^2}, \tag{3.15}$$

for all $i = 1, \dots, t$. Since γ^* is the unique zero of the gradient of ω, we conclude that it belongs to Ω and solves (3.10).

■

We note that the optimal ω-preconditioner for the rank one update in Theorem 3.2 is obtained from (3.11) when $t = 1$. On the other hand, we can also employ the Cholesky decomposition of A to derive the optimal ω-preconditioner in Theorem 3.5. We state this in the following corollary.

Corollary 3.6. *Given A and U as in Theorem 3.5. Let $A = LL^T$ be the Cholesky decomposition of A. Then, the formula for the optimal ω-preconditioner γ^* in (3.11) holds with the replacement*

$$w_i \leftarrow L^{-1} u_i, \quad i = 1, \dots, t.$$

Proof. The proof follows similarly to the one of Theorem 3.5 and thus is omitted.

■

With the same assumptions as in Theorem 3.5, we now consider the problem of finding the optimal ω-preconditioner in the box $[0,1]^t$, i.e.,

$$\bar{\gamma} = \arg \min_{\substack{\gamma \in [0,1]^t \\ A(\gamma) \succ 0}} \omega(\gamma). \tag{3.16}$$

For the rank one update ($t = 1$), Corollary 3.4 shows that the solution to (3.16) can be obtained by first computing the minimum of the unconstrained problem, whose explicit expression was given in Theorem 3.2, and then projecting onto the box constraint, which in that case was the interval $[0,1]$. However, this simple projection can fail in general for the low rank update, as we now show in Example 3.8 below.

The illustration of this phenomenon will require considering a constrained pseudoconvex minimization problem. In the following Fact 3.7, see, e.g., [24, Chapter 10], we recall the sufficient optimality conditions for this class of optimization problems. We note that no constraint qualification is needed for *sufficiency*.

Fact 3.7 (Sufficient optimality conditions for pseudoconvex programming)**.** *Let $\Omega \subseteq \mathbb{R}^n$ be nonempty open and convex. Let $f : \Omega \to \mathbb{R}$ be a pseudoconvex function and $(g_i)_{i=1}^m : \Omega \to \mathbb{R}$ a family of differentiable and quasiconvex functions. Consider the optimization problem*

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & g_i(x) \leqslant 0, \quad i = 1, \ldots, m \\ & x \in \Omega. \end{array} \tag{3.17}$$

Let $\bar{x} \in \Omega, \bar{\lambda} \in \mathbb{R}^m$, be a KKT primal-dual pair, i.e., the following KKT conditions hold:

$$\begin{aligned} \nabla f(\bar{x}) + \sum_{i=1}^m \bar{\lambda}_i \nabla g_i(\bar{x}) &= 0 \\ \bar{\lambda}_i &\geqslant 0, \quad i = 1, \ldots, m \\ \bar{\lambda}_i g_i(\bar{x}) &= 0, \quad i = 1, \ldots, m \\ \bar{x} \in \Omega \text{ and } g_i(\bar{x}) &\leqslant 0, \quad i = 1, \ldots, m. \end{aligned} \tag{3.18}$$

Then $\bar{x}$ solves (3.17).

Example 3.8 (Failure of projection for constrained problem (3.16))**.** *Let $n = 3$, $t = 2$ and consider the following initial data for the ω-minimization problem:*

$$A := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} \quad \text{and} \quad U := \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ \frac{-1}{\sqrt{2}} & 0 \\ 0 & 1 \end{bmatrix}.$$

Then, we get the following:

- *From (3.15) and Theorem 3.5, the ω-optimal preconditioner is $\gamma^* = \frac{1}{3}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$;*

- *projecting onto* $[0,1]^2$ *yields* $\gamma_p^* = \frac{1}{3}\begin{pmatrix}1\\0\end{pmatrix}$, *where* $\omega(\gamma_p^*) = 16/(9\sqrt[3]{5})$;

- *however, with* $\bar{\gamma} := \frac{1}{2}\begin{pmatrix}1\\0\end{pmatrix}$, *we get a lower value:*

$$\omega(\bar{\gamma}) = 1/\left(3\sqrt[3]{(2/11)^2}\right) \approx 1.0386 < 1.0397 \approx 16/(9\sqrt[3]{5});$$

  and $\bar{\gamma}$ *is the* ω*-optimal preconditioner in* $[0,1]^2$, *as we now show.*

To prove the last statement, note that (3.16) *can be written as the pseudoconvex program in* (3.17) *by setting* $f := \omega : \mathbb{R}^2 \to \mathbb{R}$, $g_1(\gamma) = -\gamma_1$, $g_2(\gamma) = -\gamma_2$, $g_3(\gamma) = \gamma_1 - 1$, $g_4(\gamma) = \gamma_2 - 2$ *and* Ω *defined as in* (3.13). *In particular, the only active constraint for* $\bar{\gamma} = (1/2, 0)^T$ *is* $g_2(\gamma) = 0$, *so the KKT conditions become*

$$0 = \frac{\partial \omega(\bar{\gamma})}{\partial \gamma_1},$$
$$0 = \frac{\partial \omega(\bar{\gamma})}{\partial \gamma_2} - \bar{\lambda}_2,$$

for some $\bar{\lambda}_2 \geqslant 0$. *This can be verified by simply substituting using the expressions of the partial derivatives of* ω *obtained in* (3.14). *By Fact 3.7, we conclude that for the given data,* $\bar{\gamma}$ *is the solution of* (3.16).

As done in the previous example, obtaining the ω-optimal preconditioner in the box $[0,1]^t$ would require obtaining a KKT point for the constrained pseudoconvex problem (3.16). This is not an easy task. To the author's knowledge, closed formulas for this kind of box constrained minimization problems are not known even when the objective is a quadratic. Nevertheless, using the projection of γ^* onto $[0,1]^t$ as an approximation to $\bar{\gamma}$ appears to give good results in practice. We see this in our numerical tests in Section 4.

4 Numerical Tests

We now present empirics for: the various preconditioners Section 4.1; and the optimal preconditioned low rank updates Section 4.2. The experiments were done on: Intel Core i7-12700H 2.30 GHz with 16GB RAM, under Windows 11 (64-bit). We used MATLAB version 2024a. The MATLAB source code and data of all the experiments is available at https://github.com/DavidTBelen/omega-condition-number.

4.1 Comparisons of Preconditioners for Sparse Positive Definite Linear Systems

In this section, we analyze the performance of an iterative method for approximately solving positive definite linear systems subject to different preconditioning strategies. Specifically,

we compare the ω-optimal diagonal and incomplete upper triangular ω-optimal preconditioners introduced above with state-of-the-art preconditioners, e.g., the incomplete Cholesky preconditioner. Our test enviroment follows the line of the extensive numerical comparisons presented in the survey [14].

4.1.1 Test Enviroment

The problems used in our experiment are all constructed with data from the SuiteSparse Matrix Collection [23]. We consider the symmetric positive definite matrices in this repository whose number of rows (columns) range from $5,000$ to $30,000$; but without "duplicates" (i.e., without similar matrices belonging to the same group). The right hand side of our linear system $b = e$, is always set as the vector of all ones.

As the iterative method for solving the positive definite linear systems, we consider the implementation of the *Preconditioned Conjugate Gradients Method* given by **pcg** MATLAB's in-built function. This is MATLAB's benchmark solver for positive definite linear systems. In all our experiments, our stopping criterion for **pcg** is when the relative residual reaches a tolerance smaller than 10^{-6}, i.e.,

$$\frac{\|Wx - b\|}{\|b\|} < 10^{-6}.$$

Finally, in order to avoid "trivialities", we discard matrices that generate problems that can be solved to the desired tolerance in less than 10 seconds, by **pcg** with *no preconditioner*. This leaves a subset of 16 matrices whose specific characteristics are detailed in, for instance, Table A.1. In the following we use P to denote the set of these 16 problems.

4.1.2 Preconditioning Strategies

We use the following strategies (with acronyms):

- **No preconditioning** (NONE).
- The ω-**optimal diagonal preconditioner** (DIAG) given by (2.1).
- The ω-**optimal incomplete triangular preconditioner** (ITRIU) given by (2.5). The dimension k of the triangular block is chosen according to the nonzero entries $nnz(W)$ of the matrix of interest W as

$$k = \left\lceil \frac{0.1}{2}\left(1 + \sqrt{1 + 4nnz(W)}\right)\right\rceil + 1,$$

  where $\lceil a \rceil$ stands for the minimum integer upper bound of $a \in \mathbb{R}$. The motivation on this choice resides in obtaining a preconditioner with fewer nonzero entries than in W, i.e., $t(k-1) << nnz(W)$. The last summand 1 ensures that the preconditioner is not diagonal.

- **Incomplete Cholesky factorization** (ICHOL). This preconditioning strategy consists in considering a Cholesky factorization of W, given by LL^T, but where some of the entries of L are ignored agreeing with the sparsity pattern of W. The preconditioned system then becomes
$$L^{-1}WL^{-T}y = L^{-1}b, \quad y = L^T x.$$
We use MATLAB's **ichol** to construct L. To ensure that the process does not break down (which can happen if a non positive pivot is encountered) we shift W and obtain an approximation of $W + \alpha \operatorname{Diag}(\operatorname{diag} W)$. To choose α we follow the recommended procedure in the MATLAB Help Center.

4.1.3 Performance Profile

Besides illustrating the output from the experiments as displayed in Tables A.1 to A.4, we also employ performance profile plots, e.g., [11]. These plots are constructed as follows. Let $\Gamma := \{\text{NONE, DIAG, ITRIU, ICHOL}\}$ be the set of preconditioners for our comparisons. For each $p \in P$ and $\gamma \in \Gamma$, we denote as $t_{p,\gamma}$ the measure we want to compare. In particular, we will separately consider the number of iterations and the time required for solving the system (to the desired tolerance) for the preconditioned linear system described in Section 4.1.1. In the cases where we consider a preconditioned system (i.e., all except NONE), the time for computing the preconditioner is also included in $t_{p,\gamma}$, i.e.,

$$\begin{aligned} t_{p,\gamma} = &\{\text{time for computing the preconditioner}\} \\ &+ \{\text{time for solving the preconditioned problem by } \mathbf{pcg}\}. \end{aligned}$$

Then, for every problem $p \in P$ and every $\gamma \in \Gamma$, we define the performance ratio as

$$r_{p,\gamma} := \begin{cases} \frac{t_{p,\gamma}}{\min\{t_{p,\gamma} : \gamma \in \Gamma\}} & \text{if convergence test passed,} \\ +\infty & \text{if convergence test failed.} \end{cases}$$

In our experiments, a convergence test *passed* if it succeeded in solving the linear system with the required relative residual tolerance in less than $100,000$ iterations, and otherwise it *failed*. Note that the best performing preconditioner with respect to the measure under study (time or number of iterations), say $\tilde{\gamma}$, for problem p will have performance ratio $r_{p,\tilde{\gamma}} = 1$. In contrast, if the preconditioner γ underperforms in comparison with $\tilde{\gamma}$, but still manages to pass the test, then

$$r_{p,\gamma} = \frac{t_{p,\gamma}}{t_{p,\tilde{\gamma}}} > 1$$

is the ratio between the overall time (number of iterations) required for solving the problem p for this particular choice and the time (number of iterations) employed by $\tilde{\gamma}$. Consequently, the larger the value of $r_{p,\gamma}$, the worse the preconditioner γ performed for problem p.

Finally, the performance profile of $\gamma \in \Gamma$ is defined as

$$\rho_\gamma(\tau) := \frac{1}{|P|} \operatorname{size}\{p \in P \,:\, r_{p,\gamma} \leqslant \tau\},$$

where $|P|$ is the number of problems in P. This can be understood as the relative portion of times that the performance ratio $r_{p,\gamma}$ is within a factor of $\tau \geqslant 1$ of the best possible performance ratio. In particular, $\rho_\gamma(1)$ represents the number of problems where γ is the best choice. Also, the existence of a $\tau \geqslant 1$ such that $\rho_\gamma(\tau) = 1$, indicates that γ passed the convergence test for every single problem in P. In Figure 4.1, we display our performance profiles, with $\log_2$ scale on τ.

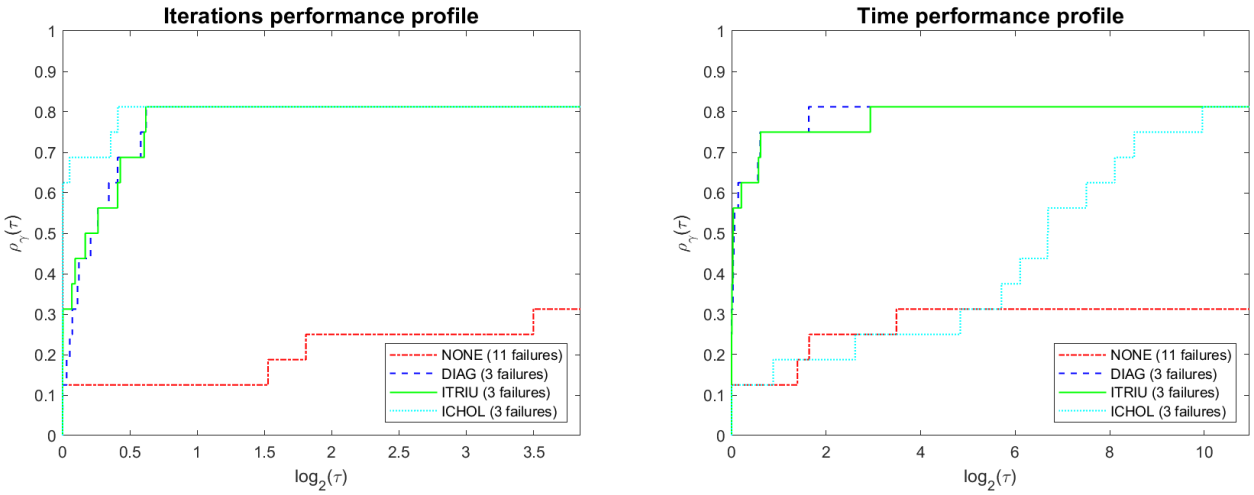

Figure 4.1: Iterations and time performance profiles for solving the system with the different choices of preconditioner.

4.1.4 Summary of the Empirics

Our empirics suggest that the diagonal (DIAG) and the incomplete upper diagonal ω-optimal (ITRIU) preconditioners have very similar behaviour. More precisely, ITRIU seems to do slightly better than DIAG, both time and number of iterations. The incomplete Cholesky (ICHOL) appears to be the best solver for reducing the number of iterations, but this does not translate into a reduction in time. This phenomenon has already been observed previously (see, e.g., [14] and the references therein). In fact, the times for ICHOL is substantially large in comparison with the other two preconditioning strategies. Finally, the residuals obtained by each one of the methods can be checked in Table A.3. This shows that the ω-optimal preconditioners also outperform the ICHOL in this aspect.

4.2 ω-Optimal Low Rank Updates for Generalized Jacobians

We now present tests with different choices of γ for efficient iterative solutions of linear systems of the form $\boxed{A(\gamma)x = b}$, where $A(\gamma)$ is given in (4.1). We use MATLAB's builtin preconditioned conjugate gradient function **pcg**. We focus our attention on the case where $A(\gamma) \in \mathbb{S}^n_{++}$ is a low rank update that appears in choosing subgradients in nonsmooth Newton

methods, see Example 3.1. Our aim is to lower conditioning to improve convergence, thus we call this γ *conditioning*.

4.2.1 Problem Generation

Specifically, we generate random instances as follows:

- Set
$$A(\gamma) := A + \epsilon I + U\,\mathrm{Diag}(\gamma)U^T; \tag{4.1}$$
- ϵ is a random number in the interval $[10^{-7}, 10^{-9}]$;
- $A = A_0^T A_0$ with $A_0 \in \mathbb{R}^{r\times n}$ a normally distributed random sparse matrix with density at most $0.5/\log(n)$; $r \in [n/2+1, n-1]$ is a random integer;
- $t \in [2, r/2]$ is the randomly chosen rank of the update, $U \in \mathbb{R}^{n\times t}$ is a normally distributed random sparse matrix of density at most $1/\log(n)$;
- The right hand side, b, is chosen as the sum of two random vectors in the range of A and U, respectively. More precisely,
$$b = A\,b^1 + U\,b^2,$$
with $b^1 \in \mathbb{R}^n$ and $b^2 \in \mathbb{R}^t$ vectors randomly generated using the standard normal distribution.

As explained in Example 3.1, in this application the γ for conditioning is required to belong to the hypercube $[0,1]^t$. Therefore, in our experiments we test the performance of four different choices of γ conditioning:

- The zero vector ($\gamma = 0$).
- The vector of ones ($\gamma = e$).
- Another common choice consists in setting the ith component of γ as
$$\gamma_i = \min\{1, 1/\|u_i\|^2\},$$
where we recall u_i denotes the ith column of U. In order to simplify notation, we use $\gamma = u^{-2}$ in the plots for this choice.
- Finally, we project the ω-optimal ($\gamma = \gamma_p^*$) obtained in Theorem 3.5 onto $[0,1]^t$. We recall that this is not necessarily the ω-optimal γ in the set $[0,1]^t$, i.e., it is not the solution of (3.16); but rather it is a heuristic approximation of it.

4.2.2 Descriptions of Parameters and Outputs

For each dimension choice $n \in \{100, 200, 500, 1000, 2000\}$, we generate 10 instances of random problems (50 problems in total) and solve the corresponding systems with the four different choices of γ conditioning and with MATLAB's **pcg**.

Table 4.1 shows the average over the 10 instances of: κ- and ω-condition numbers of every $A(\gamma)$; relative residual; number of iterations; and time used by **pcg** for every choice of γ. We stop if a tolerance of 10^{-12} is reached or the maximum $50,000$ iterations is exceeded. We use the origin as our initial starting point. Note that **pcg** can stop early if two consecutive iterations are the same. This often happens for $\gamma = 0$. The two last columns of the tables indicate the time required for computing γ_p^* by making use of the spectral and the Cholesky decompositions, respectively. Regarding the difference in time, we want to mention that although obtaining the Cholesky decomposition $A = LL^T$ is in general less costly than computing its eigenvalue decomposition, the computation of the ω-optimal preconditioner in this case requires solving the system $LW = U$, see Corollary 3.6. This means that, for larger dimensions, employing the spectral decomposition for computing γ^* is seen to be more time efficient.

n	γ	$\kappa(A(\gamma))$	$\omega(A(\gamma))$	Rel. Residual	No. Iterations	Time	T. γ^* Spec	T. γ^* Chol
100	0	5.1176e+10	1.3955e+04	6.8822e-08	174.20	0.0016	-	-
	e	6.2576e+10	1.5794e+03	5.5075e-13	123.60	0.0005	-	-
	u^{-2}	5.1860e+10	1.5917e+03	4.5831e-13	141.00	0.0006	-	-
	γ_p^*	5.2773e+10	1.5055e+03	4.8912e-13	121.80	0.0003	0.0012	0.0006
200	0	2.8445e+10	9.4045e+03	2.3621e-08	242.10	0.0026	-	-
	e	3.9524e+10	3.1707e+02	8.6685e-13	169.30	0.0017	-	-
	u^{-2}	2.6057e+10	3.6045e+02	8.1646e-13	253.00	0.0018	-	-
	γ_p^*	2.9029e+10	2.9642e+02	8.5278e-13	165.10	0.0010	0.0021	0.0018
500	0	1.1976e+11	5.3664e+03	3.7855e-08	442.40	0.0288	-	-
	e	1.0145e+11	2.4445e+02	8.8041e-13	345.60	0.0296	-	-
	u^{-2}	5.6245e+10	2.8308e+02	9.0425e-13	728.30	0.0084	-	-
	γ_p^*	6.5105e+10	2.1025e+02	8.8884e-13	304.30	0.0031	0.0138	0.0205
1000	0	8.5673e+11	1.0529e+04	5.2252e-08	343.40	0.1128	-	-
	e	7.4309e+11	2.2239e+03	9.3920e-13	326.00	0.1065	-	-
	u^{-2}	7.1303e+11	2.4369e+03	9.3184e-13	809.50	0.0319	-	-
	γ_p^*	7.5403e+11	2.2234e+03	8.8928e-13	325.90	0.0124	0.0539	0.0928
2000	0	4.6865e+11	1.4188e+04	8.4903e-08	663.60	0.6598	-	-
	e	2.0223e+12	2.6540e+03	9.2101e-13	224.80	0.6963	-	-
	u^{-2}	4.7477e+11	2.2786e+03	9.1504e-13	418.20	0.3186	-	-
	γ_p^*	5.7969e+11	1.9914e+03	9.4093e-13	144.50	0.1117	0.6658	1.5234

Table 4.1: For different dimensions n, every choice of γ conditioning, average of 10 instances: κ- and ω-condition numbers of $A(\gamma)$; residual; number of iterations; solve time. Last two columns: time for computing γ_p^*, with spectral and Cholesky decomposition.

We also use performance profiles to compare the different choices of γ; details in Section 4.1.3. Again, let P denote the set of problems, and now set $\Gamma := \{0, e, u^{-2}, \gamma_p^*\}$ as the set of γ conditioners. We separately consider the number of iterations and the time required

for solving the system $A(\gamma)\,x = b$. We set the time

$$t_{p,\gamma_p^*} = \{\text{time for solving the system } A(\gamma)\,x = b\} + \{\text{time for computing } \gamma_p^*\}.$$

The latter quantity is taken as the minimum between the spectral and Cholesky approach. For constructing the performance ratio in this setting, we consider that a convergence test passed, rather than failed, if it succeeded in solving the linear system with the required tolerance in less than $50,000$ iterations. The output appears in Figure 4.2.

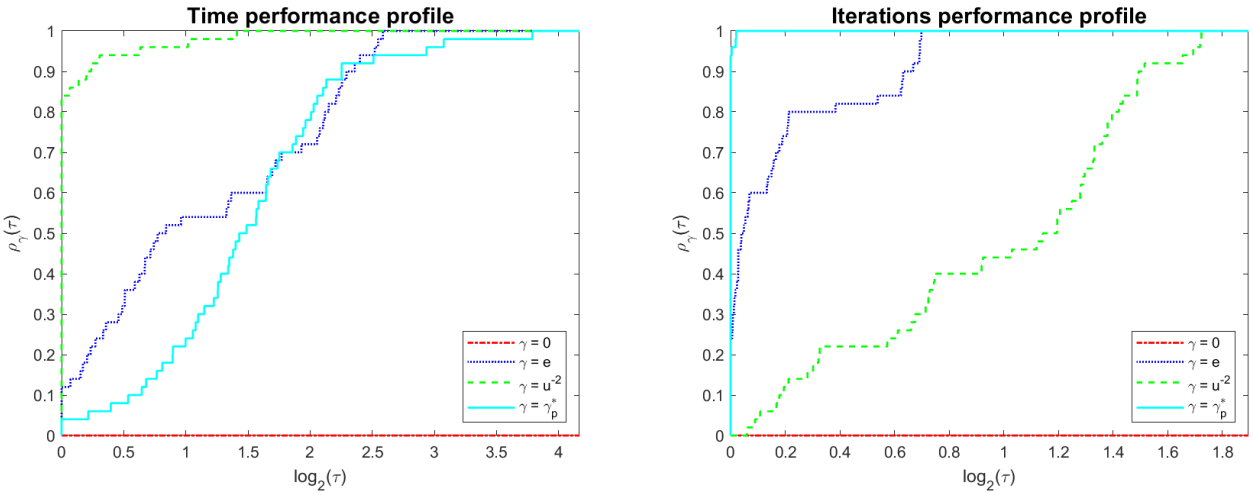

Figure 4.2: Peformance profiles for the time and number of iterations required for solving the system $A(\gamma) = b$ with the different choices of preconditioner γ using MATLAB's **pcg**.

4.2.3 Summary of Empirics

The performance profiles reveal that, in more than 90% of the tested instances, the choice $\gamma = \gamma_p^*$ leads to a problem that can be solved with the least number of iterations. Table 4.1 confims that γ_p^* is also the best choice for cpu time for **pcg**, for every dimension n. However, we cannot conclude that in practical applications γ_p^* should be chosen over, for instance, $\gamma = u^{-2}$, due to the time cost of computing γ_p^*. Nonetheless, our empirics for this application suggest that the minimization and/or reduction of the ω-condition number translates into an enhancement of the performance of the iterative solver. This is the main point we want to convey in this manuscript.

5 Conclusion

In this paper we have studied the nonclassical matrix *ω-condition number*, i.e., the ratio of the arithmetic and geometric means of eigenvalues. We have shown that this condition number has many properties that are advantageous over the classic *κ-condition number* that is the ratio of the largest to smallest eigenvalue. In particular, the differentiability of $\omega(A)$

facilitates finding optimal parameters for improving condition numbers. This was illustrated by characterizing the optimal parameters for low rank updates of positive definite matrices that arise in the context of nonsmooth Newton methods. As well as for obtaining ω-optimal preconditioning matrices for positivde definite linear systems. We empirically show that the ω-optimal preconditioners obtained in this work improve the performance of iterative methods.

The ω-condition number, when compared to the classical κ-condition number, is significantly more closely correlated to reducing the number of iterations and time for iterative methods for positive definite linear systems. This matches known results that show that preconditioning for clustering of eigenvalues helps in iterative methods, i.e., using all the eigenvalues rather than just the largest and smallest is desirable. This is further evidenced by the empirics that show that $\omega(A)$ is a significantly better estimate of the true conditioning of a linear system, i.e., how perturbations in the data A, b effect the solution x.

Finally, we have shown that an exact evaluation of $\omega(A)$ can be found using either the Cholesky or LU factorization. This is in contrast to the evaluation of $\kappa(A)$ that requires either a spectral decomposition or $\|A\|\|A^{-1}\|$ evaluation.

The results we presented here can be extended beyond A positive definite by replacing eigenvalues with singular values in the definition of $\omega(A)$.

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Declarations

Conflict of interest The authors declare they have no conflict of interest.

A Tables

We now present the tables for the empirics for the three preconditioners in Section 4.1. We use matrices from the SuiteSparse Matrix Collection.

name	n	$nnz(W)$	NONE	DIAG	ITRIU	ICHOL
mhd4800b	4800	27520	>97633	26	26	26
s3rmt3m3	5357	207123	>99172	14283	14300	14275
ex15	6867	98671	>98296	46299	46798	44614
bcsstk38	8032	355460	-	10104	9302	9289
aft01	8205	125567	>8452	786	786	592
nd3k	9000	3279690	6012	9245	9228	7993
bloweybq	10001	49999	-	-	-	-
msc10848	10848	1229776	56719	5274	5016	5200
t2dah_e	11445	176117	>99495	33	35	26
olafu	16146	1015156	>90196	28028	27448	27472
gyro	17361	1021159	28942	11605	11287	10044
nd6k	18000	6897316	6589	9857	10033	8439
raefsky4	19779	1316789	-	82865	81846	76736
LFAT5000	19994	79966	-	>4984	>5008	>4985
msc23052	23052	1142686	-	>91699	>91374	>91378
smt	25710	3749582	9764	3343	3345	2787

Table A.1: preconditioners; number of iterations

name	n	$nnz(W)$	NONE	DIAG	ITRIU	ICHOL
mhd4800b	4800	27520	>2.62	0.01	0.01	0.00
s3rmt3m3	5357	207123	>8.89	1.27	1.27	2.33
ex15	6867	98671	>6.17	2.79	2.86	769.15
bcsstk38	8032	355460	>21.52	2.19	2.02	1.99
aft01	8205	125567	>0.77	0.07	0.07	25.91
nd3k	9000	3279690	13.40	20.39	20.50	383.22
bloweybq	10001	49999	>5.93	>5.85	>6.15	>2142.80
msc10848	10848	1229776	44.50	4.10	3.97	24.31
t2dah_e	11445	176117	>11.95	0.01	0.01	5.72
olafu	16146	1015156	>62.84	17.32	16.60	1719.67
gyro	17361	1021159	20.44	7.78	7.92	1412.04
nd6k	18000	6897316	31.35	46.07	46.51	1639.17
raefsky4	19779	1316789	>80.52	67.88	66.46	4575.00
LFAT5000	19994	79966	>11.18	>11.11	>11.09	>11.85
msc23052	23052	1142686	>81.67	>81.52	>81.57	>81.03
smt	25710	3749582	27.78	8.91	8.94	915.44

Table A.2: preconditioners: total time

name	n	$nnz(W)$	NONE	DIAG	ITRIU	ICHOL
mhd4800b	4800	27520	-	5.860e-02	5.860e-02	5.882e-02
s3rmt3m3	5357	207123	-	5.149e-02	4.779e-02	5.162e-02
ex15	6867	98671	-	2.327e+00	2.163e+00	2.297e+00
bcsstk38	8032	355460	-	1.148e-01	1.144e-01	8.114e-02
aft01	8205	125567	-	2.083e-04	2.287e-04	3.049e-04
nd3k	9000	3279690	9.084e-05	1.089e-04	1.120e-04	1.152e-04
bloweybq	10001	49999	-	-	-	-
msc10848	10848	1229776	8.705e-05	2.156e-03	2.106e-03	3.433e-03
t2dah_e	11445	176117	-	1.338e-04	1.825e-04	1.871e-04
olafu	16146	1015156	-	2.182e-03	5.365e-04	7.858e-04
gyro	17361	1021159	1.289e-04	1.955e-04	2.035e-04	2.187e-04
nd6k	18000	6897316	1.324e-04	1.602e-04	1.680e-04	1.678e-04
raefsky4	19779	1316789	-	2.273e-01	2.917e-01	2.133e-01
LFAT5000	19994	79966	-	-	-	-
msc23052	23052	1142686	-	-	-	-
smt	25710	3749582	1.450e-04	2.729e-04	2.759e-04	3.224e-04

Table A.3: preconditioners: residual $\|Wx - b\|$

name	n	$nnz(W)$	DIAG	ITRIU	ICHOL
mhd4800b	4800	27520	4.694e-03	1.379e-02	7.880e-04
s3rmt3m3	5357	207123	6.284e-04	2.198e-03	2.075e-03
ex15	6867	98671	6.214e-04	1.532e-03	6.319e-01
bcsstk38	8032	355460	9.071e-04	3.398e-03	1.283e-02
aft01	8205	125567	8.676e-04	3.218e-03	1.510e+00
nd3k	9000	3279690	3.347e-03	1.974e-02	5.378e-01
bloweybq	10001	49999	9.636e-04	8.833e-04	9.084e-01
msc10848	10848	1229776	1.492e-03	8.205e-03	1.236e-01
t2dah_e	11445	176117	5.934e-04	1.529e-03	3.362e+00
olafu	16146	1015156	1.861e-03	6.930e-03	1.174e+00
gyro	17361	1021159	1.633e-03	7.153e-03	7.287e+00
nd6k	18000	6897316	1.177e-02	5.410e-02	4.203e+00
raefsky4	19779	1316789	5.265e-03	1.356e-02	3.667e+00
LFAT5000	19994	79966	2.633e-03	1.139e-03	2.662e-02
msc23052	23052	1142686	2.285e-03	8.209e-03	7.267e-03
smt	25710	3749582	3.570e-03	2.368e-02	1.769e+01

Table A.4: Times (cpu) for computing the preconditioners

B Proof of Theorem 2.6

Define the transformations (isometries) $\mathrm{Triu} : \mathbb{R}^{t(k)} \to \mathbb{R}^{k\times k}$ and $\mathrm{Triu_k} : \mathbb{R}^{t(k)} \to \mathbb{R}^{n\times n}$ according to (2.18). We denote the adjoints by triu and $\mathrm{triu_k}$, respectively, and note that

$$\mathrm{triu}^\dagger = \mathrm{triu}^*,\ \mathrm{Triu}^\dagger = \mathrm{Triu}^*\,.$$

Hence,

$$\begin{aligned} D_{+k}(d,\alpha) &= \mathrm{Diag}(d) + \mathrm{Triu_k}(\alpha) \\ &= \begin{bmatrix}\mathrm{Diag} & \mathrm{Triu_k}\end{bmatrix}\begin{pmatrix} d \\ \alpha \end{pmatrix}. \end{aligned}$$

Denote

$$\begin{aligned} \omega_k(d,\alpha) &:= \omega\big(D_{+k}(d,\alpha)^T W D_{+k}(d,\alpha)\big) \\ &= \frac{\mathrm{tr}\left(D_{+k}(d,\alpha)^T W D_{+k}(d,\alpha)\right)/n}{\det\left(D_{+k}(d,\alpha)^T W D_{+k}(d,\alpha)\right)^{1/n}} \\ &= \frac{\mathrm{tr}\left(D_{+k}(d,\alpha)^T W D_{+k}(d,\alpha)\right)}{\det(W)^{1/n}\prod_{i=1}^n d_i^{2/n}}. \end{aligned}$$

For the numerator of ω_k we use

$$\begin{aligned} f(d,\alpha) &:= \tfrac{1}{n}\,\mathrm{tr}\left(D_{+k}(d,\alpha)^T W D_{+k}(d,\alpha)\right) \\ &= \tfrac{1}{n}\big\langle D_{+k}(d,\alpha), W D_{+k}(d,\alpha)\big\rangle \\ &= \tfrac{1}{n}\left\langle \begin{pmatrix} d \\ \alpha \end{pmatrix}, D_{+k}^*\big(W D_{+k}(d,\alpha)\big)\right\rangle \\ &= \tfrac{1}{n}\begin{pmatrix} d \\ \alpha \end{pmatrix}^T D_{+k}^*\big(W D_{+k}(d,\alpha)\big) \\ &= \tfrac{1}{n}\begin{pmatrix} d \\ \alpha \end{pmatrix}^T \begin{bmatrix}\mathrm{diag} \\ \mathrm{triu_k}\end{bmatrix}\big(W D_{+k}(d,\alpha)\big) \\ &= \tfrac{1}{n}\begin{pmatrix} d \\ \alpha \end{pmatrix}^T \begin{bmatrix}\mathrm{diag}\, W\big(\mathrm{Diag}(d) + \mathrm{Triu_k}(\alpha)\big) \\ \mathrm{triu_k}\, W\big(\mathrm{Diag}(d) + \mathrm{Triu_k}(\alpha)\big)\end{bmatrix} \\ &= \tfrac{1}{n}\begin{pmatrix} d \\ \alpha \end{pmatrix}^T \begin{bmatrix}\mathrm{diag}\, W\,\mathrm{Diag} & \mathrm{diag}\, W\,\mathrm{Triu_k} \\ \mathrm{triu_k}\, W\,\mathrm{Diag} & \mathrm{triu_k}\, W\,\mathrm{Triu_k}\end{bmatrix}\begin{pmatrix} d \\ \alpha \end{pmatrix}. \end{aligned}$$

and the gradient is therefore

$$\nabla f(d,\alpha) = \frac{2}{n}\begin{bmatrix}\mathrm{diag}\, W\,\mathrm{Diag} & \mathrm{diag}\, W\,\mathrm{Triu_k} \\ \mathrm{triu_k}\, W\,\mathrm{Diag} & \mathrm{triu_k}\, W\,\mathrm{Triu_k}\end{bmatrix}\begin{pmatrix} d \\ \alpha \end{pmatrix}.$$

The denominator of ω_k is

$$g(d,\alpha) := \det(W)^{1/n}\prod_{i=1}^n d_i^{2/n}$$

and thus

$$\nabla g(d,\alpha) = \frac{2}{n} g(d,\alpha)\begin{pmatrix} 1/d_1 \\ 1/d_2 \\ \vdots \\ 1/d_n \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

For simplicity, denote $\bar{d}^{-1} := (1/\bar{d}_1, 1/\bar{d}_2, \ldots, 1/\bar{d}_n)^T \in \mathbb{R}^n$. Then,

$$\begin{aligned} \nabla\omega_k(d,\alpha) &= \tfrac{1}{g(d,\alpha)^2}\big(g(d,\alpha)\nabla f(d,\alpha) - f(d,\alpha)\nabla g(d,\alpha)\big) \\ &= \tfrac{1}{g(d,\alpha)}\left(\nabla f(d,\alpha) - \tfrac{2}{n} f(d,\alpha)\begin{pmatrix} d^{-1} \\ 0_{t(k)} \end{pmatrix}\right). \end{aligned}$$

Finally, the proof follows from noticing that

$$\begin{aligned} (\bar{d},\bar{\alpha}) \text{ satisfies (2.20) and (2.21)} &\iff \tfrac{n}{2}\nabla f(\bar{d},\bar{\alpha}) = \begin{pmatrix} \bar{d}^{-1} \\ 0_{t(k)} \end{pmatrix} \\ &\implies f(\bar{d},\bar{\alpha}) = 1. \end{aligned}$$

Hence, (2.20) and (2.21) implies $\nabla\omega_k(\bar{d},\bar{\alpha}) = 0$, i.e., $(\bar{d},\bar{\alpha})$ is optimal.

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