Randomized Numerical Linear Algebra
Lecture 1

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Planned course Outlook

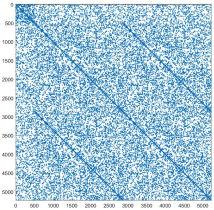
1. Review of numerical linear algebra and probability theory
2. Trace estimation and Schatten p-norm estimation (M.C. methods)
3. Sampling to approximate matrices (matrix multiplication)
4. Randomized linear embedding
5. Randomized techniques to find subspace that is aligned with the range of a matrix
6. Randomized algorithms for computing matrix factorizations
7. Solving linear systems with randomized techniques

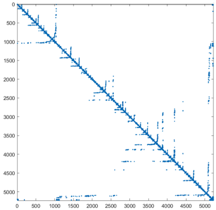
What to expect!

- The course is centered primarily on computational aspects
- Aimed at equipping you with a robust set of computational skills
- Proofs will be included occasionally, but only at a high level
- The course aims to impart an understanding of the key ideas behind proofs rather than delving into exhaustive, fully worked-out proofs

numerical linear algebra

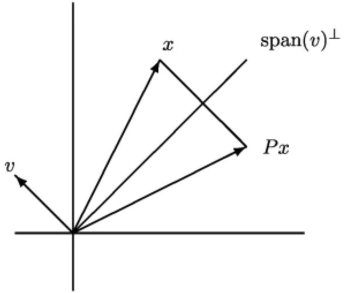
- solving dense and sparse linear systems





numerical linear algebra

- solving dense and sparse linear systems
- orthogonalization, least square & Tikhonov regularization



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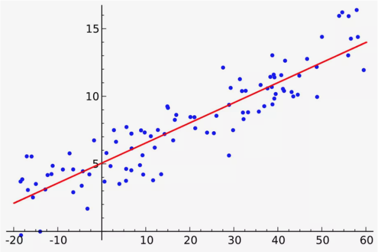

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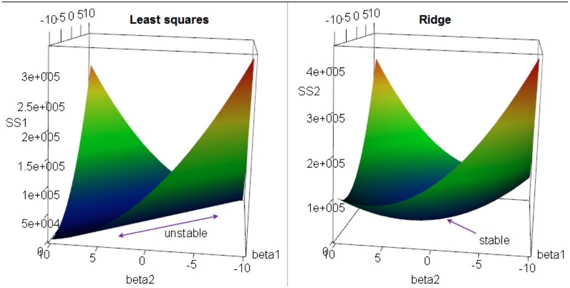

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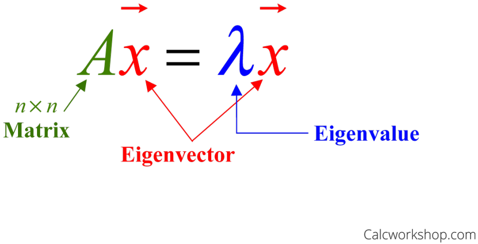
- determination of eigenvalues & eigenvectors, invariant subspaces



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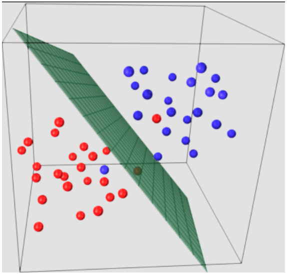
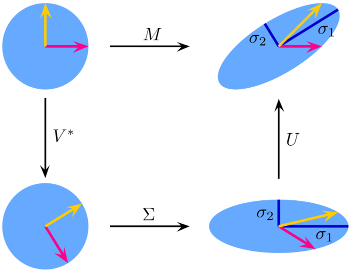


numerical linear algebra

- solving dense and sparse linear systems
- orthogonalization, least square & Tikhonov regularization
- determination of eigenvalues & eigenvectors, invariant subspaces
- singular value decomposition (SVD)



$$M = U \cdot \Sigma \cdot V^*$$

Numerical linear algebra

What is the problem?

$\Rightarrow$ Large scaling problems!

Numerical linear algebra

"Randomized" linear algebra offers novel tools addressing these challenges

Randomized algorithms

1. Monte Carlo (M.C.) algorithms ($\sim$1940)
   · Last resort methods
   · M.C. converges slowly
   · Hesitation: Two runs should produce the same number
2. Randomized algorithms in numerical linear algebra ($\sim$1980)
   · Power method, random initialization (Dixon 1983)
   · M. C. methods for trace estimation (Girard 1989 & Hutchinson 1990)
   · Randomized transformations can avoid pivoting steps in Gaussian elimination (Parker 1995)
3. Practical randomized algorithms for low-rank matrix approximation and least-squares problems (mid-2000s)
   · First computational evidence that randomized algorithms outperform classical NLA algorithms for particular classes of problems

Review:
Classical Numerical Linear Algebra

- L. N. Trefethen and D. Bau III, Numerical linear algebra, Vol. 50, SIAM
- G. Stewart, Matrix Algorithms Volume 1: Basic Decompositions, SIAM
- G. W. Stewart, Matrix algorithms volume 2: eigensystems, Vol. 2, SIAM
- G. H. Golub and C. F. Van Loan, Matrix computations
- R. A. Horn and C. R. Johnson, Matrix analysis
- R. Bhatia, Matrix analysis, Vol. 169 of Graduate Texts in Mathematics

Basics – Notation I

- Algebraic field: $\mathbb{C}$, $\mathbb{R}$, $\mathbb{F}$
- Scalars: $a, b, ...$ or $\alpha, \beta, ...$
- Vectors are elements of $\mathbb{F}^n$, $n \in \mathbb{N}$: $\mathbf{a}, \mathbf{b}, ...$ or $\boldsymbol{\alpha}, \boldsymbol{\beta}, ...$
- Special vectors $\mathbf{0}, \mathbf{1}, \boldsymbol{\delta}_i \in \mathbb{F}^n$:

$$\mathbf{0} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \mathbf{1} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \quad \boldsymbol{\delta}_i = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

- Vector element:

$$(\mathbf{a})_i = \mathbf{a}(i) \qquad i\text{th coordinate of } \mathbf{a}$$

- Colon notation: $(\mathbf{a})_{1:i} = \mathbf{a}(1 : i)$

Basics – Notation II

- A matrix is an element of $\mathbb{F}^{m\times n}$, $m, n \in \mathbb{N}$: $\mathbf{A}, \mathbf{B}, \ldots$ or $\boldsymbol{\Lambda}, \boldsymbol{\Delta}, \ldots$
- Matrix element:

$$(\mathbf{A})_{ij} = \mathbf{A}(ij) \qquad (i,j)\text{th coordinate of } \mathbf{A}$$

- Special matrices $\mathbf{0}, \mathbf{I} \in \mathbb{F}^{m\times n}$:

$$\mathbf{0} = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{pmatrix} \quad \mathbf{I} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & 1 & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}$$

- Colon notation: $(\mathbf{A})_{i:} \equiv i$th row and $(\mathbf{A})_{:j}$ jth column of $\mathbf{A}$

Basics – Notation III

- $*$ is the conjugate transpose
- $\mathbb{H}_n = \mathbb{H}_n(\mathbb{F}) = \{\mathbf{A} \in \mathbb{F}^{n\times n} \ : \ \mathbf{A} = \mathbf{A}^*\}$
- $\dagger$ is the Moor–Penrose (pseudo)inverse: $\mathbf{A}^\dagger$ is the MP inverse of $\mathbf{A}$ iff

$$\begin{array}{llll} (i) & \mathbf{A}\mathbf{A}^\dagger\mathbf{A} = \mathbf{A} & (iii) & (\mathbf{A}\mathbf{A}^\dagger)^* = \mathbf{A}\mathbf{A}^\dagger \\ (ii) & \mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger & (iv) & (\mathbf{A}^\dagger\mathbf{A})^* = \mathbf{A}^\dagger\mathbf{A} \end{array}$$

If $\mathbf{A}$ has full column rank, then $\mathbf{A}^\dagger = (\mathbf{A}^*\mathbf{A})^{-1}\mathbf{A}^*$
If $\mathbf{A}$ attains an inverse then

$$\mathbf{A}^\dagger = \mathbf{A}^{-1}$$

Eigenvalues and singular values

- PSD$= \{\mathbf{A} \in \mathbb{H}_n \ : \ \mathbf{x}^\top \mathbf{A} \mathbf{x} \geq 0 \text{ for } \mathbf{x} \neq 0\}$
- PD$= \{\mathbf{A} \in \mathbb{H}_n \ : \ \mathbf{x}^\top \mathbf{A} \mathbf{x} > 0 \text{ for } \mathbf{x} \neq 0\}$
- $\preccurlyeq$ denotes the semidefinte order on $\mathbb{H}_n$, i.e.

$$\mathbf{A} \preccurlyeq \mathbf{B} \Leftrightarrow 0 \preccurlyeq \mathbf{B} - \mathbf{A}$$

- $\prec$ denotes the semidefinte order on $\mathbb{H}_n$, i.e.

$$\mathbf{A} \prec \mathbf{B} \Leftrightarrow 0 \prec \mathbf{B} - \mathbf{A}$$

- Eigenvalues of $\mathbf{A} \in \mathbb{H}_n$: $\lambda_1 \geq \lambda_2 \geq \dots$
- Singular values of $\mathbf{A} \in \mathbb{F}^{m \times n}$: $\sigma_1 \geq \sigma_2 \geq \dots$
- Let $f : \mathbb{R} \to \mathbb{R}$. We extend f to spectral function $f : \mathbb{H}_n \to \mathbb{H}_n$

$$f(\mathbf{A}) := \sum_{i=1}^{n} f(\lambda_i) \mathbf{u}_i \mathbf{u}_i^* \quad \text{where} \quad \mathbf{A} = \sum_{i=1}^{n} \lambda_i \mathbf{u}_i \mathbf{u}_i^*$$

Inner products and geometry I

- Equip $\mathbb{F}^n$ with standard scalar product and associated ℓ^2-norm. Let $\mathbf{a}, \mathbf{b} \in \mathbb{F}^n$ then

$$\langle \mathbf{a}, \mathbf{b} \rangle := \mathbf{a} \cdot \mathbf{b} = \mathbf{a}^* \mathbf{b} = \sum_{i=1}^{n} (\mathbf{a})_i^* (\mathbf{b})_i$$

  and

$$\|\mathbf{a}\|^2 := \langle \mathbf{a}, \mathbf{a} \rangle$$

- Unit sphere in $\mathbb{F}^n$: $\mathbb{S}^{n-1} = \mathbb{S}^{n-1}(\mathbb{F})$

Inner products and geometry II

- The trace of $\mathbf{A} \in \mathbb{F}^{n \times n}$:

$$\mathrm{Tr}(\mathbf{A}) = \mathrm{trace}(\mathbf{A}) = \sum_{i=1}^{n} (\mathbf{A})_{ii}$$

  Nonlinear functions bind before the trace.

- Equip $\mathbb{F}^{m \times n}$ with the standard trace inner product and Frobenius norm:
  Let $\mathbf{A}, \mathbf{B} \in \mathbb{F}^{m \times n}$ then

$$\langle \mathbf{A}, \mathbf{B} \rangle := \mathrm{Tr}(\mathbf{A}^* \mathbf{B})$$

  and

$$\|\mathbf{A}\|_F^2 = \langle \mathbf{A}, \mathbf{A} \rangle$$

- $\mathbf{U} \in \mathbb{F}^{m \times n}$ is orthonormal iff $\mathbf{U}^* \mathbf{U} = \mathbf{I}_n$.
  $\mathbf{U}$ is unitary ($\mathbb{F} = \mathbb{C}$) or orthogonal ($\mathbb{F} = \mathbb{R}$) if $m = n$.

Matrix norms I

- Let $\| \cdot \|_\alpha$ be a norm on $\mathbb{F}^n$ and $\| \cdot \|_\beta$ be a norm on $\mathbb{F}^m$. Then

$$\| \cdot \|_{\alpha,\beta} : \mathbb{F}^{m\times n} \to \mathbb{R}; \mathbf{A} \mapsto \sup_{\substack{\mathbf{x}\in\mathbb{F}^n \\ \|\mathbf{x}\|_\alpha \neq 0}} \frac{\|\mathbf{A}\mathbf{x}\|_\beta}{\|\mathbf{x}\|_\alpha}$$

  Induces a norm on $\mathbb{F}^{m\times n}$.

- Alternatively, we may define any function

$$\| \cdot \| : \mathbb{F}^{m\times n} \to \mathbb{R}$$

  that fulfills:
  1. $0 \leq \|\mathbf{A}\|,\ \forall \mathbf{A} \in \mathbb{F}^{m\times n}$ and $\|\mathbf{A}\| = 0 \Leftrightarrow \mathbf{A} = \mathbf{0}$
  2. $\|a\mathbf{A}\| = |a|\|\mathbf{A}\|,\ \forall \mathbf{A} \in \mathbb{F}^{m\times n}$, and $\forall a \in \mathbb{F}$
  3. $\|\mathbf{A} + \mathbf{B}\| \leq \|\mathbf{A}\| + \|\mathbf{B}\|,\ \forall \mathbf{A}, \mathbf{B} \in \mathbb{F}^{m\times n}$

- $\| \cdot \|$ is an induced matrix norm iff

Matrix norms II

Several matrix norms will be used. Let $\mathbf{A} \in \mathbb{F}^{m \times n}$

- The unadorned norm $\|\cdot\|$ is the spectral norm

$$\|\mathbf{A}\| = \sigma_1 = \|\mathbf{A}\|_{\ell^2}$$

- $\|\cdot\|_*$ is the nuclear/trace norm

$$\|\mathbf{A}\|_* = \sum_{k=1}^{\min(m,n)} \sigma_k$$

- $\|\cdot\|_F$ is the Frobenius norm

$$\|\mathbf{A}\|_F^2 = \sum_{i=1}^{m} \sum_{j=1}^{n} |(A)_{ij}|^2 = \sum_{k=1}^{\min(m,n)} \sigma_k^2 = \mathrm{Tr}(\mathbf{A}^* \mathbf{A})$$

Matrix norms III

- $\|\cdot\|_p$ is the Schatten p-norm for $p \in [1, \infty]$

$$\|\mathbf{A}\|_p = \left(\sum_{k=1}^{\min(m,n)} \sigma_k^p \right)^{\frac{1}{p}}$$

- $\|\cdot\|_{K,p}$ is the Ky Fan p-norm for $p \leq \min(m, n)$

$$\|\mathbf{A}\|_{K,p} = \sum_{k=1}^{p} \sigma_k$$

Note:

$$\|\cdot\|_* = \|\cdot\|_{K,\min(m,n)} = \|\cdot\|_1$$

$$\|\cdot\|_F = \|\cdot\|_2$$

$$\|\cdot\| = \|\cdot\|_{K,1} = \|\cdot\|_\infty$$

Intrinsic Dimension

Let $\mathbf{A} \in \mathbb{H}_n$ be PSD. We define the intrinsic dimension as

$$\operatorname{intdim}(\mathbf{A}) := \frac{\operatorname{Tr}(\mathbf{A})}{\|\mathbf{A}\|}$$

Note:

$$1 \leq \operatorname{intdim}(\mathbf{A}) \leq \operatorname{rank}(\mathbf{A})$$

The upper bound is saturated if $\mathbf{A}$ is an orthogonal projector i.e.

1. $\mathbf{A} \in \mathbb{F}^{m \times m}$ and $\mathbf{A}^2 = \mathbf{A}$
2. $\mathbf{A}$ is projector and $\mathbf{A} \in \mathbb{H}_n$

The intrinsic rank can be interpreted as a continuous measure of the rank

Stable rank

Let $\mathbf{B} \in \mathbb{F}^{m \times n}$. We define the stable rank as

$$\mathrm{srank}(\mathbf{A}) := \mathrm{intdim}(\mathbf{B}^*\mathbf{B}) = \frac{\|\mathbf{B}\|_F^2}{\|\mathbf{B}\|^2}$$

Schur complement

Let

$$\mathbf{M} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} \in \mathbb{F}^{m \times m}$$

with $\mathbf{A} \in \mathbb{F}^{n \times n}$.
If $\mathbf{D}$ is invertible the Schur complement of $\mathbf{D}$ in $\mathbf{M}$ is

$$\mathbf{M}/\mathbf{D} := \mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}$$

If $\mathbf{A}$ is invertible the Schur complement of $\mathbf{A}$ in $\mathbf{M}$ is

$$\mathbf{M}/\mathbf{A} := \mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B}$$

The latter is used for Cholesky factorization.

What if $\mathbf{D}$ of $\mathbf{A}$ are singular or not square?

Generalized Schur complement

Let $\mathbf{M} \in \mathbb{F}^{m\times n}$ and

$$\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_k) \subseteq [\![m]\!] \quad \text{and} \quad \boldsymbol{\alpha}^c = [\![m]\!] \setminus \boldsymbol{\alpha}$$

and

$$\boldsymbol{\beta} = (\beta_1, ..., \beta_\ell) \subseteq [\![n]\!] \quad \text{and} \quad \boldsymbol{\beta}^c = [\![n]\!] \setminus \boldsymbol{\beta}.$$

We denote

$$\mathbf{M}[\boldsymbol{\gamma}, \boldsymbol{\delta}]$$

the $(\boldsymbol{\gamma}, \boldsymbol{\delta})$-block in $\mathbf{M}$.
The Schur complement of $\mathbf{M}[\boldsymbol{\alpha}, \boldsymbol{\beta}]$ in $\mathbf{M}$ is

$$\mathbf{M}/\mathbf{M}[\boldsymbol{\alpha}, \boldsymbol{\beta}] = \mathbf{M}[\boldsymbol{\alpha}^c, \boldsymbol{\beta}^c] - \mathbf{M}[\boldsymbol{\alpha}^c, \boldsymbol{\beta}] \left(\mathbf{M}[\boldsymbol{\alpha}, \boldsymbol{\beta}]\right)^\dagger \mathbf{M}[\boldsymbol{\alpha}, \boldsymbol{\beta}^c]$$

F. Zhang, The Schur complement and its applications, Vol. 4 of Numerical Methods and Algorithms, Springer-Verlag, New York.

Approximation in the spectral norm

We will mostly establish spectral norm errors.

- Suppose $\mathbf{A} \in \mathbb{F}^{m \times n}$ and $\hat{\mathbf{A}} \in \mathbb{F}^{m \times n}$ is an approximation

  $$\|\mathbf{A} - \hat{\mathbf{A}}\| \leq \varepsilon$$

  then
  1. $|\langle \mathbf{F}, \mathbf{A} \rangle - \langle \mathbf{F}, \hat{\mathbf{A}} \rangle| \leq \varepsilon \|\mathbf{F}\|_*$ for every matrix $\mathbf{F} \in \mathbb{F}^{m \times n}$
  2. $|\sigma_j(\mathbf{A}) - \sigma_j(\hat{\mathbf{A}})| \leq \varepsilon, \ \forall j$

How do spectral norm errors compare with Frobenius norm error measures?