MONTE CARLO METHOD FOR ESTIMATING EIGENVALUES OF SYMMETRIC MATRICES

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Abstract. In this paper, we reveal a new relationship between Rayleigh quotients and residual errors associated with symmetric matrices and unit vectors. We show that for a fixed value of the Rayleigh quotient, the Euclidean norm of the corresponding residual vectors admits both upper and lower bounds. These bounds are related to the eigenvalues of the matrix under consideration. Furthermore, we demonstrate how the derived upper bound can be used to construct a simple Monte Carlo algorithm for estimating the minimum and maximum eigenvalues.

1. Introduction

In this paper, we make use of well-known concepts and theorems related to matrix eigenvalues and their estimation, which can be found in classical references such as [1], [2], and [3]. For problems concerning the eigenvalues of symmetric matrices, we recommend the texts [5] and [6]. In this section, we briefly review the definitions used and some important statements related to our work.

Let us consider the \mathbb{R}^n Euclidean space endowed with the common inner product:

$$\langle x, y \rangle := x^T y = \sum_{i=1}^n x_i y_i \qquad (x, y \in \mathbb{R}^n).$$

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Here x^T denotes the transpose of a vector or a matrix. The Euclidean norm is induced by the inner product and is denoted by

$$||x|| := \sqrt{x^T x} = \sqrt{\langle x, x \rangle}.$$

In the following, we will investigate the spectrum of symmetric matrices, i.e. $A \in \mathbb{R}^{n \times n}$ real matrices for which $A = A^T$. There are some fundamental results worth mentioning regarding the estimation of eigenvalues of symmetric matrices.

Proposition 1.1. The eigenvalues of a symmetric matrix are real, and therefore they can be ordered as follows:

$$\lambda_{\min} := \lambda_1 \le \lambda_2 \le \dots \le \lambda_{n-1} \le \lambda_n =: \lambda_{\max}.$$

Definition 1.1. The set of eigenvalues is called the spectrum of the matrix A, and the quantity

$$\varrho\left(A\right) := \max_{i=1}^{n} |\lambda_{i}|$$

is called the spectral radius of the matrix.

The spectral radius is an important quantity that characterizes the linear transformation represented by the matrix, and its determination or estimation plays a crucial role in analyzing the convergence of iterative methods. Another important eigenvalue is the one with the smallest absolute value since the ratio of the largest to the smallest absolute eigenvalue is proportional to the condition number of the matrix, which is the key metric for assessing the stability of numerical algorithms involving the matrix. Since the eigenvalue with the smallest absolute value is equal to $\varrho\left(A^{-1}\right)$, most methods designed to estimate the spectral radius can be adapted with minor modifications to estimate the eigenvalue of the smallest absolute value as well.

1.1. Classical eigenvalue estimates

It is known that any matrix norm provides an upper bound for the spectral radius.

Proposition 1.2. If $\|.\|$ is a sub-multiplicative matrix norm then

$$\varrho\left(A\right) \leq \left\|A\right\|.$$

Another widely applicable eigenvalue estimate is given by the Gershgorin circle theorem, whose special case for symmetric matrices can be formulated as follows.

Proposition 1.3. Let $A \in \mathbb{R}^{n \times n}$ be a matrix, and define

$$R_i := \sum_{j \neq i} |a_{ij}|, \quad G_i := [a_{ii} - R_i, \ a_{ii} + R_i].$$

Then the eigenvalues of the matrix A lie within the union of the intervals G_i , i.e.

$$\lambda_j \in \bigcup_{i=1}^n G_i \qquad (j=1,\ldots,n).$$

This again provides a useful estimate for the spectral radius.

Corollary 1.1.

$$\varrho\left(A\right) \leq \max_{i=1}^{n} \left(a_{ii} + R_{i}\right).$$

Suppose that λ is an eigenvalue of the matrix A with corresponding eigenvector v. Then, for the eigenvalues (v, λ) , we clearly have

$$Av = \lambda v \iff Av - \lambda v = 0.$$

Notice, that if $v' \approx v$ and $\lambda' \approx \lambda$, then

$$Av' - \lambda'v' \approx 0.$$

Following this pattern, we can introduce the so-called residual vector for an approximate eigenvalue μ and the corresponding approximate eigenvector u.

Definition 1.2. The residual vector corresponding to an approximate eigenvalues (μ, u) is defined as

$$r := r(A, \mu, u) := Au - \mu u.$$

Clearly, for a true eigenvalues (λ, v) , we have r = 0. Moreover, for any approximate eigenpair (μ, u) , the smaller the norm ||r||, the closer (μ, u) is to an actual eigenpair of the matrix A.

For symmetric matrices, a particularly useful eigenvalue estimate is given by the so-called Rayleigh quotient.

Definition 1.3. Let $A \in \mathbb{R}^{n \times n}$ be symmetric matrix: $A = A^T$, and $0 \neq u \in \mathbb{R}^n$ be a vector. The Rayleigh quotient for A and u is defined as

$$\mu := \mu(A,u) := \frac{\langle Au,u\rangle}{\langle u,u\rangle} = \frac{\langle Au,u\rangle}{\left\|u\right\|^2}.$$

Proposition 1.4. Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix, and let $u \in \mathbb{R}^n$ be an arbitrary vector. Then the Rayleigh quotient $\mu := \mu(A, u)$ lies between the smallest and largest eigenvalues, that is

$$\lambda_{\min} \le \mu \le \lambda_{\max}$$
.

Proposition 1.5. Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix, and let $u \in \mathbb{R}^n$ be an arbitrary vector. Then the Rayleigh quotient $\mu := \mu(A, u)$ minimizes the Euclidean norm of the residual vector, i.e.

$$\forall \eta \in \mathbb{R}$$
 : $||Au - \eta u|| \ge ||Au - \mu u||$.

This latter result means the following: suppose that the matrix is symmetric and we already have an approximate eigenvector, denoted by u. Then the Rayleigh quotient provides the best (in the Euclidean sense) eigenvalue approximation corresponding to u.

1.2. Foreword

This article is part of a volume dedicated to the memory of Ferenc Schipp. Professor Schipp had a deep and enduring interest in visual patterns, beautiful illustrations, and the mathematics that underlies them. Relationships between patterns and the conjectures they inspire were frequent topics in his seminars and celebratory departmental meetings. The hyperbolic fractal shown in Figure 1, for example, was generated by a program he wrote himself and shared as a Christmas greeting with the staff of the Department of Numerical Analysis at Eötvös Loránd University in 2023.



Figure 1. Christmas tree generated by a hyperbolic fractal. The figure was created by Ferenc Schipp using a program he wrote himself.

It is perhaps thanks to Professor Schipp's influential teaching and inspiring curiosity that I approached the writing of this article with such enthusiasm. My primary aim has been to explore the mathematical structure underlying a striking pattern recently encountered, and to provide an explanation for its emergence.

In April 2023, during the Numerical Methods 2 course, we administered the first midterm exam, which included a programming task. Together with my colleague Anna Krebsz, we aimed to design an exercise related to eigenvalue computation that would result in a visually compelling plot. The task we proposed was the following:

- Let A be a symmetric matrix.
- Generate a set of random unit vectors u_i , and for each vector compute the Rayleigh quotient μ_i with respect to A.
- Next, compute the residual r_i corresponding to the eigenvalue approximation μ_i and eigenvector approximation u_i .

• Plot the points $(\mu_i, ||r_i||)$ in a Cartesian coordinate system, where the horizontal axis corresponds to the Rayleigh quotient and the vertical axis shows the norm of the residual.

Figure 2 illustrates the result for 100, 500, and 2500 randomly selected unit vectors u_i applied in the case of the same 4×4 symmetric matrix. As can be seen, the resulting points form a strikingly regular structure. At the time of the exam, we found this phenomenon intriguing, though we did not yet have a full explanation for it. In the present article, we analyze the underlying geometric and algebraic reasons for the patterns seen in Figure 2, and we demonstrate how this structure can be leveraged to estimate the eigenvalues of symmetric matrices.

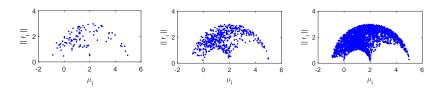


Figure 2. An interesting pattern emerges when plotting the Euclidean norm of the residual vectors as a function of the Rayleigh quotients corresponding to randomly chosen unit vectors u_i .

2. Upper and lower estimates

For many randomly chosen unit vectors u_i , a careful examination of Figure 3 reveals the emergence of semicircular patterns. In the example considered, the eigenvalues of the matrix A are -1,0,2,5, and based on the figure, we may conjecture that the intersection points of the semicircles with the x-axis are precisely the eigenvalues. We can examine the figure from another perspective. Suppose we fix the Rayleigh quotient μ . It is clear that infinitely many vectors u can yield the same Rayleigh quotient, but different vectors may lead to different residual vectors. Note that we can establish both a lower and an upper bound for the length of the residual vector in this case. The lower bound is determined by the arc of the circle that intersects the x-axis at the eigenvalues closest to μ . The upper bound is given by the arc of the circle intersecting the axis at the smallest and largest eigenvalues. In this section, we prove that these conjectures are indeed correct.

Lemma 2.1. If
$$||u|| = 1$$
 then

$$\mu^2 + ||r||^2 = ||Au||^2,$$

that is, for any unit vector u, the point $(\mu, ||r||)$ lies on a circle centered at the origin with radius ||Au||.

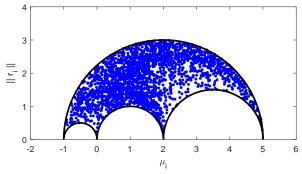


Figure 3. The points $(\mu_i, ||r_i||)$ are bounded from above by a semicircle whose intersections with the x-axis correspond to the extremal eigenvalues. From below, we also observe semicircular arcs emerging, whose intersections with the axis correspond to pairs of adjacent eigenvalues of the matrix A.

Proof.

$$||r||^{2} = \langle r, r \rangle = \langle Au - \mu u, Au - \mu u \rangle =$$

$$= ||Au||^{2} - 2 \langle Au, \mu u \rangle + ||\mu u||^{2} =$$

$$= ||Au||^{2} - 2\mu \underbrace{\langle Au, u \rangle}_{\mu} + \mu^{2} \underbrace{\langle u, u \rangle}_{1} =$$

$$= ||Au||^{2} - 2\mu^{2} + \mu^{2} = ||Au||^{2} - \mu^{2} \iff \mu^{2} + ||r||^{2} = ||Au||^{2}. \quad \blacksquare$$

Lemma 2.2.

$$\min_{i=1}^{n} \lambda_i^2 \le \mu^2 + \|r\|^2 \le \max_{i=1}^{n} \lambda_i^2.$$

Proof. Due to Lemma 2.1, we have $\mu^2 + ||r||^2 = ||Au||^2$, so it is sufficient to show that the bounds in the statement hold for the quantity $||Au||^2$. Observe that

$$||Au||^2 = \langle Au, Au \rangle = \langle A^2u, u \rangle.$$

Thus, $||Au||^2$ is the Rayleigh quotient of the matrix A^2 with respect to the vector u. It follows that the values of $||Au||^2$ must lie between the smallest and largest eigenvalues of A^2 . Since the eigenvalues of A^2 are the squares of the eigenvalues of A, the claim follows.

It is well known that if a scalar $t \in \mathbb{R}$ is added to the diagonal elements of matrix A, then the eigenvalues are shifted by t as well. In the following lemma, we show that the Rayleigh quotient behaves in the same way.

Lemma 2.3. Let $t \in \mathbb{R}$ and define A' = A + tI. Let μ' and r' denote the Rayleigh quotient and the residual vector of the matrix A', respectively. Then

- (i) $\mu' = \mu + t$, and
- (ii) r' = r.

Proof. To prove (i), we use the linearity of the inner product:

$$\mu' = \langle A'u, u \rangle = \langle (A + tI)u, u \rangle = \langle Au, u \rangle + t\langle Iu, u \rangle = \mu + t.$$

Furthermore,

$$r' = A'u - \mu'u = (A + tI)u - (\mu + t)u =$$

= $Au + tu - \mu u - tu = Au - \mu u = r$,

which means that the residual error remains unchanged when the eigenvalues of A are shifted. Note that this result is consistent since both the eigenvalues and the Rayleigh quotients of A are shifted by the same amount.

In the following theorem, we prove the upper bound:

Theorem 2.1. Let

$$c := \frac{\lambda_{\min} + \lambda_{\max}}{2}$$

be the center of the spectrum and $d := \lambda_{\max} - \lambda_{\min}$ its diameter. Then

$$(\mu - c)^2 + ||r||^2 \le \left(\frac{d}{2}\right)^2$$
,

that is, for any unit vector u, the point $(\mu, ||r||)$ lies on or inside the semicircle centered at (c, 0) with diameter d.

Proof. Let A' := A - cI. Then the eigenvalues λ'_i of A' are simply those of A shifted by -c:

$$\lambda_i' = \lambda_i - c,$$

and in particular,

$$\lambda'_{\min} = \lambda_{\min} - \frac{\lambda_{\min} + \lambda_{\max}}{2} = -\frac{d}{2},$$

$$\lambda'_{\max} = \lambda_{\max} - \frac{\lambda_{\min} + \lambda_{\max}}{2} = \frac{d}{2}.$$

Applying the upper bound from Lemma 2.2 to the matrix A', we obtain:

$$(\mu')^2 + ||r'||^2 \le \max_{i=1}^n (\lambda_i')^2.$$

Using the facts that r' = r, $\mu' = \mu - c$, and $\max_i (\lambda_i')^2 = (d/2)^2$, the claim follows.

Finally, we prove the lower bound:

Theorem 2.2. Let $c_i := \frac{\lambda_i + \lambda_{i+1}}{2}$ and $d_i := \lambda_{i+1} - \lambda_i$ for $i = 1, \dots, n-1$. Then

$$(\mu - c_i)^2 + ||r||^2 \ge \left(\frac{d_i}{2}\right)^2$$
,

that is, for any unit vector u, the point $(\mu, ||r||)$ lies on or outside the circle centered at c_i with diameter d_i .

Proof. Let $A' := A - c_i I$. Note that the eigenvalues of the transformed matrix satisfy:

$$\lambda_i' = \lambda_i - \frac{\lambda_i + \lambda_{i+1}}{2} = -\frac{d_i}{2},$$
$$\lambda_{i+1}' = \lambda_{i+1} - \frac{\lambda_i + \lambda_{i+1}}{2} = \frac{d_i}{2}.$$

Due to the ordering of the eigenvalues, we have $\min_i |\lambda_i'| = d_i/2$. Applying the lower bound from Lemma 2.2 to A', we obtain:

$$||r'||^2 + (\mu')^2 = ||r||^2 + (\mu - c_i)^2 \ge \min_{i=1}^n (\lambda_i')^2 = \left(\frac{d_i}{2}\right)^2.$$

3. Monte Carlo eigenvalue estimation

Using the inequalities derived in the previous section, we gain the ability to simultaneously estimate the largest and smallest eigenvalues of a symmetric matrix, and thus its spectral radius as well. As a consequence of Theorem 2.1, any point $(\mu_i, ||r_i||)$ lies inside the semicircular disk centered at (c, 0) with diameter d. It is easy to see that if we consider the set of all points corresponding to unit vectors $u_i \in \mathbb{R}^n$, then this circle is the smallest semicircle covering the point set. Based on this observation, we can reinterpret the task outlined in the introduction in a constructive manner as follows:

- 1. Select a few random unit vectors $u_i \in \mathbb{R}^n$.
- 2. Compute the corresponding Rayleigh quotients μ_i and norms of residual vectors $||r_i||$.
- 3. Determine the smallest semicircle covering the resulting set of points. Let its center be $(\tilde{c}, 0)$ and its diameter \tilde{d} .

In other words, we generate points from randomly selected vectors and then fit the smallest semicircle covering the resulting set. If we use a sufficiently large number of samples, we may expect that $\tilde{c} \approx c$ and $\tilde{d} \approx d$, which leads to the following simple approximations for the smallest and largest eigenvalues of the matrix:

$$\lambda_{\min} \approx \widetilde{c} - \widetilde{d}/2,$$

$$\lambda_{\max} \approx \widetilde{c} + \widetilde{d}/2,$$

and for the spectral radius:

$$\varrho(A) \approx \widetilde{\varrho}(A) := \max \left\{ \left| \widetilde{c} - \widetilde{d}/2 \right|, \ \left| \widetilde{c} + \widetilde{d}/2 \right| \right\}.$$

Note that our estimate is very similar to the spectral radius approximation induced by the Gershgorin circle theorem.

To apply the method presented above, it is necessary to determine the smallest semicircle that covers the set of points $(\mu_i, ||r_i||)$. Computing the minimal enclosing circle for a set of points is a well-studied problem with several known algorithms. In our case, we used a modified version of Welzl's algorithm to compute the smallest enclosing semicircle.

3.1. Welzl's algorithm

Welzl's algorithm is a randomized, recursive method for computing the smallest enclosing circle of a finite set of points in the plane [7, 4]. The algorithm proceeds as follows.

- 1. Shuffle the input set P of points to ensure random processing order.
- 2. Recursively compute the minimal circle enclosing all the points in P except a randomly chosen $p \in P$.
- 3. If p lies inside the current circle, return it unchanged.
- 4. If p lies outside, compute a new minimal enclosing circle that includes p and the subset $R \subset P$ of points known to lie on the boundary with $|R| \leq 2$.
- 5. Continue recursion with updated R, until a unique circle defined by up to three boundary points is found.

A pseudocode of this method can be seen in Algorithm 1, where SEC(R) returns the trivial enclosing circle of 3 or fewer points.

```
Algorithm 1 Welzl(P, R)
```

10: **end if**

```
Ensure: Smallest circle enclosing all points in P.

1: if |P| = 0 or |R| = 3 then

2: return SEC(R)

3: end if

4: Choose random p \in P

5: C \leftarrow \text{Welzl}(P \setminus \{p\}, R)

6: if C encloses p then

7: return C

8: else

9: return Welzl(P \setminus \{p\}, R \cup \{p\})
```

Require: Set of points P and R on the boundary.

Calling Welzer(P,\emptyset), the algorithm terminates with the smallest enclosing circle with expected linear time complexity. In the following, we show how

Welzl's algorithm can be modified to solve the minimal enclosing semicircle problem.

3.2. Modified Welzl's algorithm

Welzl's original algorithm relies on the fact that the smallest enclosing circle (SEC) of a point set is defined by at most three points. Therefore, at each step of the recursive algorithm, one must be able to compute the smallest enclosing circle determined by 1, 2, or 3 points. In the case of the smallest enclosing semicircles (SESC), the recursion can proceed in the same manner; however, we observe that the center of the SESC must necessarily lie on the x-axis. This constraint simplifies the problem: to compute the SESC, at most 2 points are required. There is no need for a 3rd defining point, unlike in the general (full-circle) case.

Now suppose that $P_1 := (x_1, y_1)$ and $P_2 := (x_2, y_2)$ are two points in the plane with $y_1, y_2 \ge 0$, and we want to construct the SESC. Let us denote the center of the circle by $P_0 := (x_0, 0)$, and let the radius be R. We will show that, eventually there are just two cases, as can be seen in Figure 4.

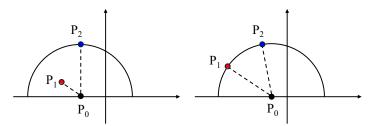


Figure 4. The geometric problem arising in the fitting of the smallest enclosing semicircle (SESC) involves constructing a circle passing through two given points, with the constraint that its center lies on the x-axis. The illustrations show the two possible cases: when SESC is defined by one single point or two points.

For a single point, the SESC is trivial. Now assume that $y_2 \ge y_1$. In the case of the SESC corresponding to P_2 , clearly $x_0 = x_2$ and $R = y_2$. It is easy to see that if in this case the semicircle also contains P_1 , then the SESC for the point set $\{P_1, P_2\}$ is the same semicircle. This condition is satisfied if P_1 lies closer to the center than the radius, that is

$$(x_1 - x_0)^2 + (y_1 - 0)^2 \le R^2 \iff (x_1 - x_2)^2 \le y_2^2 - y_1^2.$$

Note that due to the condition $y_2 \geq y_1$, the SESC of P_1 cannot contain P_2 . Therefore, if the above inequality is not satisfied, then the SESC will be the semicircle that passes through both points P_1 and P_2 . This can be computed as follows. We may assume that $x_1 \neq x_2$, since if they were equal, one of the

semicircles would necessarily contain the other point. So we have two equations:

$$(x_i - x_0)^2 + y_i^2 = R^2$$
 $(i = 1, 2).$

Subtracting one from the other:

$$(x_1 - x_0)^2 + y_1^2 = (x_2 - x_0)^2 + y_2^2,$$

$$x_1^2 - 2x_1x_0 + x_0^2 + y_1^2 = x_2^2 - 2x_2x_0 + x_0^2 + y_2^2,$$

$$2(x_2 - x_1)x_0 = x_2^2 - x_1^2 + y_2^2 - y_1^2,$$

$$x_0 = \frac{x_1 + x_2}{2} + \frac{y_2^2 - y_1^2}{2(x_2 - x_1)}.$$

Knowing x_0 , R can be easily determined e.g. as

$$R = \sqrt{(x_1 - x_0)^2 + y_1^2}.$$

Using the formulas above, we can construct the modified Welzl's algorithm for computing SESC as follows. The changed parts are highlighted in red.

- 1. Shuffle the input set P of points to ensure random processing order.
- 2. Recursively compute the minimal semicircle enclosing all the points in P except a randomly chosen $p \in P$.
- 3. If p lies inside the current semicircle, return it unchanged.
- 4. If p lies outside, compute a new minimal enclosing circle that includes p and the subset $R \subset P$ of points known to lie on the boundary with $|R| \leq 1$.
- 5. Continue recursion with updated R, until a unique semicircle defined by up to two boundary points is found.

An illustration of the algorithm in action is shown in Figure 5. As seen there, fitting a semicircle can, in favorable cases, quickly provide a good approximation for the minimal and maximal eigenvalues. However, one can also observe (see, e.g., the middle image) that the method may overestimate the maximal eigenvalue, but now we show a formula that quantifies the error of this approximation ¹.

Theorem 3.1. Let $\widetilde{\varrho}(A)$ be a Monte Carlo eigenvalue estimation of the spectral radius, as we introduced it at the beginning of Section 3. Then

$$\widetilde{\varrho}(A) \le \sqrt{2} \ \varrho(A).$$

¹I would like to thank the reviewer of the article for the idea.

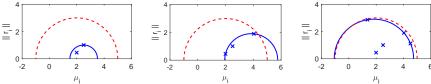


Figure 5. To simultaneously estimate the minimal and maximal eigenvalues, we fit a circle to the $(\mu_i, ||r_i||)$ points corresponding to randomly chosen u_i vectors. In the example, the matrix is 4×4 , with minimal and maximal eigenvalues -1 and 5, respectively. The red dashed circle shows the theoretical upper bound. The circles fitted to the point set are drawn in blue. From left to right, the results of the semicircle fitting are shown after inserting the 2nd, 3rd, and 5th points, respectively.

Proof. For simplicity, let us suppose, that $c = (0,0) \in \mathbb{R}^2$ and $\tilde{c} \approx c$ and $\tilde{d} \approx d$ are the approximate center and diameter of the spectrum. Let us examine how the worst possible estimate can arise. First, recall that the SESC corresponding to a point set obtained from the Monte Carlo procedure either hits a single point or passes through at least two. We may assume the first setting, since any covering semicircle passing through two points would certainly yield a better approximation, resulting in an SESC with a smaller radius. Furthermore, we may also assume that the point under consideration lies on the boundary of the theoretical, exact SESC, as this maximizes the radius of the semicircle. Therefore, let (x_1, y_1) be a point in the set such that

$$x_1^2 + y_1^2 = \left(\frac{d}{2}\right)^2 =: R^2, \quad y_1 \ge 0.$$

Then (x_1, y_1) can be written as $R(\cos \alpha, \sin \alpha)$ for some suitable $\alpha \in [0, \pi]$, and the SESC defined by this point has center $\tilde{c} = R \cos \alpha$ and diameter $\tilde{d} = 2R \sin \alpha$. The corresponding estimate for the spectral radius is therefore

$$\widetilde{\varrho}(A) = \max \big\{ R \big| \cos \alpha + \sin \alpha \big|, \quad R \big| \cos \alpha - \sin \alpha \big| \big\} \leq R \sqrt{2} = \sqrt{2} \ \varrho(A).$$

By using the translation invariance of eigenvalues and the spectral radius estimates, it follows that the above result holds for any center c, which completes the proof.

4. Conclusion

In our experiments, we tested the scalability of the Monte Carlo eigenvalue estimation. While smaller matrices yielded relatively accurate approximations fairly quickly, for larger matrices we observed inaccurate estimates that only improved with a very large number of test vectors. This issue may stem from the distribution of the random unit vectors. In high dimensions, vectors with uniformly random components rarely produce extremely large residuals: yet

such points are precisely what would be needed to improve estimates of the extremal eigenvalues. Consequently, we find this estimation method to be more suitable for theoretical settings.

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