Applied Linear Algebra

by
Dr.Dinesh Naik
(B.E, M.Tech, Ph.D)

Assistant Professor, Dept. of Information Technology
National Institute of Technology Karnataka, Surathkal

April 14, 2023

Acknowledgement

- I would like to express my sincere gratitude Stephen Boyd, Department of Electrical Engineering Stanford University

- I also thank Lieven Vandenberghe Department of Electrical and Computer Engineering University of California, Los Angeles

Flop counts

- computers store (real) numbers in *floating-point format*
- basic arithmetic operations (addition, multiplication, ...) are called *floating point operations* or flops
- complexity of an algorithm or operation: total number of flops needed, as function of the input dimension(s)
- this can be *very grossly approximated*
- crude approximation of time to execute: (flops needed)/(computer speed)
- current computers are around 1Gflop/sec (10^9 flops/sec)
- but this can vary by factor of 100

Complexity of vector addition, inner product

- $x + y$ needs n additions, so: n flops
- $x^T y$ needs n multiplications, $n - 1$ additions so: $2n - 1$ flops
- we simplify this to $2n$ (or even n) flops for $x^T y$
- and much less when x or y is sparse

Superposition and linear functions

- $f : \mathbf{R}^n \to \mathbf{R}$ means f is a function mapping n-vectors to numbers
- f satisfies the *superposition property* if

$$f(\alpha x + \beta y) = \alpha f(x) + \beta f(y)$$

  holds for all numbers α, β, and all n-vectors x, y
- be sure to parse this very carefully!
- a function that satisfies superposition is called *linear*

The inner product function

- with a an n-vector, the function

$$f(x) = a^T x = a_1 x_1 + a_2 x_2 + \cdots + a_n x_n$$

  is the *inner product function*
- $f(x)$ is a weighted sum of the entries of x
- the inner product function is linear:

$$\begin{aligned} f(\alpha x + \beta y) &= a^T(\alpha x + \beta y) \\ &= a^T(\alpha x) + a^T(\beta y) \\ &= \alpha(a^T x) + \beta(a^T y) \\ &= \alpha f(x) + \beta f(y) \end{aligned}$$

...and all linear functions are inner products

- suppose $f : \mathbf{R}^n \to \mathbf{R}$ is linear
- then it can be expressed as $f(x) = a^T x$ for some a
- specifically: $a_i = f(e_i)$
- follows from

$$\begin{aligned} f(x) &= f(x_1 e_1 + x_2 e_2 + \cdots + x_n e_n) \\ &= x_1 f(e_1) + x_2 f(e_2) + \cdots + x_n f(e_n) \end{aligned}$$

Affine functions

- a function that is linear plus a constant is called *affine*
- general form is $f(x) = a^T x + b$, with a an n-vector and b a scalar
- a function $f : \mathbf{R}^n \to \mathbf{R}$ is affine if and only if

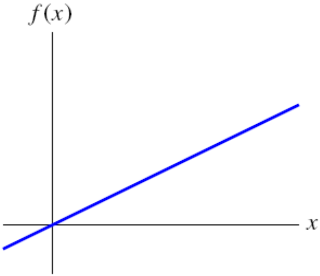
$$f(\alpha x + \beta y) = \alpha f(x) + \beta f(y)$$

  holds for all α, β with $\alpha + \beta = 1$, and all n-vectors x, y

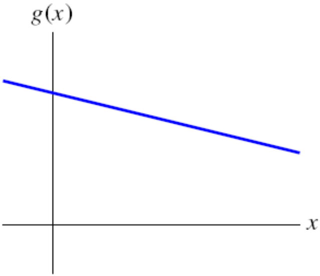
- sometimes (ignorant) people refer to affine functions as linear

Linear versus affine functions

f is linear



g is affine, not linear



First-order Taylor approximation

- suppose $f : \mathbf{R}^n \to \mathbf{R}$
- *first-order Taylor approximation* of f, near point z:

$$\hat{f}(x) = f(z) + \frac{\partial f}{\partial x_1}(z)(x_1 - z_1) + \cdots + \frac{\partial f}{\partial x_n}(z)(x_n - z_n)$$

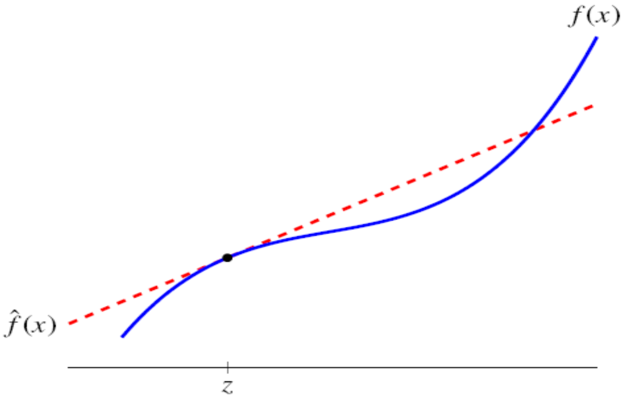
- $\hat{f}(x)$ is *very* close to $f(x)$ when x_i are all near z_i
- $\hat{f}$ is an affine function of x
- can write using inner product as

$$\hat{f}(x) = f(z) + \nabla f(z)^T (x - z)$$

where n-vector $\nabla f(z)$ is the *gradient* of f at z,

$$\nabla f(z) = \left(\frac{\partial f}{\partial x_1}(z), \ldots, \frac{\partial f}{\partial x_n}(z) \right)$$

Example



Regression model

- *regression model* is (the affine function of x)

$$\hat{y} = x^T \beta + v$$

- x is a feature vector; its elements x_i are called *regressors*
- n-vector β is the *weight vector*
- scalar v is the *offset*
- scalar $\hat{y}$ is the *prediction*
  (of some actual outcome or *dependent variable*, denoted y)

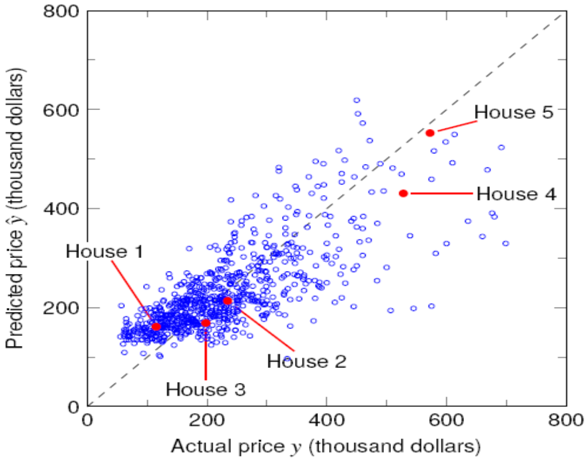
Example

- y is selling price of house in $\$1000$ (in some location, over some period)
- regressor is
$$x = (\text{house area}, \#\ \text{bedrooms})$$
(house area in 1000 sq.ft.)
- regression model weight vector and offset are
$$\beta = (148.73, -18.85), \qquad v = 54.40$$
- we'll see later how to guess β and v from sales data

Example

House	x_1 (area)	x_2 (beds)	y (price)	$\hat{y}$ (prediction)
1	0.846	1	115.00	161.37
2	1.324	2	234.50	213.61
3	1.150	3	198.00	168.88
4	3.037	4	528.00	430.67
5	3.984	5	572.50	552.66

Example


800
600
400
200
0
0
200
400
600
800
Predicted price $\hat{y}$ (thousand dollars)
Actual price y (thousand dollars)
House 1
House 2
House 3
House 4
House 5

Norm

- the *Euclidean norm* (or just *norm*) of an n-vector x is

$$\|x\| = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} = \sqrt{x^T x}$$

- used to measure the size of a vector
- reduces to absolute value for $n = 1$

Properties

for any n-vectors x and y, and any scalar β

- *homogeneity:* $\|\beta x\| = |\beta|\|x\|$
- *triangle inequality:* $\|x + y\| \leq \|x\| + \|y\|$
- *nonnegativity:* $\|x\| \geq 0$
- *definiteness:* $\|x\| = 0$ only if $x = 0$

easy to show except triangle inequality, which we show later

RMS value

- *mean-square value* of n-vector x is

$$\frac{x_1^2 + \cdots + x_n^2}{n} = \frac{\|x\|^2}{n}$$

- *root-mean-square value* (RMS value) is

$$\mathbf{rms}(x) = \sqrt{\frac{x_1^2 + \cdots + x_n^2}{n}} = \frac{\|x\|}{\sqrt{n}}$$

- $\mathbf{rms}(x)$ gives 'typical' value of $|x_i|$
- *e.g.*, $\mathbf{rms}(\mathbf{1}) = 1$ (independent of n)
- RMS value useful for comparing sizes of vectors of different lengths

Norm of block vectors

- suppose a, b, c are vectors
- $\|(a,b,c)\|^2 = a^T a + b^T b + c^T c = \|a\|^2 + \|b\|^2 + \|c\|^2$
- so we have

$$\|(a,b,c)\| = \sqrt{\|a\|^2 + \|b\|^2 + \|c\|^2} = \|(\|a\|, \|b\|, \|c\|)\|$$

(parse RHS very carefully!)

- we'll use these ideas later

Chebyshev inequality

- suppose that k of the numbers $|x_1|, \ldots, |x_n|$ are $\geq a$
- then k of the numbers $x_1^2, \ldots, x_n^2$ are $\geq a^2$
- so $\|x\|^2 = x_1^2 + \cdots + x_n^2 \geq ka^2$
- so we have $k \leq \|x\|^2 / a^2$
- number of x_i with $|x_i| \geq a$ is no more than $\|x\|^2/a^2$
- this is the *Chebyshev inequality*
- in terms of RMS value:

$$\text{fraction of entries with } |x_i| \geq a \text{ is no more than } \left(\frac{\mathbf{rms}(x)}{a}\right)^2$$

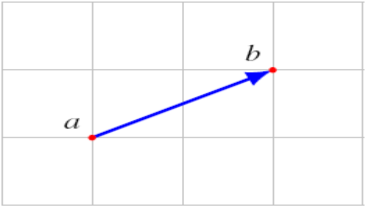
- example: no more than 4% of entries can satisfy $|x_i| \geq 5\ \mathbf{rms}(x)$

Distance

- (Euclidean) *distance* between n-vectors a and b is

$$\mathbf{dist}(a, b) = \|a - b\|$$

- agrees with ordinary distance for $n = 1, 2, 3$



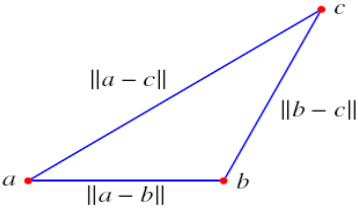
- $\mathbf{rms}(a - b)$ is the *RMS deviation* between a and b

Triangle inequality

- triangle with vertices at positions a, b, c
- edge lengths are $\|a-b\|$, $\|b-c\|$, $\|a-c\|$
- by triangle inequality

$$\|a-c\| = \|(a-b)+(b-c)\| \leq \|a-b\| + \|b-c\|$$

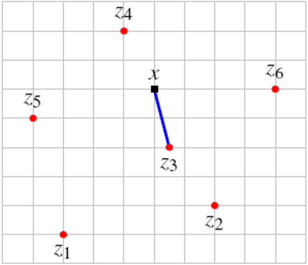
i.e., third edge length is no longer than sum of other two



Feature distance and nearest neighbors

- if x and y are feature vectors for two entities, $\|x - y\|$ is the *feature distance*
- if $z_1, \ldots, z_m$ is a list of vectors, z_j is the *nearest neighbor* of x if

$$\|x - z_j\| \leq \|x - z_i\|, \quad i = 1, \ldots, m$$



- these simple ideas are very widely used

Document dissimilarity

- 5 Wikipedia articles: 'Veterans Day', 'Memorial Day', 'Academy Awards', 'Golden Globe Awards', 'Super Bowl'
- word count histograms, dictionary of 4423 words
- pairwise distances shown below

	Veterans Day	Memorial Day	Academy Awards	Golden Globe Awards	Super Bowl
Veterans Day	0	0.095	0.130	0.153	0.170
Memorial Day	0.095	0	0.122	0.147	0.164
Academy A.	0.130	0.122	0	0.108	0.164
Golden Globe A.	0.153	0.147	0.108	0	0.181
Super Bowl	0.170	0.164	0.164	0.181	0

Standard deviation

- for n-vector x, $\mathbf{avg}(x) = \mathbf{1}^T x/n$
- *de-meaned vector* is $\tilde{x} = x - \mathbf{avg}(x)\mathbf{1}$ (so $\mathbf{avg}(\tilde{x}) = 0$)
- *standard deviation* of x is

$$\mathbf{std}(x) = \mathbf{rms}(\tilde{x}) = \frac{\|x - (\mathbf{1}^T x/n)\mathbf{1}\|}{\sqrt{n}}$$

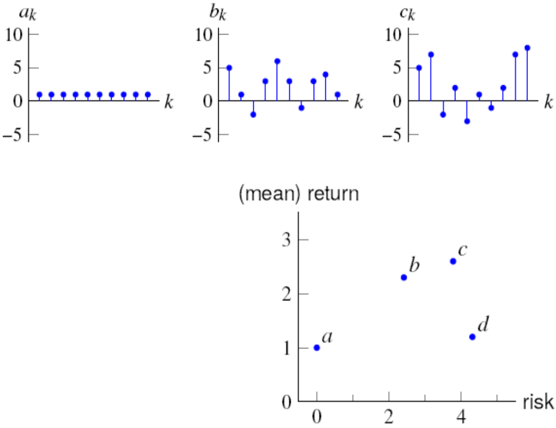
- $\mathbf{std}(x)$ gives 'typical' amount x_i vary from $\mathbf{avg}(x)$
- $\mathbf{std}(x) = 0$ only if $x = \alpha\mathbf{1}$ for some α
- greek letters μ, σ commonly used for mean, standard deviation
- a basic formula:

$$\mathbf{rms}(x)^2 = \mathbf{avg}(x)^2 + \mathbf{std}(x)^2$$

Mean return and risk

- x is time series of returns (say, in %) on some investment or asset over some period
- $\mathbf{avg}(x)$ is the mean return over the period, usually just called *return*
- $\mathbf{std}(x)$ measures how variable the return is over the period, and is called the *risk*
- multiple investments (with different return time series) are often compared in terms of return and risk
- often plotted on a *risk-return plot*

Risk-return example



Chebyshev inequality for standard deviation

- x is an n-vector with mean $\mathbf{avg}(x)$, standard deviation $\mathbf{std}(x)$
- rough idea: most entries of x are not too far from the mean
- by Chebyshev inequality, fraction of entries of x with

$$|x_i - \mathbf{avg}(x)| \geq \alpha \ \mathbf{std}(x)$$

  is no more than $1/\alpha^2$ (for $\alpha > 1$)
- for return time series with mean 8% and standard deviation 3%, loss ($x_i \leq 0$) can occur in no more than $(3/8)^2 = 14.1\%$ of periods

Cauchy–Schwarz inequality

- for two n-vectors a and b, $|a^T b| \leq \|a\|\|b\|$
- written out,

$$|a_1 b_1 + \cdots + a_n b_n| \leq \left(a_1^2 + \cdots + a_n^2\right)^{1/2} \left(b_1^2 + \cdots + b_n^2\right)^{1/2}$$

- now we can show triangle inequality:

$$\begin{aligned} \|a+b\|^2 &= \|a\|^2 + 2a^T b + \|b\|^2 \\ &\leq \|a\|^2 + 2\|a\|\|b\| + \|b\|^2 \\ &= (\|a\| + \|b\|)^2 \end{aligned}$$

Derivation of Cauchy–Schwarz inequality

- it's clearly true if either a or b is 0
- so assume $\alpha = \|a\|$ and $\beta = \|b\|$ are nonzero
- we have

$$\begin{aligned} 0 &\leq \|\beta a - \alpha b\|^2 \\ &= \|\beta a\|^2 - 2(\beta a)^T(\alpha b) + \|\alpha b\|^2 \\ &= \beta^2\|a\|^2 - 2\beta\alpha(a^T b) + \alpha^2\|b\|^2 \\ &= 2\|a\|^2\|b\|^2 - 2\|a\|\,\|b\|(a^T b) \end{aligned}$$

- divide by $2\|a\|\,\|b\|$ to get $a^T b \leq \|a\|\,\|b\|$
- apply to $-a$, b to get other half of Cauchy–Schwarz inequality

Angle

- *angle* between two nonzero vectors a, b defined as

$$\angle(a,b) = \arccos\left(\frac{a^T b}{\|a\|\,\|b\|}\right)$$

- $\angle(a,b)$ is the number in $[0,\pi]$ that satisfies

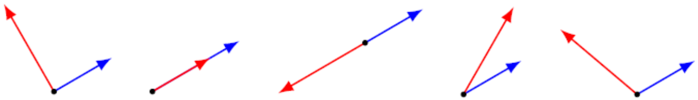
$$a^T b = \|a\|\,\|b\|\cos\left(\angle(a,b)\right)$$

- coincides with ordinary angle between vectors in 2-D and 3-D

Classification of angles

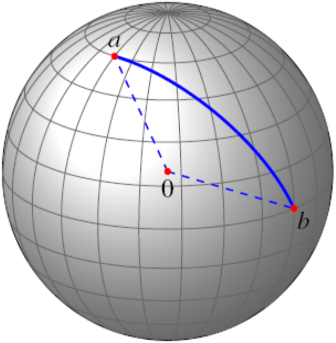
$\theta = \angle(a,b)$

- $\theta = \pi/2 = 90°$: a and b are *orthogonal*, written $a \perp b$ ($a^T b = 0$)
- $\theta = 0$: a and b are *aligned* ($a^T b = \|a\| \|b\|$)
- $\theta = \pi = 180°$: a and b are *anti-aligned* ($a^T b = -\|a\| \|b\|$)
- $\theta \leq \pi/2 = 90°$: a and b make an *acute angle* ($a^T b \geq 0$)
- $\theta \geq \pi/2 = 90°$: a and b make an *obtuse angle* ($a^T b \leq 0$)



Spherical distance

if a, b are on sphere of radius R, distance *along the sphere* is $R\angle(a,b)$



Document dissimilarity by angles

- measure dissimilarity by angle of word count histogram vectors
- pairwise angles (in degrees) for 5 Wikipedia pages shown below

	Veterans Day	Memorial Day	Academy Awards	Golden Globe Awards	Super Bowl
Veterans Day	0	60.6	85.7	87.0	87.7
Memorial Day	60.6	0	85.6	87.5	87.5
Academy A.	85.7	85.6	0	58.7	85.7
Golden Globe A.	87.0	87.5	58.7	0	86.0
Super Bowl	87.7	87.5	86.1	86.0	0

Correlation coefficient

- vectors a and b, and de-meaned vectors

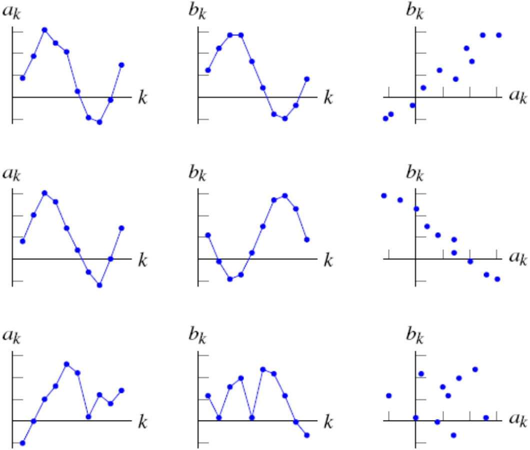
$$\tilde{a} = a - \mathbf{avg}(a)\mathbf{1}, \qquad \tilde{b} = b - \mathbf{avg}(b)\mathbf{1}$$

- *correlation coefficient* (between a and b, with $\tilde{a} \neq 0$, $\tilde{b} \neq 0$)

$$\rho = \frac{\tilde{a}^T \tilde{b}}{\|\tilde{a}\| \, \|\tilde{b}\|}$$

- $\rho = \cos \angle(\tilde{a}, \tilde{b})$
  - $\rho = 0$: a and b are *uncorrelated*
  - $\rho > 0.8$ (or so): a and b are *highly correlated*
  - $\rho < -0.8$ (or so): a and b are *highly anti-correlated*
- very roughly: highly correlated means a_i and b_i are typically both above (below) their means together

Examples



$\rho = 97\%$

$\rho = -99\%$

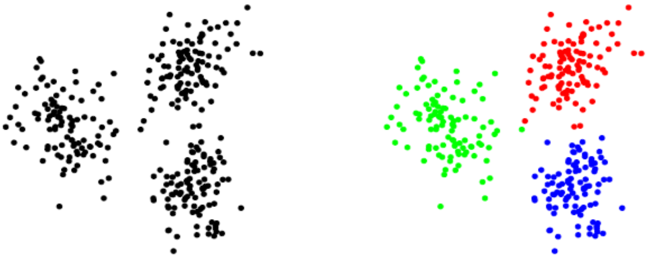
$\rho = 0.4\%$

Examples

- highly correlated vectors:
  - rainfall time series at nearby locations
  - daily returns of similar companies in same industry
  - word count vectors of closely related documents (*e.g.*, same author, topic, . . .)
  - sales of shoes and socks (at different locations or periods)
- approximately uncorrelated vectors
  - unrelated vectors
  - audio signals (even different tracks in multi-track recording)
- (somewhat) negatively correlated vectors
  - daily temperatures in Palo Alto and Melbourne

Clustering

- given N n-vectors $x_1, \ldots, x_N$
- goal: partition (divide, cluster) into k groups
- want vectors in the same group to be close to one another



Example settings

- topic discovery and document classification
  - x_i is word count histogram for document i
- patient clustering
  - x_i are patient attributes, test results, symptoms
- customer market segmentation
  - x_i is purchase history and other attributes of customer i
- color compression of images
  - x_i are RGB pixel values
- financial sectors
  - x_i are n-vectors of financial attributes of company i

Clustering objective

- $G_j \subset \{1, \ldots, N\}$ is group j, for $j = 1, \ldots, k$
- c_i is group that x_i is in: $i \in G_{c_i}$
- group *representatives*: n-vectors $z_1, \ldots, z_k$
- clustering objective is

$$J^{\text{clust}} = \frac{1}{N} \sum_{i=1}^{N} \|x_i - z_{c_i}\|^2$$

  mean square distance from vectors to associated representative
- J^{clust} small means good clustering
- goal: choose clustering c_i and representatives z_j to minimize J^{clust}

Partitioning the vectors given the representatives

- suppose representatives $z_1, \ldots, z_k$ are given
- how do we assign the vectors to groups, *i.e.*, choose $c_1, \ldots, c_N$?

- c_i only appears in term $\|x_i - z_{c_i}\|^2$ in J^{clust}
- to minimize over c_i, choose c_i so $\|x_i - z_{c_i}\|^2 = \min_j \|x_i - z_j\|^2$
- *i.e., assign each vector to its nearest representative*

Choosing representatives given the partition

- given the partition $G_1, \ldots, G_k$, how do we choose representatives $z_1, \ldots, z_k$ to minimize J^{clust}?
- J^{clust} splits into a sum of k sums, one for each z_j:

$$J^{\text{clust}} = J_1 + \cdots + J_k, \qquad J_j = (1/N) \sum_{i \in G_j} \|x_i - z_j\|^2$$

- so we choose z_j to minimize mean square distance to the points in its partition
- this is the mean (or average or centroid) of the points in the partition:

$$z_j = (1/|G_j|) \sum_{i \in G_j} x_i$$

k-means algorithm

- alternate between updating the partition, then the representatives
- a famous algorithm called *k-means*
- objective J^{clust} decreases in each step

---

given $x_1, \ldots, x_N \in \mathbf{R}^n$ and $z_1, \ldots, z_k \in \mathbf{R}^n$

repeat

Update partition: assign i to G_j, $j = \operatorname{argmin}_{j'} \|x_i - z_{j'}\|^2$

Update centroids: $z_j = \frac{1}{|G_j|} \sum_{i \in G_j} x_i$

until $z_1, \ldots, z_k$ stop changing

Convergence of k-means algorithm

- J^{clust} goes down in each step, until the z_j's stop changing
- but (in general) the k-means algorithm *does not find the partition that minimizes* J^{clust}
- k-means is a *heuristic*: it is not guaranteed to find the smallest possible value of J^{clust}
- the final partition (and its value of J^{clust}) can depend on the initial representatives
- common approach:
  - run k-means 10 times, with different (often random) initial representatives
  - take as final partition the one with the smallest value of J^{clust}

Linear dependence

- set of n-vectors $\{a_1, \ldots, a_k\}$ (with $k \geq 1$) is *linearly dependent* if

$$\beta_1 a_1 + \cdots + \beta_k a_k = 0$$

  holds for some $\beta_1, \ldots, \beta_k$, that are not all zero
- equivalent to: at least one a_i is a linear combination of the others
- we say '$a_1, \ldots, a_k$ are linearly dependent'

- $\{a_1\}$ is linearly dependent only if $a_1 = 0$
- $\{a_1, a_2\}$ is linearly dependent only if one a_i is a multiple of the other
- for more than two vectors, there is no simple to state condition

Example

- the vectors

$$a_1 = \begin{bmatrix} 0.2 \\ -7 \\ 8.6 \end{bmatrix}, \qquad a_2 = \begin{bmatrix} -0.1 \\ 2 \\ -1 \end{bmatrix}, \qquad a_3 = \begin{bmatrix} 0 \\ -1 \\ 2.2 \end{bmatrix}$$

  are linearly dependent, since $a_1 + 2a_2 - 3a_3 = 0$

- can express any of them as linear combination of the other two, *e.g.*,

$$a_2 = (-1/2)a_1 + (3/2)a_3$$

Linear independence

- set of n-vectors $\{a_1, \ldots, a_k\}$ (with $k \geq 1$) is *linearly independent* if it is not linearly dependent, *i.e.*,

$$\beta_1 a_1 + \cdots + \beta_k a_k = 0$$

  holds only when $\beta_1 = \cdots = \beta_k = 0$
- we say '$a_1, \ldots, a_k$ are linearly independent'
- equivalent to: no a_i is a linear combination of the others
- example: the unit n-vectors $e_1, \ldots, e_n$ are linearly independent

Linear combinations of linearly independent vectors

- suppose x is linear combination of linearly independent vectors $a_1, \ldots, a_k$:

$$x = \beta_1 a_1 + \cdots + \beta_k a_k$$

- the coefficients $\beta_1, \ldots, \beta_k$ are *unique*, *i.e.*, if

$$x = \gamma_1 a_1 + \cdots + \gamma_k a_k$$

  then $\beta_i = \gamma_i$ for $i = 1, \ldots, k$

- this means that (in principle) we can deduce the coefficients from x
- to see why, note that

$$(\beta_1 - \gamma_1)a_1 + \cdots + (\beta_k - \gamma_k)a_k = 0$$

  and so (by linear independence) $\beta_1 - \gamma_1 = \cdots = \beta_k - \gamma_k = 0$

Independence-dimension inequality

- *a linearly independent set of n-vectors can have at most n elements*
- put another way: *any set of $n+1$ or more n-vectors is linearly dependent*

Basis

- a set of n linearly independent n-vectors $a_1, \ldots, a_n$ is called a *basis*
- any n-vector b can be expressed as a linear combination of them:

$$b = \beta_1 a_1 + \cdots + \beta_n a_n$$

  for some $\beta_1, \ldots, \beta_n$
- and these coefficients are unique
- formula above is called *expansion of b in the $a_1, \ldots, a_n$ basis*
- example: $e_1, \ldots, e_n$ is a basis, expansion of b is

$$b = b_1 e_1 + \cdots + b_n e_n$$

Orthonormal vectors

- set of n-vectors $a_1, \ldots, a_k$ are *(mutually) orthogonal* if $a_i \perp a_j$ for $i \neq j$
- they are *normalized* if $\|a_i\| = 1$ for $i = 1, \ldots, k$
- they are *orthonormal* if both hold
- can be expressed using inner products as

$$a_i^T a_j = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

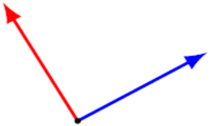
- orthonormal sets of vectors are linearly independent
- by independence-dimension inequality, must have $k \leq n$
- when $k = n$, $a_1, \ldots, a_n$ are an *orthonormal basis*

Examples of orthonormal bases

- standard unit n-vectors $e_1, \ldots, e_n$
- the 3-vectors

$$\begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}, \qquad \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \qquad \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$$

- the 2-vectors shown below



Orthonormal expansion

- if $a_1, \ldots, a_n$ is an orthonormal basis, we have for any n-vector x

$$x = (a_1^T x)a_1 + \cdots + (a_n^T x)a_n$$

- called *orthonormal expansion of* x (in the orthonormal basis)
- to verify formula, take inner product of both sides with a_i

Gram–Schmidt (orthogonalization) algorithm

- an algorithm to check if $a_1, \ldots, a_k$ are linearly independent

Gram–Schmidt algorithm

---

given n-vectors $a_1, \ldots, a_k$

for $i = 1, \ldots, k$

1. *Orthogonalization:* $\tilde{q}_i = a_i - (q_1^T a_i)q_1 - \cdots - (q_{i-1}^T a_i)q_{i-1}$
2. *Test for linear dependence:* if $\tilde{q}_i = 0$, quit
3. *Normalization:* $q_i = \tilde{q}_i / \|\tilde{q}_i\|$

- if G–S does not stop early (in step 2), $a_1, \ldots, a_k$ are linearly independent
- if G–S stops early in iteration $i = j$, then a_j is a linear combination of $a_1, \ldots, a_{j-1}$ (so $a_1, \ldots, a_k$ are linearly dependent)