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

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Vector Spaces

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

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

which satisfy a list of properties

Vector Space Axioms

- $x + y = y + x, \forall x, y \in \mathcal{V}$ — *+ is commutative*
- $(x + y) + z = x + (y + z), \forall x, y, z \in \mathcal{V}$ — *+ is associative*
- $0 + x = x, x \in \mathcal{V}$ — *0 is additive identity*
- $\forall x \in \mathcal{V} \quad \exists (-x) \in \mathcal{V}$ s.t. $x + (-x) = 0$ — *existence of additive inverse*
- $(\alpha\beta)x = \alpha(\beta x), \quad \forall \alpha, \beta \in \mathbb{R} \quad \forall x \in \mathcal{V}$ — *scalar mult. is associative*
- $\alpha(x + y) = \alpha x + \alpha y, \quad \forall \alpha \in \mathbb{R} \;\; \forall x, y \in \mathcal{V}$ — *right distributive rule*
- $(\alpha + \beta)x = \alpha x + \beta x, \quad \forall \alpha, \beta \in \mathbb{R} \quad \forall x \in \mathcal{V}$ — *left distributive rule*
- $1x = x, \quad \forall x \in \mathcal{V}$ — *1 is mult. identity*

Examples

- $\mathcal{V}_1 = \mathbb{R}^n$, with standard (componentwise) vector addition and scalar multiplication
- $\mathcal{V}_2 = \{0\}$ (where $0 \in \mathbb{R}^n$)
- $\mathcal{V}_3 = \textbf{span}(v_1, v_2, \ldots, v_k)$ where
  $$\textbf{span}(v_1, v_2, \ldots, v_k) = \{\alpha_1 v_1 + \cdots + \alpha_k v_k | \alpha_i \in \mathbb{R}\}$$
  and $v_1, \ldots, v_k \in \mathbb{R}^n$

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 $\mathcal{V}_1, \mathcal{V}_3, \mathcal{V}_3$ above are subspaces of $\mathbb{R}^n$

Vector Spaces of Functions

- $\mathcal{V}_4 = \{x : \mathbb{R}_+ \to \mathbb{R}^n | x \text{is differentiable}\}$, 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 $\mathbb{R}^n$)
- $\mathcal{V}_5 = \{x \in \mathcal{V}_4 | \dot{x} = Ax\}$
(*points* in $\mathcal{V}_5$ are *trajectories* of the linear system $\dot{x} = Ax$)
- $\mathcal{V}_5$ is a subspace of $\mathcal{V}_4$

Basis and Dimension

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

$$\mathcal{V} = \textbf{span}(v_1, v_2, \ldots, v_k)$$
and
$$\{v_1, v_2, \ldots, v_k\} \text{ is independent}$$

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

$$v = \alpha_1 v_1 + \cdots + \alpha_k v_k$$

- 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 $\mathcal{V}$, denoted $\textbf{dim}\, V$

Nullspace of a Matrix

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

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

- $\mathbf{null}(A)$ is set of vectors mapped to zero by $y = Ax$
- $\mathbf{null}(A)$ 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,

- 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. $BA = I$
- $A^T A$ is invertible

Range of a Matrix

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

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

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 $\mathcal{R}(A)$

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  - 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:

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

- 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
- 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

$$x^T A x = x^T V D V^T x = y^T D y = \sum_{i=1}^{n} \lambda_i y_i^2$$

  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
$$x^T A x = x^T V D V^T x = y^T D y = \sum_{i=1}^{n} \lambda_i y_i^2$$
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

- 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*:

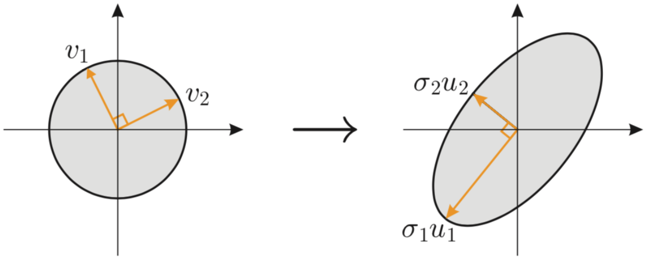
$$\sigma(A) = \{\lambda \in \mathbb{C} : \lambda I - A \text{ is singular}\}$$

Spectral Theory

- the magnitude of the largest eigenvalue (in magnitude) is called the spectral radius
$$\rho(A) = \mathsf{max}\{|\lambda_1|, \ldots, |\lambda_n|\}$$

Outline

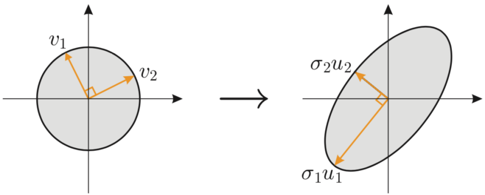
Geometry of Linear Maps



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

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

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 $u_1, \ldots, u_n$ are called the *left* or *ourput singular vectors* of A. These are *unit vectors* along the principal semiaxes of AS
- the vectors $v_1, \ldots, v_n$ 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

$$Av_i = \sigma_i u_i \text{ for } 1 \le i \le n$$

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

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

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

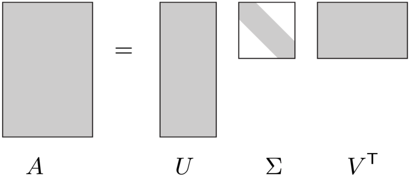
$$A = U\Sigma V^T$$

called the *thin SVD* of A

Thin SVD

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

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



here

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

SVD and Eigenvectors

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

hence:

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

SVD and Eigenvectors

similarly,

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

hence:

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

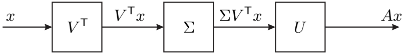
SVD and Range

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

- $u_1, \ldots, u_r$ are orthonormal basis for **range**(A)
- $v_1, \ldots, v_r$ are orthonormal basis for **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

- compute coefficients of x along input directions $v_1, \ldots, v_r$
- scale coefficients by σ_i
- 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,

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

  gives the least-squares approximate solution $x_{ls} = A^\dagger y$
- if A is fat and full rank,

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

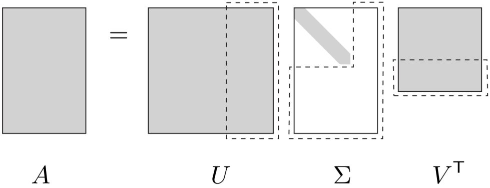
  gives the least-norm solution $x_{ln} = A^\dagger y$

Full SVD

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

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

Add extra columns to U and 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

$$A = U_1\Sigma_1 V_1^T = \left[\begin{array}{c|c} U_1 & U_2 \end{array}\right] \left[\begin{array}{c|c} \Sigma_i & 0_{r\times(n-r)} \\ \hline 0_{(m-r)\times r} & 0_{(m-r)\times(n-r)} \end{array}\right] \left[\begin{array}{c} V_1^T \\ \hline V_2^T \end{array}\right]$$

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 $i > r$)
- zero-pad (if $m > n$) or truncate (if $m < n$) to get m-vector
- rotate (by U)

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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

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

- vectors are $m \times 1$ matrices

Matrix Calculus – the Gradient (first-order derivative)

Gradient operator ∇ is linear:

- $\nabla_x(f(x) + g(x)) = \nabla_x f(x) + \nabla_x g(x)$
- 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,

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

- 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 $f(x) = x^T Ax$ 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 $f(x) = x^T Ax$

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

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

Summary of Matrix Calculus

- $\nabla_x b^T x = b$
- $\nabla_x^2 b^T x = 0$
- $\nabla_x x^T A x = Ax + A^T x$ (if A not symmetric)
- $\nabla_x x^T A x = 2Ax$ (if A symmetric)
- $\nabla_x x^T A x = A + A^T$ (if A not symmetric)
- $\nabla_x x^T A x = 2A$ (if A symmetric)