# A Tour of the Lanczos Algorithm and its Convergence Guarantees through the Decades


Qiaochu Yuan

Department of Mathematics
UC Berkeley

*Joint work with Prof. Ming Gu, Bo Li*


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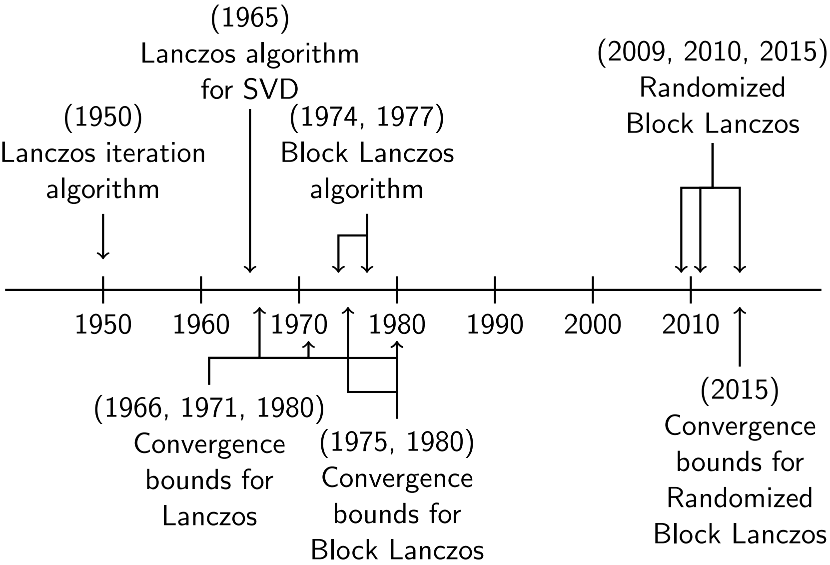
# Timeline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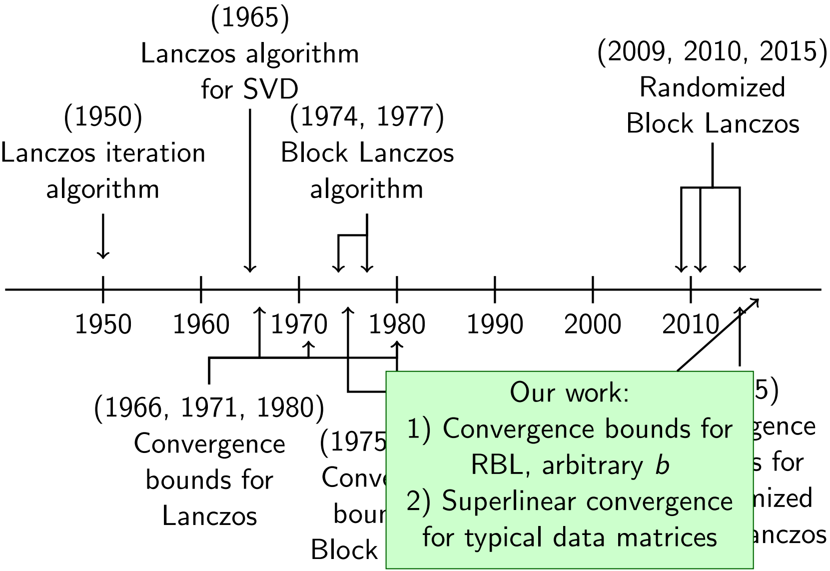

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1) Convergence bounds for
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2) Superlinear convergence
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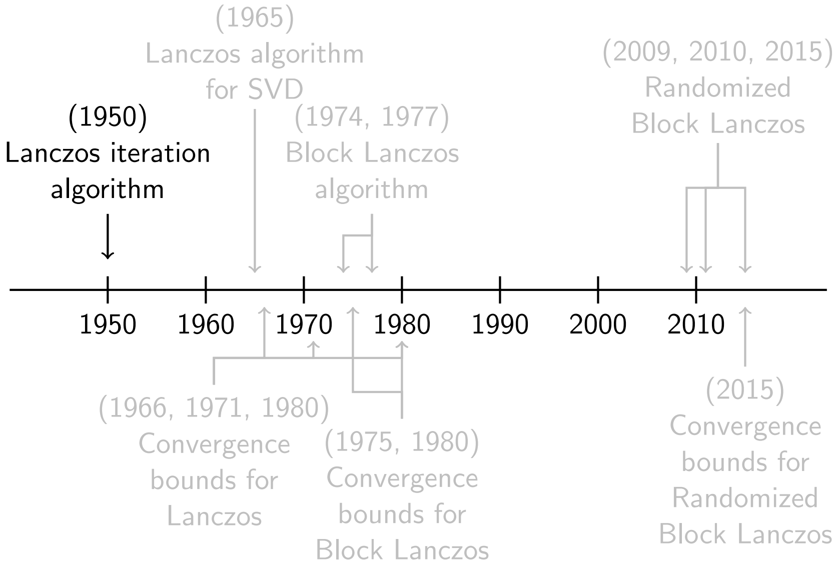
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# Lanczos Iteration Algorithm

Developed by Lanczos in 1950 [Lan50].

Widely used iterative algorithm for computing the extremal eigenvalues and corresponding eigenvectors of a large, sparse, symmetric matrix $\mathbf{A}$.

## Goal

Given a symmetric matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, with eigenvalues $\lambda_1 > \lambda_2 > \cdots > \lambda_n$ and associated eigenvectors $\mathbf{u}_1, \cdots, \mathbf{u}_n$, want to find approximations for

- $\lambda_i$, $i = 1, \cdots, k$, the $k$ largest eigenvalues of $\mathbf{A}$
- $\mathbf{u}_i$, $i = 1, \cdots, k$, the associated eigenvectors

where $k \ll n$.

# Lanczos - Details

General idea:

1. Select an initial vector $\mathbf{v}$.
2. Construct Krylov subspace $\mathcal{K}(\mathbf{A}, \mathbf{v}, k) = \mathrm{span}\{\mathbf{v}, \mathbf{A}\mathbf{v}, \mathbf{A}^2\mathbf{v}, \cdots, \mathbf{A}^{k-1}\mathbf{v}\}$.
3. Restrict and project $\mathbf{A}$ to the Krylov subspace, $\mathbf{T} = \mathrm{proj}_{\mathcal{K}} \mathbf{A}|_{\mathcal{K}}$
4. Use eigen values and vectors of $\mathbf{T}$ as approximations to those of $\mathbf{A}$.

In matrices:

$$\mathbf{K}_k = \begin{bmatrix} \mathbf{v} & \mathbf{A}\mathbf{v} & \cdots & \mathbf{A}^{k-1}\mathbf{v} \end{bmatrix} \in \mathbb{R}^{n \times k}$$

$$\mathbf{Q}_k = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_k \end{bmatrix} \leftarrow \mathrm{qr}(\mathbf{K}_k)$$

$$\mathbf{T}_k = \mathbf{Q}_k^T \mathbf{A} \mathbf{Q}_k \in \mathbb{R}^{k \times k}$$

# Lanczos - Details

$$\mathbf{A}\begin{bmatrix}\mathbf{q}_1 & \cdots & \mathbf{q}_j\end{bmatrix} = \left[\begin{array}{ccc|c}\mathbf{q}_1 & \cdots & \mathbf{q}_j & \mathbf{q}_{j+1}\end{array}\right]\left[\begin{array}{cccc}\alpha_1 & \beta_1 & & \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{j-1} \\ & & \beta_{j-1} & \alpha_j \\ \hline & & & \beta_j\end{array}\right]$$

At each step $j = 1, \cdots, k$ of Lanczos iteration:

$$\mathbf{A}\mathbf{Q}_j = \mathbf{Q}_j\mathbf{T}_j + \beta_j \mathbf{q}_{j+1}\mathbf{e}_{j+1}^T$$

Use the three-term recurrence:

$$\mathbf{A}\mathbf{q}_j = \beta_{j-1}\mathbf{q}_{j-1} + \alpha_j\mathbf{q}_j + \beta_j\mathbf{q}_{j+1}$$

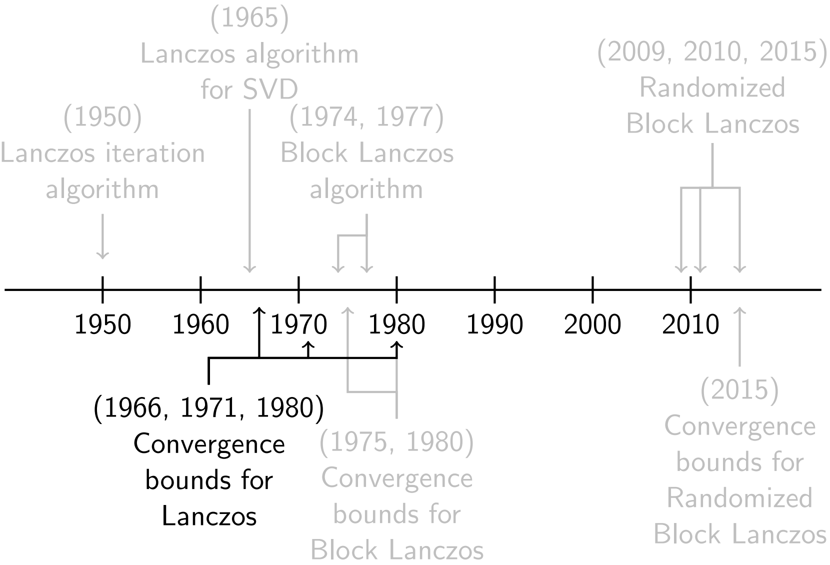
Calculate the $\alpha$s, $\beta$s as:

$$\alpha_j = \mathbf{q}_j^T\mathbf{A}\mathbf{q}_j \tag{1}$$

$$\mathbf{r}_j = (\mathbf{A} - \alpha_j\mathbf{I})\,\mathbf{q}_j - \beta_{j-1}\mathbf{q}_j \tag{2}$$

$$\beta_j = \|\mathbf{r}_j\|_2,\ \mathbf{q}_{j+1} = \mathbf{r}_j/\beta_j \tag{3}$$

# Timeline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# Convergence of Lanczos

How well does $\lambda_i^{(k)}$, the eigenvalues of $\mathbf{T}_k$, approximate $\lambda_i$, the eigenvalues of $\mathbf{A}$, for $i = 1, \cdots, k$?

First answered by Kaniel in 1966 [Kan66] and Paige in 1971 [Pai71].

**Theorem (Kaniel-Paige Inequality)**

*If* $\mathbf{v}$ *is chosen to be not orthogonal to the eigenspace associated with* $\lambda_1$*, then*

$$0 \leq \lambda_1 - \lambda_1^{(k)} \leq (\lambda_1 - \lambda_n) \frac{\tan^2 \theta(\mathbf{u}_1, \mathbf{v})}{T_{k-1}^2(\gamma_1)} \tag{4}$$

*where* $T_i(x)$ *is the Chebyshev polynomial of degree* $i$*,* $\theta(\cdot, \cdot)$ *is the angle between two vectors, and*

$$\gamma_1 = 1 + 2\frac{\lambda_1 - \lambda_2}{\lambda_2 - \lambda_n}$$

# Convergence of Lanczos

Later generalized by Saad in 1980 [Saa80].

## Theorem (Saad Inequality)

*For* $i = 1, \cdots, k$, *if* $\mathbf{v}$ *is chosen such that* $\mathbf{u}_i^T \mathbf{v} \neq 0$, *then*

$$0 \leq \lambda_i - \lambda_i^{(k)} \leq (\lambda_i - \lambda_n) \left( \frac{L_i^{(k)} \tan \theta (\mathbf{u}_i, \mathbf{v})}{T_{k-i}(\gamma_i)} \right)^2 \tag{5}$$

*where* $T_i(x)$ *is the Chebyshev polynomial of degree* $i$, $\theta(\cdot, \cdot)$ *is the angle between two vectors, and*

$$\gamma_i = 1 + 2 \frac{\lambda_i - \lambda_{i+1}}{\lambda_{i+1} - \lambda_n}$$

$$L_i^{(k)} = \begin{cases} \prod_{j=1}^{i-1} \frac{\lambda_j^{(k)} - \lambda_n}{\lambda_j^{(k)} - \lambda_i} & \textit{if } i \neq 1 \\ 1 & \textit{if } i = 1 \end{cases}$$

# Aside - Chebyshev Polynomials

Recall

$$T_j(x) = \frac{1}{2}\left(\left(x + \sqrt{x^2 - 1}\right)^j + \left(x - \sqrt{x^2 - 1}\right)^j\right) \quad (6)$$

When $j$ is large,

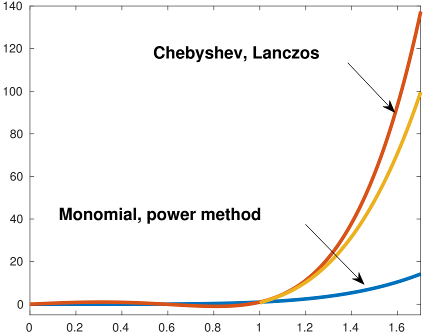
$$T_j(x) \approx \frac{1}{2}\left(x + \sqrt{x^2 - 1}\right)^j$$

and when $g$ is small,

$$T_j(1+g) \approx \frac{1}{2}\left(1 + g + \sqrt{2g}\right)^j$$

determines the convergence of Lanczos with

$$g = \Theta\left(\frac{\lambda_i - \lambda_{i+1}}{\lambda_{i+1} - \lambda_n}\right)$$



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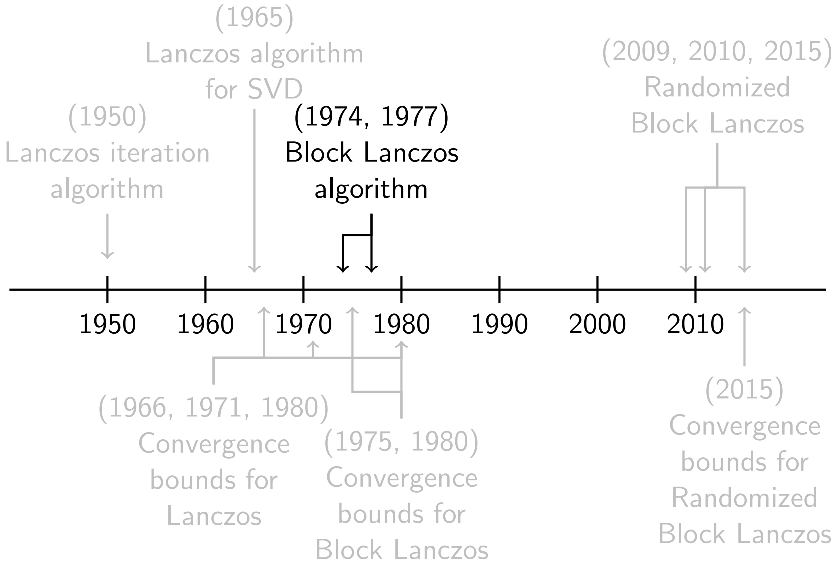

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# Block Lanczos Algorithm

Introduced by Golub and Underwood in 1977 [GU77] and Cullum and Donath in 1974 [CD74].

The block generalization of the Lanczos method uses, instead of a single initial vector $\mathbf{v}$, a block of $b$ vectors $\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \cdots & \mathbf{v}_b \end{bmatrix}$, and builds the Krylov subspace in $q$ iterations as $\mathcal{K}_q(\mathbf{A}, \mathbf{V}, q) = \mathrm{span}\left\{\mathbf{V}, \mathbf{AV}, \cdots, \mathbf{A}^{q-1}\mathbf{V}\right\}$.

$k \leq b$, $bq \ll n$.

Compared to classical Lanczos, block Lanczos

- is more memory and cache efficient, using BLAS3 operations.
- has the ability to converge to eigenvalues with cluster size $> 1$.
- has faster convergence with respect to number of iterations.

# Block Lanczos Algorithm - Details

$$\mathbf{A}\begin{bmatrix}\mathbf{Q}_1 & \cdots & \mathbf{Q}_j\end{bmatrix} = \left[\begin{array}{ccc|c}\mathbf{Q}_1 & \cdots & \mathbf{Q}_j & \mathbf{Q}_{j+1}\end{array}\right]\left[\begin{array}{cccc}\mathcal{A}_1 & \mathcal{B}_1^T & & \\ \mathcal{B}_1 & \ddots & \ddots & \\ & \ddots & \ddots & \mathcal{B}_{j-1}^T \\ & & \mathcal{B}_{j-1} & \mathcal{A}_j \\ \hline & & & \mathcal{B}_j\end{array}\right]$$

At each step $j = 1, \cdots, k$ of Lanczos iteration:

$$\mathbf{AQ} = \mathbf{QT}_j + \mathbf{Q}_{j+1}\begin{bmatrix}\mathbf{0} & \cdots & \mathbf{0} & \mathcal{B}_j\end{bmatrix}$$

Use the three-term recurrence:

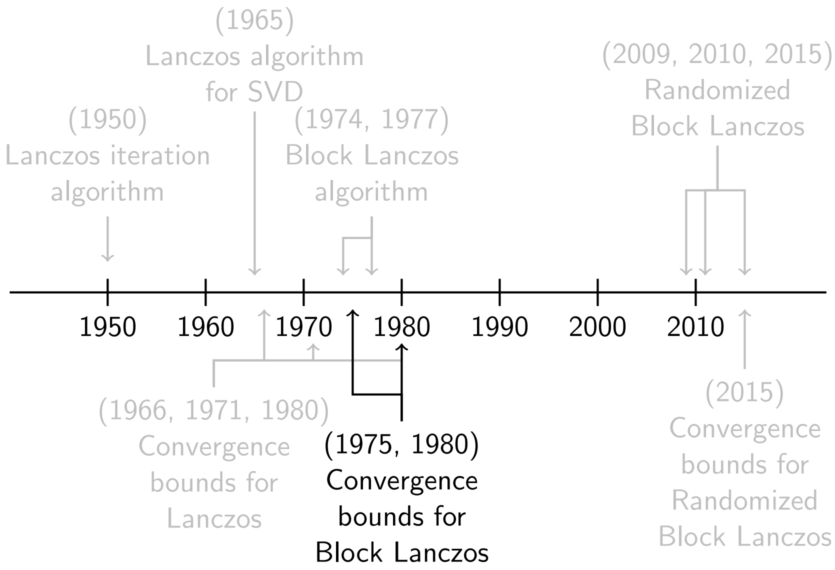
$$\mathbf{AQ}_j = \mathbf{Q}_{j-1}\mathcal{B}_{j-1}^T + \mathbf{Q}_j\mathcal{A}_j + \mathbf{Q}_{j+1}\mathcal{B}_j$$

Calculate the $\mathcal{A}$s, $\mathcal{B}$s as:

$$\mathcal{A}_j = \mathbf{Q}_j^T\mathbf{AQ}_j \tag{7}$$

$$\mathbf{Q}_{j+1}\mathcal{B}_j \leftarrow \mathrm{qr}\left(\mathbf{AQ}_j - \mathbf{Q}_j\mathcal{A}_j - \mathbf{Q}_j\mathcal{B}_{j-1}^T\right) \tag{8}$$

# Timeline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# Convergence of Block Lanczos

First analyzed by Underwood in 1975 [Und75] with the introduction of the algorithm.

## Theorem (Underwood Inequality)

*Let* $\lambda_i$, $\mathbf{u}_i$, $i = 1, \cdots, n$ *be the eigenvalues and eigenvectors of* $\mathbf{A}$ *respectively. Let* $\mathbf{U} = \begin{bmatrix} \mathbf{u}_1 & \cdots & \mathbf{u}_b \end{bmatrix}$. *If* $\mathbf{U}^T\mathbf{V}$ *is of full rank* $b$, *then for* $i = 1, \cdots, b$

$$0 \leq \lambda_i - \lambda_i^{(q)} \leq (\lambda_1 - \lambda_n) \frac{\tan^2 \Theta(\mathbf{U}, \mathbf{V})}{T_{q-1}^2(\rho_i)} \tag{9}$$

*where* $T_i(x)$ *is the Chebyshev polynomial of degree* $i$, $\cos \Theta(\mathbf{U}, \mathbf{V}) = \sigma_{\min}\left(\mathbf{U}^T\mathbf{V}\right)$, *and*

$$\rho_i = 1 + 2\frac{\lambda_i - \lambda_{b+1}}{\lambda_{b+1} - \lambda_n}$$

# Convergence of Block Lanczos

## Theorem (Saad Inequality [Saa80])

*Let* $\lambda_j$, $\mathbf{u}_j$, $j = 1, \cdots, n$ *be the eigenvalues and eigenvectors of* $\mathbf{A}$ *respectively. Let* $\mathbf{U}_i = \begin{bmatrix} \mathbf{u}_i & \cdots & \mathbf{u}_{i+b-1} \end{bmatrix}$. *For* $i = 1, \cdots, b$, *if* $\mathbf{U}_i^T \mathbf{V}$ *is of full rank* $b$, *then*

$$0 \leq \lambda_i - \lambda_i^{(q)} \leq (\lambda_i - \lambda_n) \left( \frac{L_i^{(q)} \tan \Theta \left( \mathbf{U}_i, \mathbf{V} \right)}{T_{q-i} \left( \hat{\gamma}_i \right)} \right)^2 \tag{10}$$

*where* $T_i(x)$ *is the Chebyshev polynomial of degree* $i$, $\cos \Theta \left( \mathbf{U}, \mathbf{V} \right) = \sigma_{\min} \left( \mathbf{U}^T \mathbf{V} \right)$, *and*

$$\hat{\gamma}_i = 1 + 2 \frac{\lambda_i - \lambda_{i+b}}{\lambda_{i+b} - \lambda_n}$$

$$L_i^{(q)} = \begin{cases} \prod_{j=1}^{i-1} \frac{\lambda_j^{(q)} - \lambda_n}{\lambda_j^{(q)} - \lambda_i} & \textit{if } i \neq 1 \\ 1 & \textit{if } i = 1 \end{cases}$$

# Aside - Block Size

Recall, when $j$ is large and $g$ is small

$$T_j(1+g) \approx \frac{1}{2}\left(1+g+\sqrt{2g}\right)^j \tag{11}$$

$$\text{classical: } g = \Theta\left(\frac{\lambda_i - \lambda_{i+1}}{\lambda_{i+1} - \lambda_n}\right)$$

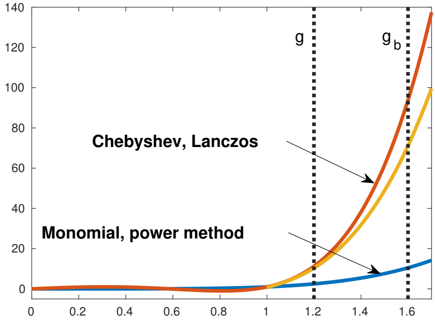
$$\text{block: } g_b = \Theta\left(\frac{\lambda_i - \lambda_{i+b}}{\lambda_{i+b} - \lambda_n}\right)$$

Suppose eigenvalue distributed as $\lambda_j > (1+\epsilon)\lambda_{j+1}$ for all $j$:

$$g_b \approx \frac{1-(1+\epsilon)^{-b}}{(1+\epsilon)^{-b}} \cdot \lambda_i$$

$$\approx b \cdot \lambda_i \epsilon$$

$$\approx b \cdot g$$



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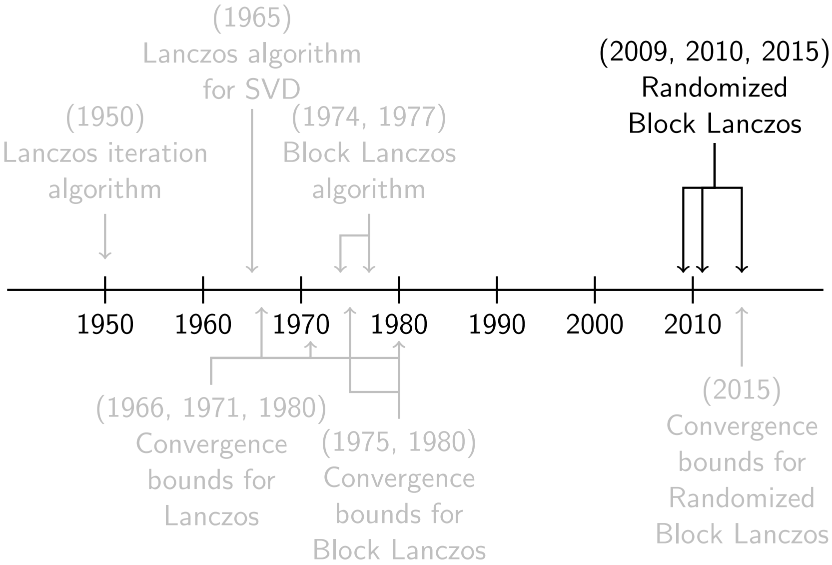
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# Randomized Block Lanczos

In recent years, there has been increased interest in algorithms to compute low-rank approximations of matrices, with

- high computational efficiency requirement, running on large matrices
- low approximation accuracy requirement, 2-3 digits of accuracy

Applications mostly in big-data computations

- compression of data matrices
- matrix processing techniques, e.g. PCA
- optimization of the nuclear norm objective function

# Randomized Block Lanczos

Grew out of work done in randomized algorithms, in particular Randomized Subspace Iteration, by

- Rokhlin, Szlam, and Tygert in 2009 [RST09]
- Halko, Martinsson, and Tropp in 2011 [HMST11]
- Gu [Gu15], and Musco [MM15] in 2015

Idea: Instead of taking any initial set of vectors $\mathbf{V}$, an unfortunate choice of which could result in poor convergence, choose $\mathbf{V} = \mathbf{A\Omega}$, a random projection of the columns of $\mathbf{A}$, to better capture the range space.

# RSI & RBL Pseudocode

**Algorithm 1** Randomized Subspace Iteration (RSI) pseudocode

**Input:** $\mathbf{A} \in \mathbb{R}^{m \times n}$, target rank $k$, block size $b$, number of iter. $q$

**Output:** $\mathbf{B}_k \in \mathbb{R}^{m \times n}$ , a rank-$k$ approximation

1: Draw $\mathbf{\Omega} \in \mathbb{R}^{n \times b}$. $\omega_{ij} \sim \mathcal{N}(0, 1)$.

2: Form $\mathbf{K} = (\mathbf{A}\mathbf{A}^T)^{q-1}\mathbf{A}\mathbf{\Omega}$.

3: Orthogonalize $\mathrm{qr}(\mathbf{K}) \to \mathbf{Q}$.

4: $\mathbf{B}_k = (\mathbf{Q}\mathbf{Q}^T\mathbf{A})_k = \mathbf{Q}(\mathbf{Q}^T\mathbf{A})_k$.

$*$ $(\mathbf{M})_k$ indicates the $k$-truncated SVD of matrix $\mathbf{M}$.

**Algorithm 2** Randomized Block Lanczos (RBL) pseudocode

**Input:** $\mathbf{A} \in \mathbb{R}^{m \times n}$, target rank $k$, block size $b$, number of iter. $q$

**Output:** $\mathbf{B}_k \in \mathbb{R}^{m \times n}$, a rank-$k$ approximation

1: Draw $\mathbf{\Omega} \in \mathbb{R}^{n \times b}$. $\omega_{ij} \sim \mathcal{N}(0, 1)$.

2: Form $\mathbf{K} = [\mathbf{A}\mathbf{\Omega}, (\mathbf{A}\mathbf{A}^T)\mathbf{A}\mathbf{\Omega}, \cdots, (\mathbf{A}\mathbf{A}^T)^{q-1}\mathbf{A}\mathbf{\Omega}]$.

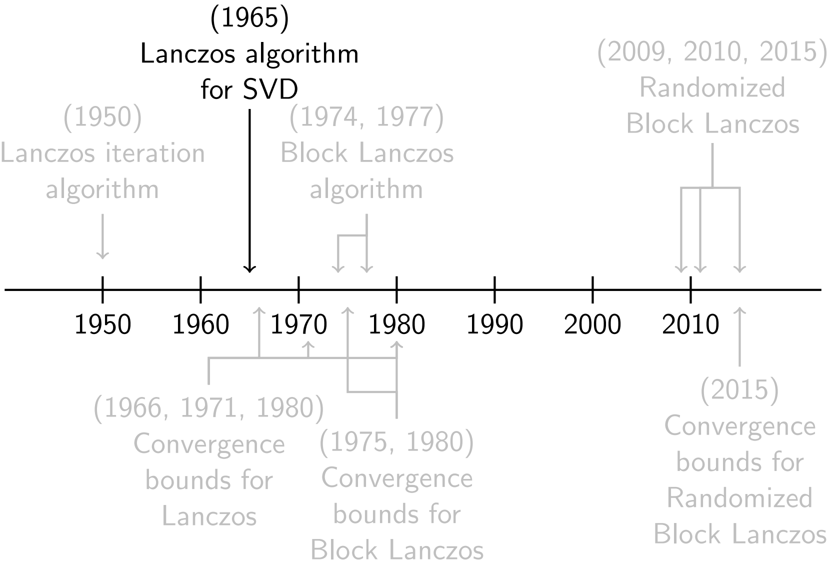
3: Orthogonalize $\mathrm{qr}(\mathbf{K}) \to \mathbf{Q}$.

4: $\mathbf{B}_k = (\mathbf{Q}\mathbf{Q}^T\mathbf{A})_k = \mathbf{Q}(\mathbf{Q}^T\mathbf{A})_k$.

$*$ requires $bq \geq k$.

$**$ numerically unstable.

# Timeline



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# Lanczos for SVD

A modification of the Lanczos algorithm can be used to find the extremal singular value pairs of a non-symmetric matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$.

Utilizing the connections between the singular value decomposition of $\mathbf{A}$ and the eigen decompositions of $\mathbf{A}\mathbf{A}^T$ and $\mathbf{A}^T\mathbf{A}$,

1. Select a block of initial vectors $\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \cdots & \mathbf{v}_b \end{bmatrix}$.
2. Construct Krylov subspaces $\mathcal{K}_V\left(\mathbf{A}^T\mathbf{A}, \mathbf{V}, q\right)$ and $\mathcal{K}_U\left(\mathbf{A}\mathbf{A}^T, \mathbf{A}\mathbf{V}, q\right)$.
3. Restrict and project $\mathbf{A}$ to form $\mathbf{B} = \mathrm{proj}_{\mathcal{K}_U}\mathbf{A}|_{\mathcal{K}_V}$
4. Use singular values and vectors of $\mathbf{B}$ as approximations to those of $\mathbf{A}$.

# Golub-Kahan Bidiagonalization [GK65]

$$\mathbf{A}\begin{bmatrix}\mathbf{V}_1 & \cdots & \mathbf{V}_j\end{bmatrix} = \begin{bmatrix}\mathbf{U}_1 & \cdots & \mathbf{U}_j\end{bmatrix}\begin{bmatrix}\mathcal{A}_1 & \mathcal{B}_1^T & & \\ & \ddots & \ddots & \\ & & \ddots & \mathcal{B}_{j-1}^T \\ & & & \mathcal{A}_j\end{bmatrix}$$

$$\mathbf{A}^T\begin{bmatrix}\mathbf{U}_1 & \cdots & \mathbf{U}_j\end{bmatrix} = \begin{bmatrix}\mathbf{V}_1 & \cdots & \mathbf{V}_j \,|\, \mathbf{V}_{j+1}\end{bmatrix}\begin{bmatrix}\mathcal{A}_1 & & & \\ \mathcal{B}_1 & \ddots & & \\ & \ddots & \ddots & \\ & & \mathcal{B}_{j-1} & \mathcal{A}_j \\ \hline & & & \mathcal{B}_j\end{bmatrix}$$

At each step $j = 1, \cdots, k$ of the bidiagonalization, calculate $\mathcal{A}$s and $\mathcal{B}$s as:

$$\mathbf{U}_j\mathcal{A}_j \leftarrow \mathrm{qr}\left(\mathbf{A}\mathbf{V}_j - \mathbf{U}_{j-1}\mathcal{B}_{j-1}^T\right) \tag{12}$$

$$\mathbf{V}_{j+1}\mathcal{B}_j \leftarrow \mathrm{qr}\left(\mathbf{A}^T\mathbf{U}_j - \mathbf{V}_j\mathcal{A}_j\right) \tag{13}$$

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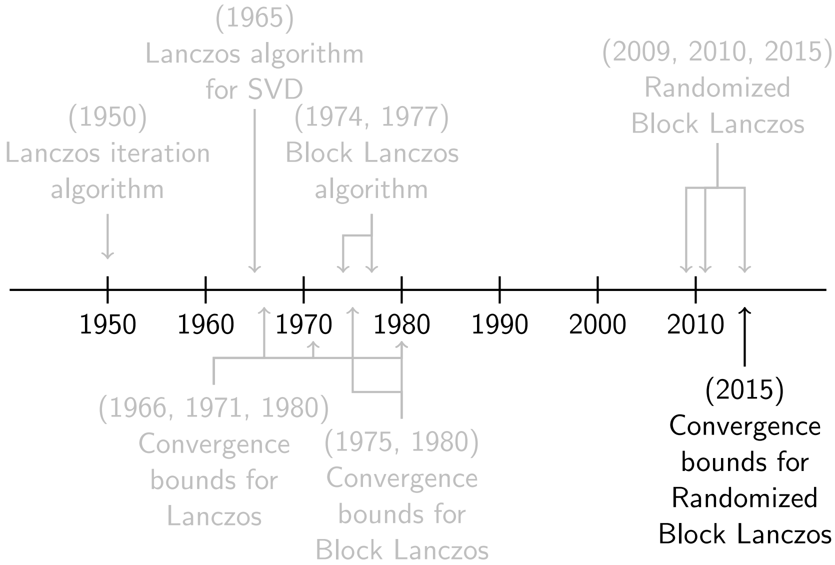
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# Convergence of RBL

Analyzed by Musco and Musco in 2015 [MM15].

**Theorem**

*For block size* $b \geq k$, *in* $q = \Theta\left(\frac{\log n}{\epsilon}\right)$ *iterations of RSI and* $q = \Theta\left(\frac{\log n}{\sqrt{\epsilon}}\right)$ *iterations of RBL, with constant probability* 99/100, *the following inequalities bounds are satisfied:*

$$|\sigma_i^2 - \sigma_i^2(\mathbf{B}_k)| \leq \epsilon\sigma_{k+1}^2, \ , \textit{for } i = 1, \cdots, k \tag{14}$$

*In the event that* $\sigma_{b+1} \leq c\sigma_k$ *with* $c < 1$, *taking* $q = \Theta\left(\frac{\log(n/\epsilon)}{\min(1, \sigma_k/\sigma_{b+1} - 1)}\right)$ *and* $q = \Theta\left(\frac{\log(n/\epsilon)}{\sqrt{\min(1, \sigma_k/\sigma_{b+1} - 1)}}\right)$ *suffices for RSI and RBL respectively.*

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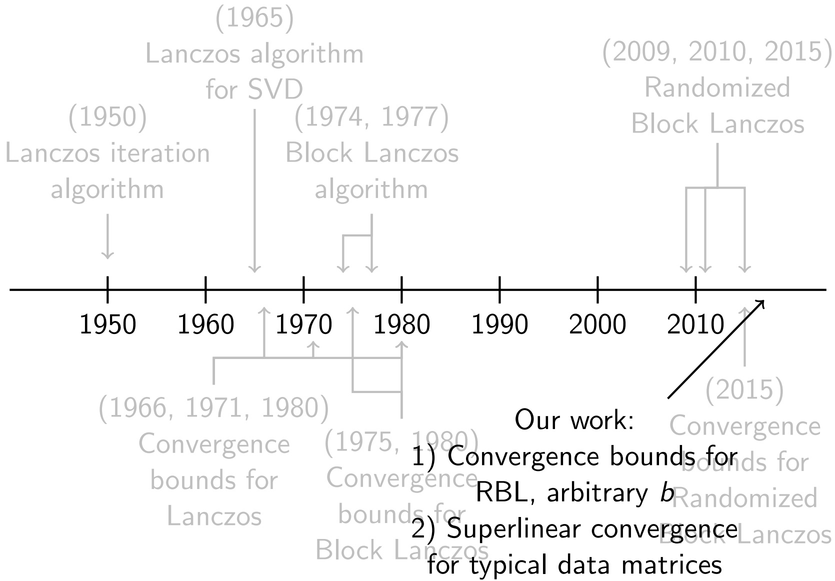

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# Aside: Convergence of RSI

Many of our analysis techniques are similar to those used by Gu to analyze RSI [Gu15]. The bounds for RBL resulting from the current work will be similar in form to the bounds for RSI.

**Theorem (RSI convergence)**

*Let $\mathbf{B}_k$ be the approximation returned by the RSI algorithm on $\mathbf{A} = \mathbf{U\Sigma V}^T$, with target rank $k$, block size $b \geq k$, and $q$ iterations. If $\hat{\mathbf{\Omega}}_1$ has full row rank in $\mathbf{V}^T\mathbf{\Omega} = \begin{bmatrix} \hat{\mathbf{\Omega}}_1^T & \hat{\mathbf{\Omega}}_2^T \end{bmatrix}^T$, then*

$$\sigma_j \geq \sigma_j(\mathbf{B}_k) \geq \frac{\sigma_j}{\sqrt{1 + \|\hat{\mathbf{\Omega}}_2\|_2^2 \|\hat{\mathbf{\Omega}}_1^\dagger\|_2^2 \left(\frac{\sigma_{b+1}}{\sigma_j}\right)^{4q+2}}} \tag{15}$$

# Current Work - Core Ideas

The core pieces of our analysis are:

1. the growth behavior of Chebyshev polynomials,
2. the choice of a clever orthonormal basis for Krylov subspace,
3. the creation of a spectrum "gap", by separating the spectrum of $\mathbf{A}$ into those singular values that are "close" to $\sigma_k$, and those that are sufficiently smaller in magnitude.

## Setup & Notation

For block size $b$, random Gaussian matrix $\mathbf{\Omega} \in \mathbb{R}^{n \times b}$, we are interested in the column span of

$$\mathbf{K}_q = \left[\mathbf{A\Omega} \quad \left(\mathbf{AA}^T\right)\mathbf{A\Omega} \quad \cdots \quad \left(\mathbf{AA}^T\right)^{q-1}\mathbf{A\Omega}\right]$$

Let the SVD of $\mathbf{A} \in \mathbb{R}^{m \times n}$ be $\mathbf{U\Sigma V}^T$. For any $0 \leq p \leq q$, define

$$\begin{aligned}\hat{\mathbf{K}}_p :&= \mathbf{U}T_{2p+1}(\mathbf{\Sigma})\left[\hat{\mathbf{\Omega}} \quad \mathbf{\Sigma}^2\hat{\mathbf{\Omega}} \quad \cdots \quad \mathbf{\Sigma}^{2(q-p-1)}\hat{\mathbf{\Omega}}\right] \\ &= \mathbf{U}T_{2p+1}(\mathbf{\Sigma})\mathbf{V}_{q-p}\end{aligned}$$

Note $\mathbf{V}_{q-p} \in \mathbb{R}^{n \times b(q-p)}$. We require $b(q-p) \geq k$, the target rank.

**Lemma**

*With $\hat{\mathbf{K}}_p$ and $\mathbf{K}_q$ as previously defined,*

$$\operatorname{span}\{\mathbf{K}_q\} \supseteq \operatorname{span}\left\{\hat{\mathbf{K}}_p\right\} \tag{16}$$

# Convergence of RBL

**Theorem (Main Result)**

*Let $\mathbf{B}_k$ be the approximation returned by the RBL algorithm. With notation as previously defined, if the random starting $\mathbf{\Omega}$ is initialized such that the block Vandermonde formed by the sub-blocks of $\mathbf{V}_{q-p}$ is invertible, then for all $1 \leq j \leq k$, and all choices[a] of $s, r$,*

$$\sigma_j \geq \sigma_j(\mathbf{B}_k) \geq \frac{\sigma_{j+s}}{\sqrt{1 + \mathcal{C}^2 T_{2p+1}^{-2} \left(1 + 2 \cdot \frac{\sigma_j - \sigma_{j+s+r+1}}{\sigma_{j+s+r+1}}\right)}} \tag{17}$$

*where $p = q - \frac{k+r}{b}$, and $\mathcal{C}$ is a constant independent of $q$.*

[a] $s$ is chosen to be non-zero to handle multiple singular values, and can be set to zero otherwise.

# Summary of Convergence Bounds

Rewriting bounds in comparable forms:

| citation | bound | req. on b |
|---|---|---|
| Saad [Saa80] | $\lambda_j^{(q)} \geq \frac{\lambda_j}{1+L_j^{(q)^2}\tan^2\Theta(\mathbf{U},\mathbf{V})\,T_{q-j}^{-2}\left(1+2\frac{\lambda_j-\lambda_{j+b}}{\lambda_{j+b}}\right)}$ | $b \geq k$ |
| Musco [MM15] spec. indep. | $\sigma_j^{(q)} \geq \frac{\sigma_j}{\sqrt{1+\mathcal{C}_1^2\log^2(n)\,q^{-2}\frac{\sigma_{k+1}^2}{\sigma_j^2}}}$ | $b \geq k$ |
| Musco [MM15] spec. dep. | $\sigma_j^{(q)} \geq \frac{\sigma_j}{\sqrt{1+\mathcal{C}_2 n e^{-q\sqrt{\min(1,\sigma_k/\sigma_{b+1}-1)}}\frac{\sigma_{k+1}^2}{\sigma_j^2}}}$ | $b \geq k$ |
| Current Work | $\sigma_j^{(q)} \geq \frac{\sigma_j}{\sqrt{1+\mathcal{C}_3^2\,T_{2q+1-2(k+r)/b}^{-2}\left(1+2\frac{\sigma_j-\sigma_{j+r+1}}{\sigma_{j+r+1}}\right)}}$ | $b \geq 1$<br>$bq \geq k+r$ |

# Typical Case - Superlinear Convergence

Recall: $\{a_q\}$ convergence *superlinearly* to $a$ if

$$\lim_{q\to\infty} \frac{|a_{q+1} - a|}{|a_q - a|} = 0 \tag{18}$$

- In practice, Lanczos algorithms (classical, block, randomized) often exhibit superlinear convergence behavior.
- It has been shown that classical Lanczos iteration is theoretically superlinearly convergent under certain assumptions about the singular spectrum [saa94, Li10].
- We show this for block Lanczos algorithms, i.e., that under certain assumptions about the singular spectrum, block Lanczos produces rank $k$ approximations $\mathbf{B}_k$ such that $\sigma_j(\mathbf{B}_k) \to \sigma_j$ superlinearly.

# Typical Case - Superlinear Convergence

A typical data matrix might have singular value spectrum decaying to 0, i.e., $\sigma_j \to 0$. In this case our bound suggests that convergence is governed by

$$a_q := \left(\mathcal{C}(r) T_p^{-1}(1+g)\right)^2 \approx \left(\mathcal{C}(r) \cdot \frac{1}{2}\left(1+g+\sqrt{2g}\right)^{-p}\right)^2 \qquad \to 0$$

with

$$g = 2\frac{\sigma_j - \sigma_{j+r+1}}{\sigma_{j+r+1}} = 2\left(\frac{\sigma_j}{\sigma_{j+r+1}} - 1\right) \to \infty$$

$$p = 2\left(q - \frac{k+r}{b}\right) + 1 = 2q + \left(1 - 2\frac{k+r}{b}\right)$$

We argue that $a_{q+1}/a_q \to 0$ as follows: for all $\epsilon > 0$, choose[1] $r$ so that $1 + g \geq \epsilon^{-\frac{1}{2}}$. Then,

$$\frac{a_{q+1}}{a_q} \leq \epsilon$$

[1] Recall 1) our main result holds for all $r$; 2) $k + r = (q-p)b$, and so choosing $r$ amounts to choosing $q$.

# Effect of $r$

There is some optimal value of $r$, typically non-zero, which achieves the best convergence factor. The balance is between larger (smaller) values of $r$, which implies lower (higher) Chebyshev degree but bigger (smaller) gap.

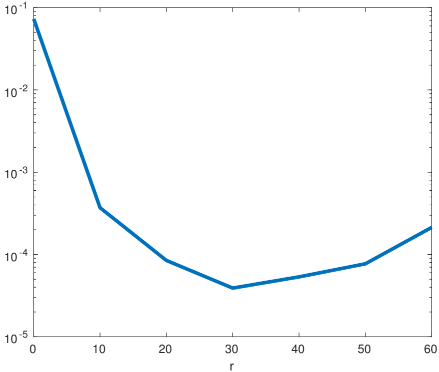
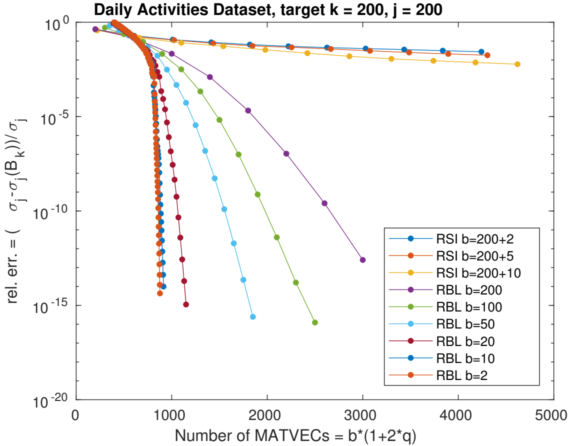



Figure: Value of reciprocal convergence factor $T^{-1}_{2q+1-2((k+r)/b)}\left(1+2\frac{\sigma_j-\sigma_{j+r+1}}{\sigma_{j+r+1}}\right)$ as $r$ varies, for Daily Activities and Sports Dataset, $k=j=100$, $b=10$, $q=20$.

# Numerical Example

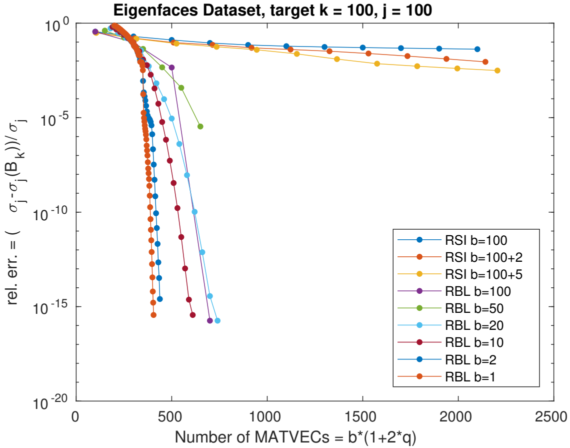
Experimentally, choices of smaller block sizes $1 \leq b < k$ appear favorable with superlinear convergence for all block sizes.

Figure: Daily Activities and Sports Dataset - $\mathbf{A} \in \mathbb{R}^{9120 \times 5625}$.



# Numerical Example

Figure: Eigenfaces Dataset - $\mathbf{A} \in \mathbb{R}^{10304 \times 400}$.



# Conclusions

- Both the theoretical analysis and numerical evidence suggest that, holding the number of matrix vector operations constant, RBL with smaller block size $b$ is better.
- For matrices with decaying spectrum, RBL achieves superlinear convergence.
- However the preference for smaller $b$ must be balanced with the advantages of a larger $b$ for computational efficiency and numerical stability reasons in a practical implementation, and should be further investigated.

# References I


- Jane Cullum and William E Donath, *A block lanczos algorithm for computing the q algebraically largest eigenvalues and a corresponding eigenspace of large, sparse, real symmetric matrices*, Decision and Control including the 13th Symposium on Adaptive Processes, 1974 IEEE Conference on, vol. 13, IEEE, 1974, pp. 505–509.
- Gene Golub and William Kahan, *Calculating the singular values and pseudo-inverse of a matrix*, Journal of the Society for Industrial and Applied Mathematics, Series B: Numerical Analysis **2** (1965), no. 2, 205–224.
- Gene Howard Golub and Richard Underwood, *The block lanczos method for computing eigenvalues*, Mathematical software, Elsevier, 1977, pp. 361–377.

# References II


- Ming Gu, *Subspace iteration randomization and singular value problems*, SIAM Journal on Scientific Computing **37** (2015), no. 3, A1139–A1173.
- Nathan Halko, Per-Gunnar Martinsson, Yoel Shkolnisky, and Mark Tygert, *An algorithm for the principal component analysis of large data sets*, SIAM Journal on Scientific computing **33** (2011), no. 5, 2580–2594.
- Shmuel Kaniel, *Estimates for some computational techniques in linear algebra*, Mathematics of Computation **20** (1966), no. 95, 369–378.
- Cornelius Lanczos, *An iteration method for the solution of the eigenvalue problem of linear differential and integral operators*, United States Governm. Press Office Los Angeles, CA, 1950.

# References III


- Ren-Cang Li, *Sharpness in rates of convergence for the symmetric lanczos method*, Mathematics of Computation **79** (2010), no. 269, 419–435.
- Cameron Musco and Christopher Musco, *Randomized block krylov methods for stronger and faster approximate singular value decomposition*, Advances in Neural Information Processing Systems, 2015, pp. 1396–1404.
- Christopher Conway Paige, *The computation of eigenvalues and eigenvectors of very large sparse matrices.*, Ph.D. thesis, University of London, 1971.
- Vladimir Rokhlin, Arthur Szlam, and Mark Tygert, *A randomized algorithm for principal component analysis*, SIAM Journal on Matrix Analysis and Applications **31** (2009), no. 3, 1100–1124.

# References IV


Yousef Saad, *On the rates of convergence of the lanczos and the block-lanczos methods*, SIAM Journal on Numerical Analysis **17** (1980), no. 5, 687–706.

*Theoretical error bounds and general analysis of a few lanczos-type algorithms*, 1994.

Richard Underwood, *An iterative block lanczos method for the solution of large sparse symmetric eigenproblems*, Tech. report, 1975.