Diagonal Preconditioning: Theory and Algorithms

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Abstract Diagonal preconditioning has been a staple technique in optimization and machine learning. It often reduces the condition number of the design or Hessian matrix it is applied to, thereby speeding up convergence. However, rigorous analyses of how well various diagonal preconditioning procedures improve the condition number of the preconditioned matrix and how that translates into improvements in optimization are rare. In this paper, we first provide an analysis of a popular diagonal preconditioning technique based on column standard deviation and its effect on the condition number using random matrix theory. Then we identify a class of design matrices whose condition numbers can be reduced significantly by this procedure. We then study the problem of optimal diagonal preconditioning to improve the condition number of any full-rank matrix and provide a bisection algorithm and a potential reduction algorithm with $O(\log(\frac{1}{\epsilon}))$ iteration complexity, where each iteration consists of an SDP feasibility problem and a Newton update using the Nesterov-Todd direction, respectively. Finally, we extend the optimal diagonal preconditioning algorithm to an adaptive setting and compare its empirical performance at reducing the condition number and speeding up convergence for regression and classification problems with that of another adaptive preconditioning technique, namely batch normalization, that is essential in training machine learning models.

Key words: Diagonal Preconditioning, Condition Number, Linear Systems, Interior Point Method, Batch Normalization.

1. Introduction

Preconditioning in general and diagonal preconditioning in particular is a popular technique used in a wide range of disciplines and problems, sometimes under different names and in different forms. In optimization, the simplest form of preconditioning is used to speed up the convergence and improve the accuracy of iterative solvers of linear systems such as the Jacobi method (Saad (2003)) and conjugate gradient (CG), which is often used in the Newton step in interior point algorithms (Nocedal and Wright (2006)). Many other first order optimization methods also involve some form of (diagonal) preconditioning or benefit from preconditioning. These include

the ADMM method (Lin et al. (2016, 2018), Takapoui and Javadi (2016), Boyd et al. (2011)) and steepest descent methods with preconditioned gradients such as mirror descent with quadratic distance functions (Beck and Teboulle (2003)), online Newton methods, and Quasi-Newton methods (Broyden (1970), Goldfarb (1970)). Diagonal preconditioners in particular are widely used in adaptive gradient methods such as AdaGrad (Duchi et al. (2011)) and Adam (Kingma and Ba (2014)), because they can adapt to the geometry of the problem and not only accelerate the rate of convergence, but also achieve low regret for problems with certain geometries (Levy and Duchi (2019)). In machine learning, it is widely acknowledged that adaptive normalization techniques such as batch normalization (Ioffe and Szegedy (2015)) and layer normalization (Ba et al. (2016)) are essential for achieving good empirical performance in terms of convergence speed of training, as well as better generalization power on test sets. Such methods can be understood as a form of adaptive diagonal preconditioning on the outputs of intermediate layers of a neural network.

Intuitively, preconditioning changes the local landscape of the objective function by making it more "rounded" so that local minima are more accessible. To understand the benefit of preconditioning more precisely and to motivate the current paper, we start with the simple setting of solving linear systems with iterative methods. Consider the problem of solving

$$Ax = b$$

given a full-rank matrix $A \in \mathbb{R}^{n \times p}$ and $b \in \mathbb{R}^p$. For large and sparse systems iterative methods based on factorization are preferred to direct methods such as matrix inversion or Gaussian elimination. The following iterative methods are commonly used to solve large linear systems, and under appropriate conditions they converge linearly with rates of convergence depending explicitly on the condition number $\kappa(A)$ of A, defined as the ratio of the largest and smallest singular values of A:

$$\kappa(A) := \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$$

Jacobi Method The Jacobi method for solving linear system Ax = b is the iteration

$$x^{(k+1)} = D^{-1}(b - Rx^{(k)})$$

where A = D + R and D is the diagonal of A. When A is diagonally dominant, the method converges linearly with a rate of $\rho(D^{-1}R) = \rho(I - D^{-1}A)$, which is bounded above by $\frac{\kappa(A) - 1}{\kappa(A) + 1}$ Arioli and Romani (1985).

Gauss-Seidel Method The Gauss-Seidel method to solve the system Ax = b is similar to the Jacobi method. Instead of using the decomposition A = D + R, it uses the decomposition A = L + U where U is the strict upper triangular part of A. The iteration then consists of

$$x^{(k+1)} = L^{-1}(b - Ux^{(k)})$$

	Jacobi	Gauss-Seidel	Kaczmarz	Steepest Descent	Conjugate Gradient
linear convergence rates	$\frac{\kappa(A)-1}{\kappa(A)+1}$	$\frac{\kappa(A)-1}{\kappa(A)+1}$	$\frac{1}{1-\kappa(A)^{-2}}$	$\left(\frac{\kappa(A)-1}{\kappa(A)+1}\right)^2$	$\frac{\sqrt{\kappa(A)}-1}{\sqrt{\kappa(A)}+1}$

Table 1 Rates of linear convergence of various iterative and first order methods for solving the system Ax = b, under respective conditions such as diagonal dominance for Jacobi and Gauss-Seidel.

where the inverse operation can done through forward substitution due to the triangular structure of L_* . Like the Jacobi method, two sufficient conditions for convergence are A is symmetric positive definite, or strictly diagonally dominant. In such cases, the linear convergence rate is again given by $\frac{\kappa(A)-1}{\kappa(A)+1}$.

Kaczmarz Method The Kaczmarz iteration to solve the linear system Ax = b consists of the updates

$$x^{(k+1)} = x^{(k)} + \frac{b_i - \langle a_i, x^{(k)} \rangle}{\|a_i\|^2} a_i$$

where $i = k \mod m$, and m is the number of rows of A, and a_i is the ith row of A. A randomized version that chooses the update with a_i at each step with probability proportional to $||a_i||^2$ has been shown to converge linearly in expectation with a rate of $\frac{1}{1-\kappa(A)^{-2}}$ Strohmer and Vershynin (2009). Other variants of the Kaczmarc method such as the block Kaczmarz method and sketch-and-project methods have been shown to have similar convergence rates Needell and Rebrova (2019). Gradient Methods First order optimization methods can also be applied to solve the square linear system Ax = b, which is equivalent to minimizing the quadratic objective $f(x) = \frac{1}{2}x^TAx - x^Ty$. Steepest descent with optimal step size has linear convergence given by

$$||x^{(k)} - x^*||_A \le \left(\frac{\kappa(A) - 1}{\kappa(A) + 1}\right)^{2k} ||x^{(0)} - x^*||_A$$

where $||v||_A = v^T A v$ Luenberger et al. (1984). Similarly, conjugate gradient (CG) has a linear convergene rate of $\frac{\sqrt{\kappa(A)}-1}{\sqrt{\kappa(A)}+1}$.

Quasi-Newton Methods Quasi-Newton methods such as BFGS and Anderson mixing accelerate the gradient method by premultiplying $\nabla f(x)$ with an approximate inverse Hessian B. The exact dependence of convergence rate on the condition number of B is not well-studied, but it has been known that when B is ill-conditioned, the algorithm suffers slowdown or divergence.

We see that the linear rates of convergence of iterative methods applied to solve Ax = b are better when the matrix A has a small condition number $\kappa(A)$. This phenomenon is not limited to linear systems. For general optimization problems, it is well known that the condition number of the Hessian matrix of the objective plays a similar role in the rate of convergence of first order methods. For example, for general strongly convex objectives, gradient descent has the same asymptotic linear convergence rate of $(\frac{\kappa(A)-1}{\kappa(A)+1})^2$ where A is now the Hessian of the objective at optimal point x^* ,

i.e. $A = \nabla^2 f(x^*)$. Thus the larger the condition number of A, the slower the convergence. In order to accelerate the convergence of iterative solvers and optimization methods, it is then essential to ensure that the condition number of the coefficient or Hessian matrix is small. Preconditioning achieves this by multiplying the a matrix A by matrices D and E, such that the matrices DA, AE, or DAE have a smaller condition number than A. For example, the preconditioned conjugate gradient method solves the equivalent system

$$M^{-1}(Ax) = M^{-1}b$$

with M given by the incomplete Cholesky factorization of A, often resulting in $\kappa(M^{-1}A) \ll \kappa(A)$.

A large class of preconditioning methods uses matrices D, E that are diagonal. Diagonal preconditioners have the advantage that they are easy to implement and there exist many heuristics for finding good diagonal preconditioners to achieve reductions in condition number. We mention the following commonly used diagonal preconditioning procedures:

- Jacobi preconditioner: $A \to A/\text{diag}(A)$ is the simplest diagonal preconditioner, and it works well when A is diagonally dominant.
- Matrix equilibriation Bradley (2010): find diagonal matrices D, E such that columns of DAE have equal ℓ_p norms, and rows of DAE have equal ℓ_p norms. The diagonal matrices can be found by for example the Sinkhorn-Knopp algorithm Sinkhorn (1964).
- Column (row) normalization: $A \to A \cdot D$ where D is the diagonal matrix of column standard deviations or column ℓ_2 norms.

The third method is also commonly used as a normalization procedure for data augmentation/processing. Compared to matrix equilibriation, it is easier to compute. It also has an interesting connection with the method of batch normalization that is ubiquitous in machine learning. Even though these preconditioning methods are popular in practice, they are heuristics and do not always guarantee a reduction in the condition number of the transformed matrix. It is thus important for the practitioner to know when these heuristics work well. Moreover, when they cannot effectively reduce the condition number of a particular matrix, one may need an efficient algorithm that provides a diagonal preconditioner that guarantees that the preconditioned matrix has smaller condition number. Finally, in stochastic optimization settings, lack of access to the full matrix requires adaptive diagonal preconditioners that make use of data accessed so far. In this paper, we attempt to address these problems. We first study the problem of when the column normalization method is effective at reducing the condition number of the data matrix. We provide a concentration result for the condition number of sub-Gaussian matrices and show that the reduction in condition number using column normalization is on the order of the ratio between

the condition numbers of the population covariance matrix and the population correlation matrix, and then give sufficient conditions on when this ratio is large, i.e. diagonal preconditioning with column norm/standard deviation is effective. Then we study the problem of finding an optimal diagonal preconditioner given a fixed matrix. We develop bisection and interior point algorithms with $O(\log \frac{1}{\epsilon})$ iteration complexities that finds a diagonal scaling that guarantees a condition number within ϵ of the smallest possible condition number achievable by diagonal preconditioning. We also give results on the effect of reduction in condition number of the data matrix on the condition number of a class of strongly convex and smooth functions. Finally, we extend our optimal diagonal preconditioner to an adaptive setting, and compare it with batch normalization, a common adaptive preconditioning method used in machine learning, on regression and classification problems, and find that gradient methods with adaptive optimal diagonal preconditioning generally requires fewer iterations compared to batch normalization. The tradeoff is that the computation of the optimal diagonal conditioner requires using a full-rank matrix, and that its practical implementation based on the bisection algorithm may take a long time.

2. Diagonal Preconditioning and Reduction in Condition Number

In this section, we study the problem of when applying the diagonal preconditioning method with normalization by column norm is effective at reducing the condition number. When applying such methods, the matrix being transformed is often a data or design matrix with i.i.d. rows drawn from some common distribution. In this case the condition number can also be viewed as a random variable. We first use matrix concentration to show that with high probability, the reduction of condition number using column normalization is close to that achieved by transforming the population covariance matrix to the population correlation matrix. Then we give sufficient conditions on when the corresponding procedure on the population covariance matrix reduces condition number significantly.

2.1. Concentration of Condition Numbers

We consider the setting where each row of the $n \times p$ design matrix X is an i.i.d. observation of a p-dimensional sub-Gaussian vector. We are interested in how the procedure of normalizing by column norm/standard deviation affects the condition number of the design matrix. Because the condition number is a random variable in this setting, we would like to simplify the analysis by first proving that it concentrates around the condition number of population parameters with high probability, from which we can conclude how much the condition number can be reduced with this procedure.

For ease of presentation, we assume for now that the sub-Gaussian vector has mean zero and covariance matrix Σ . One of the most common diagonal preconditioning procedures is to normalize each column of X by its mean or standard deviation. Thus we first analyze the concentration behavior of the condition number under this particular diagonal preconditioning, which takes the form

$$X_0 = XD^{-\frac{1}{2}}$$

where D is the diagonal matrix with

$$D_{jj} = \frac{1}{n-1} \sum_{i=1}^{n} (X_{ij} - \mu_j)^2$$
$$\mu_j = \frac{1}{n} \sum_{i=1}^{n} X_{ij} \text{ or } \mu_j \equiv 0$$

corresponding to column variance or norm squared.

We recall the definition of sub-Gaussian random vectors and some results from matrix concentration and analysis that are useful in the proof of our main result.

DEFINITION 1. Define the sub-Gaussian norm of a random variable x to be

$$||x||_{\psi_2} = \sup_{p \ge 1} p^{-1/2} (\mathbb{E}|x|^p)^{1/p}$$

and the sub-Gaussian norm of a random vector $X \in \mathbb{R}^n$ to be

$$||X||_{\psi_2} = \sup_{x \in S^{n-1}} ||\langle X, x \rangle||_{\psi_2}$$

Equivalently, the sub-Gaussian norm of X is given by the smallest K such that

$$\mathbb{E}\left[\exp(s \cdot u^T X)\right] \le \exp(K^2 s^2 / 2), \forall s \in \mathbb{R}, ||u|| = 1$$

LEMMA 1. (sub-Gaussian matrix concentration Rudelson and Vershynin (2010)) Let X be an $n \times p$ random matrix with n > p and i.i.d sub-Gaussian rows X_i with sub-Gaussian norm $K = \|X_i\|_{\psi_2}$ and $\Sigma = \mathbb{E}X_i^T X_i = \frac{1}{n} \mathbb{E}X^T X$ its second moment matrix. Then with probability at least $1 - 2\exp(-\frac{ct^2}{K^4})$,

$$\|\frac{1}{n}X^TX - \Sigma\|_{op} \le \max(\delta, \delta^2)$$
$$\delta = CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

where c and C are universal constants. Moreover, the above also implies

$$\sqrt{n} - (CK^2)\sqrt{p} - t \le \sigma_{\min}(X) \le \sigma_{\max}(X) \le \sqrt{n} + (CK^2)\sqrt{p} + t$$

LEMMA 2. (Weyl inequality) Let $\lambda_i(X)$ be the i-th eigenvalue of a self-adjoint matrix X. Then

$$|\lambda_i(X) - \lambda_i(Y)| \le ||X - Y||_{op}$$

for all i. In other words, the eigenvalue map is 1-Lipschitz on the space of self-adjoint matrices with respect to the metric induced by the operator norm.

Our main result is that the condition number of $X_0^T X_0$ where $X = X_0 D^{-\frac{1}{2}}$ concentrates around that of $D^{-\frac{1}{2}} \Sigma D^{-\frac{1}{2}}$, where D is the diagonal of Σ , i.e. $D^{-\frac{1}{2}} \Sigma D^{-\frac{1}{2}}$ is the population correlation matrix. Since $\kappa(X_0^T X_0) = \kappa(X_0)^2$, this implies that $\frac{\kappa(X)}{\kappa(X_0)}$ is on the order of $\frac{\sqrt{\kappa(\Sigma)}}{\sqrt{\kappa(D^{-\frac{1}{2}} \Sigma D^{-\frac{1}{2}})}}$ with high probability.

Theorem 1. Let X be an $n \times p$ random matrix with n > p and i.i.d. sub-Gaussian rows X_i with $K = \|X_i\|_{\psi_2}$ the sub-Gaussian norm of its rows, $\mathbb{E}X_i = 0$, and let $\Sigma = \mathbb{E}X_i^T X_i = \frac{1}{n} \mathbb{E}X^T X_i$ be the population covariance matrix. Let \hat{D} be the diagonal matrix with $\hat{D}_{ii} = (X^T X)_{ii}$, i.e. \hat{D}_{ii} is the norm squared of the i-th column of X, and let $X_0 := X \hat{D}^{-\frac{1}{2}}$ be the matrix normalized with diagonal entries of \hat{D} . Then with probability at least $1 - 2 \exp(-\frac{ct^2(\min_i(\Sigma)_{ii})^2}{K^4}) - 2 \exp(-\frac{ct^2}{K^4}) - 2 \exp(-\frac{ct^2}{K^4})$, we have

$$\begin{split} |\frac{\kappa(X^TX)}{\kappa(\Sigma)} - \frac{\kappa(X_0^TX_0)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}| &\leq \frac{2}{(1-(CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot \left[CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] \\ &+ \frac{2}{(1-(C\frac{K^2}{\min_i(\Sigma):i})\sqrt{\frac{p}{n}} - 3\frac{t}{\sqrt{n}})^2} \cdot \left[C\frac{K^2}{\min_i(\Sigma)_{ii}}\sqrt{\frac{p}{n}} + 3\frac{t}{\sqrt{n}}\right] \end{split}$$

Proof See the appendix.

If we assume that the diagonal of Σ is lower bounded, we can further simplify the bound.

COROLLARY 1. Same assumptions as the previous theorem, and additionally $\min_i(\Sigma)_{ii} \geq 1$. Then

$$\left| \frac{\kappa(X^{T}X)}{\kappa(\Sigma)} - \frac{\kappa(X_{0}^{T}X_{0})}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})} \right| \leq \frac{6}{(1 - (CK^{2})\sqrt{\frac{p}{n}} - 3\frac{t}{\sqrt{n}})^{2}} \cdot \left[CK^{2}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}} \right]$$

with probability at least

$$1 - 4\exp(-\frac{ct^2}{K^4}) - 2p\exp(-\frac{c}{K^4}\left[K^2 + \frac{t}{\sqrt{p}}\right]^2)$$

It is straightforward to extend these results to the case of sub-Gaussian matrices with independent rows and non-zero mean. The above results imply that with high probability, the "reduction" in condition number of a sub-Gaussian design matrix with column normalization is on the order of $\sqrt{\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}}$. Therefore we can shift the focus of our analysis to the problem of comparing the condition numbers of population covariance and correlation matrices.

Proof Strategy Because the scaling matrix $D = \hat{D}$ is a function of sample statistics, namely the column-wise sample standard deviations or column norm, the analysis with \hat{D} directly is cumbersome. Our strategy for showing the main result is to start with the simplest possible case for D and gradually increase the complexity of the scaling matrix. More precisely, we show a sequence of concentration results, each one built on top of the other, with the following scaling matrices:

- D is equal to the population covariance matrix Σ , with general non-diagonal Σ .
- D is the sample column-wise standard deviation, under the assumption that Σ is diagonal.
- D is the diagonal of the population covariance matrix, with general non-diagonal Σ .
- D is the sample standard deviation, with general non-diagonal Σ .

For details of the proof, see the appendix.

REMARK 1. The diagonal preconditioning considered in the above results is widely used in practice. It is common knowledge that when variables have different scales, the condition number of the design matrix (whose columns correspond to variables) tends to be large. This can be alleviated by rescaling the columns of the design matrix by its norm, so that each column has norm 1. This procedure does not guarantee, however, that there is always a significant reduction in condition number. In the next subsection, we study conditions under which such a procedure does result in a significant reduction in condition number, or equivalently that $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})} \gg 1$.

2.2. Diagonal Dominance and Condition Number

In the previous subsection, we showed that diagonal pre-conditioning with sample column norms yields matrices with condition numbers close to the population correlation matrix, so that $\frac{\kappa(X^TX)}{\kappa(\Sigma)}$ and $\frac{\kappa(X_0^TX_0)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}$ are both close to 1 with high probability. In other words, the reduction in condition number by diagonal preconditioning is on the order of $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}$. This ratio, however, is not always large. In fact, it is not even bounded below by 1. To study when the diagonal preconditioning procedure is effective in reducing condition number, we pose the next question in our analysis of diagonal preconditioning and condition numbers:

QUESTION 1. For what covariance matrices Σ is the ratio $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}$ large, where $D = \operatorname{diag}(\Sigma)$? It is well-known that a matrix whose columns have different scales tends to have a large condition number. This is the reason behind normalization procedures used to process data in a variety of contexts such as PCA and first order optimization methods. However, the answer to our question about whether the correlation matrix has a much smaller condition number will depend on the structure of the correlation matrix as well.

As a first step to explore this dependence, we randomly generate some covariance matrices and look for those with small ratio $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}$. In Table 2 we present some examples of covariance

Σ	$D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}}$		
$\begin{bmatrix} 0.17 - 0.49 - 0.19 - 0.36 \\ 2.34 & 0.71 & 1.79 \\ 0.32 & 0.53 \\ 1.44 \end{bmatrix}$	$\begin{bmatrix} 1 & -0.77 & -0.80 & -0.73 \\ 1 & 0.81 & 0.97 \\ & 1 & 0.78 \\ & & 1 \end{bmatrix}$		
$\begin{bmatrix} 1.76 & -0.41 & -0.61 & -1.86 \\ 0.21 & -0.11 & -0.45 \\ 0.28 & 0.64 \\ 1.99 \end{bmatrix}$	$\begin{bmatrix} 1 & -0.66 & -0.86 & 0.99 \\ 1 & -0.47 & -0.68 \\ 1 & 0.85 \\ 1 \end{bmatrix}$		

Table 2 Examples of covariance matrices whose corresponding correlation matrices have larger condition number.

matrices with $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}$ < 1, i.e. the correlation matrix is more ill-conditioned than the covariance matrix.

We see that the correlation matrices with large condition numbers all have off-diagonal entries that are close to 1, which is confirmed by other examples.

In this section, we show that if a covariance matrix Σ has columns (and rows) that are of different scales, but its corresponding correlation matrix is diagonally dominant, then diagonal preconditioning can achieve a reduction in condition number on the order of $\kappa(D)$ with high probability, where D is the matrix consisting of the diagonal entries of Σ . To put the result in perspective, note that $\kappa(\Sigma) \leq \kappa(D) \cdot \kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})$ is always true. We are interested in sufficient conditions that guarantee a matching lower bound, so that $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})} \approx \kappa(D)$, i.e. the reduction is on the order of $\kappa(D)$ with high probability for a class of matrices.

REMARK 2. One useful tool that helps us to understand the condition numbers of correlation and covariance matrices is the Cholesky decomposition: any positive definite matrix M can be written as $M = LL^T$ where L is a lower triangular matrix with non-negative diagonal entries.

Let Σ_0 be a correlation matrix, that is Σ_0 is positive definite with diagonal entries equal to 1 and off-diagonal entries in [-1,1] and let D be a diagonal matrix with strictly positive entries. Then $D^{\frac{1}{2}}\Sigma_0 D^{\frac{1}{2}}$ defines a covariance matrix whose diagonal is equal to D.

Let $\Sigma_0 = LL^T$ be the Cholesky decomposition of Σ_0 . This decomposition gives us some intuition about when a correlation matrix is ill-conditioned. Since Σ_0 has diagonal entries equal to 1, the norm of every row of L is 1. Suppose $(\Sigma_0)_{ij}$ has large magnitude for some i < j. Since $(\Sigma_0)_{ij} = \ell_i^T \ell_j$ where ℓ_i denotes the ith row of Σ_0 , and $L_{ij} = 0$ for j > i because L is lower triangular, $|\ell_i^T \ell_j|$ is large only if the first i entries of ℓ_j has large norm, which forces L_{jj} to be small. The condition number of L, $\kappa(L)$, is not equal to $\frac{\max_i |L_{ii}|}{\min_i |L_{ii}|}$, which is only true for diagonal matrices. However, as we have seen, $\kappa(L) \ge \frac{\max_i |L_{ii}|}{\min_i |L_{ii}|}$, which implies that $\kappa(L)$ is likely to be large, i.e. Σ_0 is ill-conditioned. This heuristic argument will be made rigorous, but it provides the main intuition that a correlation matrix is ill-conditioned if and only if it has off-diagonal term with magnitude close to 1.

By the basic properties of condition number, $\kappa(\Sigma_0) = \kappa^2(L) = \kappa^2(L^T)$ and

$$\kappa(\Sigma) = \kappa(D^{\frac{1}{2}}\Sigma_0D^{\frac{1}{2}}) = \kappa^2(L^TD^{\frac{1}{2}}) = \kappa^2(D^{\frac{1}{2}}L)$$

Again, since $\kappa(D^{\frac{1}{2}}L) \geq \frac{\max_i |L_{ii}D_{ii}^{\frac{1}{2}}|}{\min_i |L_{ii}D_{ii}^{\frac{1}{2}}|}$ and L_{ii} are bounded above by 1, the right hand side will be dominated by $\frac{\max_i (D_{ii}^{\frac{1}{2}})}{\min_i (D_{ii}^{\frac{1}{2}})} = \kappa(D^{\frac{1}{2}})$ if $\max_i (D_{ii}^{\frac{1}{2}}) \gg 1$ and $\frac{\max_i L_{ii}}{\min_i L_{ii}}$ is not too large. On the other hand, if $\frac{\max_i L_{ii}}{\min_i L_{ii}}$ is large, in which case Σ_0 is ill conditioned, then the right hand side may well be dominated by this quantity instead of $\kappa(D^{\frac{1}{2}})$.

So the intuition here is that the condition number of a covariance matrix also depends on the scale difference between the largest standard deviation and smallest standard deviation. If the diagonal matrix D of variances is ill-conditioned but the correlation matrix is well conditioned, the condition number of the covariance matrix is close to that of its diagonal.

The Cholesky decomposition has thus provided us with the following two intuitions. First, a correlation matrix is ill conditioned if it has off diagonal entries with magnitude close to 1. Second, if the diagonal of a covariance matrix has a large condition number, then likely so does the covariance matrix itself. We now make these intuitions rigorous.

We start with a result on the condition number of diagonally dominant matrices.

LEMMA 3. Assume $M \in \mathbb{R}^{p \times p}$ is square invertible with $|M_{ii}| \ge \alpha \sum_{j \ne i} |M_{ij}|$ for all i and some $\alpha > 1$, then

$$\kappa_{\infty}(M) \le \frac{\alpha+1}{\alpha-1} \cdot \frac{\max_{i} |M_{ii}|}{\min_{i} |M_{ii}|}$$

for κ_{∞} defined based on the sup norm $||M||_{\infty} = \sup_{i,j} |M_{ij}|$, and

$$\kappa_q(M) \le p^{2/q} \frac{\alpha + 1}{\alpha - 1} \cdot \frac{\max_i |M_{ii}|}{\min_i |M_{ii}|}$$

for κ_q defined based on the q-norm $\|M\|_q = \sup_{\|v\|_q = 1} \|Mv\|_q$ for $1 \le q < \infty$.

Proof For a fixed vector $x \in \mathbb{R}^p$, let $||x||_{\infty} = |x_i|$. We have

$$\begin{split} |(Mx)_i| &\geq |M_{ii}||x_i| - \sum_{j \neq i} |M_{ij}||x_j| \geq |M_{ii}||x_i| - \sum_{j \neq i} |M_{ij}||x_i| \\ &\geq (1 - \frac{1}{\alpha})|M_{ii}||x_i| = (1 - \frac{1}{\alpha})|M_{ii}||x||_{\infty} \geq (1 - \frac{1}{\alpha}) \min_{i} |M_{ii}||x||_{\infty} \end{split}$$

which implies $\frac{\|Mx\|_{\infty}}{\|x\|_{\infty}} \ge (1 - \frac{1}{\alpha}) \min_i |M_{ii}|$, so that

$$||M^{-1}||_{\infty} = \max_{x \neq 0} \frac{||M^{-1}x||_{\infty}}{||x||_{\infty}} = \max_{x \neq 0} \frac{||M^{-1}Mx||_{\infty}}{||Mx||_{\infty}}$$
$$= \max_{x \neq 0} \frac{||x||_{\infty}}{||Mx||_{\infty}} \le \frac{\alpha}{\alpha - 1} \cdot \frac{1}{\min_{i} |M_{ii}|}$$

On the other hand,

$$||M_i||_{\infty} \le \sum_{j} |M_{ij}| \le (1 + \frac{1}{\alpha})|M_{ii}| \le (1 + \frac{1}{\alpha}) \max_{i} |M_{ii}|$$

from which we can conclude that $\kappa_{\infty}(M) \leq \frac{\alpha+1}{\alpha-1} \frac{\max_i |M_{ii}|}{\min_i |M_{ii}|}$.

Based on the upper bound for κ_{∞} and equivalence of matrix norms, we can obtain upper bounds for condition numbers based on q-norms. By Holder's inequality, $\|M\|_q \leq n^{1/q-1/q'} \|M\|_{q'}$ for $q \leq q' \leq \infty$. This suggests that $\|M\|_q \leq n^{1/q} \|M\|_{\infty}$ and so

$$\kappa_q(M) \le p^{2/q} \kappa_\infty(M) \le p^{2/q} \cdot \frac{\alpha + 1}{\alpha - 1} \frac{\max_i |M_{ii}|}{\min_i |M_{ii}|}$$

To understand the above lemma in the context of covariance and correlation matrices, compare $\kappa(\Sigma) \leq \kappa(\Sigma_0) \cdot \kappa(D)$ with the bound

$$\kappa(\Sigma) \le p \frac{\alpha + 1}{\alpha - 1} \frac{\max_{i} |\Sigma_{ii}|}{\min_{i} |\Sigma_{ii}|} = p \frac{\alpha + 1}{\alpha - 1} \cdot \kappa(D)$$

from the lemma. We can see $\frac{\alpha+1}{\alpha-1}$ as a proxy of the condition number $\kappa(\Sigma_0)$ of the correlation matrix. The larger α is, the closer Σ_0 is to the identity matrix, and the closer its condition number is to 1. In the limit, we should have $\lim_{\alpha\to\infty} \kappa(\Sigma_0) = 1 = \lim_{\alpha\to\infty} \frac{\alpha+1}{\alpha-1}$.

We shall use the above result to give a sufficient condition on when the ratio $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}$ is large, i.e. when diagonal preconditioning with column standard deviation/norm achieves a significant reduction in condition number with high probability.

More specifically, we show that if the correlation matrix is diagonally dominant, then the ratio $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}$ is bounded below by $\frac{1}{p}(\frac{\alpha-1}{\alpha+1})^2\kappa(D)$.

THEOREM 2. For a covariance matrix Σ , if $\sqrt{\Sigma_{ii}} \geq \alpha \sum_{j \neq i} \left| \frac{\Sigma_{ij}}{\sqrt{\Sigma_{ij}}} \right|$, then we have

$$\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})} \geq \frac{1}{p}(\frac{\alpha-1}{\alpha+1})^2\kappa(D)$$

Proof Let $\Sigma_0 = D^{-\frac{1}{2}} \Sigma D^{-\frac{1}{2}}$. The conditions $\sqrt{\Sigma_{ii}} \ge \alpha \sum_{j \ne i} |\frac{\Sigma_{ij}}{\sqrt{\Sigma_{jj}}}|$ imply that Σ_0 is diagonally dominant, so that by the previous lemma $\kappa(\Sigma_0) \le p \frac{\alpha+1}{\alpha-1}$ since Σ_0 has diagonal equal to 1.

The main ingredient of the proof is to use the Cholesky decomposition of the correlation matrix and the fact that for a triangular matrix L, the following condition holds:

$$\kappa(L) \ge \frac{\max_i L_{ii}}{\min_i L_{ii}}$$

Now let $\Sigma_0 = L_0 L_0^T$ be the Cholesky factorization of Σ_0 where L_0 is a lower triangular matrix. It then follows that $\Sigma = LL^T$ where $L = D^{\frac{1}{2}}L_0$ is also a lower triangular matrix. We have

$$(\frac{\alpha+1}{\alpha-1})^{2} \cdot \kappa(\Sigma) = (\frac{\alpha+1}{\alpha-1})^{2} \cdot (\kappa(D^{\frac{1}{2}}L_{0}))^{2} \ge (\frac{\alpha+1}{\alpha-1})^{2} \cdot (\frac{\max_{i}(D^{\frac{1}{2}}L_{0})_{ii}}{\min_{i}(D^{\frac{1}{2}}L_{0})_{ii}})^{2}$$

$$\ge (\frac{\alpha+1}{\alpha-1})^{2} \cdot (\frac{\max_{i}(D^{\frac{1}{2}})_{ii}}{\min_{i}(D^{\frac{1}{2}})_{ii}})^{2} \cdot (\frac{\min_{i}(L_{0})_{ii}}{\max_{i}(L_{0})_{ii}})^{2}$$

$$= (\frac{\alpha+1}{\alpha-1})^{2} \cdot \kappa^{-2}(L_{0}) \cdot \kappa^{2}(D^{\frac{1}{2}}) = (\frac{\alpha+1}{\alpha-1})^{2} \cdot \kappa^{-1}(\Sigma_{0}) \cdot \kappa(D)$$

$$\ge (\frac{\alpha+1}{\alpha-1}) \cdot \kappa(D) \ge \frac{1}{p} \kappa(\Sigma_{0}) \cdot \kappa(D)$$

where we have used the inequality $||f \cdot g||_{\infty} \ge ||f||_{\infty}/||g^{-1}||_{\infty}$ for vectors $f, g \in \mathbb{R}^p_{++}$ and $f \cdot g$ is element-wise multiplication.

Rewriting the inequality gives the desired inequality

$$\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})} \ge \frac{1}{p}(\frac{\alpha-1}{\alpha+1})^2\kappa(D)$$

We have thus shown that when the correlation matrix Σ_0 is α -diagonally dominant, the ratio of condition numbers $\frac{\kappa(D^{\frac{1}{2}}\Sigma_0D^{\frac{1}{2}})}{\kappa(\Sigma_0)}$ is bounded below by $\frac{1}{p}(\frac{\alpha-1}{\alpha+1})^2\kappa(D)$. For a design matrix with sub-Gaussian rows with covariance matrix satisfying this condition, the reduction of condition number is on the order of $\sqrt{\kappa(D)}$ with high probability.

3. Optimal Diagonal Preconditioning

We have shown that when the population correlation matrix is diagonally dominant, diagonal preconditioning of design matrix by sample standard deviations yields a reduction in condition number on the order of $\sqrt{\kappa(D)}$ with high probability. However, many population correlation matrices are not diagonally dominant, or we may not be able to easily verify this condition. In such cases, we need an efficient method to obtain a diagonal conditioner that does reduce the condition number of any fixed design matrix X. We turn to this problem in this section.

Given a fixed design matrix $X \in \mathbb{R}^{n \times p}$, we are interested in the optimal diagonal preconditioning matrix D, that gives the minimal condition number of

$$\min_{D \text{ diagonal, } D\succeq 0} XD^{-\frac{1}{2}}$$

among all diagonal preconditioners. We first reformulate the problem to a quasi-convex SDP problem that can be solved with bisection, and then provide a faster potential reduction algorithm with guarantee on convergence. The purpose of studying the optimal diagonal preconditioning procedure is the following:

- 1. In settings where diagonal preconditioning helps to reduce condition number, we would like to compare the performances of diagonal preconditioning using column standard deviation/norm studied in the previous section with that of the optimal diagonal preconditioning, to see how much gap there is between the two.
- 2. In situations where diagonal preconditioning with sample standard deviation/norm does not actually reduce the condition number, we may instead use the optimal diagonal preconditioning procedure.
- 3. We are also interested in how the result of adaptive diagonal preconditioning procedures, such as batch normalization, compares with the optimal diagonal preconditioning. This may help us understand the nature of such adaptive preconditioning procedures.

3.1. Optimal Diagonal Preconditioning

Writing $M = X^T X \in \mathbb{R}^{p \times p}$ and rewriting $D^{-\frac{1}{2}}$ as D, the optimal diagonal preconditioning problem is

$$\min_{D \text{ diagonal}} \kappa(DMD)$$

We can rewrite it as

$$\min_{D,\kappa} \kappa$$
$$I \prec DMD \prec \kappa I$$

The inequality constraints can be further simplified to $D^{-2} \leq M \leq \kappa D^{-2}$. The problem can thus be reformulated as

$$\min_{\kappa,D} \kappa$$

$$s.t.M \succeq D$$

$$\kappa D \succeq M$$

where D is a diagonal matrix with strictly positive entries.

We may solve this problem using bisection as follows. First find a large fixed κ_0 such that the convex feasiblity SDP problem

$$\min_{D \succeq 0} 0$$

$$s.t.M \succeq D$$

$$\kappa_0 D \succeq M$$

has a solution. In practice, we can start with $\kappa_0 = \kappa(M)$, or if we have some prior information that there exists some D_0 that satisfies

$$\kappa(D_0MD_0) < \kappa(M)$$

we can set $\kappa_0 = \kappa(D_0 M D_0)$ as a warm start. Often the choice $D_0 \equiv (\operatorname{diag}(M))^{-1/2}$ or $D_0 \equiv (\operatorname{diag}(\operatorname{std}(M)))^{-1/2}$ yields a smaller upper bound.

Then, solve the feasibility problem

$$\min_{D \succeq 0} 0$$

$$s.t.M \succeq D$$

$$\frac{\kappa_0}{2} D \succeq M$$

If it is feasible, then we know the optimal objective value is in $[1, \frac{\kappa_0}{2}]$, otherwise it is in $[\frac{\kappa_0}{2}, \kappa_0]$. We can find an ϵ -optimal solution in $O(\log \frac{1}{\epsilon})$ iterations.

There is also a geometric interpretation of the feasibility problem with parameter κ : it looks for an ellipsoid E with axes of symmetry the coordinate axes, such that it is inscribed in the ellipsoid defined by M, and such that a multiple κ of E includes the ellipsoid defined by M. Such inscribing and containing ellipsoids have been used the ellipsoid method, where the ellipsoids are not constrained to be symmetric along coordinate axes. The geometric interpretation also makes it clear that the optimal value $\kappa^* \geq 1$ is achieved.

Algorithm 1 Step 0. Start with $\kappa^0 > \kappa^*$ such that

$$\min_{D \succeq 0} 0$$

$$s.t.M \succeq D$$

$$\kappa_0 D \succ M$$

is feasible. Set $\kappa_{min} = 1$, $\kappa_{max} = \kappa_0$. Step 1. Solve the feasibility problem

$$\begin{aligned} \min_{D\succeq 0} 0 \\ s.t.M \succeq D \\ \frac{\kappa_{\max} + \kappa_{\min}}{2} D \succeq M \end{aligned}$$

If it is feasible, then set $\kappa_{max} \leftarrow \frac{\kappa_{max} + \kappa_{min}}{2}$. Otherwise, set $\kappa_{min} \leftarrow \frac{\kappa_{max} + \kappa_{min}}{2}$. Step 2. If $\kappa_{max} - \kappa_{min} > \epsilon$, return to Step 1.

We next develop an interior point method that finds an ϵ -optimal diagonal scaling in $O(\log \frac{1}{\epsilon})$ iterations, where each iteration consists of a Newton update step. This is in contrast with the bisection algorithm, which also has $O(\log \frac{1}{\epsilon})$ iterations, but each iteration consists of solving a SDP feasibility problem. The formulation and proof borrows ideas from interior point methods for linear programming and semidefinite programming, in particular Mizuno (1992), Ye (1992, 1995), Nesterov and Todd (1997), most notable of which are the work of Nesterov and Todd (Nesterov and Todd (1997)) on Newton updates in SDP and the work of Ye (Ye (1995)) on the "von Neumann economic growth problem".

3.2. Interior Point Algorithms with Potential Reduction

Recall the reformulated optimal diagonal preconditioning problem

$$\min_{D \succeq 0} \kappa$$

$$s.t.M \succeq D$$

$$\kappa D \succ M$$

Following Ye (1995), we define the potential function as

$$P(\kappa) = \sum_{i} \log \lambda_{i} (M - D^{\kappa}) + \sum_{i} \log \lambda_{i} (\kappa D^{\kappa} - M) + \sum_{i} \log D_{ii}^{\kappa}$$

where D^{κ} is the analytic center of the feasible region

$$\Gamma(\kappa) = \{D \succeq 0 : D \text{ diagonal}; M \succeq D; \kappa D \succeq M\}$$

which is simply the unique maximizer of the strictly concave problem

$$\max_{D\succeq 0 \text{ diagonal}} \sum_{i} \log \lambda_{i}(M-D) + \sum_{i} \log \lambda_{i}(\kappa D-M) + \sum_{i} \log D_{ii}$$

$$\max_{D\succeq 0 \text{ diagonal}} \log \det(M-D) + \log \det(\kappa D - M) + \log \det D$$

See also Mizuno et al. (1993), Luo et al. (1998), Sturm and Zhang (1999) for the use of analytic centers in path-following and potential reduction interior point algorithms for LP and SDP problems.

The geometric interpretation of the problem makes it clear that if the feasible region $\Gamma(\kappa^0)$ has a non-empty interior for some $\kappa^0 < \infty$, then the feasible region $\Gamma(\kappa)$ has a non-empty interior for all $\kappa \geq \kappa^0$, so that the analytic center is well defined. At the optimal objective value $\kappa^* \geq 1$, however, the solution set has no interior because it must be the case that $\lambda_p(\kappa D - M) = 0$ for any D in the solution set, where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$ are the eigenvalues of a matrix, and so perturbing D in some direction by any amount will violate the constraint $M \succeq D$.

LEMMA 4. For M > 0, the feasible set of the feasibility problem

$$\min_{D \succeq 0} 0$$

$$s.t.M \succeq D$$

$$\kappa D \succeq M$$

has bounded non-empty interior for all $\kappa > \kappa^*$.

Next we show that the potential function is monotonic in κ , and that it is bounded away from $P(\kappa^*)$, for any κ large, so that it is a reasonable measure of the progress of the problem: we just need to be able to reduce the potential function by a constant amount at every step and terminate when the potential function is reduced below a certain threshold determined by accuracy ϵ .

PROPOSITION 1. If $\kappa_0 > \kappa_1 > \kappa^*$, then $P(\kappa_0) > P(\kappa_1)$.

Proof See the appendix.

PROPOSITION 2. Let t satisfy $\kappa^* \leq 2^t$, then for any $\overline{\kappa} > \kappa^* + 2^{-t}$, we have

$$P(\overline{\kappa}) > -Cpt$$

for some universal constant that only depends on M.

Proof See the appendix.

These two results imply that if $P(\kappa) < O(-pt)$, then we must have $\kappa \le \kappa^* + 2^{-t}$. Therefore if we can find a D whose associated potential is below the threshold of $O(p \log \epsilon)$, we have found an approximate solution that yields a condition number that is within ϵ of the optimal condition number. Our goal is then to design an algorithm that achieves constant reduction of the potential at every iteration, which would guarantee an iteration complexity of $O(\log \frac{1}{\epsilon})$.

In the next two subsections, we develop potential reduction algorithms based on this idea, using exact and and approximate analytic centers, respetively. Before doing so, we show that the analytic center satisfies an equality condition that is useful in the proof of the reduction of potential function. This is essentially the first order condition of the convex optimization problem, but because it also serves an important role in the Newton reduction step, we state it is a particular form in the next lemma.

LEMMA 5. The analytic center D of the feasible region $\Gamma(\kappa)$ satisfies

$$Z + \kappa Y = X$$

where

$$X = R^{-1}, Y = S^{-1}, Z = D^{-1}, R = M - D, S = \kappa D - M$$

Proof Since D solves the convex problem

$$\max_{D} \log \det(M-D) + \log \det(\kappa D - M) + \log \det D$$

The first order condition implies

$$-(M-D)^{-1} + \kappa(\kappa D - M)^{-1} + D^{-1} = 0$$

so if we define R = M - D and $S = \kappa D - M$, and

$$X = R^{-1}, Y = S^{-1}, Z = D^{-1}$$

then we have $Z + \kappa Y = X$ and moreover $R + S = (\kappa - 1)D$.

3.3. Analysis of Potential Reduction with Exact Analytic Center

Let D^0, D^1 be the analytic centers of $\Gamma^0 = \Gamma(\kappa^0)$ and $\Gamma^1 = \Gamma(\kappa^1)$. With a suitable choice of $\Delta \kappa = \kappa^0 - \kappa^1 > 0$, we show that the analytic centers D^0 and D^1 are close, and that

$$P(\kappa^1) \le P(\kappa^0) - \Omega(1)$$

so that we can achieve constant reduction of the potential function by going from D^0 to D^1 . To obtain D^1 from D^0 , we can use symmetrized versions of Newton iterations with a quadratic convergence rate. The exact form of the Newton iteration is deferred to the next subsection, where we propose a practical potential algorithm using approximate analytic centers and only one Newton step.

THEOREM 3. Let $\kappa^* \in [1, \infty)$ be the solution of

$$\min_{D \succeq 0} \kappa$$

$$s.t.M \succeq D$$

$$\kappa D \succeq M$$

and let $\overline{\kappa}$ be a known upper bound of κ^* , i.e.

$$\min_{D \succeq 0} 0$$

$$s.t.M \succeq D$$

$$\overline{\kappa}D \succ M$$

is feasible.

Let D^0 and D^1 be the analytic centers of $\Gamma^0 = \Gamma(\kappa^0)$ and $\Gamma^1 = \Gamma(\kappa^1)$ for $\kappa^0, \kappa^1 \in (\kappa^*, \overline{\kappa})$. If $\Delta \kappa = \kappa^0 - \kappa^1 > 0$ satisfies

$$\Delta \kappa = \frac{\beta}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})}$$
$$= \frac{\beta}{e^T D^0 \operatorname{diag}((\kappa^0 D^0 - M)^{-1})e}$$

for some sufficiently small $\beta \in (0,1)$ that only depends on $\overline{\kappa}, M$, then

$$\begin{split} &\sqrt{Tr((D^1)^{1/2}(D^0)^{-1}(D^1)^{1/2}-I)^2} \leq c \cdot \beta \\ &\sqrt{Tr((D^0)^{1/2}(D^1)^{-1}(D^0)^{1/2}-I)^2} \leq c \cdot \beta \end{split}$$

for some constant c and

$$P(\kappa^1) \le P(\kappa^0) - \beta$$

Proof See the appendix.

We have thus obtained a conceptual algorithm, which uses the exact analytic center, summarized in Algorithm 2.

Algorithm 2 Step 0. Let D^0 be analytic center of $\Gamma(\kappa^0)$ with $\kappa^0 > \kappa^*$. Set k = 0. Step 1. Let

$$\Delta \kappa^k = \frac{\beta}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})}$$

for some small constant $0 < \beta < 1$ and let $\kappa^{k+1} = \kappa^k - \Delta \kappa^k$. Then use Newton's method described in the next section to generate the axact analytic center D^{k+1} of $\Gamma(\kappa^{k+1})$.

Step 2. If $P(\kappa^{k+1}) > O(-pt)$, set $k \leftarrow k+1$ and return to Step 1.

3.4. Algorithm with Approximate Analytic Center

Given step size $\Delta \kappa$, in order to apply the potential reduction algorithm, we still need to find the new analytic center D^1 corresponding to $\kappa^0 - \Delta \kappa$. This can be achieved using Newton iterations. However, it is not necessary to use exact analytic centers. Instead, we can use an approximate analytic center obtained from only one Newton update step, and show that the max-potential still reduces by a constant amount. Moreover, if we start from an approximate analytic center, one Newton step with the appropriate step size $\Delta \kappa$ yields an approximate center that still achieves this constant reduction in potential. We develop these results in this subsection.

By an approximate analytic center, we mean a set of variables (R, S, D, X, Y, Z) that satisfy the optimality conditions

$$R = M - D \succeq 0,$$

$$S = \kappa D - M \succeq 0$$

$$D \succeq 0$$

$$Z + \kappa Y = X$$

but instead of requiring RX = SY = DZ = I as is true for the exact analytic center, we allow the products to be close to the identity I.

We define a measure of proximity of the products as follows

$$\begin{split} \delta(A,B) &:= \sqrt{Tr(B^{1/2}AB^{1/2}-I)^2} \\ &= \|B^{1/2}AB^{1/2}-I\|_F = \|A^{1/2}BA^{1/2}-I\|_F \end{split}$$

where the equality follows from the fact that the Frobenius norm is a spectral property for symmetric matrices. We may also check that

$$\delta(A,B) = \sqrt{Tr((AB-I)^2)} = \sqrt{Tr((BA-I)^2)}$$

As we will see in the following results, this is the appropriate measure of proximity. The first result we show is that starting from an analytic center for $\Gamma(\kappa^0)$, we can obtain a feasible point in $\Gamma(\kappa^1)$ that is an $O(\beta)$ approximate analytic center.

PROPOSITION 3. Let D^0 be the exact analytic center of κ^0 . Define $R_0 = M - D_0$, $S_0 = \kappa_0 D_0 - M$ and $X_0 = R_0^{-1}, Y_0 = S_0^{-1}, Z_0 = D_0^{-1}$.

Further, let $\Delta \kappa = \kappa^0 - \kappa^1$ with $\Delta \kappa = \frac{\beta}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})}$ where $\beta \in (0,1)$ is a sufficiently small constant, and

$$\overline{R}^0 = R^0, \overline{S}^0 = -\Delta \kappa D^0 + S^0, \overline{D}^0 = D^0$$

$$\overline{X}^0 = X^0, \overline{Y}^0 = Y^0, \overline{Z}^0 = \Delta \kappa Y^0 + Z^0$$

Then, the new variables satisfy

$$\overline{R}^0 = M - \overline{D}^0 \succeq 0$$

$$\overline{S}^0 = \kappa^1 \overline{D}^0 - M \succeq 0$$

$$\overline{D}^0 \succeq 0$$

and
$$\overline{Z}^0 + \kappa^1 \overline{Y}^0 = \overline{X}^0$$
. Moreover, $\delta(\overline{S}^0, \overline{Y}^0) \leq \beta, \delta(\overline{D}^0, \overline{Z}^0) \leq \beta, \delta(\overline{R}^0, \overline{X}^0) = 0$.

Proof We can readily verify that the new variables satisfy the desired equalities. When $\Delta \kappa$ is appropriately chosen as in the previous theorem, we can guarantee that $\overline{S}^0 \succeq 0$. Now

$$\begin{split} \delta(\overline{S}^0, \overline{Y}^0)^2 &= Tr((\overline{S}^0 \overline{Y}^0 - I)^2) = Tr((-\Delta \kappa D^0 + S^0) Y^0 - I)^2 \\ &= Tr(-\Delta \kappa D^0 Y^0)^2 \\ &= Tr(-\Delta \kappa D^0 (\kappa_0 D_0 - M)^{-1})^2 \\ &\leq (Tr(-\Delta \kappa D^0 (\kappa_0 D_0 - M)^{-1}))^2 = \beta^2 \end{split}$$

where we have used $Tr(A^2) = (TrA)^2 - 2\sigma_2(A)$ where $\sigma_2(A) = \sum_{i < j} \lambda_i \lambda_j$ and λ_i are the eigenvalues of A. Therefore, $\delta(\overline{S}^0, \overline{Y}^0) \leq \beta$. Similarly, $\delta(\overline{D}^0, \overline{Z}^0) \leq \beta$ and since $\overline{R}^0 = R^0, \overline{X}^0 = X^0$, we have $\delta(\overline{D}^0, \overline{Z}^0) = 0$

Next we show that this set of variables $(\overline{R}^0, \overline{S}^0, \overline{D}^0, \overline{X}^0, \overline{Y}^0, \overline{Z}^0)$ can be used as an initial set to generate a new $O(\beta^2)$ approximate center for κ^1 , using a Newton step. This also implies that starting from an approximate analytic center we can obtain an exact analytic center by applying the Newton iterations with quadratic convergence. Here to ensure the symmetry of updates in the Newton step, we use the Nesterov-Todd direction Todd et al. (1998), Nesterov and Todd (1997).

PROPOSITION 4. Let Let $(\overline{R}^0, \overline{S}^0, \overline{D}^0, \overline{X}^0, \overline{Y}^0, \overline{Z}^0)$ be any set that satisfy

$$\overline{R}^0 = M - \overline{D}^0 \succeq 0$$

$$\overline{S}^0 = \kappa^1 \overline{D}^0 - M \succeq 0$$

$$\overline{D}^0 \succeq 0$$

and $\overline{Z}^0 + \kappa^1 \overline{Y}^0 = \overline{X}^0$, with

$$\delta(\overline{R}^0, \overline{X}^0) = \|(\overline{R}^0)^{\frac{1}{2}} \overline{X}^0 (\overline{R}^0)^{\frac{1}{2}} - I\|_F \le \beta$$

$$\delta(\overline{D}^0, \overline{Z}^0) = \|(\overline{D}^0)^{\frac{1}{2}} \overline{Z}^0 (\overline{D}^0)^{\frac{1}{2}} - I\|_F \le \beta$$

$$\delta(\overline{S}^0, \overline{Y}^0) = \|(\overline{S}^0)^{\frac{1}{2}} \overline{Y}^0 (\overline{S}^0)^{\frac{1}{2}} - I\|_F \le \beta$$

for some $\beta \in (0,1)$.

Let $X^1, Y^1, Z^1, R^1, S^1, D^1$ be defined by

$$X^{1} = \overline{X}^{0} + \Delta X, Y^{1} = \overline{Y}^{0} + \Delta Y, Z^{1} = \overline{Z}^{0} + \Delta Z$$
$$R^{1} = \overline{R}^{0} + \Delta R, S^{1} = \overline{S}^{0} + \Delta S, D^{1} = \overline{D}^{0} + \Delta D$$

where the increments Δs are given by the Newton step

$$\Delta Z + W^{-1} \Delta D W^{-1} = (\overline{D}^0)^{-1} - \overline{Z}^0$$
$$\Delta X + U^{-1} \Delta R U^{-1} = (\overline{R}^0)^{-1} - \overline{X}^0$$
$$\Delta Y + V^{-1} \Delta S V^{-1} = (\overline{S}^0)^{-1} - \overline{Y}^0$$

and

$$\Delta R = -\Delta D, \Delta S = \kappa^1 \Delta D, \Delta X = \Delta Z + \kappa^1 \Delta Y$$

where U, V, W are the geometric means

$$U = (\overline{R}^{0})^{1/2} ((\overline{R}^{0})^{1/2} \overline{X}^{0} (\overline{R}^{0})^{1/2})^{-1/2} (\overline{R}^{0})^{1/2}$$

$$V = (\overline{S}^{0})^{1/2} ((\overline{S}^{0})^{1/2} \overline{Y}^{0} (\overline{S}^{0})^{1/2})^{-1/2} (\overline{S}^{0})^{1/2}$$

$$W = (\overline{D}^{0})^{1/2} ((\overline{D}^{0})^{1/2} \overline{Z}^{0} (\overline{D}^{0})^{1/2})^{-1/2} (\overline{D}^{0})^{1/2}$$

to ensure that updates are symmetric.

Then we have

$$\delta(R^{1}, X^{1}) = \|(R^{1})^{\frac{1}{2}} X^{1} (R^{1})^{\frac{1}{2}} - I\|_{F} \le \frac{1}{2} \frac{\beta^{2}}{1 - \beta}$$

$$\delta(S^{1}, Y^{1}) = \|(S^{1})^{\frac{1}{2}} Y^{1} (S^{1})^{\frac{1}{2}} - I\|_{F} \le \frac{1}{2} \frac{\beta^{2}}{1 - \beta}$$

$$\delta(D^{1}, Z^{1}) = \|(D^{1})^{\frac{1}{2}} Z^{1} (D^{1})^{\frac{1}{2}} - I\|_{F} \le \frac{1}{2} \frac{\beta^{2}}{1 - \beta}$$

and

$$\|(\overline{D}^0)^{-\frac{1}{2}}D^1(\overline{D}^0)^{-\frac{1}{2}} - I\|_F \le \frac{\beta}{1-\beta}$$

Proof See the appendix.

Our next result shows that starting from an $O(\delta)$ approximate center $(R^0, S^0, D^0, X^0, Y^0, Z^0)$ instead of an exact center for κ^0 , by following the procedures described in Proposition 3 to form the initial set $(\overline{R}^0, \overline{S}^0, \overline{D}^0, \overline{X}^0, \overline{Y}^0, \overline{Z}^0)$ for κ^1 , this initial set also satisfies the closeness conditions

$$\delta(\overline{R}^0, \overline{X}^0) \le \delta', \delta(\overline{D}^0, \overline{Z}^0) \le \delta', \delta(\overline{S}^0, \overline{Y}^0) \le \delta'$$

for $\delta' = \beta + \delta$, i.e. it is an $O(\beta + \delta)$ approximate analytic center for κ^1 , for δ sufficiently small. This $O(\beta + \delta)$ approximate center can then be used in the Newton iteration in Proposition 4 to obtain an $O((\beta + \delta)^2) = O(\delta)$ approximate center for κ^1 , thus ensuring that we can go from an $O(\delta)$ approximate center for κ^0 to an $O(\delta)$ approximate center for κ^1 with a Newton step.

Proposition 5. Suppose that $(R^0, S^0, D^0, X^0, Y^0, Z^0)$ satisfy

$$R^{0} = M - D^{0} \succeq 0$$

$$S^{0} = \kappa^{0} S^{0} - M \succeq 0$$

$$D^{0} \succeq 0$$

$$Z^{0} + \kappa^{0} Y^{0} = X^{0}$$

 $with \ \delta(R^0,X^0) \leq \delta, \delta(D^0,Z^0) \leq \delta, \delta(S^0,Y^0) \leq \delta \ for \ some \ \delta \in (0,1). \ Further, \ let \ \Delta \kappa = \kappa^0 - \kappa^1 \ with \ \delta(R^0,X^0) \leq \delta + \delta(R^0,X^0) \leq \delta(R$

$$\Delta \kappa = \frac{\beta}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})}$$

where $\beta \in (0,1)$ is a sufficiently small constant, then with

$$\overline{R}^0 = R^0, \overline{S}^0 = -\Delta \kappa D^0 + S^0, \overline{D}^0 = D^0$$

$$\overline{X}^0 = X^0, \overline{Y}^0 = Y^0, \overline{Z}^0 = \Delta \kappa Y^0 + Z^0$$

we have $\overline{R}^0 = M - \overline{D}^0 \succeq 0$, $\overline{S}^0 = \kappa^1 \overline{D}^0 - M \succeq 0$, $\overline{D}^0 \succeq 0$, $\overline{Z}^0 + \kappa^1 \overline{Y}^0 = \overline{X}^0$, and $\delta(\overline{R}^0, \overline{X}^0) \leq \beta$, $\delta(\overline{S}^0, \overline{Y}^0) \leq \delta + \beta$, $\delta(\overline{D}^0, \overline{Z}^0) \leq \delta + \beta$.

Proof See the appendix.

The above three results guarantee that if we start from an $O(\delta)$ approximate center for κ^0 , by taking a small but constant step $\Delta \kappa$, a Newton update step yields an $O(\delta)$ approximate center for $\kappa^1 = \kappa^0 - \Delta \kappa$, and we may iteratively generate approximate centers in this fashion. In the next result, we show that approximate centers, as the name suggests, yields a potential that is close to that of the exact center, and so we have an algorithm with approximate centers, such that the reduction in potential at every step is constant, and the termination criterion is when the potential evaluated at the approximate center drops below some threshold.

THEOREM 4. Let \overline{D}^0 and \overline{D}^1 be approximate centers for κ^0 and $\kappa^1 = \kappa^0 - \frac{\beta}{Tr(\overline{D}^0 \cdot (\kappa^0 \overline{D}^0 - M)^{-1})}$ respectively, obtained using the procedures in Proposition 3 to generate feasible point and the Newton update with Nesterov-Todd direction for β sufficiently small. If

$$\delta(\overline{R}^0, \overline{X}^0) \le \delta, \delta(\overline{D}^0, \overline{Z}^0) \le \delta, \delta(\overline{S}^0, \overline{Y}^0) \le \delta$$

for δ a small universal constant, then

$$\delta(\overline{R}^1, \overline{X}^1) \le \delta, \delta(\overline{D}^1, \overline{Z}^1) \le \delta, \delta(\overline{S}^1, \overline{Y}^1) \le \delta$$

and $P(\overline{D}^1, \kappa^1) \leq P(\overline{D}^0, \kappa^0) - c\beta$ for $c \in (0, 1)$ a universal constant.

Proof See the appendix.

Algorithm 3 Step 0. Let \overline{D}^0 be an $O(\beta)$ approximate analytic center of $\Gamma(\kappa^0)$ with $\kappa^0 > \kappa^*$. Set k = 0.

Step 1. Let $\Delta \kappa^k = \frac{\beta}{Tr(\overline{D}^0 \cdot (\kappa^0 \overline{D}^0 - M)^{-1})}$ for some small constant $0 < \beta < 1$ and let $\kappa^{k+1} = \kappa^k - \Delta \kappa^k$. Update

$$\overline{S}^0 \leftarrow -\Delta \kappa \overline{D}^0 + \overline{S}^0$$
$$\overline{Z}^0 \leftarrow \Delta \kappa Y^0 + \overline{Z}^0$$

to obtain feasible point for κ^{k+1} .

- Step 2. Use Newton's update to generate approximate analytic center \overline{D}^{k+1} of $\Gamma(\kappa^{k+1})$.
- Step 3. If $P(\kappa^{k+1}) > O(-pt)$, set $k \leftarrow k+1$ and return to Step 1.

The above result thus guarantees that if we start from an approximate center that is accurate enough, we can always ensure that the updated approximate center obtained from a Newton step with Nesterov-Todd direction remain as accurate, given small but constant step size. Our results in this section provided us with two algorithms that generate optimal diagonal preconditioners that guarantee reduction in condition number, given any fixed matrix. In practice, we observe that running the bisection algorithm or Newton update for a few itereations already generates a good preconditioner, and that is what we implement when comparing with other preconditioning methods.

4. Diagonal Preconditioning and Stochastic Convex Optimization

So far we have focused on diagonal preconditioning of design matrices. We studied how preconditioning affects the condition number of the design matrices, and also developed algorithms to compute optimal diagonal preconditioners. These results have direct implications on the convergence rates of iterative solvers of linear systems and first order methods applied to quadratic objectives, since convergence rates depend explicitly on the condition number of the (constant) Hessian matrix X^TX .

For general convex objective functions, convergence rates of first order methods depend on the smoothness and convexity constants of the function. It is therefore more challenging to study the impact of preconditioning on the design matrix on the convergence of first order methods on general convex objective functions, as we need to investigate how the reduction in condition number of the design matrix translates to improvements in the smoothness and convexity constants of the objective function. In this section, we first give such a result for a class of objective functions f that correspond to the (regularized) loss of an empirical risk minimization problem (Shalev-Shwartz and Zhang (2013)), and show that when f is smooth and strongly convex, reductions in the condition number of the objective is on the order of $\frac{\kappa(X)}{\kappa(X_0)}$ where X is the design matrix and X_0 is any preconditioned design matrix with smaller condition number. For other more general classes of convex objectives, we leave to future work to quantify theoretically the impact of condition number on convergence rates. However, we make the case that the optimal diagonal preconditioning algorithms developed in the previous section is not limited to being applied to fixed design matrices. We establish the connection of batch normalization, a popular technique in machine learning, to adaptive preconditioning, and develop an adaptive version of the optimal diagonal preconditioning algorithm. We then conduct numerical experiments that demonstrate the

	Lipschitz continuous	Smooth	Smooth&Strongly Convex
Full Gradient	$O(\frac{1}{\epsilon^2})$	$O(\frac{L}{\sqrt{\epsilon}})$	$O(\sqrt{\kappa}\log\frac{1}{\epsilon})$
Stochastic Gradient	$O(\frac{1}{\epsilon^2})$	$O(\frac{1}{\epsilon^2})$	$O(\frac{1}{\lambda \epsilon})$

Table 3 Optimal iteration complexity of convex optimization. L and λ are the moduli of smoothness and convexity, i.e. $\lambda \leq \|\nabla_{\theta}^2 f\| \leq L$, and $\kappa = L/\lambda$ is the condition number.

Nesterov	EMGD	SAG $(n \ge 8\kappa)$	SDCA
$O(\sqrt{\kappa}n\log\frac{1}{\epsilon})$	$O((n+\kappa^2)\log\frac{1}{\epsilon})$	$O(n\log\frac{1}{\epsilon})$	$O((n+\kappa)\log\frac{1}{\epsilon})$

Table 4 Computational complexity of stochastic first order methods for minimizing $f = \frac{1}{n} \sum_{i=1}^{n} f_i + g_{\lambda}$.

effectiveness of the optimal diagonal preconditioning algorithm at speeding up first order methods in regression and classification problems in the next section.

4.1. Convergence Rates for General Convex Problems

The relationship between the complexity of first order methods and the smoothness and convexity properties of the objective function has been well established in the optimization literature. Here the complexity is usually expressed in terms of the number of iterations required to obtain an ϵ -optimal solution. We summarize the corresponding iteration complexities of solving

$$\min_{\theta} f(\theta, X)$$

in Table 3, taken from Zhang et al. (2013).

The iteration complexity in stochastic optimization is generally polynomial in $\frac{1}{\epsilon}$. However, when f is of the form

$$f = \frac{1}{n} \sum_{i=1}^{n} f_i + g_{\lambda}$$

where f_i are convex and L-smooth, while g_{λ} is L-smooth and λ -strongly convex, the complexity can be improved to be logarithmic in $\frac{1}{\epsilon}$. For example, the stochastic average gradient (SAG) method has iteration complexity $O(n\log\frac{1}{\epsilon})$ provided $n \geq 8\kappa$, the stochastic dual coordinate ascent (SDCA) method (Shalev-Shwartz and Zhang (2013)) has iteration complexity $O((n+\kappa)\log\frac{1}{\epsilon})$, and the epoch mixed gradient descent (EMGD) method (Zhang et al. (2013)) has the complexity $O((n+\kappa^2)\log\frac{1}{\epsilon})$. Of the three, EMGD can be applied to general strongly convex and smooth functions, in which case it requires $O(\log\frac{1}{\epsilon})$ full gradient queries and $O(\kappa^2\log\frac{1}{\epsilon})$ stochastic gradient queries. Table 4 compares these stochastic gradient algorithms with the accelerated gradient descent of Nesterov applied to stochastic gradient descent.

We note the distinction between the condition number of a function and a matrix. For a function $f(\theta, X)$, where X denotes data and θ denotes parameter, the condition number is given by L/λ where

$$\lambda \le \|\nabla_{\theta}^2 f(\theta, X)\| \le L$$

for all $\theta \in \Theta$ the parameter space. When $f(\theta, X, Y) = \frac{1}{n} ||X\theta - Y||_2^2$, the Hessian is a fixed quantity, namely the Wishart matrix $X^T X$. In general, the Hessian is parameterized by θ and λ and L are the upper and lower bounds of the largest and smallest eigenvalues of the Hesisan, respectively.

In this section, we are interested in how diagonal preconditioning procedures on the design matrix affect the iteration complexity through reducing the condition number of the objective function.

4.2. Accelerating Optimization through Preconditioning

To motivate the discussion, we first examine the least squares problem

$$\min_{\theta} \frac{1}{n} \|X\theta - Y\|_2^2$$

where $X \in \mathbb{R}^{n \times p}$ which has smoothness and strong convexity moduli of $\lambda_1(X^TX)$ and $\lambda_n(X^TX)$, respectively. Here we assume that n > p, so that X^TX is invertible and hence the objective function is both smooth and strongly convex. For the least squares problem, an analytic solution is available, but we consider first order methods mainly because the quadratic form makes the effect of preconditioning procedures obvious. We may also imagine a setting where potentially n, p are large so that direct computation of $(X^TX)^{-1}$ is costly, so that we can only resort to (stochastic) first order methods. In any case, given the least squares problem, we are interested in how diagonal preconditioning procedures speed up the convergence of first order methods.

There are potentially two levels of stochasticity. The data matrix is assumed to have i.i.d. rows from some distribution. Our earlier results show that the condition number $\kappa(X^TX)$ of sub-Gaussian data matrices concentrate around that of the population covariance matrix Σ , and that for a class of population covariance matrices, preconditioning with column standard deviation reduces the condition number of the data matrix by a factor on the order of $\sqrt{\kappa(\mathrm{diag}(\Sigma))}$ with high probability. So for full gradient methods, a reduction in computational complexity is achieved through the reduction of the condition number on the order of $\sqrt{\kappa(\mathrm{diag}(\Sigma))}$ with high probability if we assume sub-Gaussian data distribution with well-behaved covariance matrix Σ , or $\sqrt{\frac{\kappa(X^TX)}{\kappa(D^{-1}X^TXD^{-1})}}$ using optimal diagonal preconditioning methods developed in the previous section, for the least squares problem.

For general smooth and strongly convex objectives $f(\theta, X)$ the condition number $\kappa(\nabla_{\theta}^2 f(\theta, X))$ of the Hessian of the objective function is not constant, but depends on the current estimate θ^k of the parameter. Here there are two types of preconditioning that can be performed. The first type is that done on the data matrix X, using a variety of conditioning algorithms including the usual data normalization procedure, batch normalization, or the optimal diagonal preconditioning algorithm developed in this paper. It can be done on the entire X once before the optimization procedure, or for stochastic systems, on the sub design matrix formed by the minibatch of samples. If we are

using first order methods, only the above preconditioning on the (sub)design matrix is possible. If we can efficiently calculate or approximate the inverse Hessian, then a second preconditioning option is to precondition directly on the (approximate) Hessian or inverse Hessian, evaluated at the current estimate θ^k . As discussed earlier, Quasi-Newton methods and other accelerated gradient methods such as Anderson mixing (Zhang et al. (2018)) and Adagrad (Duchi et al. (2011)) rely crucially on some form of approximate inverse Hessian or Jacobian. When the approximate inverse Hessian is ill-conditioned, the methods are known to slow down or diverge both in theory and in practice (Shanno and Kettler (1970)). Preconditioning the approximate inverse Hessian has been considered in as early as (Shanno (1970)). Here we simply note that our optimal diagonal algorithm can also be applied to the quasi-Newton update formulae to improve the condition number of the approximate inverse Hessian.

We focus on the case of preconditioning on the data/design matrix X, and study how the reduction in $\kappa(X^TX)$ translates into that of κ_f , where

$$\kappa_f = \frac{L_f}{\lambda_f}$$

$$L_f = \sup_{\theta} \|\nabla_{\theta}^2 f(X, \theta)\|$$

$$\lambda_f = \inf_{\theta} \|\nabla_{\theta}^2 f(X, \theta)\|$$

In order to analyze how preconditioning of the data matrix affects the condition number of the Hessian at θ^k , we need to make assumptions about the structure of the objective function f. For example, if f is of the form $f_0(X\theta)$ for some f_0 with condition number κ_0 , then the Hessian of the objective function satisfies

$$\kappa(\nabla_{\theta}^{2} f) = \kappa(X^{T} \cdot \nabla^{2} f_{0}(X\theta) \cdot X)$$

and we should expect improvements on the condition number of X^TX to improve the condition number of the Hessian as well. In the following result, we focus on the case when f corresponds to the (regularized) loss of an empirical risk minimization problem (Shalev-Shwartz and Zhang (2013)). In this case, the reduction in κ_f is on the order of $\sqrt{\kappa(X^TX)/\kappa(DX^TXD)}$ for smooth and strongly convex objectives. This reduction then implies the corresponding improvements in iteration complexities of first order methods, thorugh their dependences on κ_f .

THEOREM 5. If $f(X, w) = \frac{1}{n} \sum_i f_i(w^T x_i)$ for scalar λ -strongly convex and L-smooth functions f_i . Then replacing x_i with Dx_i , where D is a diagonal matrix such that $\kappa(DX^T XD) \leq \kappa(X^T X)$, we have

(i) For general $f_i(z)$,

$$\kappa(\nabla_w^2 f(XD, w)) \le \frac{\kappa(\nabla_w^2 f(X, w))}{\kappa(X^T X) / \kappa(DX^T XD)} \kappa_0^2$$

where $\kappa_0 = \frac{L}{\lambda}$, i.e. when f_i are well-conditioned so κ_0 is small, the reduction in condition number of the objective function with preconditioning is on the order of $\kappa(X^TX)/\kappa(DX^TXD)$.

(ii) When $f_i(z) = z^2$, the result reduces to the special case of linear regression, where the reduction in condition number is lower bounded by exactly $\kappa(X^TX)/\kappa(DX^TXD)$.

Proof We have

$$\nabla_w^2 f(X, w) = \frac{1}{n} \sum_i \nabla^2 f_i(w^T x_i) x_i x_i^T$$

Moreover,

$$\frac{1}{n}LX^TX \succeq \frac{1}{n}\sum_{i} \nabla^2 f_i(w^Tx_i)x_ix_i^T \succeq \frac{1}{n}\lambda X^TX$$

so that

$$\begin{split} \kappa(\nabla_w^2 f(XD, w)) &\leq \kappa(DX^T XD) \cdot \kappa_0 \\ &= \frac{\kappa(DX^T XD)}{\kappa(X^T X)} \cdot \kappa(X^T X) \cdot \kappa_0 \\ &\leq \kappa_0^2 \cdot \kappa(\nabla_w^2 f(X, w)) \cdot \frac{\kappa(DX^T XD)}{\kappa(X^T X)} \end{split}$$

The above result separates out the effect of the design matrix on the condition number of the objective function. If the objective function itself is smooth and strongly convex, then diagonal preconditioning on a badly-conditioned design matrix results in a reduction of the condition number of the objective function on the order of $\sqrt{\kappa(X^TX)/\kappa(DX^TXD)}$, which then implies improvements on the complexities of first order methods through their dependences on the condition number.

4.3. Adaptive Diagonal Preconditioning

So far, we have focused on preconditioning with a fixed preconditioner D when we have acces to all the data at once in the form of the design matrix, where D is obtained from data matrix X, e.g. column-wise standard deviation of X or optimal diagonal preconditioning obtained using methods discussed in the previous section. However, in practice such a preconditioner may not be available. For example, in stochastic gradient descent or online learning, we may not have prior access to the full data matrix X, instead only drawing random subsets of all samples. In such settings, it is still possible to speed up the convergence with adaptive preconditioning procedures applied to

first order methods. In fact, many first order methods can be understood to involve some form of adaptive preconditioning. For example, BFGS method (Broyden (1970), Goldfarb (1970)) and AdaGrad (Duchi et al. (2011)) pre-multiply the gradient with some approximate (diagonal) inverse Hessian. Other adaptive gradient methods that perform local optimization with an adaptive metric constructed from observed iterates have become increasingly popular in deep learning with benefits to the convergence speed as well as statistical properties of the iterative optimization procedures. For example, Levy and Duchi (2019) show that when the "scale" of the gradients varies across dimensions, adaptive gradient methods such as AdaGrad (Duchi et al. (2011)) achieves lower regret compared to vanilla stochastic gradient methods.

A popular normalization technique used in deep learning, called batch normalization (Ioffe and Szegedy (2015)), can also be understood as a form of adaptive (diagonal) conditioning. For general neural networks, let $x^{(m,k)} \in \mathbb{R}^{n \times p_m}$ denote the output of the m-th layer, consisting of n p_m -dimensional vectors, at the kth iteration of stochastic gradient descent. Batch normalization involves applying a centering operation and a scaling operation to $x^{(m,k)}$, followed by reverse

$$\tilde{x}_i^{(m,k)} = \frac{(x_i^{(m,k)} - \mu_i)}{\sigma_i} \cdot \gamma_i + \beta_i$$

operations with parameters $\gamma \in \mathbb{R}^{p_m}_{++}, \beta \in \mathbb{R}^{p_m}$, to obtain

for the *i*th column of $x^{(m,k)}$, where μ_i is the mean of the *i*th column, and σ_i is the standard deviation. The parameters γ, β are updated through SGD together with the original parameters of the neural network. The point is that population statistics for intermediate layers are not known a priori, so γ and β serve as adaptive parameters that are updated at each step of the training.

Specialized to the least squares problem, it effectively solves the problem $\min_{\theta,D} \frac{1}{n} ||XD\theta - y||_2^2$ by alternating between θ and D during each iteration, i.e. at the kth iteration, given $D^{(k)}$, one solves the problem $\min_{\theta} \frac{1}{n} ||XD^{(k)}\theta - y||_2^2$ and then find $D_1^{(k+1)}$ by solving $\min_{D} \frac{1}{n} ||XD\theta^{(k+1)} - y||_2^2$.

This alternating optimization procedure is present in many other convex optimization problems with special structures, for example the ADMM method for minimizing the sum of convex functions with block variables (Lin et al. (2015), Wen et al. (2010)). It is also used in non-convex formulations of convex problems, most notably low-rank matrix and tensor factorization Chi et al. (2019), Aswani (2016), Zhao et al. (2015), where alternating minimization of the objective is employed to solve a non-convex formulation of the problem. Besides convergence issues, another recent focus of the latter literature is on the "implicit regularization" (Wu et al. (2019)) of the alternating minimization algorithm associated with the non-convex formulation.

It is similarly possible to extend our optimal diagonal preconditioning procedure to the stochastic setting. Suppose each iteration we observe subsets of rows of a design matrix X. At each iteration

we update our estimate of X^TX based on samples drawn from X so far. Then we can compute the optimal diagonal preconditioner D based on the current estimate of X^TX . As the number of iterations increases, our estimate of X^TX becomes more accurate, and D should approach the appropriate optimal diagonal preconditioner given X^TX . This gives the following algorithm.

Algorithm 4 (Adaptive optimal diagonal preconditioning) Let $\overline{X}^{(0)} = []$ and at the kth iteration, form the cumulative design matrix $\overline{X}^{(k)}$ by concatenating the k-th batch $X^{(k)}$ with $\overline{X}^{(k-1)}$ and retaining unique rows. If $\overline{X}^{(k)}$ is full rank, then find $D_1^{(k)}$ that minimizes $\kappa(D(\overline{X}^{(k)T}\overline{X}^{(k)}D))$ and perform the preconditioning $X^{(k)}D_1^{(k)}$. Alternatively, we can perform the optimal diagonal scaling every m iterations, where m is chosen to balance the tradeoff between computational cost and convergence speed.

A natural next step is to compare the performance of the optimal diagonal preconditioning with that of batch normalization on regression and classification problems. We take up this in the next section. We also note that although batch normalization speeds up the convergence of first order methods and can be viewed as a form of adaptive diagonal preconditioning, it is not the case that the effective condition numbers of Hessian matrices under batch normalization are reduced, since the diagonal conditioner is selected so as to minimze the objective loss rather than the condition number of the preconditioned matrix. This is in contrast to our adaptive optimal preconditioning algorithm, which speeds up convergence by reducing the effective condition number of the design matrix. Thus it remains to further investigate the mechanism through which batch normalization speeds up the convergence of first order methods.

We also mention that other adaptive methods, such adaptive regularization of objective (Jiang et al. (2017)) and adaptive step size Gao and Goldfarb (2019), are also effective in speeding up the convergence of first order methods. These methods are often applied to quasi-Newton methods and the step size is determined based on information on the local curvature of the objective function, e.g. the damped Newton method Nesterov (2013) of Nesterov, who derived convergence results for self-concordant functions Nesterov and Nemirovskii (1994). As a possible extension of the optimal preconditioning framework, it may be interesting to consider using an approximate optimal preconditioner of the approximate inverse Hessian, and to explore potential connections with adaptive step size approaches for self-concordant functions.

5. Numerical Experiments

In this section, we perform numerical experiments to compare the performance of diagonal preconditioning methods at accelerating gradient and stochastic gradient descent applied to regression and classification problems.

5.1. Simulated Dataset

For our simulated dataset, we randomly generate design matrix X whose rows are i.i.d. Gaussian vectors with covariance matrix Σ . The covariance matrix itself is generated using the sklearn package in python, and has condition numbers in the range of 100-1000. We consider the regression problem

$$\min_{\theta} \frac{1}{n} \|X\theta - Y\|_2^2$$

where Y is generated using a ground-truth parameter θ^* , and we assess the speed of convergence by looking at the distance of estimate to the optimal solution of the quadratic problem, namely the OLS estimate θ_{OLS} of θ : we declare convergence when $\|\theta^{(k)} - \theta_{OLS}\|_2 / \|\theta_{OLS}\|_2$ is below some threshold, usually set to be 0.01.

We consider the following modified problem

$$\min_{\tilde{\theta}} \frac{1}{n} \|XD\tilde{\theta} - D_0Y\|_2^2$$

where D is one of the following diagonal preconditioners:

- \bullet Normalization: D is the diagonal matrix of column standard deviations or norms of X.
- Optimal diagonal preconditioning: D minimizes $\kappa(DX^TXD)$ among all positive diagonal matrices.
- (full) Batch normalization: $D_0 = I$, and $D_1^{(0)}$ is the diagonal matrix of column standard deviations of X. At the kth iteration, update $\theta^{(k+1)}$ by solving $\min_{\theta} \frac{1}{n} ||XD^{(k)}\theta y||_2^2$ and then form $D_1^{(k+1)}$ by solving $\min_{D} \frac{1}{n} ||XD\theta^{(k+1)} y||_2^2$.

We compare the convergence speeds of gradient and stochastic gradient descent methods with these preconditioners. Step size is determined by backtracking line search using the Armijo-Goldstein conditions.

For stochastic gradient descent, since X is not directly available, we use the corresponding adaptive versions of the above procedures:

- Normalization: D is the diagonal matrix of column standard deviations or norms of $X^{(k)}$, the batch of data in the k-th iteration.
- Adaptive optimal diagonal preconditioning: at kth iteration, form the cumulative design matrix $\overline{X}^{(k)}$ by concatenating $X^{(k)}$ with $\overline{X}^{(k-1)}$ and retaining unique rows, and find D that minimizes $\kappa(D(\overline{X}^{(k)T}\overline{X}^{(k)}D)$.
- Batch normalization: $D^{(0)} = I$. At the kth iteration, update $\theta^{(k+1)}$ by solving $\min_{\theta} \frac{1}{n} \|X^{(k)} D^{(k)} \theta y\|_2^2$ and then form $D^{(k+1)}$ by solving $\min_{D} \frac{1}{n} \|X^{(k)} D \theta^{(k+1)} y\|_2^2$ where $X^{(k)}$ is the batch of samples at the kth iteration.

(n,p)	(1000, 20)		(1000, 40)		(1000, 100)	
	iterations	κ	iterations	κ	iterations	κ
No preconditioning	44529	278.30	39709	870.81	72795	1129.80
Fixed preconditioning	16639	230.36	148954	909.80	62915	1087.84
Optimal preconditioning	10230	144.81	29835	746.99	29881	858.46
Batch normalization	11721	470.12	31032	1226.79	47654	1192.45

Table 5 Number of iterations till convergence for preconditioning methods for gradient descent, with step size determined through backtracking line search. Convergence is declared when $\|\theta-\theta^*\|$ is within a small constant factor of $\|\theta^*\|$, where θ^* is the OLS solution, and θ is the effective coefficient taking into account the preconditioning on X. The covariance matrix Σ is randomly generated using python package sklearn and the condition number of the effective design matrix $X \sim \mathcal{N}(0, \Sigma)$ is also reported above as κ . For example, for preconditioning with diagonal matrix D, the condition number of XD is given. For batch normalization, since the condition number of the effective deisgn matrix changes every iteration, the median of those numbers are given. We see that preconditioning with column standard deviation does not always reduce the condition number of the design matrix, and indeed in such cases convergence of steepest descent is slowed down.

Tables 5 and 6 summarize the number of iterations before convergence for various methods and problems of various sizes. We note that in many cases the optimal diagonal preconditioner returns a preconditioned matrix with significantly smaller condition number, as guaranteed by our theoretical analyses. This is also manifested through the acceleration in convergence of steepest descent. On the other hand, preconditioning with column statistics does not always guarantee reduction in condition number. In general, steepest descent with optimal diagonal preconditioning achieves comparable performance to batch normalization when it performs well. On the other hand, there are specific cases where stochastic gradient descent with batch normalization takes considerably longer time than optimal preconditioning. The tradoff here is that for large matrices (p large), finding an approximate optimal diagonal preconditioner may take a non-negligible amount of time, whereas batch normalization only adds one extra step of gradient update for the preconditioner D. The numerical simulations also confirm that although batch normalization speeds up first order optimization methods, the effective condition number of the design matrix is not actually decreased. This suggests that although the performance of batch normalization is comparable to that of optimal diagonal preconditioning, the exact mechanism through which it speeds up convergence remains to be investigated further.

5.2. MNIST Dataset

To compare the preconditioning procedures on a real dataset, we use the MNIST handwritten digit classification dataset, consisting of 70000 handwritten digits in the format of 28×28 binary pixel photos, with a train-validation split of 6:1. As a preprocessing step, we reshape each two-dimensional datapoint into a 784-dimensional vector. As the design matrix is rank-deficient due to linear dependency and duplicate rows, we select the subset of linearly independent columns,

(n,p)	(1000, 20)		(1000, 40)		(1000, 100)	
	iterations	κ	iterations	κ	iterations	κ
No preconditioning	12350	166.53	43712	986.51	96619	1637.54
Fixed preconditioning	11825	140.86	100547	1149.97	54646	1594.44
Optimal preconditioning	10791	126.07	31202	868.13	47310	1313.44
Batch normalization	11189	251.85	35999	1280.45	48448	2012.47

Table 6 Number of iterations till convergence for adaptive preconditioning methods for mini-batch stochastic gradient descent, with step size determined through backtracking line search. Batch size is between 10-20% of the training set size. The last two preconditioning methods, i.e. optimal preconditioning and batch normalization, are adaptive, whereas the first two only requires preconditioning once before the start of the optimization routine. For adaptive optimal diagonal preconditioning, the diagonal preconditioner is updated once every 100 iterations, using the most up to date cumulative design matrix. All reported condition numbers are medians of the sequence of condition numbers of the effective design matrix during training.

(n,p)	iterations	log-gap
No preconditioning	2000	-2.74
Fixed preconditioning	1823	-2.90
Optimal preconditioning	1503	-3.12
Batch normalization	1621	-3.35

Table 7 Number of iterations till convergence of diagonal preconditioning methods for gradient descent and the log-gap at convergence. We see that while the log-gaps are comparable among the three diagonal conditioners, the number of iterations required is the smallest for optimal diagonal preconditioner.

and also perturb the entries with iid Gaussian noise with standard deviation 0.01. The resulting design matrix has a condition number of 73288.03, i.e. a very ill-conditioned system. Applying the optimal diagonal preconditioner yields a design matrix with condition number 102.27, a significant reduction. To assess the convergence speeds of gradient and stochastic gradient descent methods, we run multinomial logistic regression with cross-entropy loss, $f(\theta) = \frac{1}{n} \sum_{i=1}^{n} -\log p_i^{y_i}$ where p_i^k is the probability of the k-th class of the ith sample, predicted by the model: $p_i^k = \frac{\exp(\theta_k^T x_i)}{\sum_{k=1}^K \exp(\theta_k^T x_i)}$, with the descent direction given by $\nabla_{\theta_k} f(\theta) = -\frac{1}{n} \sum_{y_i = k} x_i + \frac{1}{n} \sum_i \frac{x_i \exp(\theta_k^T x_i)}{\sum_{k=1}^K \exp(\theta_k^T x_i)}$.

Because the problem is non-convex, we declare convergence when the number of iterations reached a maximum value, or when the norm of gradient drops below the threshold 0.001. We then report the log-gap $\log(f(\theta) - f(\theta^*))$ of the various methods, where θ^* is a pre-computed optimal solution.

We see that while the log-gaps are comparable among the three diagonal conditioners, the number of iterations required till convergence is the smallest for optimal diagonal preconditioner. All methods are able to achieve a test accuracy of at least 88%.

6. Conclusion

In this paper, we studied diagonal preconditioning and its impact on the condition number and convergence speed of linear systems and quadratic and general convex optimization problems. We

first showed that the popular preconditioning technique of normalization by column standard deviation/norm reduces the condition number of the design matrix X by $\sqrt{\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}}$ for X with independent sub-Gaussian rows and convariance matrix Σ , where $D = \operatorname{diag}(\Sigma)$. We then gave a diagonal dominance condition that guarantees that this reduction is large. Next, for any fixed design matrix, we developed bisection and interior point algorithms that guarantee a diagonal preconditioner that reduces the condition number of the preconditioned matrix, with $O(\frac{1}{\epsilon})$ iteration complexity, and each iteration consists of an SDP feasibility problem or a Newton update step with Nesterov-Todd directions. These results have direct implications for the effect of preconditioning on speeding up the convergence of iterative algorithms for linear systems and first order methods for quadratic optimization problems, as the linear convergence rates have explicit dependence on the condition number. For general convex optimization problems, it is less clear how improvements in the condition number of the design matrix translate into speedup of first order methods. We showed that for a particular class of strongly convex and smooth objectives, the reduction in the condition number of the objective function enjoys the same order $\sqrt{\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}}$ of reduction as that of the design matrix. Finally, we established connections of batch normalization to adaptive preconditioning, and extended our optimal diagonal preconditioning algorithm to an adaptive setting compatible with stochastic first order methods. Numerical experiments on real and simulated datasets with regression and classification tasks show that the optimal diagonal preconditioner speeds up convergence compared to preconditioning with heuristics such as column standard deviation, and is comparable to the performance of batch normalization. On the other hand, batch normalization does not seem to reduce the effective condition number of the system, so its mechanism of speeding up convergence remains to be investigated further.

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Appendix A: Basic Facts about the Condition Number

Let $\|\cdot\|$ be any matrix norm on the space of matrices $\mathbb{R}^{m\times n}$. Then the condition number associated with this norm is defined as

$$\kappa(A) := ||A|| \cdot ||A^{-1}||$$

where A^{-1} is the pseudo-inverse of a non-singular A.

When $\|\cdot\|$ is the 2-norm defined as

$$||A|| = \sup_{\|v\|_2 = 1} ||Av||_2$$

the condition number can be alternatively written

$$\kappa(A) = \frac{\max_{i} \sigma_{i}(A)}{\min_{i} \sigma_{i}(A)}$$

where $\{\sigma_i\}_{i=1}^{m \wedge n}$ are the non-zero singular values of A. Moreover, if A is symmetric positive definite, then we can replace singular values with eigenvalues in the definition.

The condition number is a measure of how close a matrix is to being singular. Alternatively, it also describes the amount of distortion that the matrix transformation causes when applied to the unit sphere.

Because matrix norms are equivalent, in the sense that for any two norms $\|\cdot\|_a$ and $\|\cdot\|_b$, there exist constants c, C such that

$$c||A||_a \le ||A||_b \le C||A||_a$$

we see that the condition numbers defined by the two norms are also equivalent, i.e.

$$c^2 \kappa_a(A) \le \kappa_b(A) \le C^2 \kappa_a(A)$$

Condition number is invariant under scaling by constants, and from definition, $\kappa(A) = \kappa(A^{-1})$. Since $||AB|| \le ||A|| ||B||$ for matrix norms, $\kappa(AB) \le \kappa(A) \cdot \kappa(B)$, and this also implies $\kappa(A) \ge 1$ for any matrix A.

Because the Cholesky factorization will be important in the proof of our results on the reduction in condition number, we show the following fact about the condition number of a lower triangular matrix.

Lemma 1 Let $L \in \mathbb{R}^{n \times n}$ be a lower triangular matrix with full rank. Then $\kappa_p(L) \ge \frac{\max_i |L_{ii}|}{\min_i |L_{ii}|}$ for any $p \ge 1$.

Proof Note that

$$||L||_{p} = \max_{\|v\|_{p}=1} ||Lv||_{p} \ge \max_{i,j} ||e_{i}^{T} L e_{j}||_{p}$$
$$= \max_{i,j} |L_{ij}| \ge \max_{i} |L_{ii}|$$

and similarly

$$||L^{-1}||_p \ge \max_i |(L^{-1})_{ii}| \ge (L^{-1})_{11}$$
$$= L_{11} \ge \min_i |L_{ii}|$$

In other words, for triangular matrices, the condition number is lower bounded by the condition number of the diagonal matrix.

Lastly, for condition numbers defined with matrix p-norms, we have

$$\kappa(A^T A) = \kappa(A^T) \cdot \kappa(A)$$
$$= \kappa(A)^2$$

since

$$\max_{\|v\|=1} \|A^T A v\| = \max_{\|u\|=1, \|v\|=1} \langle u, A^T A v \rangle$$
$$\geq \max_{\|v\|=1} \langle A v, A v \rangle = \|A\|^2$$

and so in fact $||A^T A|| = ||A||^2$.

Appendix B: Results with Omitted Proofs for Condition Number Concentration

In this section we provide a sequence of results culminating in Theorem 1 of the main paper, which states that the diagonal preconditioning procedure given by

$$X_0 = XD^{-\frac{1}{2}} \tag{1}$$

where D is the diagonal matrix with

$$D_{jj} = \frac{1}{n-1} \sum_{i=1}^{n} (X_{ij} - \mu_j)^2$$
$$\mu_j = \frac{1}{n} \sum_{i=1}^{n} X_{ij}$$

results in a reduction of condition number on the order of $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}$ with high probability.

Because the scaling matrix D is a function of sample statistics, namely the column-wise sample standard deviations or column norm, the analysis with D directly is cumbersome. Our strategy for showing the main result is to start with the simplest possible case for D and gradually increase the complexity of the scaling matrix. More precisely, we show a sequence of concentration results, each one built on top of the other, with the following scaling matrices:

- D is equal to the population covariance matrix Σ , with general non-diagonal Σ .
- D is the sample column-wise standard deviation, under the assumption that Σ is diagonal.

- D is the diagonal of the population covariance matrix, with general non-diagonal Σ .
- D is the sample standard deviation, with general non-diagonal Σ .

We start with the case $D = \Sigma$. Even though Σ is not diagonal in general, we will see that its concentration result on condition numbers is the easiest to prove, and will also be useful for later steps. Let

$$X_0 = X \Sigma^{-\frac{1}{2}}$$

Observe that

$$||X^T X||_{op} \le ||X_0^T X_0||_{op} \cdot ||\Sigma||_{op}$$
$$||(X^T X)^{-1}||_{op} \le ||(X_0^T X_0)^{-1}||_{op} \cdot ||(\Sigma)^{-1}||_{op}$$

so that

$$\kappa(X^TX) \leq \kappa(X_0^TX_0) \cdot \kappa(\Sigma)$$

holds true for any positive definite Σ . We want to show that when X has independent sub-Gaussian rows with second moment Σ , the gap in the inequality is small with high probability, i.e.

$$\kappa(X^TX) \approx \kappa(X_0^TX_0) \cdot \kappa(\Sigma)$$

with high probability. The intuition is that tall matrices X are approximate isometries, so that X_0 will be close to the identity matrix with high probability.

Our first result is the closeness of the two quantities $\kappa(X_0^T X_0)$ and $\frac{\kappa(X^T X)}{\kappa(\Sigma)}$. Intuitively, since $\mathbb{E} X_0^T X_0 = \Sigma^{-\frac{1}{2}} \mathbb{E}(X^T X) \Sigma^{-\frac{1}{2}} = n \cdot I$, we should expect the condition number $\kappa(X_0^T X_0)$ to concentrate around 1, and similarly for $\kappa(X^T X)$ to concentrate around $\kappa(\Sigma)$, so this closeness result is essentially a result of the concentration of condition numbers, but its particular form is useful for later results.

Theorem 1 Let X be an $n \times p$ random matrix with i.i.d. sub-Gaussian rows X_i with sub-Gaussian norm $K = ||X_i||_{\psi_2}$, $\mathbb{E}X_i = 0$, and let $\Sigma = \mathbb{E}X_i^T X_i = \frac{1}{n} \mathbb{E}X^T X$ be positive definite. Let $X_0 = X \Sigma^{-\frac{1}{2}}$ be the matrix normalized by population covariance matrix. Then for universal constants c, C, with probability at least $1 - 2\exp(-\frac{ct^2}{K^4}) - 2\exp(-\frac{ct^2\sigma_{\min}^2(\Sigma)}{K^4})$,

$$\begin{split} |\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| &\leq \frac{2}{(1 - (C\frac{K^2}{\sigma_{\min}(\Sigma)})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (C\frac{K^2}{\sigma_{\min}(\Sigma)}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \\ &+ \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \end{split}$$

Proof Note that

$$\frac{1}{n} \mathbb{E} X_0^T X_0 = \frac{1}{n} \Sigma^{-\frac{1}{2}} \mathbb{E} X^T X \Sigma^{-\frac{1}{2}}$$
$$= I$$

and that X_0 has i.i.d sub-Gaussian rows with sub-Gaussian norm at most $\|\Sigma^{-\frac{1}{2}}\|K$. This is because the *i*-th row of X_0 , which is equal to $X_i\Sigma^{-\frac{1}{2}}$, satisfies

$$\begin{split} \|X_i \Sigma^{-\frac{1}{2}}\|_{\psi_2} &= \|\Sigma^{-\frac{1}{2}} X_i^T\|_{\psi_2} \\ &= \sup_{\|x\|_2 \le 1} \|\langle \Sigma^{-\frac{1}{2}} X_i^T, x \rangle\|_{\psi_2} \\ &= \sup_{\|x\|_2 \le 1} \|\langle X_i^T, \Sigma^{-\frac{1}{2}} x \rangle\|_{\psi_2} \\ &= \sup_{\|x\|_2 \le 1} \|\langle X_i^T, x \rangle\|_{\psi_2} \cdot \|\Sigma^{-\frac{1}{2}}\|_{op} \\ &= \|X_i\|_{\psi_2} \cdot \|\Sigma^{-\frac{1}{2}}\|_{op} \le \|\Sigma^{-\frac{1}{2}}\|K \end{split}$$

Applying the sub-Gaussian concentration result , we see that for n sufficiently large,

$$\|\frac{1}{n}X^{T}X - \Sigma\|_{op} \le CK^{2}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

$$\|\frac{1}{n}X_{0}^{T}X_{0} - I\|_{op} \le C\frac{K^{2}}{\sigma_{\min}(\Sigma)}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

jointly with probability at least $1 - 2\exp(-\frac{ct^2}{K^4}) - 2\exp(-\frac{ct^2\sigma_{\min}^2(\Sigma)}{K^4})$. The eigenvalue stability result then implies

$$\begin{split} |\sigma_{\max}(\frac{1}{n}X^TX) - \sigma_{\max}(\Sigma)| &\leq CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}} \\ |\sigma_{\min}(\frac{1}{n}X^TX) - \sigma_{\min}(\Sigma)| &\leq CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}} \end{split}$$

and

$$|\sigma_{\max}(\frac{1}{n}X_0^TX_0) - 1| \le C \frac{K^2}{\sigma_{\min}(\Sigma)} \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

$$|\sigma_{\min}(\frac{1}{n}X_0^TX_0) - 1| \le C \frac{K^2}{\sigma_{\min}(\Sigma)} \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

It then follows that

$$\begin{split} |\kappa(X^TX) - \kappa(\Sigma)| &= |\frac{\sigma_{\max}(\frac{1}{n}X^TX)}{\sigma_{\min}(\frac{1}{n}X^TX)} - \frac{\sigma_{\max}(\Sigma)}{\sigma_{\min}(\Sigma)}| \\ &= |\frac{\sigma_{\max}(\frac{1}{n}X^TX) \cdot \sigma_{\min}(\Sigma) - \sigma_{\max}(\Sigma)\sigma_{\min}(\frac{1}{n}X^TX)}{\sigma_{\min}(\frac{1}{n}X^TX)\sigma_{\min}(\Sigma)}| \\ &\leq |\frac{\sigma_{\max}(\frac{1}{n}X^TX) \cdot \sigma_{\min}(\Sigma) - \sigma_{\max}(\Sigma) \cdot \sigma_{\min}(\Sigma)}{\sigma_{\min}(\frac{1}{n}X^TX)\sigma_{\min}(\Sigma)}| + \\ |\frac{\sigma_{\max}(\Sigma) \cdot \sigma_{\min}(\Sigma) - \sigma_{\max}(\Sigma)\sigma_{\min}(\frac{1}{n}X^TX)}{\sigma_{\min}(\frac{1}{n}X^TX)\sigma_{\min}(\Sigma)}| \\ &\leq |\frac{\sigma_{\max}(\frac{1}{n}X^TX) - \sigma_{\max}(\Sigma)}{\sigma_{\min}(\frac{1}{n}X^TX)}| + \kappa(\Sigma)|\frac{\sigma_{\min}(\Sigma) - \sigma_{\min}(\frac{1}{n}X^TX)}{\sigma_{\min}(\frac{1}{n}X^TX)}| \\ &\leq \frac{n}{(\sqrt{n} - (CK^2)\sqrt{p} - t)^2} \cdot \left[CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right](\kappa(\Sigma) + 1) \end{split}$$

and similarly

$$|\kappa(X_0^T X_0) - 1| = \left| \frac{\sigma_{\max}(\frac{1}{n} X^T X)}{\sigma_{\min}(\frac{1}{n} X^T X)} - 1 \right|$$

$$\begin{split} &=|\frac{\sigma_{\max}(\frac{1}{n}X^TX)-\sigma_{\min}(\frac{1}{n}X^TX)}{\sigma_{\min}(\frac{1}{n}X^TX)}|\\ &\leq 2\frac{C\frac{K^2}{\sigma_{\min}(\Sigma)}\sqrt{\frac{p}{n}}+\frac{t}{\sqrt{n}}}{\frac{(\sqrt{n}-(C\frac{K^2}{\sigma_{\min}(\Sigma)})\sqrt{p}-t)^2}} = \frac{2n}{(\sqrt{n}-(C\frac{K^2}{\sigma_{\min}(\Sigma)})\sqrt{p}-t)^2}(C\frac{K^2}{\sigma_{\min}(\Sigma)}\sqrt{\frac{p}{n}}+\frac{t}{\sqrt{n}}) \end{split}$$

Therefore

$$\begin{split} |\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| &\leq \frac{2n}{(\sqrt{n} - (C\frac{K^2}{\sigma_{\min}(\Sigma)})\sqrt{p} - t)^2} \cdot (C\frac{K^2}{\sigma_{\min}(\Sigma)}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \\ &+ \frac{2n}{(\sqrt{n} - (CK^2)\sqrt{p} - t)^2} \cdot (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \\ &= \frac{2}{(1 - (C\frac{K^2}{\sigma_{\min}(\Sigma)})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (C\frac{K^2}{\sigma_{\min}(\Sigma)}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \\ &+ \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \end{split}$$

and if $\sigma_{\min}(\Sigma) \geq 1$, then the bound further simplifies to

$$|\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| \leq \frac{4}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2 \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})$$

Corollary 1 If in addition to the conditions in the theorem above, the population covariance matrix Σ satisfies $\sigma_{\min}(\Sigma) \geq 1$, the bound further simplifies to

$$|\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| \le \frac{4}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2 \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})$$

with probability at least $1 - 4\exp(-\frac{ct^2}{K^4})$.

The same result holds if the sub-Gaussian vector has non-zero mean μ .

Corollary 2 Same assumptions as in the previous theorem, but now with $\mathbb{E}X_i = \mu$, $\Sigma = \mathbb{E}X_i^T X_i$, and

$$X_0 = (X - \mu)(\Sigma - \mu^T \mu)^{-\frac{1}{2}}$$

Then with probability at least $1-2\exp(-\frac{ct^2}{K^4})-2\exp(-\frac{ct^2\sigma_{\min}^2(\Sigma)}{K^4})$,

$$\begin{split} |\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| &\leq \frac{2}{(1 - (C\frac{K^2}{\sigma_{\min}(\Sigma)})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (C\frac{K^2}{\sigma_{\min}(\Sigma)}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \\ &+ \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \end{split}$$

So far we have shown that the condition number $\kappa(X^TX)$ is close to $\kappa(\Sigma) \cdot \kappa(X_0^TX_0)$ with high probability. Our next step is to prove a similar result for normalization using batch statistics, in the special case when Σ is diagonal, i.e. the columns of X are also independent.

When the columns of X are also independent, a similar concentration holds for sub-Gaussian random matrices, and as a consequence, the condition number of a matrix normalized with sample statistics is also smaller by $\kappa(\Sigma)$ with high probability.

Lemma 2 (Rudelson and Vershynin (2010))Let X be an $n \times p$ matrix with $n \ge p$ whose columns X_j are i.i.d. sub-gaussian random vectors with $||X_j||_2 = \sqrt{n}$ almost surely, $K = ||X_j||_{\psi_2}$, and $\frac{1}{n}\mathbb{E}X^TX = I$. Then for universal constants c, C and every $t \ge 0$, with probability at least $1 - 2\exp(-\frac{ct^2}{K^4})$,

$$\left\|\frac{1}{n}X^TX - I\right\|_{op} \le CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

and

$$\sqrt{n} - (CK^2)\sqrt{p} - t \le \sigma_{\min}(X) \le \sigma_{\max}(X) \le \sqrt{n} + (CK^2)\sqrt{p} + t$$

Theorem 2 Let X be an $n \times p$ random matrix with i.i.d. sub-Gaussian rows X_i , $\mathbb{E}X_i = 0$, and let $\Sigma = \mathbb{E}X_i^T X_i = \frac{1}{n} \mathbb{E}X^T X$ be diagonal and positive definite. Let $\hat{\Sigma}$ be the diagonal matrix with $\hat{\Sigma}_{jj} = \frac{1}{n} (X^T X)_{jj}$. Let $X_0 := X \hat{\Sigma}^{-\frac{1}{2}}$ be the normalized matrix. Then for universal constants c, C, and $K = \max_j \|X_j\|_{\psi_2}$ where X_j is the j-th column of X, with probability at least $1 - 4 \exp(-\frac{ct^2}{K^4}) - 2 \exp(-\frac{ct^2\sigma_{\min}^2(\Sigma) - (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})}{K^4})$,

$$\begin{split} |\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| &\leq \frac{2}{(1 - (\frac{K^2}{\sigma_{\min}(\Sigma) - (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (C\frac{K^2}{\sigma_{\min}(\Sigma) - (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \\ &+ \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) \end{split}$$

Proof First note that since Σ is diagonal, the entries of X are independent. As a result, the sub-Gaussian norm of each row X_i of X is bounded above by the sub-Gaussian norm of the maximum of the sub-Gaussian norm of its entries, which is in turn bounded above by K.

Matrix concentration 1 then implies with probability at least $1 - 2\exp(-\frac{ct^2}{K^4})$,

$$\|\frac{1}{n}X^TX - \Sigma\|_{op} \le CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

On the other hand,

$$\mathbb{E}\frac{1}{n}X_0^T X_0 = I$$

where now X_0 has independent columns but not independent rows. In addition, for each row i of X_0 , it holds true that

$$\mathbb{E}(X_0)_i^T(X_0)_i = I$$

This is because of the identity

$$\sum_{i} (X_0)_i^T (X_0)_i = X_0^T X_0$$

and by symmetry,

$$\mathbb{E}(X_0)_i^T(X_0)_i = \mathbb{E}(X_0)_i^T(X_0)_i$$

for all i, j.

Note also that each column of X_0 satisfies $||(X_0^T)_j||_2 = \sqrt{n}$ by construction, and the columns are independent. In order to apply the concentration result 2 on matrices with independent columns, we need a bound on the sub-Gaussian norm of the columns of X_0 .

Since $X_0 = X\hat{\Sigma}^{-\frac{1}{2}}$, the rows of X_0 have sub-Gaussian norm of at most $\sqrt{\frac{K^2}{\sigma_{\min}(\hat{\Sigma})}}$. Moreover, since $\hat{\Sigma}$ is diagonal, the columns of X_0 also have sub-Gaussian norm of at most $\sqrt{\frac{K^2}{\sigma_{\min}(\hat{\Sigma})}}$. The entries of each column of X_0 are no longer independent, due to normalization, but are still uncorrelated, as their products have symmetric distributions. Recall that $\hat{\Sigma}_{jj} = \frac{1}{n}(X^TX)_{jj}$. The relationship between infinity and operator norm implies

$$\|\hat{\Sigma} - \Sigma\|_{op} = \|\hat{\Sigma} - \Sigma\|_{\infty} \le \|\frac{1}{n}X^TX - \Sigma\|_{\infty} \le \|\frac{1}{n}X^TX - \Sigma\|_{op} \le CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

We can conclude that the sub-Gaussian norm of columns of $X\hat{\Sigma}^{-\frac{1}{2}}$ is bounded above by $\sqrt{\frac{K^2}{\sigma_{\min}(\Sigma) - (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})}}$, with probability at least $1 - 2\exp(-\frac{ct^2}{K^4})$. Thus the concentration result on random matrices with independent columns apply, and with probability at least $1 - 2\exp(-\frac{ct^2}{K^4}) - 2\exp(-\frac{ct^2\sigma_{\min}^2(\Sigma) - (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})}{K^4})$,

$$\|\frac{1}{n}X_0^T X_0 - I\|_{op} \le C \frac{K^2}{\sigma_{\min}(\Sigma) - (CK^2 \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})} \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

This combined with

$$\|\frac{1}{n}X^TX - \Sigma\|_{op} \leq CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

lets us conclude that with probability $1-4\exp(-\frac{ct^2}{K^4})-2\exp(-\frac{ct^2\sigma_{\min}^2(\Sigma)-(CK^2\sqrt{\frac{P}{n}}+\frac{t}{\sqrt{n}})}{K^4})$,

$$|\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| \leq \frac{2}{(1 - (\frac{K^2}{\sigma_{\min}(\Sigma) - (CK^2 \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (C\frac{K^2}{\sigma_{\min}(\Sigma) - (CK^2 \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}) + \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2 \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})$$

and as before, with sufficiently large n and $\sigma_{\min}(\Sigma) \geq 1$, the bound simplifies to

$$|\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| \le \frac{4}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2 \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})$$

Corollary 3 If in addition to the conditions in the theorem above, the population covariance matrix Σ satisfies $\sigma_{\min}(\Sigma) \geq 1$, the bound further simplifies to

$$|\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| \le \frac{4}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2 \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})$$

 $\label{eq:with probability at least 1-4exp} with \ probability \ at \ least \ 1-4\exp(-\frac{ct^2}{K^4}) - 2\exp(-\frac{ct^2-(CK^2\sqrt{\frac{p}{n}}+\frac{t}{\sqrt{n}})}{K^4}).$

Corollary 4 Same assumptions as in the previous theorem, but now with $\mathbb{E}X_i = \mu$, $\Sigma = \mathbb{E}X_i^T X_i$. Let $\hat{\mu} = \frac{1}{n} \sum_i X_i$ be the sample mean of the columns, and \hat{D} be the diagonal matrix with entries $\hat{D}_{ii} = \frac{1}{n} \sum_j (X_{ji} - \hat{\mu}_i)^2$, or equivalently \hat{D} is the diagonal of the empirical covariance matrix $\frac{1}{n}(X - \hat{\mu})^T(X - \hat{\mu})$. If we center and normalize X with sample statistics:

$$X_0 = (X - \hat{\mu})\hat{D}^{-\frac{1}{2}}$$

 $Then \ with \ probability \ at \ least \ 1 - 4\exp(-\frac{ct^2}{K^4}) - 2\exp(-\frac{ct^2\sigma_{\min}^2(\Sigma) - (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})}{K^4}),$

$$|\kappa(X_0^T X_0) - \frac{\kappa(X^T X)}{\kappa(\Sigma)}| \leq \frac{2}{(1 - (C\frac{K^2}{\sigma_{\min}(\Sigma)})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (C\frac{K^2}{\sigma_{\min}(\Sigma)}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})$$

$$+ \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot (CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}})$$

So far our two results state that

- On one hand, for data matrix X with general covariance matrix not necessarily diagonal, if we have access to the population covariace Σ itself, then preconditioning X by $\Sigma^{-\frac{1}{2}}$ reduces the condition number by $\kappa(\Sigma)$ with high probability.
- On the other hand, if we don't have access to the population covariance Σ but we know Σ is diagonal, then preconditioning X by $\hat{\Sigma}^{-\frac{1}{2}}$, where $\hat{\Sigma}$ is the diagonal matrix with entries equal to the norms squared of each column, also reduces the condition number by $\kappa(\Sigma)$ with high probability.

To work towards the ultimate goal of preconditioning with the column sample standard deviations, we next consider the setting where the covariance matrix Σ is not necessarily diagonal, and show that preconditioning by the diagonal matrices $D = \operatorname{diag}(\Sigma)$ still results in the concentration of the condition number of the preconditioned matrix $XD^{-\frac{1}{2}}$, this time towards that of $\sqrt{\frac{\kappa(\Sigma)}{\kappa(D)}}$.

Theorem 3 Let X be an $n \times p$ random matrix with i.i.d. sub-Gaussian rows X_i with $K = ||X_i||_{\psi_2}$, $\mathbb{E}X_i = 0$, and let $\Sigma = \mathbb{E}X_i^T X_i = \frac{1}{n} \mathbb{E}X^T X$ be the population covariance matrix. Let D be the diagonal matrix with $D_{ii} = \Sigma_{ii}$, and let $X_0 := XD^{-\frac{1}{2}}$ the matrix normalized with diagonal entries of Σ . Then with probability at least $1 - 2 \exp(-\frac{ct^2(\min_i(\Sigma)_{ii})^2}{K^4}) - 2 \exp(-\frac{ct^2}{K^4})$,

$$\begin{split} |\frac{\kappa(X^TX)}{\kappa(\Sigma)} - \frac{\kappa(X_0^TX_0)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}| &\leq \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot \left[CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] \\ &+ \frac{2}{(1 - (C\frac{K^2}{\min_i(\Sigma)_{ii}})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot \left[C\frac{K^2}{\min_i(\Sigma)_{ii}}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] \end{split}$$

Proof Note that $\mathbb{E}\frac{1}{n}X_0^TX_0 = D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}}$, i.e. the population correlation matrix. Moreover, the sub-Gaussian norm of $X_0 = XD^{-\frac{1}{2}}$ is bounded above by $\|D^{-\frac{1}{2}}\|_{op}K$. By matrix concentration, with probability at least $1 - 2\exp(-\frac{ct^2(\min_i(\Sigma)_{ii})^2}{K^4}) - 2\exp(-\frac{ct^2}{K^4})$, the following two inequalities hold simultaneously

$$\|\frac{1}{n}X_0^T X_0 - D^{-\frac{1}{2}} \Sigma D^{-\frac{1}{2}}\|_{op} \le C \frac{K^2}{\min_i(\Sigma)_{ii}} \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$
$$\|\frac{1}{n}X^T X - \Sigma\|_{op} \le C K^2 \sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

and as a result

$$|\kappa(X^TX) - \kappa(\Sigma)| \leq \frac{1}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot \left[CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right](\kappa(\Sigma) + 1)$$

and similarly

$$|\kappa(X_0^TX_0) - \kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})| \leq \frac{1}{(1 - (C\frac{K^2}{\min_i(\Sigma)_{ii}})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot \left[C\frac{K^2}{\min_i(\Sigma)_{ii}}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] (\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}}) + 1)$$

Therefore

$$\begin{split} |\frac{\kappa(X^{T}X)}{\kappa(\Sigma)} - \frac{\kappa(X_{0}^{T}X_{0})}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}| &\leq \frac{2}{(1 - (CK^{2})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^{2}} \cdot \left[CK^{2}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] \\ &+ \frac{2}{(1 - (C\frac{K^{2}}{\min_{i}(\Sigma)_{ii}})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^{2}} \cdot \left[C\frac{K^{2}}{\min_{i}(\Sigma)_{ii}}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] \end{split}$$

which again simplifies to $\frac{2}{(1-(CK^2)\sqrt{\frac{p}{n}}-\frac{t}{\sqrt{n}})^2}\cdot\left[CK^2\sqrt{\frac{p}{n}}+\frac{t}{\sqrt{n}}\right]$ if the diagonal entries of Σ are bounded below by 1.

Corollary 5 Same assumptions as in the previous theorem, but now with $\mathbb{E}X_i = \mu$, $\Sigma = \mathbb{E}X_i^T X_i$. Let D be the diagonal matrix with $D_{ii} = (\Sigma - \mu^T \mu)_{ii}$. If we center and normalize X with population statistics:

$$X_0 = (X - \mu)(D)^{-\frac{1}{2}}$$

Then with probability at least $1 - 2\exp\left(-\frac{ct^2(\min_i D_{ii})^2}{K^4}\right) - 2\exp\left(-\frac{ct^2}{K^4}\right)$,

$$\begin{split} |\frac{\kappa(X^TX)}{\kappa(\Sigma)} - \frac{\kappa(X_0^TX_0)}{\kappa(D^{-\frac{1}{2}}(\Sigma - \mu^T\mu)D^{-\frac{1}{2}})}| &\leq \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot \left[CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] \\ &+ \frac{2}{(1 - (C\frac{K^2}{\min_i D_{ii}})\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot \left[C\frac{K^2}{\min_i D_{ii}}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] \end{split}$$

The above result says that if we normalize by the diagonal of the population covariance matrix, i.e. the population standard deviations, then we would get a reduction in condition number of $XD^{-\frac{1}{2}}$ on the order close to $\sqrt{\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}}$. Thus if the population covariance Σ has large condition number while the population correlation matrix $D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}}$ has small condition number, the reduction is large. However, the ratio $\frac{\kappa(\Sigma)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}$ is not always small, and in fact is not always bounded below by 1. In the next section, we analyze situations when the ratio is small for special classes of covariance matrices.

Now what is left to be proved is the most general version of condition number reduction with diagonal preconditioning, namely using sample standard deviations instead of population standard deviations.

Theorem 4 (Theorem 1 in paper) Let X be an $n \times p$ random matrix with i.i.d. sub-Gaussian rows X_i with $K = \|X_i\|_{\psi_2}$ the sub-Gaussian norm of its rows, $\mathbb{E}X_i = 0$, and let $\Sigma = \mathbb{E}X_i^T X_i = \frac{1}{n} \mathbb{E}X^T X$ be the population covariance matrix. Let \hat{D} be the diagonal matrix with $\hat{D}_{ii} = (X^T X)_{ii}$, i.e. \hat{D}_{ii} is the norm squared of the i-th column of X, and let $X_0 = X \hat{D}^{-\frac{1}{2}}$ be the matrix normalized with diagonal entries of \hat{D} . Let $D = \operatorname{diag}(\Sigma)$. Then with probability at least $1 - 2 \exp(-\frac{\operatorname{ct}^2(\min_i(\Sigma)_{ii})^2}{K^4}) - 2 \exp(-\frac{\operatorname{ct}^2}{K^4}) - 2p \exp(-\frac{\operatorname{c}}{K^4} \left[K^2 + \frac{\min_i(\Sigma)_{ii}}{\sqrt{p}} \cdot t\right]^2)$,

$$\begin{split} |\frac{\kappa(X^TX)}{\kappa(\Sigma)} - \frac{\kappa(X_0^TX_0)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}| &\leq \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot \left[CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] \\ &+ \frac{2}{(1 - (C\frac{K^2}{\min_i(\Sigma)_{ii}})\sqrt{\frac{p}{n}} - 3\frac{t}{\sqrt{n}})^2} \cdot \left[C\frac{K^2}{\min_i(\Sigma)_{ii}}\sqrt{\frac{p}{n}} + 3\frac{t}{\sqrt{n}}\right] \end{split}$$

Proof Since the rows of X are independent, its columns are sub-Gaussian vectors with independent entries with sub-Gaussian norm bounded above by K. Standard concentration result of the norm implies that with probability at least $1 - 2\exp(-\frac{cT^2}{K^4})$,

$$|\hat{D}_{ii}^{\frac{1}{2}} - D_{ii}^{\frac{1}{2}}| \le T$$

for all large T. Union bound then gives that with probability at least $1-2p\exp(-\frac{cT^2}{K^4})$,

$$|\hat{D}_{ii}^{\frac{1}{2}} - D_{ii}^{\frac{1}{2}}| \le T, \forall i$$

so that

$$|\frac{\hat{D}_{ii}^{\frac{1}{2}}}{D_{ii}^{\frac{1}{2}}} - 1| \le T \frac{1}{\sqrt{\min_{i}(\Sigma)_{ii}}}$$

For any i, j, let X_i denote the *i*th row of X, we have

$$\begin{split} |\hat{D}_{ii}^{-\frac{1}{2}}X_{i}^{T}X_{j}\hat{D}_{jj}^{-\frac{1}{2}} - D_{ii}^{-\frac{1}{2}}X_{i}^{T}X_{j}D_{jj}^{-\frac{1}{2}}| &\leq \|X_{i}^{T}\|_{2}\|X_{j}^{T}\|_{2}|\hat{D}_{ii}^{-\frac{1}{2}}\hat{D}_{jj}^{-\frac{1}{2}} - D_{ii}^{-\frac{1}{2}}D_{jj}^{-\frac{1}{2}}| \\ &= |\hat{D}_{ii}^{\frac{1}{2}}\hat{D}_{jj}^{\frac{1}{2}}| \cdot |\hat{D}_{ii}^{-\frac{1}{2}}\hat{D}_{jj}^{-\frac{1}{2}} - D_{ii}^{-\frac{1}{2}}D_{jj}^{-\frac{1}{2}}| \\ &= |1 - \frac{\hat{D}_{ii}^{\frac{1}{2}}\hat{D}_{jj}^{\frac{1}{2}}}{D_{ii}^{\frac{1}{2}}D_{jj}^{\frac{1}{2}}}| = |1 - \frac{\hat{D}_{ii}^{\frac{1}{2}}}{D_{ii}^{\frac{1}{2}}} + \frac{\hat{D}_{ii}^{\frac{1}{2}}}{D_{ii}^{\frac{1}{2}}} - \frac{\hat{D}_{ii}^{\frac{1}{2}}\hat{D}_{jj}^{\frac{1}{2}}}{D_{ii}^{\frac{1}{2}}D_{jj}^{\frac{1}{2}}}| \\ &\leq |1 - \frac{\hat{D}_{ii}^{\frac{1}{2}}}{D_{ii}^{\frac{1}{2}}}| + |\frac{\hat{D}_{ii}^{\frac{1}{2}}}{D_{ii}^{\frac{1}{2}}} - \frac{\hat{D}_{ii}^{\frac{1}{2}}\hat{D}_{jj}^{\frac{1}{2}}}{D_{ii}^{\frac{1}{2}}D_{jj}^{\frac{1}{2}}}| \\ &\leq T \frac{1}{\sqrt{\min_{i}(\Sigma)_{ii}}} (1 + \frac{\hat{D}_{ii}^{\frac{1}{2}}}{D_{ii}^{\frac{1}{2}}}) \leq 2 \frac{T^{2}}{\min_{i}(\Sigma)_{ii}} \end{split}$$

for all large T.

The relation between operator norm and maximum entry of a matrix A, $||A||_{op} \leq \sqrt{np} \cdot \max_{i,j} |A_{ij}|$ then implies that

$$\begin{split} \|\frac{1}{n}D^{-\frac{1}{2}}X^{T}XD^{-\frac{1}{2}} - \frac{1}{n}\hat{D}^{-\frac{1}{2}}X^{T}X\hat{D}^{-\frac{1}{2}}\|_{op} &\leq \sqrt{np} \cdot \frac{1}{n}\max_{i,j}|\hat{D}_{ii}^{-\frac{1}{2}}X_{i}^{T}X_{j}\hat{D}_{jj}^{-\frac{1}{2}} - D_{ii}^{-\frac{1}{2}}X_{i}^{T}X_{j}D_{jj}^{-\frac{1}{2}}|\\ &\leq 2\frac{T^{2}}{\min_{i}(\Sigma)_{ii}} \cdot \sqrt{\frac{p}{n}} \end{split}$$

Now recall the result from Theorem 5, that with probability at least $1 - 2\exp(-\frac{ct^2(\min_i(\Sigma)_{ii})^2}{K^4}) - 2\exp(-\frac{ct^2}{K^4})$, the following two inequalities hold simultaneously

$$\|\frac{1}{n}D^{-\frac{1}{2}}X^{T}XD^{-\frac{1}{2}} - D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}}\|_{op} \le C\frac{K^{2}}{\min_{i}(\Sigma)_{ii}}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$
$$\|\frac{1}{n}X^{T}X - \Sigma\|_{op} \le CK^{2}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

Now choose T such that $T^2 = K^2 + \frac{\min_i(\Sigma)_{ii}}{\sqrt{p}} \cdot t$, we see that

$$\|\frac{1}{n}D^{-\frac{1}{2}}X^{T}XD^{-\frac{1}{2}} - \frac{1}{n}\hat{D}^{-\frac{1}{2}}X^{T}X\hat{D}^{-\frac{1}{2}}\|_{op} \le 2\frac{K^{2}}{\min_{i}(\Sigma)_{ii}} \cdot \sqrt{\frac{p}{n}} + 2\frac{t}{\sqrt{n}}$$

so that

$$\|\frac{1}{n}\hat{D}^{-\frac{1}{2}}X^{T}X\hat{D}^{-\frac{1}{2}} - D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}}\|_{op} \leq C\frac{K^{2}}{\min_{i}(\Sigma)_{ii}}\sqrt{\frac{p}{n}} + 3\frac{t}{\sqrt{n}}$$
$$\|\frac{1}{n}X^{T}X - \Sigma\|_{op} \leq CK^{2}\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}$$

and eigenvalue stability result 2 allows us to conclude that

$$\begin{split} |\frac{\kappa(X^TX)}{\kappa(\Sigma)} - \frac{\kappa(X_0^TX_0)}{\kappa(D^{-\frac{1}{2}}\Sigma D^{-\frac{1}{2}})}| & \leq \frac{2}{(1 - (CK^2)\sqrt{\frac{p}{n}} - \frac{t}{\sqrt{n}})^2} \cdot \left[CK^2\sqrt{\frac{p}{n}} + \frac{t}{\sqrt{n}}\right] \\ & + \frac{2}{(1 - (C\frac{K^2}{\min_i(\Sigma)_{ii}})\sqrt{\frac{p}{n}} - 3\frac{t}{\sqrt{n}})^2} \cdot \left[C\frac{K^2}{\min_i(\Sigma)_{ii}}\sqrt{\frac{p}{n}} + 3\frac{t}{\sqrt{n}}\right] \end{split}$$

with probability at least

$$1 - 2\exp(-\frac{ct^2(\min_i(\Sigma)_{ii})^2}{K^4}) - 2\exp(-\frac{ct^2}{K^4}) - 2p\exp(-\frac{c}{K^4}\left[K^2 + \frac{\min_i(\Sigma)_{ii}}{\sqrt{p}} \cdot t\right]^2)$$

Appendix C: Results and Omitted Proofs on Optimal Diagonal Preconditioning

Proposition 1 (Proposition 1 in the paper) If $\kappa_0 > \kappa_1 > \kappa^*$, then $P(\kappa_0) > P(\kappa_1)$.

Proof Let D^0 and D^1 denote the analytic centers of $\Gamma(\kappa^0)$ and $\Gamma(\kappa^1)$, respectively. We know that D^1 is contained in the feasible region $\Gamma(\kappa^0)$, so that

$$P(\kappa_0) \ge \sum_i \log \lambda_i (M - D^1) + \sum_i \log \lambda_i (\kappa_0 D^1 - M) + \sum_i \log D^1$$

>
$$\sum_i \log \lambda_i (M - D^1) + \sum_i \log \lambda_i (\kappa_1 D^1 - M) + \sum_i \log D^1 = P(\kappa_1)$$

where the second inequality follows from the following minimax principle: for any real symmetric matrix with $\lambda_1 \geq \lambda_2 \dots$,

$$\lambda_k = \min_{C} \max_{\|C\|=1, Cx=0} \langle Ax, x \rangle$$

where C is any $(k-1) \times n$ matrix. This implies that if $A \succeq B$, $\lambda_k(A) \ge \lambda_k(B)$, since for

$$C = \arg\min_{C} \max_{\|C\|=1, Cx=0} \langle Ax, x \rangle$$

we have

$$\lambda_k(B) \leq \max_{\|C\|=1, Cx=0} \langle Bx, x \rangle \leq \max_{\|C\|=1, Cx=0} \langle Ax, x \rangle = \lambda_k(A)$$

and if $A \neq B$, then at least one inequality is strict.

Proposition 2 (Proposition 2 in the paper)Let t satisfy $\kappa^* \leq 2^t$, then for any $\overline{\kappa} > \kappa^* + 2^{-t}$, we have

$$P(\overline{\kappa}) > -Cpt$$

for some universal constant that only depends on M.

Proof Recall that

$$P(\kappa) = \max_{D \succeq 0} \log \det(M-D) + \log \det(\kappa D - M) + \log \det D$$

Since $\overline{\kappa} > \kappa^*$, $\Gamma(\overline{\kappa})$ has a bounded and nonempty interior. We claim that there exists an interior point $\overline{D} \in \Gamma(\overline{\kappa})$ such that

$$\overline{D} \succeq 2^{-Ct}I$$

$$M - \overline{D} \succeq 2^{-Ct}I$$

$$\overline{\kappa}\overline{D} - M \succ 2^{-Ct}I$$

for some C that only depends on M. We may obtain this \overline{D} by shrinking any D^* that satisfies

$$M - D^* \succeq 0$$

$$\kappa^* D^* - M \succeq 0$$

$$D^* \succeq 0$$

as follows. Given D^* satisfying the above conditions, we can first find some C such that $D^* \succeq 2^{-Ct}I$. Then for $\delta > 0$ sufficiently close to 0,

$$M - 2^{-\delta t} \cdot D^* \succeq M - D^* + (D^* - 2^{-\delta t} \cdot D^*)$$

 $\succeq (1 - 2^{-\delta t})2^{-Ct}I \succeq 2^{-C't}I$

Finally, since $\overline{\kappa} > \kappa^* + 2^{-t}$, we have

$$\overline{\kappa} 2^{-\delta t} D^* - M \succeq (\kappa^* + 2^{-t}) 2^{-\delta t} D^* - M$$
$$\succeq 2^{-(1+\delta)t} D^* \succeq 2^{-C't} I$$

so that $\overline{D} = 2^{-\delta t}D^*$ satisfies the required conditions. This implies that $P(\overline{\kappa}) \ge P(\overline{D}, \overline{\kappa}) > -Cpt$. \square Recall the following property which is useful in our proof.

Lemma 3 Let X be a symmetric matrix, ||X|| be the Frobenius norm, and $||X||_{\infty} = \max_{j} |\lambda_{j}(X)|$. Then if $||X||_{\infty} < 1$,

$$Tr(X) \ge \log \det(I+X) \ge Tr(X) - \frac{\|X\|^2}{2(1-\|X\|_{\infty})}$$

Theorem 5 (Theorem 3 in the paper) Let $\kappa^* \in [1, \infty)$ be the solution of

$$\min_{D \succeq 0} \kappa$$

$$s.t.M \succeq D$$

$$\kappa D \succeq M$$

and let $\overline{\kappa}$ be a known upper bound of κ^* , i.e.

$$\min_{D \succeq 0} 0$$

$$s.t.M \succeq D$$

$$\overline{\kappa}D \succ M$$

is feasible.

Let D^0 and D^1 be the analytic centers of $\Gamma^0 = \Gamma(\kappa^0)$ and $\Gamma^1 = \Gamma(\kappa^1)$ for $\kappa^0, \kappa^1 \in (\kappa^*, \overline{\kappa})$. If $\Delta \kappa = \kappa^0 - \kappa^1 > 0$ satisfies

$$\Delta \kappa = \frac{\beta}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})}$$
$$= \frac{\beta}{e^T D^0 \operatorname{diag}((\kappa^0 D^0 - M)^{-1})e}$$

for some sufficiently small $\beta \in (0,1)$ that only depends on $\overline{\kappa}, M$, then

$$Tr(D^1(D^0)^{-1}) \le O(1)$$

$$Tr(D^0(D^1)^{-1}) \leq O(1)$$

and

$$P(\kappa^1) \le P(\kappa^0) - \beta$$

Proof First note that the function

$$P(D, \kappa) = \log \det(M - D) + \log \det(\kappa D - M) + \log \det D$$

is jointly concave in (κ, D) on any convex set $(\underline{\kappa}, \infty) \times \mathcal{D}(\underline{\kappa})$ for any $\underline{\kappa} > \kappa^*$, and $\mathcal{D}(\kappa)$ is the set of all positive matrices such that $\kappa D - M \succ 0$. This implies that

$$\underline{P}(\kappa) = \max_{D \in \mathcal{D}(\kappa)} \log \det(M - D) + \log \det(\kappa D - M) + \log \det D$$

is a concave function on $(\underline{\kappa}, \infty)$. Note, however, that $\underline{P}(\kappa)$ is not necessarily equal to $P(\kappa)$, because for $\kappa^0 > \underline{\kappa}$, the solution D^0 of

$$\max_{D \in \mathcal{D}(\kappa^0)} \log \det(M - D) + \log \det(\kappa^0 D - M) + \log \det D$$

does not necessarily satisfy $D^0 \in \mathcal{D}(\underline{\kappa})$. Fortunately, since the optimizer $D(\kappa)$ corresponding to each κ is always in the interior of $\mathcal{D}(\kappa)$, if β is small enough, we can guarantee that $D^0 \in \mathcal{D}(\kappa^1)$ with $\kappa^1 = \kappa^0 - \Delta \kappa$ and $\Delta \kappa = \frac{\beta}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})}$. More precisely, with D^0 being the solution of

$$\max_{D \in \mathcal{D}(\kappa^0)} \log \det(M - D) + \log \det(\kappa^0 D - M) + \log \det D$$

and $\kappa^1 = \kappa^0 - \Delta \kappa$, we have

$$\begin{aligned} |\lambda_n(\kappa^1 D^0 - M) - \lambda_n(\kappa^0 D^0 - M)| &\leq \Delta \kappa \cdot \max_i D_{ii}^0 \\ &= \frac{\beta}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})} \cdot \max_i D_{ii}^0 \\ &\leq \frac{\beta}{(\min_i D_{ii}^0) \cdot \lambda_1((\kappa^0 D^0 - M)^{-1})} \cdot \max_i D_{ii}^0 \\ &= \beta \cdot \kappa(D^0) \cdot \lambda_n(\kappa^0 D^0 - M) \end{aligned}$$

where we have used Weyl's inequality and

$$Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1}) \ge Tr(\min_i D^0_{ii} \cdot I \cdot (\kappa^0 D^0 - M)^{-1})$$

 $\ge \min_i D^0_{ii} \cdot \lambda_1 ((\kappa^0 D^0 - M)^{-1})$

Since $\kappa(D^0)$ is bounded above by some universal constant that only depends on $M, \overline{\kappa}$, with β small enough, we have

$$\lambda_n(\kappa^1 D^0 - M) \ge \lambda_n(\kappa^0 D^0 - M) - \beta \cdot \kappa(D^0) \cdot \lambda_n(\kappa^0 D^0 - M)$$

$$> 0$$

so that D^0 is in the interior of $\mathcal{D}(\kappa^1)$.

Thus on any interval $[\kappa^1, \kappa^0] \subset (\kappa^*, \overline{\kappa})$ with length bounded by $\frac{\beta}{Tr(D^0, (\kappa^0 D^0 - M)^{-1})}$, the function

$$P(\kappa) = \max_{D \in \mathcal{D}(\kappa)} \log \det(M - D) + \log \det(\kappa D - M) + \log \det D$$

is concave in κ .

Now

$$P(\kappa) = P(D(\kappa), \kappa)$$

where $D(\kappa)$ is the unique maximizer corresponding to κ , so that

$$\frac{d}{d\kappa}P(\kappa) = Tr(\nabla_D P(D(\kappa), \kappa) \cdot \partial_{\kappa} D(\kappa)) + \partial_{\kappa} P(D(\kappa), \kappa)$$
$$= \partial_{\kappa} P(D(\kappa), \kappa)$$
$$= Tr(D \cdot (\kappa D - M)^{-1})$$

using the envelope theorem, or equivalently the first order condition of the maximization problem. By concavity of $P(\kappa)$, we have

$$P(\kappa^{1}) - P(\kappa^{0}) \leq \frac{d}{d\kappa} P(\kappa) \mid_{\kappa^{0}} \cdot (\kappa^{1} - \kappa^{0})$$
$$= -\Delta \kappa \cdot Tr(D^{0} \cdot (\kappa^{0}D^{0} - M)^{-1})$$
$$= -\beta$$

and since $P(\kappa)$ is increasing and concave on $[\kappa^1, \kappa^0]$

$$\begin{split} |P(\kappa^1) - P(\kappa^0)| &\leq \max_{\kappa \in [\kappa^1, \kappa^0]} |\frac{d}{d\kappa} P(\kappa)|_{\kappa} | \cdot \Delta \kappa \\ &= \Delta \kappa \cdot Tr(D^0 \cdot (\kappa^1 D^0 - M)^{-1}) \\ &= \beta \cdot \frac{Tr(D^0 \cdot (\kappa^1 D^0 - M)^{-1})}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})} \\ &\leq \beta \cdot \kappa(D^0) \cdot \frac{Tr((\kappa^1 D^0 - M)^{-1})}{Tr((\kappa^0 D^0 - M)^{-1})} \\ &= \beta \cdot \kappa(D^0) \cdot \frac{\sum_i \frac{1}{\lambda_i(\kappa^1 D^0 - M)}}{\sum_i \frac{1}{\lambda_i(\kappa^0 D^0 - M)}} \end{split}$$

$$\begin{split} &=\beta \cdot \kappa(D^0) \cdot \frac{\sum_i \frac{\lambda_1(\kappa^0 D^0 - M)}{\lambda_i(\kappa^1 D^0 - M)}}{\sum_i \frac{\lambda_1(\kappa^0 D^0 - M)}{\lambda_i(\kappa^0 D^0 - M)}} \\ &\leq \beta \cdot \kappa(D^0) \cdot \frac{\sum_i \frac{\lambda_1(\kappa^0 D^0 - M)}{\lambda_i(\kappa^1 D^0 - M)}}{n} \\ &= \beta \cdot \kappa(D^0) \cdot \frac{\sum_i \frac{\lambda_n(\kappa^1 D^0 - M)}{\lambda_i(\kappa^1 D^0 - M)}}{n} \cdot \frac{\lambda_1(\kappa^0 D^0 - M)}{\lambda_n(\kappa^1 D^0 - M)} \\ &\leq \beta \cdot \kappa(D^0) \cdot \frac{\lambda_1(\kappa^0 D^0 - M)}{\lambda_1(\kappa^1 D^0 - M)} \cdot \frac{\lambda_1(\kappa^1 D^0 - M)}{\lambda_n(\kappa^1 D^0 - M)} \\ &\leq \beta \cdot \kappa(D^0) \cdot \frac{\lambda_1(\kappa^0 D^0 - M)}{\lambda_1(\kappa^1 D^0 - M)} \cdot \frac{\lambda_1(\kappa^1 D^0 - M)}{\lambda_n(\kappa^1 D^0 - M)} \end{split}$$

and

$$\frac{\lambda_1(\kappa^0 D^0 - M)}{\lambda_1(\kappa^1 D^0 - M)} \le C(\beta, \kappa^*, \overline{\kappa})$$
$$\frac{\lambda_1(\kappa^1 D^0 - M)}{\lambda_n(\kappa^1 D^0 - M)} \le C(\beta, \kappa^*, \overline{\kappa})$$

by a similar argument as before. So there exists $\xi > 0$ depending only on $\beta, \kappa^*, \overline{\kappa}$, so that

$$-\xi - \beta \le P(\kappa^1) - P(\kappa^0) \le -\beta$$

Now we show that D^0 and D^1 are close. Recall the inequality

$$Tr(X) \ge \log \det(I+X) \ge Tr(X) - \frac{\|X\|^2}{2(1-\|X\|_{\infty})}$$

$$\begin{split} \log \det((D^0)^{-1}D^1) &\leq Tr((D^0)^{-1}(D^1 - D^0)) \\ &\leq \log \det((D^0)^{-1}D^1) + \frac{\|(D^0)^{-1}(D^1 - D^0)\|}{2(1 - \lambda_1((D^0)^{-1}(D^1 - D^0)))} \\ &\log \det(M - D^0)^{-1}(M - D^1) \leq Tr((M - D^0)^{-1}(D^0 - D^1))) \\ &\leq \log \det(M - D^0)^{-1}(M - D^1) + \frac{\|(M - D^0)^{-1}(D^0 - D^1)\|}{2(1 - \lambda_1((M - D^0)^{-1}(D^0 - D^1)))} \\ &\log \det(\kappa^0 D^0 - M)^{-1}(\kappa^1 D^1 - M) \leq Tr((\kappa^0 D^0 - M)^{-1}(\kappa^1 D^1 - \kappa^0 D^0)) \\ &\leq \log \det(\kappa^0 D^0 - M)^{-1}(\kappa^1 D^1 - M) + \frac{\|(\kappa^0 D^0 - M)^{-1}(\kappa^1 D^1 - \kappa^0 D^0)\|}{2(1 - \lambda_1((\kappa^0 D^0 - M)^{-1}(\kappa^1 D^1 - \kappa^0 D^0)))} \end{split}$$

summing the inequalities, and using

$$-(M-D^0)^{-1} + \kappa^0 (\kappa^0 D^0 - M)^{-1} + (D^0)^{-1} = 0$$

we have

$$-\Delta \kappa \cdot Tr((\kappa^0 D^0 - M)^{-1} D^1) \ge P(\kappa^1) - P(\kappa^0)$$
$$\ge -\beta - \xi$$

Recall that

$$\Delta \kappa = \frac{\beta}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})}$$

so that

$$\frac{Tr((\kappa^0 D^0 - M)^{-1} D^1)}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})} \leq 1 + \frac{\xi}{\beta}$$

and the left hand side is bounded below by

$$\begin{split} \frac{Tr((\kappa^0D^0-M)^{-1}D^1)}{Tr(D^0\cdot(\kappa^0D^0-M)^{-1})} &= \frac{Tr((\kappa^0D^0-M)^{-1}D^0\cdot(D^0)^{-1}D^1)}{Tr(D^0\cdot(\kappa^0D^0-M)^{-1})} \\ &\geq \frac{\sum_i \lambda_i((\kappa^0D^0-M)^{-1}D^0)\cdot\lambda_{n-i+1}((D^0)^{-1}D^1)}{Tr(D^0\cdot(\kappa^0D^0-M)^{-1})} \\ &\geq \frac{(\sum_i \lambda_i^2((\kappa^0D^0-M)^{-1}D^0))^{\frac{1}{2}}\cdot(\sum_i \lambda_{n-i+1}^2((D^0)^{-1}D^1))^{\frac{1}{2}}}{Tr(D^0\cdot(\kappa^0D^0-M)^{-1})} \cdot \eta \\ &= \frac{\frac{1}{n}(\sum_i \lambda_i((\kappa^0D^0-M)^{-1}D^0))\cdot(\sum_i \lambda_{n-i+1}((D^0)^{-1}D^1))}{Tr(D^0\cdot(\kappa^0D^0-M)^{-1})} \cdot \eta \\ &= Tr((D^0)^{-1}D^1)\cdot\frac{1}{n}\cdot\eta \end{split}$$

where η is upper bounded by a universal constant, so that

$$Tr(D^1(D^0)^{-1}) \le O(1)$$

Proposition 6. (Proposition 4 in the paper)Let $(\overline{R}^0, \overline{S}^0, \overline{D}^0, \overline{X}^0, \overline{Y}^0, \overline{Z}^0)$ be any set that satisfy

$$\overline{R}^0 = M - \overline{D}^0 \succeq 0$$
$$\overline{S}^0 = \kappa^1 \overline{D}^0 - M \succeq 0$$
$$\overline{D}^0 \succ 0$$

and

$$\overline{Z}^0 + \kappa^1 \overline{Y}^0 = \overline{X}^0$$

with

$$\delta(\overline{R}^0, \overline{X}^0) = \|(\overline{R}^0)^{\frac{1}{2}} \overline{X}^0 (\overline{R}^0)^{\frac{1}{2}} - I\|_F \le \beta$$

$$\delta(\overline{D}^0, \overline{Z}^0) = \|(\overline{D}^0)^{\frac{1}{2}} \overline{Z}^0 (\overline{D}^0)^{\frac{1}{2}} - I\|_F \le \beta$$

$$\delta(\overline{S}^0, \overline{Y}^0) = \|(\overline{S}^0)^{\frac{1}{2}} \overline{Y}^0 (\overline{S}^0)^{\frac{1}{2}} - I\|_F \le \beta$$

for any $\beta \in (0,1)$.

Let $X^1, Y^1, Z^1, R^1, S^1, D^1$ be defined by

$$X^{1} = \overline{X}^{0} + \Delta X$$

$$Y^{1} = \overline{Y}^{0} + \Delta Y$$

$$Z^{1} = \overline{Z}^{0} + \Delta Z$$

$$R^{1} = \overline{R}^{0} + \Delta R$$

$$S^{1} = \overline{S}^{0} + \Delta S$$

$$D^{1} = \overline{D}^{0} + \Delta D$$

where the increments Δs are given by the Newton step

$$\Delta Z + W^{-1} \Delta D W^{-1} = (\overline{D}^0)^{-1} - \overline{Z}^0$$

$$\Delta X + U^{-1} \Delta R U^{-1} = (\overline{R}^0)^{-1} - \overline{X}^0$$

$$\Delta Y + V^{-1} \Delta S V^{-1} = (\overline{S}^0)^{-1} - \overline{Y}^0$$

and

$$\Delta R = -\Delta D$$

$$\Delta S = \kappa^{1} \Delta D$$

$$\Delta Z + \kappa^{1} \Delta Y = \Delta X$$

where U, V, W are the geometric means

$$U = (\overline{R}^{0})^{1/2} ((\overline{R}^{0})^{1/2} \overline{X}^{0} (\overline{R}^{0})^{1/2})^{-1/2} (\overline{R}^{0})^{1/2}$$

$$V = (\overline{S}^{0})^{1/2} ((\overline{S}^{0})^{1/2} \overline{Y}^{0} (\overline{S}^{0})^{1/2})^{-1/2} (\overline{S}^{0})^{1/2}$$

$$W = (\overline{D}^{0})^{1/2} ((\overline{D}^{0})^{1/2} \overline{Z}^{0} (\overline{D}^{0})^{1/2})^{-1/2} (\overline{D}^{0})^{1/2}$$

to ensure that updates Δs are symmetric.

Then we have

$$\delta(R^{1}, X^{1}) = \|(R^{1})^{\frac{1}{2}} X^{1} (R^{1})^{\frac{1}{2}} - I\|_{F} \leq \frac{1}{2} \frac{\beta^{2}}{1 - \beta}$$

$$\delta(S^{1}, Y^{1}) = \|(S^{1})^{\frac{1}{2}} Y^{1} (S^{1})^{\frac{1}{2}} - I\|_{F} \leq \frac{1}{2} \frac{\beta^{2}}{1 - \beta}$$

$$\delta(D^{1}, Z^{1}) = \|(D^{1})^{\frac{1}{2}} Z^{1} (D^{1})^{\frac{1}{2}} - I\|_{F} \leq \frac{1}{2} \frac{\beta^{2}}{1 - \beta}$$

and

$$\|(\overline{D}^0)^{-\frac{1}{2}}D^1(\overline{D}^0)^{-\frac{1}{2}} - I\|_F \le \frac{\beta}{1-\beta}$$

Proof First observe that the Newton system has a unique solution. To see this, note that we can eliminate $\Delta X, \Delta Y, \Delta Z$ using $\Delta Z + \kappa^1 \Delta Y = \Delta X$. Then using

$$\Delta R = -\Delta D$$
$$\Delta S = \kappa^1 \Delta D$$

we can uniquely solve for ΔD , from which all other increments can be uniquely determined.

We have

$$\begin{split} \delta(D^1,Z^1)^2 &= \|(Z^1)^{\frac{1}{2}}D^1(Z^1)^{\frac{1}{2}} - I\|_F^2 = Tr(((Z^1)^{\frac{1}{2}}D^1(Z^1)^{\frac{1}{2}} - I)^2) \\ &= Tr((Z^1)D^1(Z^1)D^1) - 2Tr(Z^1D^1) + Tr(I) \\ &= Tr((D^1Z^1 - I)^2) \\ &\leq \left(Tr(D^1Z^1 - I)\right)^2 \end{split}$$

where we have used $Tr(A^2) = (TrA)^2 - 2\sigma_2(A)$ where

$$\sigma_2(A) = \sum_{i < j} \lambda_i \lambda_j$$

and λ_i are the eigenvalues of A.

The Newton update formula

$$\Delta Z + W^{-1} \Delta D W^{-1} = (\overline{D}^0)^{-1} - \overline{Z}^0$$

$$Z^1 = Z^0 + \Delta Z$$

$$D^1 = D^0 + \Delta D$$

and

$$W = (\overline{D}^0)^{1/2} ((\overline{D}^0)^{1/2} \overline{Z}^0 (\overline{D}^0)^{1/2})^{-1/2} (\overline{D}^0)^{1/2}$$

imply

$$\begin{split} Tr(D^1Z^1-I) &= Tr((\overline{D}^0+\Delta D)(\overline{Z}^0+\Delta Z)-I) \\ &= Tr(\overline{D}^0\overline{Z}^0+\Delta D\overline{Z}^0+\overline{D}^0\Delta Z+\Delta D\Delta Z-I) \\ &= Tr(-\overline{D}^0W^{-1}\Delta DW^{-1}+\Delta D\overline{Z}^0+\Delta D\Delta Z) \\ &= Tr(-(\overline{D}^0)^{1/2}\overline{Z}^0(\overline{D}^0)^{1/2}(\overline{D}^0)^{-1/2}\Delta D(\overline{D}^0)^{-1/2}+\Delta D\overline{Z}^0+\Delta D\Delta Z) \\ &= Tr(-\Delta D\overline{Z}^0+\Delta D\overline{Z}^0+\Delta D\Delta Z) \\ &= Tr(\Delta D\Delta Z) \end{split}$$

So that

$$\delta(D^1, Z^1) \le Tr(\Delta D \Delta Z)$$

and similarly

$$\delta(R^1, X^1) \le Tr(\Delta R \Delta X)$$

 $\delta(S^1, Y^1) \le Tr(\Delta S \Delta Y)$

Multiplying both sides of

$$\Delta Z + W^{-1} \Delta D W^{-1} = (\overline{D}^0)^{-1} - \overline{Z}^0$$

by $W^{\frac{1}{2}}$ on the left and on the right we have

$$W^{\frac{1}{2}} \Delta Z W^{\frac{1}{2}} + W^{-\frac{1}{2}} \Delta D W^{-\frac{1}{2}} = W^{\frac{1}{2}} (\overline{D}^0)^{-1} W^{\frac{1}{2}} - W^{\frac{1}{2}} \overline{Z}^0 W^{\frac{1}{2}}$$

Then squaring and taking the trace,

$$Tr(W^{\frac{1}{2}}\Delta ZW^{\frac{1}{2}}+W^{-\frac{1}{2}}\Delta DW^{-\frac{1}{2}})^2=Tr(W^{\frac{1}{2}}(\overline{D}^0)^{-1}W^{\frac{1}{2}}-W^{\frac{1}{2}}\overline{Z}^0W^{\frac{1}{2}})^2$$

and the left hand side is equal to

$$\begin{split} Tr(W^{\frac{1}{2}}\Delta ZW^{\frac{1}{2}} + W^{-\frac{1}{2}}\Delta DW^{-\frac{1}{2}})^2 &= Tr(W^{\frac{1}{2}}\Delta ZW^{\frac{1}{2}})^2 + Tr(W^{-\frac{1}{2}}\Delta DW^{-\frac{1}{2}})^2 \\ &\quad + Tr(\Delta Z\Delta D) + Tr(\Delta D\Delta Z) \end{split}$$

So we have

$$2Tr(\Delta Z \Delta D) \leq Tr(W^{\frac{1}{2}}(\overline{D}^{0})^{-1}W^{\frac{1}{2}} - W^{\frac{1}{2}}\overline{Z}^{0}W^{\frac{1}{2}})^{2}$$

Now we calculate the right hand side. Using

$$W = (\overline{D}^{0})^{1/2} ((\overline{D}^{0})^{1/2} \overline{Z}^{0} (\overline{D}^{0})^{1/2})^{-1/2} (\overline{D}^{0})^{1/2}$$
$$= (\overline{Z}^{0})^{-1/2} ((\overline{Z}^{0})^{1/2} \overline{D}^{0} (\overline{Z}^{0})^{1/2})^{1/2} (\overline{Z}^{0})^{-1/2}$$

we get

$$\begin{split} Tr(W^{\frac{1}{2}}(\overline{D}^{0})^{-1}W^{\frac{1}{2}})^{2} &= Tr(\overline{D}^{0})^{1/2}((\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2})^{-1}(\overline{D}^{0})^{1/2}(\overline{D}^{0})^{-1} \\ &= Tr(\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-1} \\ &Tr(W^{\frac{1}{2}}\overline{Z}^{0}W^{\frac{1}{2}})^{2} = Tr(\overline{Z}^{0})^{-1/2}((\overline{Z}^{0})^{1/2}\overline{D}^{0}(\overline{Z}^{0})^{1/2})^{1}(\overline{Z}^{0})^{-1/2}\overline{Z}^{0} \\ &= Tr\overline{D}^{0}\overline{Z}^{0} \\ &Tr(W^{\frac{1}{2}}(\overline{D}^{0})^{-1}W^{\frac{1}{2}})(W^{\frac{1}{2}}\overline{Z}^{0}W^{\frac{1}{2}}) = Tr(I) \\ &Tr(W^{\frac{1}{2}}\overline{Z}^{0}W^{\frac{1}{2}})(W^{\frac{1}{2}}(\overline{D}^{0})^{-1}W^{\frac{1}{2}}) = Tr(I) \end{split}$$

so that

$$\begin{split} Tr(W^{\frac{1}{2}}(\overline{D}^{0})^{-1}W^{\frac{1}{2}} - W^{\frac{1}{2}}\overline{Z}^{0}W^{\frac{1}{2}})^{2} &= Tr(\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-1} + Tr\overline{D}^{0}\overline{Z}^{0} + 2Tr(I) \\ &= Tr((\overline{D}^{0})^{-1/2}(\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-1/2}(I - 2(\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2} + ((\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2})^{2})) \\ &= Tr((\overline{D}^{0})^{-1/2}(\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-1/2}(I - (\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2})^{2}) \end{split}$$

Now recall that

$$\delta(\overline{D}^0, \overline{Z}^0) = \|(\overline{D}^0)^{\frac{1}{2}} \overline{Z}^0 (\overline{D}^0)^{\frac{1}{2}} - I\|_F \le \beta$$

and so

$$Tr((I - (\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2})^{2}) = \|(\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2} - I\|_{F}^{2}$$
$$= \delta(\overline{D}^{0}, \overline{Z}^{0})^{2} < \beta^{2}$$

and Holder's inequality yields

$$Tr((\overline{D}^{0})^{-1/2}(\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-1/2}(I - (\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2})^{2}) \leq \lambda_{1}((\overline{D}^{0})^{-1/2}(\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-1/2}) \cdot Tr(I - (\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2})^{2}) \\ \leq \lambda_{1}((\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-1})\beta^{2}$$

Recall the eigenvalue stability result

$$|\lambda_i(X) - \lambda_i(Y)| \le ||X - Y||_{op}$$

for symmetric positive definite matrices X,Y and again using

$$\begin{split} \|(\overline{D}^0)^{1/2}\overline{Z}^0(\overline{D}^0)^{1/2} - I\|_F &= \|\overline{D}^0\overline{Z}^0 - I\|_F \\ &= \sqrt{Tr(\overline{D}^0\overline{Z}^0 - I)^T(\overline{D}^0\overline{Z}^0 - I)} \le \beta \end{split}$$

and the inequality

$$||X||_{op} \le ||X||_F$$

between operator norm and Frobenius norm, we have

$$|\lambda_{n}((\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2}) - 1| = |\lambda_{n}((\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2}) - \lambda_{n}(I)|$$

$$\leq \|(\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2} - I\|_{op} \leq \|(\overline{D}^{0})^{1/2}\overline{Z}^{0}(\overline{D}^{0})^{1/2} - I\|_{F} \leq \beta$$

so that

$$\lambda_n((\overline{D}^0)^{1/2}\overline{Z}^0(\overline{D}^0)^{1/2}) \ge 1 - \beta$$

and

$$\lambda_1((\overline{D}^0)^{-1/2}(\overline{Z}^0)^{-1}(\overline{D}^0)^{-1/2}) = \frac{1}{\lambda_n((\overline{D}^0)^{1/2}\overline{Z}^0(\overline{D}^0)^{1/2})} \le \frac{1}{1-\beta}$$

This allows us to finally conclude that

$$Tr(\Delta Z \Delta D) \le \frac{1}{2} \frac{\beta^2}{1-\beta}$$

and so

$$\begin{split} \delta(D^1, Z^1) &\leq Tr(\Delta Z \Delta D) \\ &\leq \frac{1}{2} \frac{\beta^2}{1 - \beta} \end{split}$$

The same argument applied to (R^1, X^1) , (S^1, Y^1) gives

$$\delta(R^{1}, X^{1}) \leq \frac{1}{2} \frac{\beta^{2}}{1 - \beta}$$
$$\delta(S^{1}, Y^{1}) \leq \frac{1}{2} \frac{\beta^{2}}{1 - \beta}$$

Now we show that

$$\|(\overline{D}^0)^{-\frac{1}{2}}D^1(\overline{D}^0)^{-\frac{1}{2}} - I\|_F \le \frac{\beta}{1-\beta}$$

Note

$$\begin{split} \|(\overline{D}^{0})^{-\frac{1}{2}}D^{1}(\overline{D}^{0})^{-\frac{1}{2}} - I\|_{F}^{2} &= Tr(((\overline{D}^{0})^{-\frac{1}{2}}D^{1}(\overline{D}^{0})^{-\frac{1}{2}} - I)^{2}) \\ &= Tr(((\overline{D}^{0})^{-1}(D^{1} - \overline{D}^{0})(\overline{D}^{0})^{-1}(D^{1} - \overline{D}^{0}) \\ &= Tr((\overline{D}^{0})^{-1}\Delta D(\overline{D}^{0})^{-1}\Delta D) \end{split}$$

Now multiplying both sides of

$$W\Delta ZW + \Delta D = (\overline{Z}^0)^{-1} - \overline{D}^0$$

by $(\overline{D}^0)^{-\frac{1}{2}}$, we have

$$Tr(((\overline{D}^{0})^{-1}\Delta D)^{2}) \leq Tr(((\overline{D}^{0})^{-1}(\overline{Z}^{0})^{-1} - I))^{2})$$

$$= \|(\overline{D}^{0})^{-\frac{1}{2}}(\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-\frac{1}{2}} - I\|_{F}^{2}$$

$$= \|(I - (\overline{D}^{0})^{\frac{1}{2}}(\overline{Z}^{0})(\overline{D}^{0})^{\frac{1}{2}})((\overline{D}^{0})^{-\frac{1}{2}}(\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-\frac{1}{2}})\|_{F}^{2}$$

$$\leq Tr((I - (\overline{D}^{0})^{\frac{1}{2}}(\overline{Z}^{0})(\overline{D}^{0})^{\frac{1}{2}})^{2})\lambda_{1}(((\overline{D}^{0})^{-\frac{1}{2}}(\overline{Z}^{0})^{-1}(\overline{D}^{0})^{-\frac{1}{2}})^{2})$$

$$\leq \beta^{2}/(1 - \beta)^{2}$$

as desired.

PROPOSITION 7. (Proposition 5 in paper) Suppose that $(R^0, S^0, D^0, X^0, Y^0, Z^0)$ satisfy

$$R^{0} = M - D^{0} \succeq 0$$

$$S^{0} = \kappa^{0} S^{0} - M \succeq 0$$

$$D^{0} \succeq 0$$

$$Z^{0} + \kappa^{0} Y^{0} = X^{0}$$

with $\delta(R^0, X^0) \leq \delta, \delta(D^0, Z^0) \leq \delta, \delta(S^0, Y^0) \leq \delta$ for some $\delta \in (0, 1)$. Further, let $\Delta \kappa = \kappa^0 - \kappa^1$ with

$$\Delta \kappa = \frac{\beta}{Tr(D^0 \cdot (\kappa^0 D^0 - M)^{-1})}$$

where $\beta \in (0,1)$ is a sufficiently small constant, then with

$$\begin{split} \overline{R}^0 &= R^0, \overline{S}^0 = -\Delta \kappa D^0 + S^0, \overline{D}^0 = D^0 \\ \overline{X}^0 &= X^0, \overline{Y}^0 = Y^0, \overline{Z}^0 = \Delta \kappa Y^0 + Z^0 \end{split}$$

we have $\overline{R}^0 = M - \overline{D}^0 \succeq 0$, $\overline{S}^0 = \kappa^1 \overline{D}^0 - M \succeq 0$, $\overline{D}^0 \succeq 0$, $\overline{Z}^0 + \kappa^1 \overline{Y}^0 = \overline{X}^0$, and $\delta(\overline{R}^0, \overline{X}^0) \leq \beta$, $\delta(\overline{S}^0, \overline{Y}^0) \leq \delta + \beta$, $\delta(\overline{D}^0, \overline{Z}^0) \leq \delta + \beta$.

 $Proof \quad \text{We have } \delta(\overline{R}^0, \overline{X}^0) = \delta(R^0, X^0) \leq \delta \text{ and }$

$$\delta(\overline{D}^0, \overline{Z}^0) = \|(\overline{D}^0)^{\frac{1}{2}} \overline{Z}^0 (\overline{D}^0)^{\frac{1}{2}} - I\|_F \le \beta$$
$$\delta(\overline{S}^0, \overline{Y}^0) = \|(\overline{S}^0)^{\frac{1}{2}} \overline{Y}^0 (\overline{S}^0)^{\frac{1}{2}} - I\|_F \le \beta$$

$$\begin{split} \delta(\overline{S}^0, \overline{Y}^0)^2 &= Tr((\overline{S}^0 \overline{Y}^0 - I)^2) \\ &= Tr((S^0 Y^0 - \Delta \kappa D^0 Y^0 - I)^2) \\ &= Tr(((S^0)^{\frac{1}{2}} Y^0 (S^0)^{\frac{1}{2}} - \Delta \kappa (S^0)^{\frac{1}{2}} Y^0 (S^0)^{\frac{1}{2}} - I)^2) \\ &= \|(S^0)^{\frac{1}{2}} Y^0 (S^0)^{\frac{1}{2}} - I - \Delta \kappa (S^0)^{\frac{1}{2}} Y^0 (S^0)^{\frac{1}{2}} \|_F^2 \end{split}$$

so using the triangle inequality of the Frobenius norm,

$$\begin{split} \delta(\overline{S}^0, \overline{Y}^0) &= \|(S^0)^{\frac{1}{2}} Y^0(S^0)^{\frac{1}{2}} - I - \Delta \kappa (S^0)^{\frac{1}{2}} Y^0(S^0)^{\frac{1}{2}} \|_F \\ &\leq \|(S^0)^{\frac{1}{2}} Y^0(S^0)^{\frac{1}{2}} - I \|_F + \|\Delta \kappa (S^0)^{\frac{1}{2}} Y^0(S^0)^{\frac{1}{2}} \|_F \\ &\leq \delta + Tr(\Delta \kappa (S^0)^{\frac{1}{2}} Y^0(S^0)^{\frac{1}{2}}) = \delta + \beta \end{split}$$

and similarly $\delta(\overline{D}^0, \overline{Z}^0) \leq \delta + \beta$.

THEOREM 6. (Theorem 4 in the paper) Let \overline{D}^0 and \overline{D}^1 be approximate centers for κ^0 and $\kappa^1 = \kappa^0 - \frac{\beta}{Tr(\overline{D}^0 \cdot (\kappa^0 \overline{D}^0 - M)^{-1})}$ respectively, obtained using the Newton update with Nesterov-Todd direction for β sufficiently small. If

$$\delta(\overline{R}^0, \overline{X}^0) \le \delta$$
$$\delta(\overline{D}^0, \overline{Z}^0) \le \delta$$
$$\delta(\overline{S}^0, \overline{Y}^0) \le \delta$$

for δ a small universal constant, then

$$\delta(\overline{R}^1, \overline{X}^1) \le \delta$$
$$\delta(\overline{D}^1, \overline{Z}^1) \le \delta$$
$$\delta(\overline{S}^1, \overline{Y}^1) \le \delta$$

and

$$P(\overline{D}^1, \kappa^1) \le P(\overline{D}^0, \kappa^0) - c\beta$$

for $c \in (0,1)$ a universal constant.

Proof The first part of the proof consists of showing that when the approximate center is $O(\eta)$ close to the analytic center, the potential is $O(\eta^2)$ close to the max-potential, for sufficiently small η .

Recall the definition

$$P(D,\kappa) := \log \det(M-D) + \log \det(\kappa D - M) + \log \det D$$

For fixed κ , suppose we have an approximate center \overline{D} with

$$\overline{R} = M - \overline{D} \succeq 0$$

$$\overline{S} = \kappa \overline{D} - M \succeq 0$$

$$\overline{D} \succeq 0$$

$$\overline{Z} + \kappa \overline{Y} = \overline{X}$$

and

$$\delta(\overline{R}, \overline{X}) \le \eta$$
$$\delta(\overline{S}, \overline{Y}) \le \eta$$
$$\delta(\overline{D}, \overline{Z}) \le \eta$$

for some small $\eta \in (0,1)$. Let D be the analytic center with κ . The result about Newton update applied to \overline{D} implies that

$$\|(\overline{D})^{-\frac{1}{2}}D^{(1)}(\overline{D})^{-\frac{1}{2}} - I\|_F \le \frac{\eta}{1-\eta}$$

where D' is the result of one step of Newton update applied to \overline{D} . We also know that the new approximate centers have distance upper bounded by $\frac{1}{2} \frac{\eta^2}{1-\eta}$. Now the key is to iterate the Newton update so that we obtain a sequence of approximate centers $D^{(1)}, D^{(2)}, \ldots$, that converges to D. Using the upper bounds on the approximate centers, we obtain, with $\overline{D} = D^{(0)}$,

$$\begin{split} \|(\overline{D})^{-\frac{1}{2}}D(\overline{D})^{-\frac{1}{2}} - I\|_{F} &= \|(\overline{D})^{-\frac{1}{2}}D(\overline{D})^{-\frac{1}{2}} - (\overline{D})^{-\frac{1}{2}}(D^{(1)})(\overline{D})^{-\frac{1}{2}} + (\overline{D})^{-\frac{1}{2}}(D^{(1)})(\overline{D})^{-\frac{1}{2}} - I\|_{F} \\ &= \|(D^{(0)})^{-\frac{1}{2}}D(D^{(0)})^{-\frac{1}{2}} - (D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}} + (D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}} - I\|_{F} \\ &\leq \|(D^{(0)})^{-\frac{1}{2}}D(D^{(0)})^{-\frac{1}{2}} - (D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}}\|_{F} + \|(D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}} - I\|_{F} \\ &\leq \sqrt{Tr((D^{(0)})^{-1}(D - (D^{(1)}))^{2}} + \frac{\eta}{1 - \eta} \\ &= \sqrt{Tr((D^{(0)})^{-1}(D^{(1)})(D^{(0)})^{-\frac{1}{2}}) \cdot \sqrt{Tr((D^{(1)})^{-\frac{1}{2}}D(D^{(1)})^{-\frac{1}{2}} - I)^{2}} + \frac{\eta}{1 - \eta} \\ &\leq \lambda_{1}((D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}}) \cdot \sqrt{Tr((D^{(1)})^{-\frac{1}{2}}D(D^{(1)})^{-\frac{1}{2}} - I)^{2}} + \frac{\eta}{1 - \eta} \\ &= \lambda_{1}((D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}}) \cdot \|(D^{(1)})^{-\frac{1}{2}}D(D^{(1)})^{-\frac{1}{2}} - I\|_{F} + \frac{\eta}{1 - \eta} \end{split}$$

where we have used the Cauchy-Schwarz inequality

$$\sqrt{Tr(AB)} \le \sqrt{Tr(A^TA)} \cdot \sqrt{Tr(B^TB)}$$

and the Holder inequality

$$Tr(AB) \le \lambda_1(A) \cdot Tr(B)$$

to obtian the last inequality. Now since

$$\|(\overline{D})^{-\frac{1}{2}}D^{(1)}(\overline{D})^{-\frac{1}{2}} - I\|_F \le \frac{\eta}{1-\eta}$$

we have

$$|\lambda_{1}((D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}})| \leq \lambda_{1}((D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}} - I) + \lambda_{1}(I)$$

$$\leq \|(D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}} - I\|_{F} + 1$$

$$\leq \frac{1}{1-n}$$

The bound on Newton update further implies that

$$\|(D^{(1)})^{-\frac{1}{2}}D^{(2)}(D^{(1)})^{-\frac{1}{2}} - I\|_F \le \frac{\frac{1}{2}\frac{\eta^2}{1-\eta}}{1 - \frac{1}{2}\frac{\eta^2}{1-\eta}}$$

and iterating the argument above gives

$$\begin{split} \|(\overline{D})^{-\frac{1}{2}}D(\overline{D})^{-\frac{1}{2}} - I\|_{F} &\leq \lambda_{1}((D^{(0)})^{-\frac{1}{2}}(D^{(1)})(D^{(0)})^{-\frac{1}{2}}) \cdot \|(D^{(1)})^{-\frac{1}{2}}D(D^{(1)})^{-\frac{1}{2}} - I\|_{F} + \frac{\eta}{1-\eta} \\ &\leq \frac{1}{1-\eta} \cdot (\lambda_{1}((D^{(1)})^{-\frac{1}{2}}(D^{(2)})(D^{(1)})^{-\frac{1}{2}}) \cdot \|(D^{(2)})^{-\frac{1}{2}}D(D^{(2)})^{-\frac{1}{2}} - I\|_{F} + \frac{\frac{1}{2}\frac{\eta^{2}}{1-\eta}}{1-\frac{1}{2}\frac{\eta^{2}}{1-\eta}}) + \frac{\eta}{1-\eta} \\ &\leq \frac{1}{1-\eta} \cdot (\frac{1}{1-\frac{1}{2}\frac{\eta^{2}}{1-\eta}} \cdot \|(D^{(2)})^{-\frac{1}{2}}D(D^{(2)})^{-\frac{1}{2}} - I\|_{F} + \frac{\frac{1}{2}\frac{\eta^{2}}{1-\eta}}{1-\frac{1}{2}\frac{\eta^{2}}{1-\eta}}) + \frac{\eta}{1-\eta} \end{split}$$

For $\eta < 1/2$, $\frac{1}{2} \frac{\eta^2}{1-\eta} \le \eta^2 < \eta$, so we have the upper bound

$$\begin{split} \|(\overline{D})^{-\frac{1}{2}}D(\overline{D})^{-\frac{1}{2}} - I\|_{F} &\leq \frac{1}{1 - \eta} \cdot (\frac{1}{1 - \frac{1}{2}\frac{\eta^{2}}{1 - \eta}} \cdot \|(D^{(2)})^{-\frac{1}{2}}D(D^{(2)})^{-\frac{1}{2}} - I\|_{F} + \frac{\frac{1}{2}\frac{\eta^{2}}{1 - \eta}}{1 - \frac{1}{2}\frac{\eta^{2}}{1 - \eta}}) + \frac{\eta}{1 - \eta} \\ &\leq \frac{1}{1 - \eta} \cdot \frac{1}{1 - \frac{1}{2}\frac{\eta^{2}}{1 - \eta}} \cdot \|(D^{(2)})^{-\frac{1}{2}}D(D^{(2)})^{-\frac{1}{2}} - I\|_{F} + \frac{\eta^{2}}{(1 - \eta)^{2}} + \frac{\eta}{1 - \eta} \\ &\leq \frac{1}{1 - \eta} \cdot \frac{1}{1 - \eta^{2}} \cdot \|(D^{(2)})^{-\frac{1}{2}}D(D^{(2)})^{-\frac{1}{2}} - I\|_{F} + \frac{\eta^{2}}{(1 - \eta)^{2}} + \frac{\eta}{1 - \eta} \\ &\leq \sum_{k=1}^{n} (\frac{\eta}{1 - \eta})^{k} = \frac{\eta}{1 - \eta} \frac{1 - \eta}{1 - 2\eta} = \frac{\eta}{1 - 2\eta} \end{split}$$

Now by concavity of $P(D, \kappa)$ in D, we have

$$P(D,\kappa) := \log \det(M-D) + \log \det(\kappa D - M) + \log \det D$$

$$\begin{split} P(D,\kappa) - P(\overline{D},\kappa) &\leq Tr(\nabla_D P(\overline{D},\kappa) \cdot (D - \overline{D}) \\ &= Tr((-\overline{R}^{-1} + \kappa \overline{S}^{-1} + \overline{D}^{-1}) \cdot (D - \overline{D})) \\ &= Tr((-\overline{R}^{-1} + \overline{X} + \kappa \overline{S}^{-1} - \kappa \overline{Y} + \overline{D}^{-1} - \overline{Z}) \cdot (D - \overline{D})) \\ &= Tr((-\overline{R}^{-1} + \overline{X})(\overline{R} - R)) + Tr((\overline{S}^{-1} - \overline{Y})(S - \overline{S})) + Tr((\overline{D}^{-1} - \overline{Z}) \cdot (D - \overline{D})) \end{split}$$

The three quantities are all $O(\eta^2)$: For example,

$$Tr((\overline{D}^{-1} - \overline{Z}) \cdot (D - \overline{D})) = Tr((\overline{D})^{\frac{1}{2}} (\overline{D}^{-1} - \overline{Z})(\overline{D})^{\frac{1}{2}} \cdot (\overline{D})^{-\frac{1}{2}} (D - \overline{D})(\overline{D})^{-\frac{1}{2}})$$

$$\leq \|(I - (\overline{D})^{\frac{1}{2}} \overline{Z}(\overline{D})^{\frac{1}{2}})\|_{F} \cdot \|(I - (\overline{D})^{-\frac{1}{2}} D(\overline{D})^{-\frac{1}{2}}\|_{F}$$

$$\leq \eta \cdot \frac{\eta}{1 - 2\eta}$$

and similarly we have $O(\eta^2)$ bounds for the other two quantities, because of similar $O(\eta)$ bounds for $\|(\overline{R})^{-\frac{1}{2}}R(\overline{R})^{-\frac{1}{2}}-I\|_F$ and $\|(\overline{S})^{-\frac{1}{2}}S(\overline{S})^{-\frac{1}{2}}-I\|_F$.

Now let \overline{D}^0 be an approximate center for κ^0 , and \overline{D}^1 be an approximate center for κ^1 , obtained using Newton updates. Recall that $\kappa^1 = \kappa^0 - \frac{\beta}{Tr((\overline{D})^0 \cdot (\kappa^0(\overline{D})^0 - M)^{-1})}$. We have, with $\eta = \delta + \beta$,

$$\begin{split} P(\kappa^1, \overline{D}^1) - P(\kappa^0, \overline{D}^0) &= P(\kappa^1, \overline{D}^1) - P(\kappa^1, D^1) + P(\kappa^1, D^1) - P(\kappa^0, D^0) + P(\kappa^0, D^0) - P(\kappa^0, \overline{D}^0) \\ &\leq -\beta + P(\kappa^0, D^0) - P(\kappa^0, \overline{D}^0) \\ &\leq -\beta + c \cdot \eta^2 \end{split}$$

With δ and β small enough, $-\beta + c \cdot \eta^2 \le -c'\beta$ for some $c' \in (0,1)$, and

$$\delta(\overline{R}^1, \overline{X}^1) \le \frac{1}{2} \frac{(\delta + \beta)^2}{1 - (\delta + \beta)} \le \delta$$