Linear Algebra Primer (cont')

Note: the slides are based on CS131 (Juan Carlos et al) and EE263 (by Stephen Boyd et al) at Stanford. Reorganized, revised, and typed by Hao Su

Outline

- Geometry of Linear Algebra
 - Vector spaces
 - Basis, dimension
 - ► Nullspace, range
- Spectral Decomposition
 - Eigenpairs
 - Spectral theory
- Singular Value Decomposition
 - Geometry of linear maps
 - Singular values, singular vectors
 - Pseudo-inverse
- Matrix Calculus
 - Gradient

Outline

- Geometry of Linear Algebra
 - Vector spaces
 - ► Basis, dimension
 - ▶ Nullspace, range
- ► Spectral Decomposition
 - Eigenpairs
 - Spectral theory
- ► Singular Value Decomposition
 - ► Geometry of linear maps
 - ► Singular values, singular vectors
 - ► Pseudo-inverse
- Matrix Calculus
 - Gradient

Vector Spaces

a vector space or linear space (over the reals) consists of

- ▶ a set \mathcal{V}
- ▶ a vector sum $+: \mathcal{V} \times \mathcal{V} \to \mathcal{V}$
- lacktriangle a scalar multiplication: $\mathbb{R} imes \mathcal{V} o \mathcal{V}$
- lacktriangle a distinguished element $0 \in \mathcal{V}$

which satisfy a list of properties

Vector Space Axioms

$$\triangleright$$
 $x + y = y + x, \forall x, y \in \mathcal{V}$

$$(x+y)+z=x+(y+z), \forall x,y,z\in \mathcal{V}$$

$$\triangleright$$
 0 + $x = x, x \in \mathcal{V}$

$$\forall x \in \mathcal{V} \quad \exists (-x) \in \mathcal{V} \text{ s.t. } x + (-x) = 0$$

$$(\alpha\beta)x = \alpha(\beta x), \quad \forall \alpha, \beta \in \mathbb{R} \quad \forall x \in \mathcal{V}$$

$$(\alpha + \beta)x = \alpha x + \beta x, \quad \forall \alpha, \beta \in \mathbb{R} \quad \forall x \in \mathcal{V}$$

▶
$$1x = x$$
, $\forall x \in \mathcal{V}$

+ is commutative + is associative 0 is additive identity existence of additive inverse scalar mult. is associative right distributive rule left distributive rule 1 is mult. identity

Examples

- $\mathcal{V}_1 = \mathbb{R}^n$, with standard (componentwise) vector addition and scalar multiplication
- $ightharpoonup \mathcal{V}_2 = \{0\} \ (\text{where } 0 \in \mathbb{R}^n)$
- ▶ $V_3 = \operatorname{span}(v_1, v_2, \dots, v_k)$ where $\operatorname{span}(v_1, v_2, \dots, v_k) = \{\alpha_1 v_1 + \dots + \alpha_k v_k | \alpha_i \in \mathbb{R}\}$ and $v_1, \dots, v_k \in \mathbb{R}^n$

Subspaces

- a subspace of a vector space is a subset of a vector space which is itself a vector space
- roughly speaking, a subspace is closed under vector addition and scalar multiplication
- examples V_1, V_3, V_3 above are subspaces of \mathbb{R}^n

Vector Spaces of Functions

▶ $V_4 = \{x : \mathbb{R}_+ \to \mathbb{R}^n | x \text{ is differentiable} \}$, where vector sum is sum of functions:

$$(x+z)(t) = x(t) + z(t)$$

and scalar multiplication is defined by

$$(\alpha x)(t) = \alpha x(t)$$

(a *point* in \mathcal{V}_4 is a *trajectory* in \mathbb{R}^n)

- ▶ $V_5 = \{x \in V_4 | \dot{x} = Ax\}$ (points in V_5 are trajectories of the linear system $\dot{x} = Ax$)
- $ightharpoonup \mathcal{V}_5$ is a subspace of \mathcal{V}_4

Basis and Dimension

set of vectors $\{v_1, v_k, \dots, v_k\}$ is called a *basis* for a vector space $\mathcal V$ if

$$\mathcal{V} = extsf{span}(v_1, v_2, \dots, v_k)$$
 and $\{v_1, v_2, \dots, v_k\}$ is independent

ightharpoonup equivalently, every $v \in \mathcal{V}$ can be uniquely expressed as

$$\mathbf{v} = \alpha_1 \mathbf{v}_1 + \dots + \alpha_k \mathbf{v}_k$$

- lackbox for a given vector space $\mathcal V$, the number of vectors in any basis is the same
- ▶ number of vectors in any basis is called the *dimension* of V, denoted dim V

Nullspace of a Matrix

the *nullspace* of $A \in \mathbb{R}^{m \times n}$ is defined as

$$\mathbf{null}(A) = \{x \in \mathbb{R}^n | Ax = 0\}$$

- **null**(A) is set of vectors mapped to zero by y = Ax
- ▶ **null**(A) is set of vectors orthogonal to all rows of A

null(A) gives *ambiguity* in x given y = Ax:

- if y = Ax and $z \in \mathbf{null}(A)$, then y = A(x + z)
- ▶ conversely, if y = Ax and $y = A\tilde{x}$, then $\tilde{x} = x + z$ for some $z \in \mathbf{null}(A)$

 $\mathbf{null}(A)$ is also written $\mathcal{N}(A)$

Zero Nullspace

A is called *one-to-one* if 0 is the only element of its null space

$$\mathbf{null}(A) = \{0\}$$

Equivalently,

- \triangleright x can always be uniquely determined from y = Ax (i.e., the linear transformation y = Ax doesn't 'lose' information)
- mapping from x to Ax is one-to-one: different x's map to different y's
- columns of A are independent (hence, a basis for their span)
- ▶ A has a *left inverse*, i.e., there is a matrix $B \in \mathbb{R}^{n \times m}$ s.t. BA = I
- \triangleright A^TA is invertible

Range of a Matrix

the *range* of $A \in \mathbb{R}^{m \times n}$ is defined as

$$\mathsf{range}(A) = \{Ax | x \in \mathbb{R}^n\} \subseteq \mathbb{R}^m$$

range(A) can be interpreted as

- ▶ the set of vectors that can be 'hit' by linear mapping y = Ax
- ▶ the span of columns of A
- ▶ the set of vectors y for which Ax = y has a solution

range(A) is also written $\mathcal{R}(A)$

Outline

- ► Geometry of Linear Algebra
 - Vector spaces
 - ▶ Basis. dimension
 - ► Nullspace, range
- Spectral Decomposition
 - Eigenpairs
 - Spectral theory
- ► Singular Value Decomposition
 - ► Geometry of linear maps
 - Singular values, singular vectors
 - ► Pseudo-inverse
- ▶ Matrix Calculus
 - Gradient
 - ► Jacobian
 - Hessian

Eigenvector and Eigenvalue

▶ an eigenvector *x* of a linear transformation *A* is a non-zero vector that, when *A* is applied to it, does not change direction

$$Ax = \lambda x, \qquad x \neq 0.$$

▶ applying A to the vector only scales the vector by the scalar value λ , called an *eigenvalue*.

Eigenvector and Eigenvalue

we want to find all the eigenvalues of A:

$$Ax = \lambda x, \qquad x \neq 0.$$

which can be written as:

$$Ax = (\lambda I)x, \qquad x \neq 0.$$

therefore:

$$(\lambda I - A)x = 0, \qquad x \neq 0.$$

Eigenvector and Eigenvalue

we can solve for eigenvalues by solving :

$$(\lambda I - A)x = 0, \qquad x \neq 0.$$

▶ above means that $\lambda I - A$ is not full rank, thus we can instead solve the above equation as:

$$|(\lambda I - A)| = 0.$$

▶ this is called *characteristic polynomial* of an $n \times n$ matrix

Properties of Eigenvalues

▶ the trace of *A* is equal to the sume of its eigenvalues:

$$\operatorname{tr}(A) = \sum_{i=1}^n \lambda_i$$

▶ the determinant of *A* is equal to the product of its eigenvalues

$$|A| = \prod_{i=1}^n \lambda_i$$

- ▶ the rank of A is equal to the number of non-zero eigenvalues of A
- ▶ for general A, it can be proved by Schur Decomposition easily (omitted)
- ▶ for diagonalizable *A*, the proof is straightforward

Diagonalization

▶ if matrix A can be diagonalized, that is,

$$P^{-1}AP = \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix}$$

▶ then:

$$AP = P \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix}$$

• write $P = [\vec{\alpha}_1, \dots, \vec{\alpha}_n]$, the above equation can be rewritten as

$$A\vec{\alpha}_i = \lambda_i \vec{\alpha}_i$$

Diagonalization by Spectral Decomposition

- here is a sufficient (but not necessary) condition
- \blacktriangleright assuming all λ_i 's are unique, by eigenvalue equation:

$$AV = VD$$

$$A = VDV^{-1}$$

- ▶ why?
 - eigenvectors associated with different eigenvalues are linearly independent, thus A invertible
 - ▶ in fact, if A is symmetric, V could be orthonormal and $A = VDV^T$

Diagonalization (Summary)

- ▶ an $n \times n$ matrix A is diagonalizable if it has n linearly independent (in fact, orthogonal) eigenvectors.
- ▶ matrices with *n* distinct eigenvalues are diagnolizable

Symmetric Matrices

Properties

- ▶ for a real symmetric matrix A, all the eigenvalues are real
- ► A is diagonalizable
- ▶ the eigenvectors of *A* are orthonormal

$$A = VDV^T$$

Symmetric Matrices

therefore

$$x^{T}Ax = x^{T}VDV^{T}x = y^{T}Dy = \sum_{i=1}^{n} \lambda_{i}y_{i}^{2}$$

where $y = V^T x$

▶ so, if we wanted to find the vector x that

$$\max_{x \in \mathbb{R}^n} x^T A x \qquad \text{subject to } ||x||_2^2 = 1$$

Symmetric Matrices

therefore

$$x^{T}Ax = x^{T}VDV^{T}x = y^{T}Dy = \sum_{i=1}^{n} \lambda_{i}y_{i}^{2}$$

where $y = V^T x$

▶ so, if we wanted to find the vector x that

$$\max_{x \in \mathbb{R}^n} x^T A x \qquad \text{subject to } ||x||_2^2 = 1$$

is the same as finding the eigenvector that corresponds to the largest eigenvalue.

Spectral Theory

- lacktriangle we call an eigenvalue λ and an associated eigenvector an eigenpair
- ▶ the space of vectors where $(A \lambda I)x = 0$ is often called the *eigenspace* of A associated with the eigenvalue λ
- ▶ the set of all eigenvalues of *A* is called its *spectrum*:

$$\sigma(A) = \{ \lambda \in \mathbb{C} : \lambda I - A \text{ is singular} \}$$

Spectral Theory

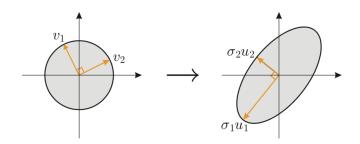
► the magnitude of the largest eigenvalue (in magnitude) is called the spectral radius

$$\rho(A) = \max\{|\lambda_1|, \dots, |\lambda_n|\}$$

Outline

- ► Geometry of Linear Algebra
 - Vector spaces
 - ► Basis, dimension
 - ► Nullspace, range
- Spectral Decomposition
 - Eigenpairs
 - Spectral theory
- Singular Value Decomposition
 - Geometry of linear maps
 - Singular values, singular vectors
 - Pseudo-inverse
- ► Matrix Calculus
 - Gradient

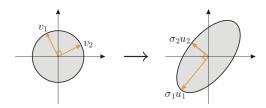
Geometry of Linear Maps



every matrix $A \in \mathbb{R}^{m \times n}$ maps the unit ball in \mathbb{R}^n to an ellipsoid in \mathbb{R}^m

$$S = \{x \in \mathbb{R}^n | ||x|| \le 1\}$$
 $AS = \{Ax | x \in S\}$

Singular Values and Singular Vectors



- ▶ first, assume $A \in \mathbb{R}^{m \times n}$ is skinny and full rank
- ▶ the numbers $\sigma_1, \ldots, \sigma_n > 0$ are called the *singular values* of A
- ▶ the vectors $u_1, ..., u_n$ are called the *left* or *ourput singular vectors* of A. These are *unit vectors* along the principal semiaxes of AS
- ▶ the vectors $v_1, ..., v_n$ are called the *right* or *input singular vectors* of A. These map to the principal semiaxes, so that

$$Av_i = \sigma_i u_i$$

Thin Singular Value Decomposition

$$Av_i = \sigma_i u_i$$
 for $1 \le i \le n$

For $A \in \mathbb{R}^{m \times n}$ with rank(A) = n, let

$$U = \begin{bmatrix} u_1 & u_2 & \dots & u_n \end{bmatrix} \qquad \Sigma = \begin{bmatrix} \sigma_1 & & & & \\ & \sigma_2 & & & \\ & & \ddots & & \\ & & & \sigma_n \end{bmatrix} \qquad V = \begin{bmatrix} v_1 & v_2 & \dots & v_n \end{bmatrix}$$

the above equation is $AV=U\Sigma$ and since V is orthogonal

$$A = U\Sigma V^T$$

called the thin SVD of A

Thin SVD

For $A \in \mathbb{R}^{m \times n}$ with $\mathbf{rank}(A) = r$, the *thin SVD* is

$$A = U\Sigma V^T = \sum_{i=1}^r \sigma_i u_i v_i^T$$

$$A \qquad U \qquad \Sigma \qquad V^{\mathsf{T}}$$

here

- ▶ $U \in \mathbb{R}^{m \times r}$ has orthonormal columns,
- $ightharpoonup \Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_r)$, where $\sigma_1 \ge \cdots \sigma_r > 0$
- ▶ $V \in \mathbb{R}^{n \times r}$ has orthonormal columns

SVD and Eigenvectors

$$A^{T}A = (U\Sigma V^{T})^{T}(U\Sigma V^{T}) = V\Sigma^{2}V^{T}$$

hence:

- \triangleright v_i are eigenvectors of A^TA (corresponding to nonzero eigenvalues)
- $ightharpoonup \sigma_i = \sqrt{\lambda_i(A^TA)} \text{ (and } \lambda_i(A^TA) = 0 \text{ for } i > r \text{)}$
- $||A|| = \sigma_1$

SVD and Eigenvectors

similarly,

$$AA^{T} = (U\Sigma V^{T})(U\Sigma V^{T})^{T} = U\Sigma^{2}U^{T}$$

hence:

- \triangleright u_i are eigenvectors of AA^T (corresponding to nonzero eigenvalues)
- $ightharpoonup \sigma_i = \sqrt{\lambda_i(AA^T)} \text{ (and } \lambda_i(AA^T) = 0 \text{ for } i > r)$

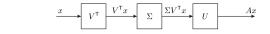
SVD and Range

$$A = U\Sigma V^T$$

- u_1, \ldots, u_r are orthonormal basis for **range**(A)
- $ightharpoonup v_1, \ldots, v_r$ are orthonormal basis for $\mathbf{null}(A)^{\perp}$

Interpretations

$$A = U\Sigma V^T = \sum_{i=1}^r \sigma_i u_i v_i^T$$



linear mapping y = Ax can be decomposed as

- ightharpoonup compute coefficients of x along input directions v_1, \ldots, v_r
- \triangleright scale coefficients by σ_i
- ightharpoonup reconstitute along output directions u_1, \ldots, u_r

difference with eigenvalue decomposition for symmetric A: input and output directions are different

General Pseudo-inverse

if $A \neq 0$ has SVD $A = U\Sigma V^T$, the *pseudo-inverse* or *Moore-Penrose* inverse of A is

$$A^{\dagger} = V \Sigma^{-1} U^T$$

▶ if A is skinny and full rank,

$$A^{\dagger} = (A^T A)^{-1} A^T$$

gives the least-squares approximate solution $x_{ls}=A^\dagger y$

▶ if A is fat and full rank,

$$A^{\dagger} = A^{T} (AA^{T})^{-1}$$

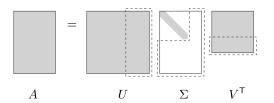
gives the least-norm solution $x_{ln} = A^{\dagger} y$

Full SVD

SVD of $A \in \mathbb{R}^{m \times n}$ with rank(A) = r

$$A = U_1 \Sigma_1 V_1^T = \begin{bmatrix} u_1 & \cdots & u_r \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r \end{bmatrix} \begin{bmatrix} v_1^T \\ \vdots \\ v_r^T \end{bmatrix}$$

Add extra columns to $\it U$ and $\it V$, and add zero rows/cols to Σ_1



Full SVD

- ▶ find $U_2 \in \mathbb{R}^{m \times (m-r)}$ such that $U = [U_1 \ U_2] \in \mathbb{R}^{m \times m}$ is orthogonal
- ▶ find $V_2 \in \mathbb{R}^{n \times (n-r)}$ such that $V = [V_1 \ V_2] \in \mathbb{R}^{n \times n}$ is orthogonal
- ▶ add zero rows/cols to Σ_1 to form $\Sigma \in \mathbb{R}^{m \times n}$

$$\Sigma = \left[\begin{array}{c|c} \Sigma_i & 0_{r \times (n-r)} \\ \hline 0_{(m-r) \times r} & 0_{(m-r) \times (n-r)} \end{array} \right]$$

then the full SVD is

$$A = U_1 \Sigma_1 V_1^T = \begin{bmatrix} U_1 \mid U_2 \end{bmatrix} \begin{bmatrix} \Sigma_i & 0_{r \times (n-r)} \\ \hline 0_{(m-r) \times r} \mid 0_{(m-r) \times (n-r)} \end{bmatrix} \begin{bmatrix} V_1^T \\ \hline V_2^T \end{bmatrix}$$

which is $A = U\Sigma V^T$

Image of Unit Ball under Linear Transformation

full SVD:

$$A = U\Sigma V^T$$

gives interpretation of y = Ax

- ▶ rotate (by V^T)
- ▶ stretch along axes by σ_i ($\sigma_i = 0$ for i > r)
- ightharpoonup zero-pad (if m > n) or truncate (if m < n) to get m-vector
- ▶ rotate (by U)

Outline

- ► Geometry of Linear Algebra
 - Vector spaces
 - ► Basis, dimension
 - ► Nullspace, range
- ► Spectral Decomposition
 - Eigenpairs
 - Spectral theory
- ► Singular Value Decomposition
 - Geometry of linear maps
 - ► Singular values, singular vectors
 - ► Pseudo-inverse
- Matrix Calculus
 - Gradient

Matrix Calculus – the Gradient (first-order derivative)

- ▶ let a function $f: \mathbb{R}^{m \times n} \to \mathbb{R}$ take as input a matrix A of size $m \times n$ and returns a real value
- ▶ then the *gradient* of *f*:

$$\nabla_{A}f(A) \in \mathbb{R}^{m \times n} = \begin{bmatrix} \frac{\partial f(A)}{\partial A_{11}} & \frac{\partial f(A)}{\partial A_{12}} & \cdots & \frac{\partial f(A)}{\partial A_{1n}} \\ \frac{\partial f(A)}{\partial A_{21}} & \frac{\partial f(A)}{\partial A_{22}} & \cdots & \frac{\partial f(A)}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \frac{\partial f(A)}{\partial A_{m2}} & \cdots & \frac{\partial f(A)}{\partial A_{mn}} \end{bmatrix}$$

i.e., an $m \times n$ matrix with

$$(\nabla_{ij}f(A))_{ij}=\frac{\partial f(A)}{\partial A_{ij}}$$

 \triangleright vectors are $m \times 1$ matrices

Matrix Calculus – the Gradient (first-order derivative)

Gradient operator ∇ is linear:

- ▶ For $t \in \mathbb{R}$, $\nabla_x(tf(x)) = t\nabla_x f(x)$

Matrix Calculus – the Hessian (second-order derivative)

▶ Consider a **vector function** f(x) defined as $f: \mathbb{R}^n \to \mathbb{R}$. The Hessian w.r.t x is an $n \times n$ matrix:

$$\nabla f(x) \in \mathbb{R}^{n \times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial^2 x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}$$

▶ In other words,

$$(\nabla_x^2 f(x))_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_i}$$

Note that Hessian is always symmetric since

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} = \frac{\partial^2 f(x)}{\partial x_j \partial x_i}$$

Gradients of Quadratic Vector Functions

▶ Consider a quadratic function $f(x) = x^T A x$ for $A \in \mathbb{S}$. Remember that

$$f(x) = \sum_{i} \sum_{j} A_{ij} x_i x_j$$

▶ If you take partial derivative, after calculation, we will have

$$\frac{\partial f(x)}{\partial x_k} = 2\sum_{i=1}^n A_{ki}x_i$$

▶ This result can be written compactly in matrix form:

$$\nabla_{x}f(x)=2Ax$$

Hessian of Quadratic Vector Functions

▶ Let's look at the Hessian of the quadratic function $f(x) = x^T A x$

$$\frac{\partial^2 f(x)}{\partial x_k \partial x_l} = \frac{\partial}{\partial x_k} \left[\frac{\partial f(x)}{\partial x_l} \right] = 2A_{lk} = 2A_{kl}$$

▶ Matrix form: $\nabla_x x^T A x = 2A$

Summary of Matrix Calculus

- $\nabla_x b^T x = b$
- $\nabla^2_x b^T x = 0$