From \Re to \Re^n .

Local Extrema for $f(x_1, x_2..., x_n)$

Definition

[Local minimum]: A function $f: \mathcal{D} \to \Re$ of n variables has a local minimum at \mathbf{x}^0 if $\exists \mathcal{N}(\mathbf{x}^0)$ such that $\forall \mathbf{x} \in \mathcal{N}(\mathbf{x}^0)$, $f(\mathbf{x}^0) \leq f(\mathbf{x})$. In other words, $f(\mathbf{x}^0) \leq f(\mathbf{x})$ whenever \mathbf{x} dies in some neighborhood around \mathbf{x}^0 . An example neighborhood is the circular disc when $\mathcal{D} = \Re^n$.

Definition

[Local maximum]: $f(\mathbf{x}^0) \ge f(\mathbf{x})$.

General Reference: Stories About Maxima and Minima (Mathematical World) by Vladimir M. Tikhomirov

Local Extrema

These definitions are exactly analogous to the definitions for a function of single variable. Figure 8 shows the plot of $f(x_1, x_2) = 3x_1^2 - x_1^3 - 2x_2^2 + x_2^4$. As can be seen in the plot, the function has several local maxima and minima.

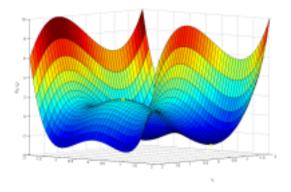


Figure 8:

Convexity and Extremum: Slopeless interpretation (SI)

Definition

A function f is convex on \mathcal{D} , *iff*

$$f(\alpha \mathbf{x}_1 + (1 - \alpha)\mathbf{x}_2) \le \alpha f(\mathbf{x}_1) + (1 - \alpha)f(\mathbf{x}_2)$$

(3)

(4)

and is strictly convex on $\mathcal{D}\text{, }\textit{iff}$

$$f(\alpha \mathbf{x}_1 + (1 - \alpha)\mathbf{x}_2) < \alpha f(\mathbf{x}_1) + (1 - \alpha)f(\mathbf{x}_2)$$

whenever $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{D}$, $\mathbf{x}_1 \neq \mathbf{x}_2$ and $0 < \alpha < 1$.

Note: This implicitly assumes that whenever $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{D}$, then their convex combinatio is also in D Prof. Ganesh Ramakrishnan (IIT Bombay) From \Re to \Re^n : CS709 26/12/2016 32 / 200 Convexity and Extremum: Slopeless interpretation (SI)

Definition

A function f is convex on \mathcal{D} , *iff*

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$$f(\alpha \mathbf{x}_1 + (1 - \alpha)\mathbf{x}_2) < \alpha f(\mathbf{x}_1) + (1 - \alpha)f(\mathbf{x}_2)$$

whenever $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{D}$, $\mathbf{x}_1 \neq \mathbf{x}_2$ and $0 < \alpha < 1$.

Note: This implicitly assumes that whenever $\mathbf{x}_1, \mathbf{x}_2 \in \mathcal{D}$, $\alpha \mathbf{x}_1 + (1 - \alpha)\mathbf{x}_2 \in \mathcal{D}$ Such a set is called a convex set

Prof. Ganesh Ramakrishnan (IIT Bombay)

From \Re to \Re^n : CS709

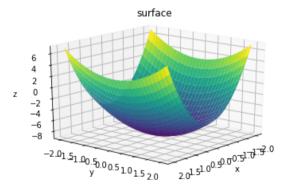
26/12/2016 32 / 200

(3)

(4)

Local Extrema

Figure 9 shows the plot of $f(x_1, x_2) = 3x_1^2 + 3x_2^2 - 9$. As can be seen in the plot, the function is cup shaped and appears to be convex everywhere in \Re^2 .





From $f(x): \Re \to \Re$ to $f(x_1, x_2 \dots x_n): \mathcal{D} \to \Re$

Need to also extend

- Extreme Value Theorem
- Rolle's theorem, Mean Value Theorem, Taylor Expansion
- Necessary and Sufficient first and second order conditions for local/extrema
- First and second order conditions for Convexity
- Need following notions/definitions in $\ensuremath{\mathcal{D}}$
 - Neighborhood and open sets/balls (Local extremum)
 - Bounded, Closed Sets, Continuity of functions (
 Extreme value theorem analysis
 - Convex Sets (Convex functions of *n* variables)
 - Directional Derivatives and Gradients (Taylor Expansion, all first order conditions)

and Hessians

Necessary and sufficient conditions for convexity

Prof. Ganesh Ramakrishnan (IIT Bombay)

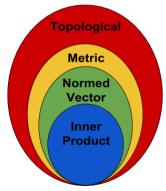
Building block

for convex

Spaces & Mathematical Structures

Contents: The Mathematical Structures called Spaces

- Topological Spaces: Notion of neighbourhood of points, open sets, continuity.
- Metric Spaces: Notion of positive distance between two points.
- Normed Vector Spaces: Notion of positive length of each point.
- Inner Product Spaces: Notion of projection of one point on another, both positive and negative.



Topological Spaces

Set of points X along with the set of neighbors $(N(\mathbf{x}))$ of each point $(\mathbf{x} \in X)$, with certain axioms required to be satisfied by the points and their neighbors.

- Definition 1: A topological space is an ordered pair (X, \mathcal{N}) , where:
 - X is a set
 - \mathcal{N} is a collection of subsets of X, satisfying the following axioms:
 - * The empty set and X itself belong to \mathcal{N} .
 - * Any (finite or infinite) union of members of $\mathcal N$ still belongs to $\mathcal N$.
 - * The intersection of any finite number of members of \mathcal{N} still belongs to \mathcal{N} .

• As per above example, which out of following are toplogies with $X = \{1, 2, 3\}$ and $\mathcal{N} =$

$$\{\{1, 2, 3\}\}$$
 yes

$$\{\{1\}, \{1\}, \{1, 2, 3\}\}$$
 ves

•
$$\{\{\}, \{1\}, \{2\}, \{1, 2\}, \{1, 2, 3\}\}$$
 yes

- ► {{},{1},{2},{1,2,3}} **no**
- ► {{},{1,2},{<u>2,3},{1,2,3}</u>} **no**

Topological Spaces

Set of points X along with the set of open sets (N) with certain axioms required to be satisfied by sets in N:

- Definition 1: A topological space is an ordered pair (X, \mathcal{N}), where:
 - ► X is a set
 - \mathcal{N} is a collection of subsets of X, satisfying the following axioms:
 - * The empty set and X itself belong to \mathcal{N} .
 - * Any (finite or infinite) union of members of $\mathcal N$ still belongs to $\mathcal N$.
 - $\star\,$ The intersection of any finite number of members of ${\cal N}$ still belongs to ${\cal N}.$
- As per above example, which out of following are toplogies with $X = \{1, 2, 3\}$ and $\mathcal{N} =$
 - ▶ $\{\{\}, \{1, 2, 3\}\}$ Yes
 - $\{\{\}, \{1\}, \{1, 2, 3\}\}$ Yes
 - $\{\{\}, \{1\}, \{2\}, \{1,2\}, \{1,2,3\}\}$ Yes
 - $\{\{\}, \{2\}, \{1,2\}, \{2,3\}, \{1,2,3\}\}$ Yes N(3) = $\{\{2,3\}, \{1,2,3\}\}$
 - ▶ {{}, {1}, {2}, {1, 2, 3}} No as {1} \cup {2} $\notin N$
 - ▶ {{}, {1,2}, {2,3}, {1,2,3}} No as {1,2} \cap {2,3} $\notin N$

Topological Spaces: Neighborhoods and Open Sets

The sets $O \in \mathcal{N}$ are basically the open sets. The neighbourhoods can be recovered by defining $N(\mathbf{x})$ to be a neighbourhood of \mathbf{x} if $N(\mathbf{x})$ includes a set O such that $\mathbf{x} \in O$. For example

- with $X = \{1, 2, 3\}$ and $\mathcal{N} = \{\{\}, \{1, 2, 3\}, \text{ each of } \{\} \text{ and } \{1, 2, 3\} \text{ is an open set } O \text{ and } N(1) = \{\{1, 2, 3\}\}$ $N(2) = \{\{1, 2, 3\}\}$ $N(3) = \{\{1, 2, 3\}\}$
- with $X = \{1, 2, 3\}$ and $\mathcal{N} = \{\{\}, \{1\}, \{1, 2, 3\}\}$, each of $\{\}, \{1\}$ and $\{1, 2, 3\}$ is an open set O and $N(1) = \{\{1\}, \{1, 2, 3\}\}$ $N(2) = \{\{1, 2, 3\}\}$ $N(3) = \{\{1, 2, 3\}\}$
- with $X = \{1, 2, 3\}$ and $\mathcal{N} = \{\{\}, \{1\}, \{2\}, \{1, 2\}, \{1, 2, 3\}\}$, each of $\{\}, \{1\}, \{2\}, \{1, 2\}$ and $\{1, 2, 3\}$ is an open set O and $N(1) = \{\{1\}, \{1, 2\}, \{1, 2, 3\}\}$ $N(2) = \{\{2\}, \{1, 2\}, \{1, 2, 3\}\}$ $N(3) = \{\{1, 2, 3\}\}$

Topological Spaces and Open Sets

• with $X = \{1, 2, 3\}$ and $\mathcal{N} = \{\{\}, \{2\}, \{1, 2\}, \{2, 3\}, \{1, 2, 3\}\}$ each of $\{\}, \{2\}, \{1, 2\}, \{2, 3\}$ and $\{1, 2, 3\}$ is an open set O and $N(1) = \{\{1, 2\}, \{1, 2, 3\}\}$ $N(2) = \{\{1, 2\}, \{2, 3\}, \{1, 2, 3\}\}$ $N(3) = \{\{2, 3\}, \{1, 2, 3\}\}$

(Alternative) Definition 2: A topological space is an ordered pair (X, N(.)), where X is a set and N(.) is a neighborhood function such that for each $\mathbf{x} \in X$, if $N(\mathbf{x})$ is a

- neighbourhood of \mathbf{x} then $\mathbf{x} \in \mathit{N}(\mathbf{x})$.
- subset of X and includes a neighbourhood of \mathbf{x} , then $N(\mathbf{x})$ is a neighbourhood of \mathbf{x} .
- neighbourhood of x, then for any other neighborhood N'(x), $N(x) \cap N'(x)$ is also a neighbourhood of x.
- neighbourhood of \mathbf{x} , then it includes a neighbourhood $N'(\mathbf{x})$ such that $N(\mathbf{x})$ is a neighbourhood of each point of $N'(\mathbf{x})$. This definition directly gives you

What topological spaces (and their special cases) give us

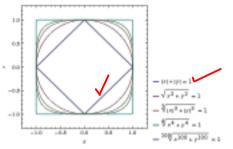
- Definition 1: A topological space is an ordered pair (X, \mathcal{N}) , where....
- Definition 2: A topological space is an ordered pair (X, N(.)), where....
- Definition 1 allows for understanding open sets as elements of \mathcal{N} .
 - We can define an open ball $B(\mathbf{x})$ to be any element of $N(\mathbf{x})$.
 - ► If additionally, we have metric d(.,.) on the space, we can define an open ball $B(\mathbf{x}, r)$ of radius r as $\{\mathbf{y} | \mathbf{d}(\mathbf{x}, \mathbf{y}) < \mathbf{r}\}$
 - A norm ball $\overline{B}(\mathbf{x}, r) = {\mathbf{y} || \mathbf{x} \mathbf{y} || < \mathbf{r}}$ also should have homogenity! That is, $\|\alpha \mathbf{x} - \alpha \mathbf{y}\| = \alpha \|\mathbf{x} - \mathbf{y}\|$
- Definition 2 allows for continuity of function \underline{f} definied from a topology X, N(.) to another topology Y, M(.). Function f is continuous if for every $\mathbf{x} \in X$ and every neighbourhood $M(f(\mathbf{x}))$ of $f(\mathbf{x})$ there is a neighbourhood $N(\mathbf{x})$ of \mathbf{x} such that $f(N(\mathbf{x})) \subseteq f(M(\mathbf{x}))$.

Metric Spaces

Set of points (X) along with a notion of distance $d(x_1, x_2)$ between any two points($x_1, x_2 \in X$) such that:

- $d(\mathbf{x}_1, \mathbf{x}_2) \ge 0$ (non-negativity).
- 2 $d(\mathbf{x}_1, \mathbf{x}_2) = 0$ iff $\mathbf{x}_1 = \mathbf{x}_2$ (identity).
- $\ \, \bullet \ \, \mathsf{d}(\mathbf{x}_1,\mathbf{x}_2)=\mathsf{d}(\mathbf{x}_2,\mathbf{x}_1) \ \, (\mathsf{symmetry}).$
- $\texttt{ d}(\mathbf{x}_1,\mathbf{x}_2) + \mathsf{d}(\mathbf{x}_2,\mathbf{x}_3) \geq \mathsf{d}(\mathbf{x}_1,\mathbf{x}_3) \text{ (triangle inequality)}.$

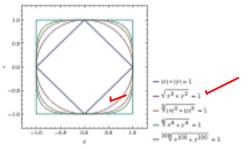
Metric Spaces: Examples



• 1-metric d_1 : The space with the taxi cab metric

•
$$d((x_1, y_1), (x_2, y_2)) = |x_1 - x_2| + |y_1 - y_2|$$

Metric Spaces: Examples



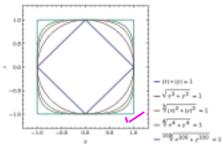
• 1-metric d_1 : The space with the taxi cab metric

•
$$d((x_1, y_1), (x_2, y_2)) = |x_1 - x_2| + |y_1 - y_2|$$

• 2-metric d_2 : The space \Re^2 with the 'usual distance' (measured using Pythagoras's theorem, a theorem we will generalize later for convex functions using Bregman divergence):

•
$$d((x_1, y_1), (x_2, y_2)) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}.$$

Metric Spaces: Examples



• 1-metric d_1 : The space with the taxi cab metric

•
$$d((x_1, y_1), (x_2, y_2)) = |x_1 - x_2| + |y_1 - y_2|$$

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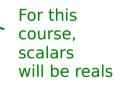
•
$$d((x_1, y_1), (x_2, y_2)) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}.$$

• Infinity metric d_{∞} : The space with the maximum metric

•
$$d((x_1, y_1), (x_2, y_2)) = max(|x_1 - x_2|, |y_1 - y_2|)$$

Normed Vector Spaces

- Vector Space: A space consisting of vectors, together with the
 - associative and commutative operation of addition of vectors,
 - associative and distributive operation of multiplication of vectors by scalars.
- Field of scalars: e.g. algebraic structure with:-
 - Addition: must be multiplicative and associative.
 - Subtraction.
 - Multiplication: must be commutative, associative and distributive.
 - Oivision: multiplicative inverse must exist.



R^n

Normed Vector Spaces

- Vector Space: A space consisting of vectors, together with the
 - associative and commutative operation of addition of vectors,
 - **2** associative and distributive operation of multiplication of vectors by scalars.
- Field of scalars: e.g. algebraic structure with:-
 - Addition: must be multiplicative and associative.
 - Subtraction.
 - Multiplication: must be commutative, associative and distributive.
 - Oivision: multiplicative inverse must exist.
- Norm: A function that assigns a strictly positive length or size to each vector in a vector space save for the zero vector, which is assigned a length of zero.
- Normed Vector Space: A vector space on which a norm is defined.

Normed Vector Spaces

A vector space on which a norm is defined.

- In any real vector space \Re^n , the length of a vector has the following properties:
 - **1** The zero vector, 0, has zero length; every other vector has a positive length.

* $\|\mathbf{x}\| \ge 0$, and $\|\mathbf{x}\| = 0$ iff $\mathbf{x} = 0$.

- Multiplying a vector by a positive number changes its length without changing its direction. Moreover,
 - * $\|\alpha \mathbf{x}\| = |\alpha| \|\mathbf{x}\|$ for any scalar α . Homogenity
- The triangle inequality holds. That is, taking norms as distances, the distance from point A through B to C is never shorter than going directly from A to C, or the shortest distance between any two points is a straight line.

★ $||\mathbf{x}_1 + \mathbf{x}_2|| \le ||\mathbf{x}_1|| + ||\mathbf{x}_2||$ for any vectors \mathbf{x}_1 and \mathbf{x}_2 .

Triangle inequality

The generalization of these three properties to more abstract vector spaces leads to the notion of norm. For example: A matrix norm. We will see examples Additionally, in the case of square matrices (thus, m = n), some (but not all) matrix norms satisfy the following condition, which is related to the fact that matrices are more than just vectors: $||AB|| \leq ||A|| ||B||$ for all matrices A and B in $K^{n\times n}$.

Homework Problems

- Intuitively construct a topological space that does not have a metric
- Intuitively construct a metric space that does not have norm

It is a vector space over a field of scalars along with an inner product.

(Conjugate) Symmetry: <x₁, x₂> = < x₂, x₁>. For reals, Conjugate of x1 = x1
 Linearity in the first argument.

- $\mathbf{P} < \mathbf{a}\mathbf{x}_1, \mathbf{x}_2 >= \mathbf{a} < \mathbf{x}_1, \mathbf{x}_2 >$
- $\blacktriangleright \ < {\bf x}_1 + {\bf x}_2, {\bf x}_3 > = < {\bf x}_1, {\bf x}_3 > + < {\bf x}_3, {\bf x}_3 >$

③ Positive definiteness: $\langle \mathbf{x}, \mathbf{x} \rangle \ge 0$, with equality iff $\mathbf{x} = 0$.

In the general case, you could have integrals instead of summations (as in the ordinary dot product)

Proof: Normed Vector Space is a Metric Space

• Normed Vector Space: A vector space on which a norm is defined. In any real vector space \Re^n , the length of a vector has the following properties:

1
$$\|\mathbf{x}\| \ge 0$$
, and $\|\mathbf{x}\| = 0$ iff $\mathbf{x} = 0$.

2 $\|\alpha \mathbf{x}\| = |\alpha| \|\mathbf{x}\|$ for any scalar α .

 $\textbf{ (} \|\mathbf{x}_1 + \mathbf{x}_2\| \leq \|\mathbf{x}_1\| + \|\mathbf{x}_2\| \text{ for any vectors } \mathbf{x}_1 \text{ and } \mathbf{x}_2.$

- ② Metric Space: Set of points (X) along with a notion of distance d(x₁, x₂) between any two points (x₁, x₂ ∈ X) such that:
 - $d(\mathbf{x}_1, \mathbf{x}_2) \geq 0$ (non-negativity).

 - $d(\mathbf{x}_1, \mathbf{x}_2) = d(\mathbf{x}_2, \mathbf{x}_1)$ (symmetry).
 - $\textbf{0} \ \ \textit{d}(\mathbf{x}_1,\mathbf{x}_2) + \textit{d}(\mathbf{x}_2,\mathbf{x}_3) \geq \textit{d}(\mathbf{x}_1,\mathbf{x}_3) \ (\text{triangle inequality}).$

Operation of Proof:

For a normed vector space with ||.||, we just need to prove that the function d(x1,x2) = ||x1-x2|| is a valid distance metric as per metric space

Proof: Normed Vector Space is a Metric Space

• Normed Vector Space: A vector space on which a norm is defined. In any real vector space \Re^n , the length of a vector has the following properties:

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$$\|\mathbf{x}\| \ge 0$$
, and $\|\mathbf{x}\| = 0$ iff $\mathbf{x} = 0$.

2 $\|\alpha \mathbf{x}\| = |\alpha| \|\mathbf{x}\|$ for any scalar α .

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 - $d(\mathbf{x}_1, \mathbf{x}_2) \geq 0$ (non-negativity).
 - $\ \ \, {\boldsymbol \partial} \ \ \, {\boldsymbol d}({\mathbf x}_1,{\mathbf x}_2)=0 \ \, {\rm iff} \ {\mathbf x}_1={\mathbf x}_2 \ \, {\rm (identity)}.$
 - $d(\mathbf{x}_1, \mathbf{x}_2) = d(\mathbf{x}_2, \mathbf{x}_1)$ (symmetry).
 - $\textbf{0} \ \ \textbf{\textit{d}}(\mathbf{x}_1,\mathbf{x}_2) + \textbf{\textit{d}}(\mathbf{x}_2,\mathbf{x}_3) \geq \textbf{\textit{d}}(\mathbf{x}_1,\mathbf{x}_3) \ \text{(triangle inequality)}.$

Operation Proof:

- In vector space, a vector $\mathbf{x} = \mathbf{x}_1 \mathbf{x}_2$ can be defined by subtraction. Define $d(\mathbf{x}_1, \mathbf{x}_2) = \|\mathbf{x}_1 \mathbf{x}_2\|$, so $1.1 \Rightarrow \|\mathbf{x}_1 \mathbf{x}_2\| \ge 0$; $\|\mathbf{x}_1 \mathbf{x}_2\| = 0$ iff $\mathbf{x}_1 \mathbf{x}_2 = 0$, hence 2.1 and 2.2 are proved.
- **2** $1.2 \Rightarrow || 1(\mathbf{x}_1 \mathbf{x}_2)|| = |-1|||\mathbf{x}_1 \mathbf{x}_2||$. So, $||\mathbf{x}_2 \mathbf{x}_1|| = ||\mathbf{x}_1 \mathbf{x}_2||$, so 2.3 is proved.
- **3** Take $\mathbf{x}_1 = \mathbf{z}_1 z_0$ and $\mathbf{x}_2 = \mathbf{z}_0 \mathbf{z}_2$, put in 1.3 to get $\|\mathbf{z}_1 \mathbf{z}_0\| + \|\mathbf{z}_0 \mathbf{z}_2\| \ge \|\mathbf{z}_1 \mathbf{z}_2\|$ so 2.4 is prooved.

The Mathematical Structures & Spaces: Some Proofs

Some Proofs For Mathematical Structures & Spaces

- Under what conditions on *P*, is $\sqrt{\mathbf{x}^T P \mathbf{x}}$ a valid Norm?
- Prove that inner product space is a normed vector space.
- What is an example of normed vector space that is not an inner product space?
- Prove that $| \langle u, v \rangle | \leq ||u||_P ||v||_P$ for any norm P.

Cauchy Shwarz inequality that results from the fact that every inner product space is a normed vector space and that the norm induced by the inner product should satisfy properties of norm. Under what conditions on P is $\sqrt{\mathbf{x}^T P \mathbf{x}}$ a valid Norm?

Assume $\mathbf{x} \in \Re^n$ and $P \in \Re^{n \times n}$.

- *P* is symmetric positive definite iff:
 - **()** Symmetric: $P^T = P$
 - 2 Positive Definite: $\forall \mathbf{x} \neq 0, \ \mathbf{x}^T P \mathbf{x} \ge 0$

Proof:

Apply eigenvalue decomposition on P

Under what conditions on P is $\sqrt{\mathbf{x}^T P \mathbf{x}}$ a valid Norm?

Assume $\mathbf{x} \in \Re^n$ and $P \in \Re^{n \times n}$.

- *P* is symmetric positive definite iff:
 - **()** Symmetric: $P^T = P$
 - 2 Positive Definite: $\forall \mathbf{x} \neq 0, \ \mathbf{x}^T P \mathbf{x} \ge 0$

Proof:

- If P is symmetric positive definite (SPD), then P can be written as:
 - $P = Q\Lambda Q^T$, (Eigenvalue decomposition) where ...
 - * Q is an orthogonal matrix whose columns are the eigenvectors of P.
 - $\star~\Lambda$ is a diagonal matrix whose positive entries are the eigenvalues of P.
- Hence, we can write $\underline{P} = SS^T$ where $\underline{S} = Q\sqrt{\Lambda}$.
- Thus we have $\mathbf{x}^T P \mathbf{x} = \mathbf{x}^T S S^T \mathbf{x} = (S^T \mathbf{x})^T (S^T \mathbf{x}) = \mathbf{y}^T \mathbf{y}$ • where $\mathbf{y} = (S^T \mathbf{x})$ and thus $\mathbf{y} \in \Re^n$.
- So, $\mathbf{x}^T P \mathbf{x} \ge 0$. Square root of eigenvalues gives you lengths of axes of ellipsoid and eigenvectors give you orientations

Proving P is $\sqrt{\mathbf{x}^T P \mathbf{x}}$ a valid Norm using Cholesky Decomposition (Optional)

Assume $\mathbf{x} \in \Re^n$ and $P \in \Re^{n \times n}$.

- *P* is symmetric positive definite iff:
 - **()** Symmetric: $P^T = P$
 - 2 Positive Definite: $\forall \mathbf{x} \neq 0, \ \mathbf{x}^T P \mathbf{x} \ge 0$

Proof:

- If P is symmetric positive definite (SPD), then P can be written as:
 - $P = LDL^{T}$, (LDL decomposition) where ...
 - \star L is lower triangular matrix with a 1 in each diagonal entry.
 - \star D is diagonal matrix with positive values.
- Hence, we can write $P = RR^T$ where $R = L\sqrt{D}$. (Cholesky Decomposition)
- Thus we have $\mathbf{x}^{T} P \mathbf{x} = \mathbf{x}^{T} R R^{T} \mathbf{x} = (R^{T} \mathbf{x})^{T} (R^{T} \mathbf{x}) = \mathbf{y}^{T} \mathbf{y}$
 - where $\mathbf{y} = (R^T \mathbf{x})$ and thus $\mathbf{y} \in \Re^n$.
- So, $\mathbf{x}^T P \mathbf{x} \ge 0$.

$\sqrt{\mathbf{x}^{T}P\mathbf{x}}$ a valid norm for psd *P*: Optional Elaborate Proof

• Normed Vector Space: A vector space on which a norm is defined. In any real vector space \Re^n , the length of a vector has the following properties:

1
$$\|\mathbf{x}\| \ge 0$$
, and $\|\mathbf{x}\| = 0$ iff $\mathbf{x} = 0$.
2 $\|\alpha \mathbf{x}\| = |\alpha| \|\mathbf{x}\|$ for any scalar α .
3 $\|\mathbf{x}_1 + \mathbf{x}_2\| \le \|\mathbf{x}_1\| + \|\mathbf{x}_2\|$ for any vectors \mathbf{x}_1 and \mathbf{x}_2 .

Proof:

- **9** By definition of PST: $\|\mathbf{x}^T P \mathbf{x}\| \ge 0$, and $\|\mathbf{x}^T P \mathbf{x}\| = 0$ iff $\mathbf{x} = 0$.
- **3** For any scalar α : $\|\alpha \mathbf{x}\|_{P} = \sqrt{(\alpha \mathbf{x})^{T} P(\alpha \mathbf{x})} = \sqrt{(\alpha^{2})(\mathbf{x}^{T} P \mathbf{x})} = \alpha \sqrt{\mathbf{x}^{T} P \mathbf{x}} = |\alpha| ||\mathbf{x}||_{P}$.
- $\textbf{0} \ \|\mathbf{x}_1 + \mathbf{x}_2\|_{P} \leq \|\mathbf{x}_1\|_{P} + \|\mathbf{x}_2\|_{P} \text{ for any vectors } \mathbf{x}_1 \text{ and } \mathbf{x}_2. \text{ Next Slide.}$

 $\sqrt{\mathbf{x}^T P \mathbf{x}}$ a valid norm for psd *P*: Optional Elaborate Proof

Proof for $\|\mathbf{x}_1 + \mathbf{x}_2\|_P \le \|\mathbf{x}_1\|_P \|\mathbf{x}_2\|_P$ For any vectors \mathbf{x}_1 and \mathbf{x}_2 :

•
$$\|\mathbf{x}_1 + \mathbf{x}_2\|_P^2 =$$

• $(\mathbf{x}_1 + \mathbf{x}_2)^T P(\mathbf{x}_1 + \mathbf{x}_2)$
• $\mathbf{x}_1^T P \mathbf{x}_1 + \mathbf{x}_2^T P \mathbf{x}_2 + \mathbf{x}_1^T P \mathbf{x}_2 + \mathbf{x}_2^T P \mathbf{x}_1$
• $u^T u + v^T v + u^T v + v^T u$ (Using $P = RR^T$, $u = R^T \mathbf{x}_1$ and $v = R^T \mathbf{x}_2$)
• $u^T u + v^T v + 2u^T v$, since $u^T v = v^T u$

2 $(\|\mathbf{x}_1\|_P + \|\mathbf{x}_2\|_P)^2 =$

$$\|\mathbf{x}_1\|_{P}^{2} + \|\mathbf{x}_2\|_{P}^{2} + 2\|\mathbf{x}_1\|_{P}\|\mathbf{x}_2\|_{P} \\ \mathbf{x}_1^{T}P\mathbf{x}_1 + \mathbf{x}_2^{T}P\mathbf{x}_2 + 2\sqrt{(\mathbf{x}_1^{T}P\mathbf{x}_1)(\mathbf{x}_2^{T}P\mathbf{x}_2)} \\ \mathbf{u}^{T}u + v^{T}v + 2\sqrt{(u^{T}u)(v^{T}v)} \\ \end{array}$$

3 By Cauchy Schwarz Inequality: $u^T v \le \sqrt{(u^T u)(v^T v)}$ ($Cos(\theta) \le 1$)

Every Inner product space is a normed vector space: Optional Elaborate Proof

By conjugate symmetry, we have $\langle \mathbf{x}, \mathbf{x} \rangle = \overline{\langle \mathbf{x}, \mathbf{x} \rangle}$. So $\langle \mathbf{x}, \mathbf{x} \rangle$ must be real. So, we can define $\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$. We need to prove that $\|\mathbf{x}\|$ is a valid norm:-

• By positive definiteness: $\langle \mathbf{x}, \mathbf{x} \rangle \ge 0$, with equality iff $\mathbf{x} = 0$. So $\|\mathbf{x}\| \ge 0$ (= iff $\mathbf{x} = 0$). • For any complex t, $\|t\mathbf{x}\| = \sqrt{\langle t\mathbf{x}, t\mathbf{x} \rangle} = \sqrt{t * t} < \mathbf{x}, \mathbf{x} > = |t| \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$ (as $|t| = \sqrt{t * t}$) So $\|t\mathbf{x}\| == |t| \|\mathbf{x}\|$ • $\|\mathbf{x}_1 + \mathbf{x}_2\| = \sqrt{\langle \mathbf{x}_1 + \mathbf{x}_2, \mathbf{x}_1 + \mathbf{x}_2 \rangle} = \sqrt{\langle \mathbf{x}_1, \mathbf{x}_1 \rangle + \langle \mathbf{x}_2, \mathbf{x}_2 \rangle + \langle \mathbf{x}_1, \mathbf{x}_2 \rangle + \langle \mathbf{x}_2, \mathbf{x}_2 \rangle}$ (by Cauchy Schwartz inequality)

Recap: Basis and Dimensions from Linear Algebra wrt $< ., . >_E$ (Eucledian Inner Product) Instructor: Prof. Ganesh Ramakrishnan

Recap: Basis and Dimensions from Linear Algebra

Recap: Basis in Linear Algebra

Basis for a space: The basis for a space is a set of vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n$ with two properties, viz., (1) The vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n$ are independent and (2) These vectors span the space.

Set of vectors that is necessary and sufficient for spanning the space. Eg: A (standard) basis for the four dimensional space \Re^4 is:

$$\begin{bmatrix} 1\\0\\0\\0 \end{bmatrix}, \begin{bmatrix} 0\\1\\0\\0 \end{bmatrix}, \begin{bmatrix} 0\\0\\1\\0 \end{bmatrix}, \begin{bmatrix} 0\\0\\1\\0 \end{bmatrix}, \begin{bmatrix} 0\\0\\0\\1 \end{bmatrix}$$
(5)

It is easy to verify that the above vectors are independent; if a combination of the vectors using the scalars in $[c_1, c_2, c_3, c_4]$ should yield the zero vector, we must have $c_1 = c_2 = c_3 = c_4 = 0$. Another way of proving this is by making the four vectors the columns of a matrix. The resultant matrix will be an identity matrix. The null space of an identity matrix is the zero

vector

This is not the only basis of \Re^4 . Consider the following three vectors

2		0		[0]
0		0		0
0	,	2	,	0
0		0		2

(6)

These vectors are certainly independent. But they do not span \Re^4 .

This can be proved by showing that the following vector in \Re^4 cannot be expressed as a linear combination of these vectors.

$$\begin{bmatrix} 0\\ 2\\ 0\\ 0 \end{bmatrix}$$
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- In fact, if the last vector on the previous slide is added to the set of three vectors in (6), together, they define another basis for \Re^4 .
- This could be proved by introducing them as columns of a matrix A, subject A to row reduction and check if there are any free variables (or equivalently, whether all columns are pivot columns). If there are no free variables, we can conclude that the vectors form a basis for \Re^4 .
- This is also equivalent to the statement that *if the matrix A is invertible, its columns form a basis for its column space.*

- We can generalize our observations to \Re^n : if an $n \times n$ matrix A is invertible, its coulumns for a basis for \Re^n .
- While there can be many bases for a space, a commonality between all the bases is that they have exactly the same number of vectors.
- This unique size of the basis is called the dimension of the space.

Dimension: The number of vectors in any basis of a vector space is called the dimension of the space.

Do the vectors in (6), form a basis for any space at all?

The vectors are independent and therefore span the space of all linear combinations of the three vectors.

The space spanned by these vectors is a hyperplane in \Re^4 .

Let A be any matrix. By definition, the columns of A span the column space C(A) of A. If there exists a $\mathbf{c} \neq \mathbf{0}$ such that, $A\mathbf{c} = 0$, then the columns of A are not linearly independent. For example, the columns of the matrix A given below are not linearly independent.

$$A = \begin{bmatrix} 1 & 2 & 3 & 1 \\ 2 & 3 & 5 & 2 \\ 3 & 4 & 7 & 3 \end{bmatrix}$$
(8)

A choice of $\mathbf{c} = \begin{bmatrix} -1 & 0 & 0 & 1 \end{bmatrix}^T$ gives $A\mathbf{c} = 0$. Thus, the columns of A do not form a basis for its columns space.

What is a basis for C(A)? A most natural choice is the first two columns of A; the thid column is the sum of the first and second columns, while the fourth column is the same as the first column. Also, column elimination¹ on A yields pivots on the first two columns. Thus, a basis for C(A) is

$$\left[\begin{array}{c}1\\2\\3\end{array}\right], \left[\begin{array}{c}2\\3\\4\end{array}\right]$$

(9)

Another basis for C(A) consists of the first and third columns. We note that the dimension of C(A) is 2. We also note that the rank of A is the number of its pivots columns, which is exactly the dimension of C(A).

¹Column elimination operations are very similar to row elimination operations.

All of this gives us a nice result.

Theorem

The rank of a matrix is the same as the dimension of its column space. That is, rank(A) = dimension(C(A)).

- What about the dimension of the null space? We already saw that $\mathbf{c} = \begin{bmatrix} -1 & 0 & 0 & 1 \end{bmatrix}^T$ is in the null space.
- Another element of the null space is c' = [1 1 − 1 0]^T. These vectors in the null space specify combinations of the columns that yield zeroes. The two vectors c and c' are obviously independent. Do these two vectors span the entire null space?
- The dimension of the null space is the same as the number of free variables, which happens to be 4-2=2 in this example. Thus the two vectors c and c' must indeed span the null space. In fact, it can be proved that the dimension of the null space of an $m \times n$ matrix A is n rank(A).

Recap: Row Space and Column Space in Linear Algebra (contd.)

- The space spanned by the rows of a matrix is called the *row space*. We can also define the row space of a matrix A as the column space of its transpose A^T . Thus the row space of A can be specified as $C(A^T)$.
- The null space of A, N(A) is often called the *right null space* of A, while the null space of A^{T} , $N(A^{T})$ is often referred to as its *left null space*.
- How do we visualize these four spaces? N(A) and $C(A^T)$ of an $m \times n$ matrix A are in \Re^n , while C(A) and $N(A^T)$ are in \Re^m .
- How can we construct bases for each of the four subspaces? We note that dimensions of C(A) and the rank of $C(A^T)$ should be the same, since row rank of a matrix is its column rank. The bases of C(A) can be obtained as the set of the pivot columns.

- Let r be the rank of A. Recall that the null space is constructed by linear combinations of the special solutions of the null space (??) and there is one special solution for each assignment of the free variables. In fact, the number of special solutions exactly equals the number of free variables, which is n r. Thus, the dimension of N(A) will be n r.
- Similarly, the dimension of $N(A^T)$ will be m r.

Let us illustrate all this on the sample matrix in (8).

$$\begin{bmatrix} 1 & 2 & 3 & 1 \\ 2 & 3 & 5 & 2 \\ 3 & 4 & 7 & 3 \end{bmatrix} \xrightarrow{E_{2,1}, E_{3,1}} \begin{bmatrix} 1 & 2 & 3 & 1 \\ 0 & -1 & -1 & 0 \\ 0 & -2 & -2 & 0 \end{bmatrix} \xrightarrow{E_{3,2}} (R=) \begin{bmatrix} 1 & 2 & 3 & 1 \\ 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$
(10)

- The reduced matrix *R* has the same row space as *A*, by virtue of the nature of row reduction. In fact, the rows of *A* can be retrieved from the rows of *R* by reversing the linear operations involved in row elimination. The first two rows give a basis for the row space of *A*.
- The dimension of $C(A^T)$ is 2, which is also the rank of A.
- To find the left null space of A, we look at the system $\mathbf{y}^T A = 0$. Recall the Gauss-Jordan elimination method from Section **??** that augments A with an $m \times m$ identity matrix, and performs row elimination on the augmented matrix.

$$[A \ I_{m \times m}] \stackrel{rref}{\Longrightarrow} [R \ E_{m \times m}]$$

The rref will consist of the reduced matrix augmented with the elimination matrix reproduced on its right.

For the example case in 10, we apply the same elimination steps to obtain the matrix E below:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \stackrel{E_{2,1},E_{3,1}}{\Longrightarrow} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -3 & 0 & 1 \end{bmatrix} \stackrel{E_{3,2}}{\Longrightarrow} (E=) \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & -2 & 1 \end{bmatrix}$$
(11)

Writing down EA = R,

$$\begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 & 1 \\ 2 & 3 & 5 & 2 \\ 3 & 4 & 7 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 & 1 \\ 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$
(12)

We observe that the last row of *E* specifies a linear combination of the rows of *A* that yields a zero vector (corresponding to the last row of *R*). This is the only vector that yields a zero row in *R* and is therefore the only element in the basis of the left null space of *A*, that is, $N(A^T)$. The dimension of $N(A^T)$ is 1.

- As another example, consider the space S of vectors $\mathbf{v} \in \Re^3$ where $\mathbf{v} = [v_1 \ v_2 \ v_3]^T$ such that $\mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_3 = \mathbf{0}$. What is the dimension of this subspace?
- Note that this subspace is the right null space N(A) of a 1×3 matrix $A = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$, since $A\mathbf{v} = 0$. The rank, r = rank(A) is 1, implying that the dimension of the right null space is n r = 3 1 = 2.
- One set of basis vectors for S is $[-1\ 1\ 0]$, $[-1\ 0\ 1]$. The column space C(A) is \Re^1 with dimension 1. The left null space $N(A^T)$ is the singleton set $\{0\}$ and as expected, has a dimension of m r = 1 1 = 0.

Recap: Matrix Spaces

We will extend the set of examples of vector spaces discussed in Section **??** with a new vector space, that of all $m \times n$ matrices with real entries, denoted by $\Re^{m \times n}$.

- It is easy to verify that the space of all matrices is closed under operations of addition and scalar multiplication. Additionally, there are interesting subspaces in the entire matrix space $\Re^{m \times n}$, *viz.*,
 - set S of all $n \times n$ symmetric matrices
 - ▶ set U of all $n \times n$ upper triangular matrices
 - ▶ set \mathcal{L} of all $n \times n$ lower triangular matrices
 - set \mathcal{D} of all $n \times n$ diagonal matrices
- Let $\mathcal{M} = \Re^{3 \times 3}$ be the space of all 3×3 matrices. The dimension of \mathcal{M} is 9. Each element of this basis has a 1 in one of the 9 positions and the remaining entries as zeroes.
- Of these basis elements, three are symmetric (those having a 1 in any of the diagonal positions). These three matrices form the basis for the subspace of diagonal matrices.
- Six of the nine basis elements of *M* form the basis of *U* while six of them form the basis of *L*.

Recap: Matrix Spaces (contd.)

- The intersection of any two matrix spaces is also a matrix space. For example, $S \cap U$ is D, the set of diagonal matrices.
- However the union of any two matrix spaces need not be a matrix space. For example, $S \cup U$ is not a matrix space; the sum S + U, $S \in S$, $U \in U$ need not belong to $S \cup U$.
- We will discuss a special set comprising all linear combinations of the elements of union of two vector spaces V₁ and V₂ (*i.e.*, V₁ ∪ V₂), and denote this set by V₁ ⊕ V₂. By definition, this set is a vector space. For example, S + U = M, which is a vector space.

Recap: Matrix Spaces (contd.)

A property fundamental to many properties of matrices is the expression for a rank 1 matrix. A rank 1 matrix can be expressed as the product of a column vector with a row vector (the row vector forming a basis for the matrix). Thus, any rank 1 matrix X can be expressed as

$$X_{m \times n} = u^{T} v = \begin{bmatrix} u_{1} \\ u_{2} \\ u_{3} \\ \vdots \\ \vdots \\ u_{m} \end{bmatrix} \begin{bmatrix} v_{1} & v_{2} & \dots & v_{n} \end{bmatrix}$$
(13)

Recap: Matrix Spaces (contd.)

Let $\mathcal{M}_{m \times n}$ be the set of all $m \times n$ matrices. Is the subset of $\mathcal{M}_{m \times n}$ matrices with rank k, a subspace? For k = 1, this space is obviously not a vector space as is evident from the sum of rank 1 matrices, A^1 and B^1 , which is not a rank 1 matrix. In fact, the subset of $\mathcal{M}_{m \times n}$ matrices with rank k is not a subspace.

$$A^{1} + B^{1} = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 1 \\ 1 & 2 & 1 \end{bmatrix} + \begin{bmatrix} 4 & 4 & 2 \\ 2 & 2 & 1 \\ 4 & 4 & 2 \end{bmatrix} = \begin{bmatrix} 5 & 6 & 3 \\ 4 & 6 & 2 \\ 5 & 6 & 3 \end{bmatrix}$$

(14)

Orthogonality and Projection

- Two vectors \mathbf{x} and \mathbf{y} are said to be orthogonal *iff*, their dot product (more generally, the inner product) is 0. In the eucledian space, the dot product of the two vectors is $x^T y$.
- The condition $x^T y = 0$ is equivalent to the pythagorous condition between the vectors \mathbf{x} and \mathbf{y} that form the perpendicular sides of a right triangle with the hypotenuse given by $\mathbf{x} + \mathbf{y}$. The pythagorous condition is $||\mathbf{x}||^2 + ||\mathbf{y}||^2 = ||\mathbf{x} + \mathbf{y}||^2$, where the norm is the eucledian norm, given by $||\mathbf{x}||^2 = \mathbf{x}^T \mathbf{x}$.
- This equivalence can be easily proved and is left to the reader as an exercise. By definition, the vector **0** is orthogonal to every other vector.

We will extend the definition of orthogonality to subspaces; a subspace \mathcal{U} is orthogonal to subspace \mathcal{V} *iff*, every vector in \mathcal{U} is orthogonal to every vector in \mathcal{V} . As an example:

Theorem

The row space $C(A^T)$ of an $m \times n$ matrix A is orthogonal to its right null space N(A).

Proof: $A\mathbf{x} = \mathbf{0}, \forall \mathbf{x} \in \mathcal{N}(A)$. On the other hand, $\forall \mathbf{y} \in \mathcal{C}(A^T), \exists z \in \Re^m, \mathbf{s.t.}, \mathbf{y} = A^T \mathbf{z}$. Therefore, $\forall \mathbf{y} \in \mathcal{C}(A^T), \mathbf{x} \in \mathcal{N}(A), \mathbf{y}^T \mathbf{x} = \mathbf{z}^T A \mathbf{x} = \mathbf{z}.\mathbf{0} = 0$.

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Orthogonality and Projection

Not only are $C(A^T)$ and the right null space N(A) orthogonal to each other, but they are also orthogonal complements in \Re^n , that is, N(A) contains all vectors that are orthogonal to some vector in $C(A^T)$.

Theorem

The null space of A and its row space are orthogonal complements.

Proof: We note, based on our discussion earlier that the dimensions of the row space and the (right) null space add up to *n*, which is the number of columns of *A*. For any vector $\mathbf{y} \in C(A^T)$, we have $\exists \mathbf{z} \in \Re^m$, $\mathbf{s.t.}$, $\mathbf{y} = A^T \mathbf{z}$. Suppose $\forall \mathbf{y} \in C(A^T)$, $\mathbf{y}^T \mathbf{x} = 0$. That is, $\forall \mathbf{z} \in \Re^m$, $\mathbf{z}^T A \mathbf{x} = 0$. This is possible only if $A \mathbf{x} = \mathbf{0}$. Thus, necessarily, $\mathbf{x} \in N(A)$.

Orthogonality and Projection

Based on preceeding theorem, we prove that there is a one-to-one mapping between the elements of row space and column space.

Theorem

If
$$\mathbf{x} \in C(A^T)$$
, $\mathbf{y} \in C(A^T)$ and $\mathbf{x} \neq \mathbf{y}$, then, $A\mathbf{x} \neq A\mathbf{y}$.

Proof: Note that $A\mathbf{x}$ and $A\mathbf{y}$ are both elements of C(A). Next, observe that $\mathbf{x} - \mathbf{y} \in C(A^T)$, which by theorem 7, implies that $\mathbf{x} - \mathbf{y} \notin N(A)$. Therefore, $A\mathbf{x} - A\mathbf{y} \neq \mathbf{0}$ or in other words, $A\mathbf{x} \neq A\mathbf{y}$.

Similarly, it can be proved that if $\mathbf{x} \in C(A)$, $\mathbf{y} \in C(A)$ and $\mathbf{x} \neq \mathbf{y}$, then, $A^T \mathbf{x} \neq A^T \mathbf{y}$. The two properties together imply a one-to-one mapping between the row and column spaces.

Projection Matrices

The projection of a vector t on a vector s is a vector $\mathbf{p} = c\mathbf{s}$, $c \in \Re$ (in the same direction as s), such that $\mathbf{t} - c\mathbf{s}$ is orthogonal to s. That is, $\mathbf{s}^T(\mathbf{t} - c\mathbf{s}) = 0$ or $\mathbf{s}^T\mathbf{t} = c\mathbf{s}^T\mathbf{s}$). Thus, the scaling factor c is given by $c = \frac{\mathbf{s}^T\mathbf{t}}{\mathbf{s}^T\mathbf{s}}$. The projection of the vector t on a vector s is then

$$\mathbf{p} = \mathbf{s} \frac{\mathbf{t}^{\mathsf{T}} \mathbf{s}}{\mathbf{s}^{\mathsf{T}} \mathbf{s}} \tag{15}$$

Using the associative property of matrix multiplication, the expression for ${\bf p}$ can be re-written as

$$\mathbf{p} = P\mathbf{t} \tag{16}$$

where, $P = ss^T \frac{1}{s^T s}$ is called the *projection matrix*.

- The rank of the projection matrix is 1 (since it is a column mutiplied by a row).
- The projection matrix is symmetric and its column space is a line through s.
- For any d ∈ ℜ, P(ds) = ds, that is, the projection of any vector in the direction of s is the same vector. Thus, P² = P.

Least Squares

- We earlier saw a method for solving the system $A\mathbf{x} = \mathbf{b}$ (A being an $m \times n$ matrix), when a solution exists. Howevever, a solution may not exist, especially when m > n, that is when the number of equations is greater than the number of variables.
- We also saw that the *rref* looks like $[I \ 0]^T$, where *I* is an $n \times n$ identity matrix. It could happen that the row reduction yields a zero submatrix in the lower part of *A*, but the corresponding elements in **b** are not zeroes.
- In other words, **b** may not be in the column space of *A*. In such cases, we are often interested in finding a 'best fit' for the system; a solution \hat{x} that satisfies $A\mathbf{x} = \mathbf{b}$ as well as possible.

We define the best fit in terms of a vector p which is the projection of b onto C(A) and solve A x̂ = p. We require that b - p is orthogonal to C(A), which means

$$A^{T}(\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{0} \tag{17}$$

• The vector $\mathbf{e} = \mathbf{b} - A\hat{\mathbf{x}}$ is the error vector and is in $N(A^T)$. The equation (82) can be rewritten as

$$(A^{T}A)\hat{\mathbf{x}} = A^{T}\mathbf{b}$$
(18)

A matrix that plays a key role in this problem is $A^T A$. It is an $n \times n$ symmetric matrix (since $(A^{T}A)^{T} = A^{T}A$). The right null space $N(A^{T}A)$ is the same as $N(A)^{2}$. It naturally follows that the ranks of $A^{T}A$ and A are the same (since, the sum of the rank and dimension of null space equal n in either case). Thus, $A^{T}A$ is invertible exactly if N(A) has dimension 0, or equivalently, A is a full column rank.

Theorem

If A is a full column rank matrix (that is, its columns are independent), A^TA is invertible.

Proof: We will show that the null space of $A^T A$ is $\{0\}$, which implies that the square matrix $A^{T}A$ is full column (as well as row) rank is invertible. That is, if $A^{T}A\mathbf{x} = \mathbf{0}$, then $\mathbf{x} = \mathbf{0}$. Note that if $A^T A \mathbf{x} = \mathbf{0}$, then $\mathbf{x}^T A^T A \mathbf{x} = ||A\mathbf{x}|| = 0$ which implies that $A\mathbf{x} = \mathbf{0}$. Since the columns of A are linearly independent, its null space is 0 and therefore, $\mathbf{x} = \mathbf{0}$. Assuming that A is full column rank, the equation (18) can be rewritten as

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$$\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b}.$$
(19)
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Therefore the expression for the projection ${\bf p}$ will be

$$\mathbf{p} = \mathcal{A}(\mathcal{A}^{\mathsf{T}}\mathcal{A})^{-1}\mathcal{A}^{\mathsf{T}}\mathbf{b}$$
(20)

This expression is the n-dimensional equivalent of the one dimensional expression for projection in (79). The projection matrix in (20) is given by $P = A(A^T A)^{-1}A^T$. We will list the solution for some special cases:

- If A is an $n \times n$ square invertible matrix, its column space is the entire \Re^n and the projection matrix will turn out to be the identity matrix.
- Also, if *b* is in the column space C(A), then $\mathbf{b} = A\mathbf{t}$ for some *t* in \Re^n and consequently, $P\mathbf{b} = A(A^TA)^{-1}(A^TA)\mathbf{t} = A\mathbf{t} = \mathbf{b}$.
- On the other hand, if b is orthogonal to C(A), it will lie in $N(A^T)$, and therefore, $A^T \mathbf{b} = 0$, implying that $\mathbf{p} = 0$.

Another equivalent way of looking at the best fit solution $\hat{\mathbf{x}}$ is a solution that minimizes the square of the norm of the error vector

$$e(\hat{\mathbf{x}}) = ||A\mathbf{x} - \mathbf{b}||^2 \tag{21}$$

Setting $\frac{de(\hat{\mathbf{x}})}{d\mathbf{x}} = 0$, we get the same expression for $\hat{\mathbf{x}}$ as in (83). The solution in 83 is therefore often called the *least squares solution*. Thus, we saw two views of finding a best fit; first was the view of projecting into the column space while the second concerned itself with minimizing the norm squared of the error vector.

We will take an example. Consider the data matrix A and the coefficient matrix \mathbf{b} as in (22).

$$Ax = \begin{bmatrix} 2 & -1 \\ -1 & 2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \\ 3 \end{bmatrix}$$

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(22)

The matrix A is full column rank and therefore $A^T A$ will be invertible. The matrix $A^T A$ is given as

$$\mathsf{A}^{\mathsf{T}}\mathsf{A} = \left[\begin{array}{cc} 6 & -3 \\ -3 & 6 \end{array} \right]$$

Substituting the value of $A^{T}A$ in the system of equations (18), we get,

$$6\hat{x}_1 - 3\hat{x}_2 = 2 \tag{23}$$

$$-3\hat{x}_1 + 6\hat{x}_2 = 8 \tag{24}$$

The solution of which is, $x_1 = \frac{4}{5}$, $x_2 = \frac{26}{15}$.

Orthonormal Vectors

A collection of vectors $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n$ is said to be orthonormal *iff* the following condition holds $\forall i, j$:

$$\mathbf{q}_{i}^{T}\mathbf{q}_{j} \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$
(25)

A large part of numerical linear algebra is built around working with orthonormal matrices, since they do not overflow or underflow. Let Q be a matrix comprising the columns q_1 through q_n . It can be easily shown that

$$Q^T Q = I_{n \times n}$$

Orthonormal Vectors (contd.)

When Q is square, $Q^{-1} = Q^{T}$. Some examples of matrices with orthonormal columns are:

The matrix $Q_{rotation}$ when multiplied to a vector, rotates it by an angle θ , whereas $Q_{reflection}$ reflects the vector at an angle of $\theta/2$.

Orthonormal Vectors (contd.)

These matrices present standard varieties of linear transformation, but in general, premultiplication by an $m \times n$ matrix transforms from an input space in \Re^m to an input space in \Re^n .

The matrix $Q_{Hadamard}$ is an orthonormal matrix consisting of only 1's and -1's. Matrices of this form exist only for specific dimensions such as 2, 4, 8, 16, *etc.*, and are called *Hadamard matrices*³.

The matrix Q_{rect} is an example rectangular matrix whose columns are orthonormal.

³An exhaustive listing of different types of matrices can be found at http://en.wikipedia.org/wiki/List_of_matrices.

Orthonormal Vectors (contd.)

Suppose a matrix Q has orthonormal columns. What happens when we project any vector onto the column space of Q? Substituting A = Q in (20), we get⁴:

$$\mathbf{p} = Q(Q^T Q)^{-1} Q^T \mathbf{b} = Q Q^T \mathbf{b}$$
(27)

Making the same substitution in (83),

$$\hat{\mathbf{x}} = (\boldsymbol{A}^{\mathsf{T}}\boldsymbol{Q})^{-1}\boldsymbol{Q}^{\mathsf{T}}\mathbf{b} = \boldsymbol{Q}^{\mathsf{T}}\mathbf{b}$$
(28)

The *i*th component of **x**, is given by $x_i = q_i^T b$.

Let Q_1 be one orthonormal basis and Q_2 be another orthonormal basis for the same space. Let A be the coefficient matrix for a set of points represented using Q_1 and B be the coefficient matrix for the same set of points represented using Q_2 . Then $Q_1A = Q_2B$, which implies that B can be computed as $B = Q_1^T Q_1 A$. This gives us the formula for changing basis. ⁴Note that $Q^TQ = I$. However, $QQ^T = I$ only if Q is a square matrix.

From \Re to \Re^n : CS709

Gram-Schmidt Orthonormalization

- The goal of the Gram-Schmidt orthonormalization process is to generate a set of orthonormal vectors $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n$, given a set of independent vectors $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$.
- The first step in this process is to generate a set of orthogonal vectors $\mathbf{t}_1, \mathbf{t}_2, \dots, \mathbf{t}_n$ from $\mathbf{a}_1, \mathbf{a}_2, \dots, \bullet a_n$. To start with, \mathbf{t}_1 is chosen to be \mathbf{a}_1 .
- Next, the vector t_2 is obtained by removing the projection of a_2 on t_1 , from a_2 , based on (79). That is,

$$\mathbf{t}_2 = \mathbf{a}_2 - \frac{1}{\mathbf{a}_1^{\mathsf{T}} \mathbf{a}_1} \mathbf{a}_1 \mathbf{a}_1^{\mathsf{T}} \mathbf{a}_2$$
(29)

• This is carried out iteratively for i = 1, 2, ..., n, using the expression below:

$$\mathbf{t}_{i} = \mathbf{a}_{i} - \frac{1}{\mathbf{t}_{1}^{T}\mathbf{t}_{1}}\mathbf{t}_{1}\mathbf{t}_{1}^{T}\mathbf{a}_{i} - \frac{1}{\mathbf{t}_{2}^{T}\mathbf{t}_{2}}\mathbf{t}_{2}\mathbf{t}_{2}^{T}\mathbf{a}_{i} - \dots - \frac{1}{\mathbf{t}_{i-1}^{T}\mathbf{t}_{i-1}}\mathbf{t}_{i-1}\mathbf{t}_{i-1}^{T}\mathbf{a}_{i}$$
(30)

Gram-Schmidt Orthonormalization (contd.)

- This iterative procedure gives us the orthogonal vectors $\mathbf{t}_1, \mathbf{t}_2, \ldots, \mathbf{t}_n$.
- Finally, the orthonormal vectors $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n$ are obtained by the simple expression

$$\mathbf{q}_i = \frac{1}{||\mathbf{t}_i||} \mathbf{t}_i \tag{31}$$

- Let A be the matrix with columns $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$ and Q, the matrix with columns $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n$.
- It can be proved that C(V) = C(Q), that is, the matrices V and Q have the same column space. The vector a_i can be expressed as

$$\mathbf{a}_{i} = \sum_{k=1}^{n} (\mathbf{a}_{i}^{T} \mathbf{q}_{k}) \mathbf{q}_{k}$$
(32)

• The *i*th column of A is a linear combination of the columns of Q, with the scalar coefficient $\mathbf{a}_i^T \mathbf{q}_k$ for the k^{th} column of Q.

Gram-Schmidt Orthonormalization (contd.)

• By the very construction procedure of the Gram-Schmidt orthonormalization process, \mathbf{a}_i is orthogonal to \mathbf{q}_k for all k > i. Therefore, (32) can be expressed more precisely as

$$\mathbf{a}_{i} = \sum_{k=1}^{i} (\mathbf{a}_{i}^{T} \mathbf{q}_{k}) \mathbf{q}_{k}$$
(33)

• Therefore, matrix A can be decomposed into the product of Q with a upper triangular matrix R; A = QR, with $R_{k,i} = \mathbf{a}_i^T \mathbf{q}_k$. Since $\mathbf{a}_i^T \mathbf{q}_k = 0$, $\forall k > i$, we can easily see that R is upper triangular.

End Recap: Basis and Dimensions from Linear Algebra wrt $< ., . >_E$ (Eucledian Inner Product)