2. Norm, distance, angle

- norm
- distance
- k-means algorithm
- angle
- complex vectors

Euclidean norm

(Euclidean) norm of vector $a \in \mathbf{R}^n$:

$$\begin{aligned} \|a\| &= \sqrt{a_1^2 + a_2^2 + \cdots + a_n^2} \\ &= \sqrt{a^T a} \end{aligned}$$

- if $n = 1$, $\|a\|$ reduces to absolute value $|a|$
- measures the magnitude of a
- sometimes written as $\|a\|_2$ to distinguish from other norms, *e.g.*,

$$\|a\|_1 = |a_1| + |a_2| + \cdots + |a_n|$$

Properties

Positive definiteness

$$\|a\| \geq 0 \quad \text{for all } a, \qquad \|a\| = 0 \quad \text{only if } a = 0$$

Homogeneity

$$\|\beta a\| = |\beta|\|a\| \quad \text{for all vectors } a \text{ and scalars } \beta$$

Triangle inequality (proved on page 2.7)

$$\|a + b\| \leq \|a\| + \|b\| \quad \text{for all vectors } a \text{ and } b \text{ of equal length}$$

Norm of block vector: if a, b are vectors,

$$\left\| \begin{bmatrix} a \\ b \end{bmatrix} \right\| = \sqrt{\|a\|^2 + \|b\|^2}$$

Cauchy–Schwarz inequality

$$|a^T b| \leq \|a\| \|b\| \quad \text{for all } a, b \in \mathbf{R}^n$$

moreover, equality $|a^T b| = \|a\| \|b\|$ holds if:

- $a = 0$ or $b = 0$; in this case $a^T b = 0 = \|a\| \|b\|$
- $a \neq 0$ and $b \neq 0$, and $b = \gamma a$ for some $\gamma > 0$; in this case

$$0 < a^T b = \gamma \|a\|^2 = \|a\| \|b\|$$

- $a \neq 0$ and $b \neq 0$, and $b = -\gamma a$ for some $\gamma > 0$; in this case

$$0 > a^T b = -\gamma \|a\|^2 = -\|a\| \|b\|$$

Proof of Cauchy–Schwarz inequality

1. trivial if $a = 0$ or $b = 0$

2. assume $\|a\| = \|b\| = 1$; we show that $-1 \leq a^T b \leq 1$

$$\begin{array}{rcl} 0 & \leq & \|a-b\|^2 \\ & = & (a-b)^T(a-b) \\ & = & \|a\|^2 - 2a^T b + \|b\|^2 \\ & = & 2(1 - a^T b) \end{array}$$

with equality only if $a = b$

$$\begin{array}{rcl} 0 & \leq & \|a+b\|^2 \\ & = & (a+b)^T(a+b) \\ & = & \|a\|^2 + 2a^T b + \|b\|^2 \\ & = & 2(1 + a^T b) \end{array}$$

with equality only if $a = -b$

3. for general nonzero a, b, apply case 2 to the unit-norm vectors

$$\frac{1}{\|a\|}a, \quad \frac{1}{\|b\|}b$$

Average and RMS value

let a be a real n-vector

- the *average* of the elements of a is

$$\mathbf{avg}(a) = \frac{a_1 + a_2 + \cdots + a_n}{n} = \frac{\mathbf{1}^T a}{n}$$

- the *root-mean-square* value is the root of the average squared entry

$$\mathbf{rms}(a) = \sqrt{\frac{a_1^2 + a_2^2 + \cdots + a_n^2}{n}} = \frac{\|a\|}{\sqrt{n}}$$

Exercise: show that $|\,\mathbf{avg}(a)| \le \mathbf{rms}(a)$

Triangle inequality from Cauchy–Schwarz inequality

for vectors a, b of equal size

$$\begin{aligned} \|a+b\|^2 &= (a+b)^T(a+b) \\ &= a^Ta + b^Ta + a^Tb + b^Tb \\ &= \|a\|^2 + 2a^Tb + \|b\|^2 \\ &\leq \|a\|^2 + 2\|a\|\|b\| + \|b\|^2 \qquad \text{(by Cauchy–Schwarz)} \\ &= (\|a\| + \|b\|)^2 \end{aligned}$$

- taking squareroots gives the triangle inequality
- triangle inequality is an equality if and only if $a^Tb = \|a\|\|b\|$ (see page 2.4)
- also note from line 3 that $\|a+b\|^2 = \|a\|^2 + \|b\|^2$ if $a^Tb = 0$

Outline

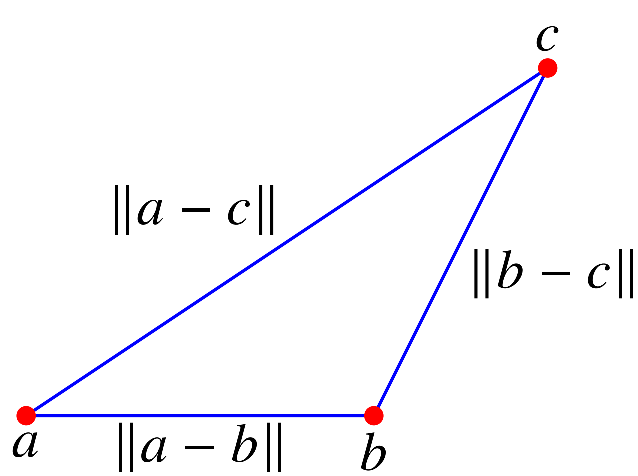
- norm
- **distance**
- k-means algorithm
- angle
- complex vectors

Distance

the (Euclidean) distance between vectors a and b is defined as $\|a - b\|$

- $\|a - b\| \geq 0$ for all a, b and $\|a - b\| = 0$ only if $a = b$
- triangle inequality

$$\|a - c\| \leq \|a - b\| + \|b - c\| \quad \text{for all } a, b, c$$



- RMS deviation between n-vectors a and b is $\mathbf{rms}(a - b) = \dfrac{\|a - b\|}{\sqrt{n}}$

Standard deviation

let a be a real n-vector

- the *de-meaned* vector is the vector of deviations from the average

$$a - \mathbf{avg}(a)\mathbf{1} = \begin{bmatrix} a_1 - \mathbf{avg}(a) \\ a_2 - \mathbf{avg}(a) \\ \vdots \\ a_n - \mathbf{avg}(a) \end{bmatrix} = \begin{bmatrix} a_1 - (\mathbf{1}^T a)/n \\ a_2 - (\mathbf{1}^T a)/n \\ \vdots \\ a_n - (\mathbf{1}^T a)/n \end{bmatrix}$$

- the *standard deviation* is the RMS deviation from the average

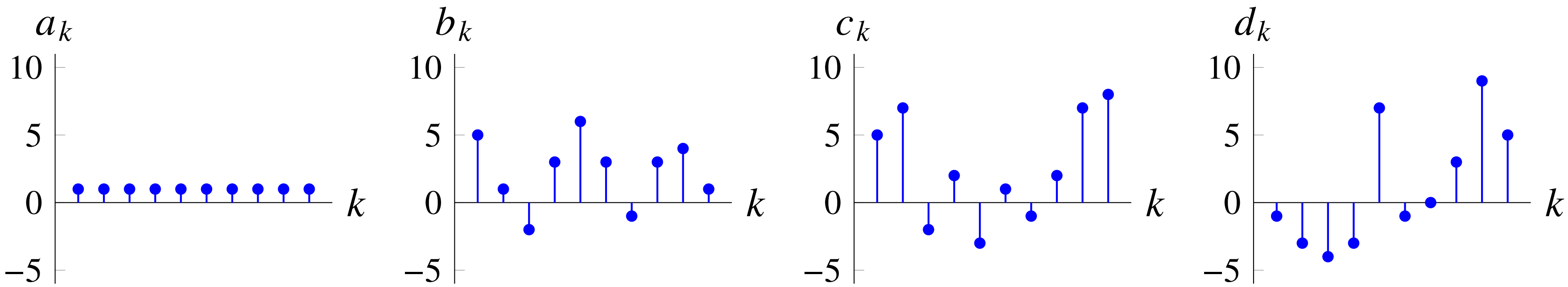
$$\mathbf{std}(a) = \mathbf{rms}(a - \mathbf{avg}(a)\mathbf{1}) = \frac{\left\| a - ((\mathbf{1}^T a)/n)\mathbf{1} \right\|}{\sqrt{n}}$$

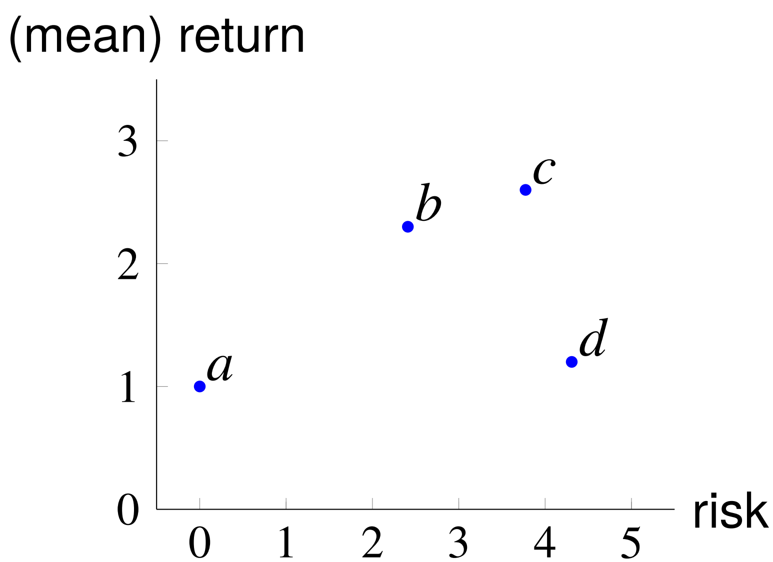
- the de-meaned vector in *standard units* is

$$\frac{1}{\mathbf{std}(a)}(a - \mathbf{avg}(a)\mathbf{1})$$

Mean return and risk of investment

- vectors represent time series of returns on an investment (as a percentage)
- average value is *(mean) return* of the investment
- standard deviation measures variation around the mean, *i.e.*, *risk*





Exercise

show that

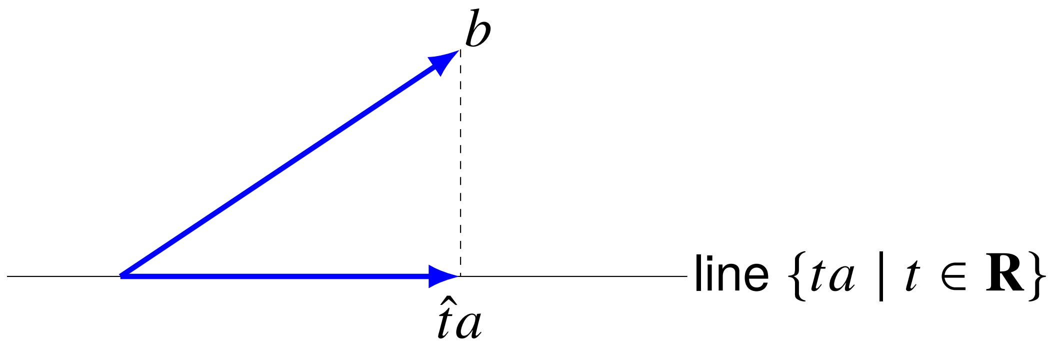
$$\mathbf{avg}(a)^2 + \mathbf{std}(a)^2 = \mathbf{rms}(a)^2$$

Solution

$$\begin{aligned}
\mathbf{std}(a)^2 &= \frac{\|a - \mathbf{avg}(a)\mathbf{1}\|^2}{n} \\
&= \frac{1}{n}\left(a - \frac{\mathbf{1}^T a}{n}\mathbf{1}\right)^T \left(a - \frac{\mathbf{1}^T a}{n}\mathbf{1}\right) \\
&= \frac{1}{n}\left(a^T a - \frac{(\mathbf{1}^T a)^2}{n} - \frac{(\mathbf{1}^T a)^2}{n} + \left(\frac{\mathbf{1}^T a}{n}\right)^2 n\right) \\
&= \frac{1}{n}\left(a^T a - \frac{(\mathbf{1}^T a)^2}{n}\right) \\
&= \mathbf{rms}(a)^2 - \mathbf{avg}(a)^2
\end{aligned}$$

Exercise: nearest scalar multiple

given two vectors $a, b \in \mathbf{R}^n$, with $a \neq 0$, find scalar multiple ta closest to b



Solution

- squared distance between ta and b is

$$\|ta - b\|^2 = (ta - b)^T(ta - b) = t^2 a^T a - 2ta^T b + b^T b$$

  a quadratic function of t with positive leading coefficient $a^T a$

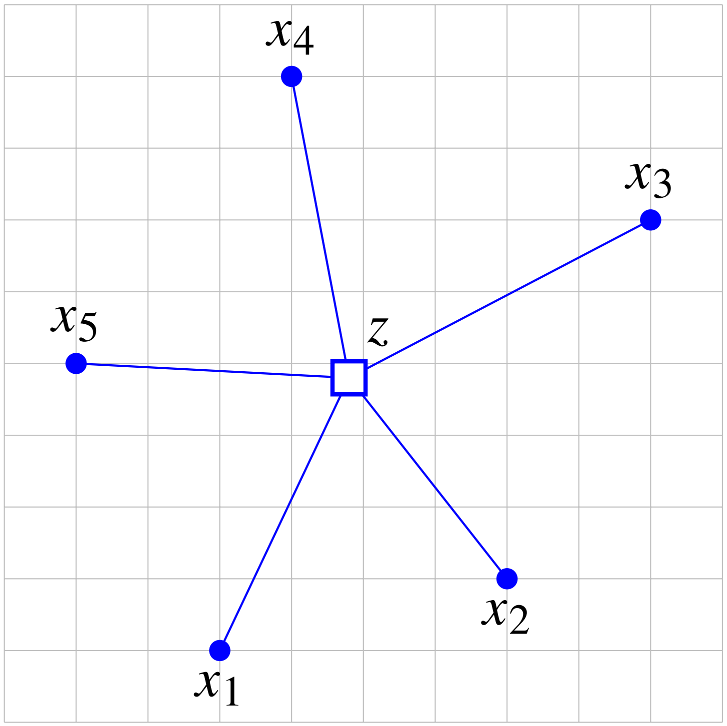
- derivative with respect to t is zero for

$$\hat{t} = \frac{a^T b}{a^T a} = \frac{a^T b}{\|a\|^2}$$

Exercise: average of collection of vectors

given N vectors $x_1, \ldots, x_N \in \mathbf{R}^n$, find the n-vector z that minimizes

$$\|z - x_1\|^2 + \|z - x_2\|^2 + \cdots + \|z - x_N\|^2$$



z is also known as the *centroid* of the points $x_1, \ldots, x_N$

Solution: sum of squared distances is

$$
\begin{aligned}
&\|z - x_1\|^2 + \|z - x_2\|^2 + \cdots + \|z - x_N\|^2 \\
&\quad = \sum_{i=1}^{n} \left((z_i - (x_1)_i)^2 + (z_i - (x_2)_i)^2 + \cdots + (z_i - (x_N)_i)^2 \right) \\
&\quad = \sum_{i=1}^{n} \left(N z_i^2 - 2 z_i \left((x_1)_i + (x_2)_i + \cdots + (x_N)_i \right) + (x_1)_i^2 + \cdots + (x_N)_i^2 \right)
\end{aligned}
$$

here $(x_j)_i$ is ith element of the vector x_j

- term i in the sum is minimized by

$$z_i = \frac{1}{N}((x_1)_i + (x_2)_i + \cdots + (x_N)_i)$$

- solution z is component-wise average of the points $x_1, \ldots, x_N$:

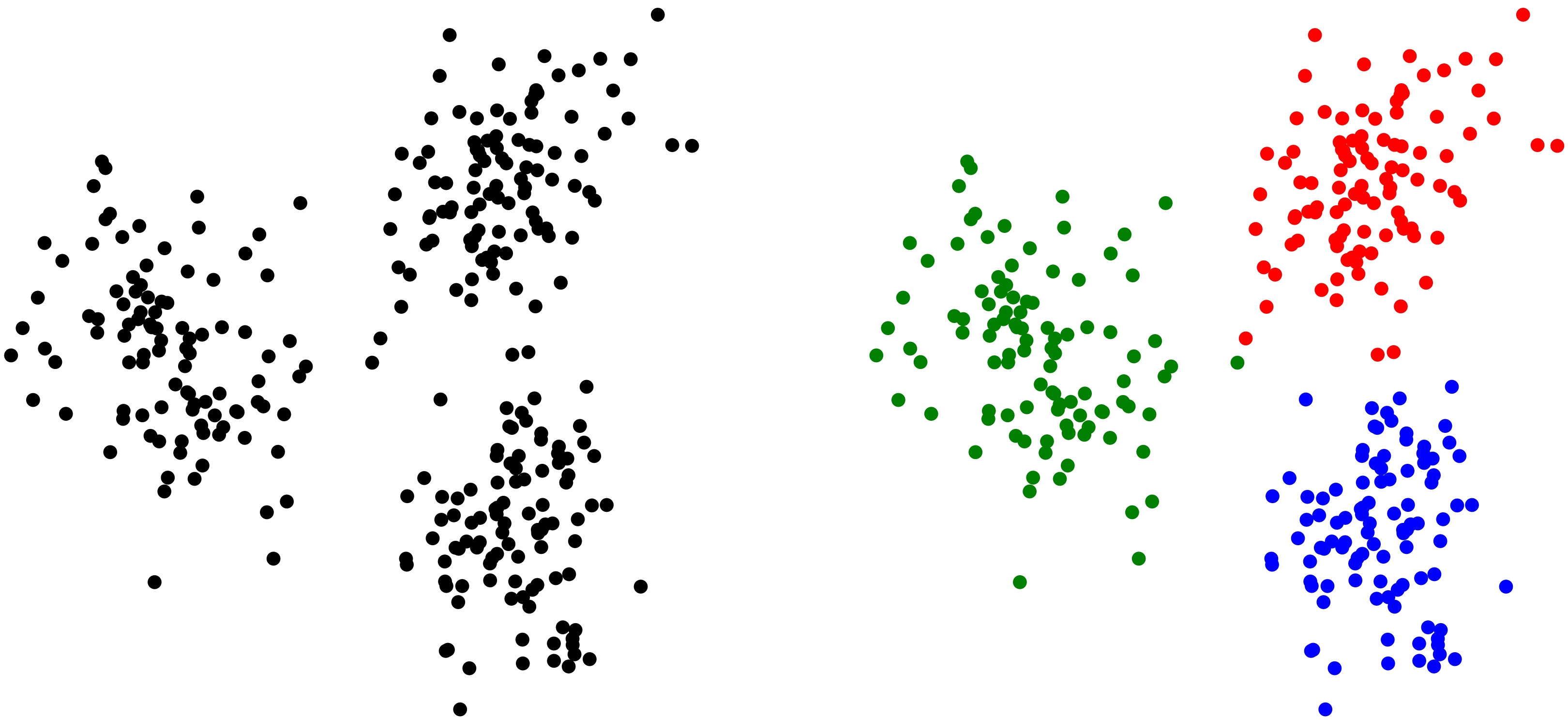
$$z = \frac{1}{N}(x_1 + x_2 + \cdots + x_N)$$

Outline

- norm
- distance
- **k-means algorithm**
- angle
- complex vectors

k-means clustering

a popular iterative algorithm for partitioning N vectors $x_1, \ldots, x_N$ in k clusters



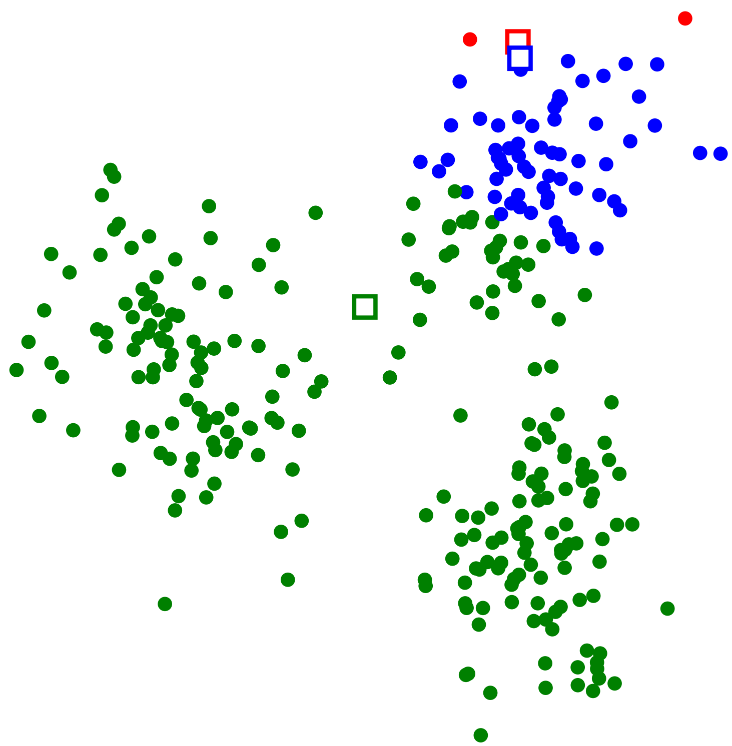
Algorithm

choose initial 'representatives' $z_1, \ldots, z_k$ for the k groups and repeat:

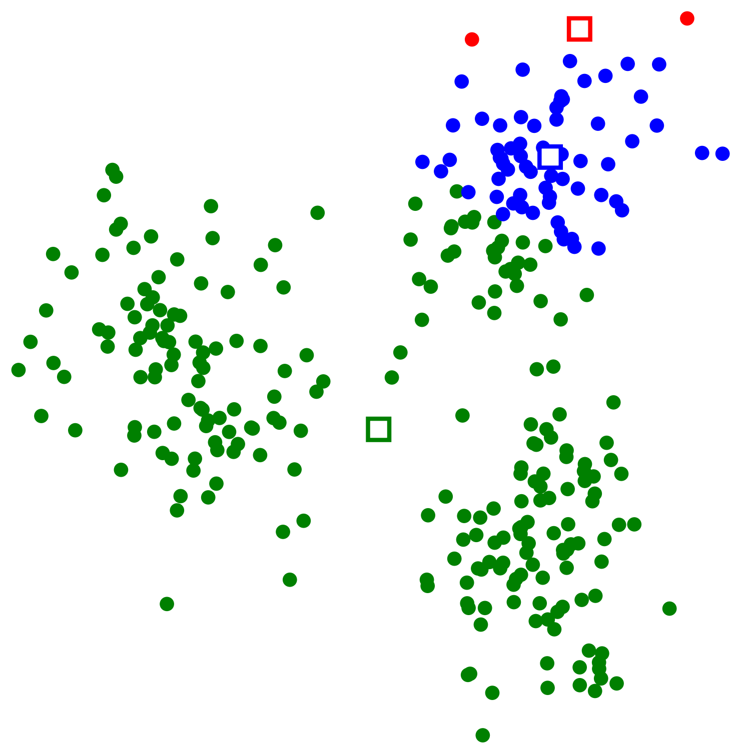
1. assign each vector x_i to the nearest group representative z_j
2. set the representative z_j to the mean of the vectors assigned to it

- initial representatives are often chosen randomly
- as a variation, choose a random initial partition and start with step 2
- solution depends on choice of initial representatives or partition
- can be shown to converge in a finite number of iterations
- in practice, often restarted a few times, with different starting points

Example: first iteration

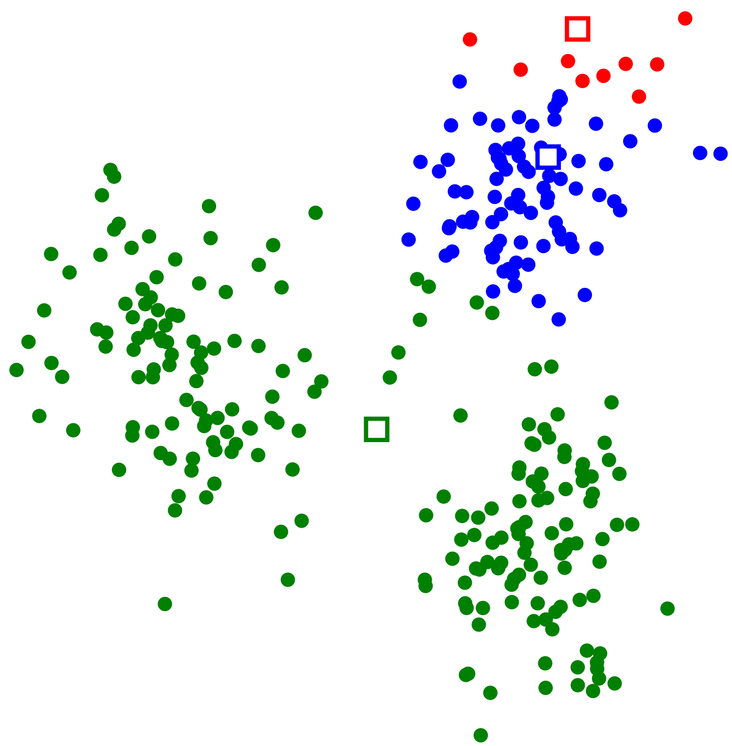


assignment to groups

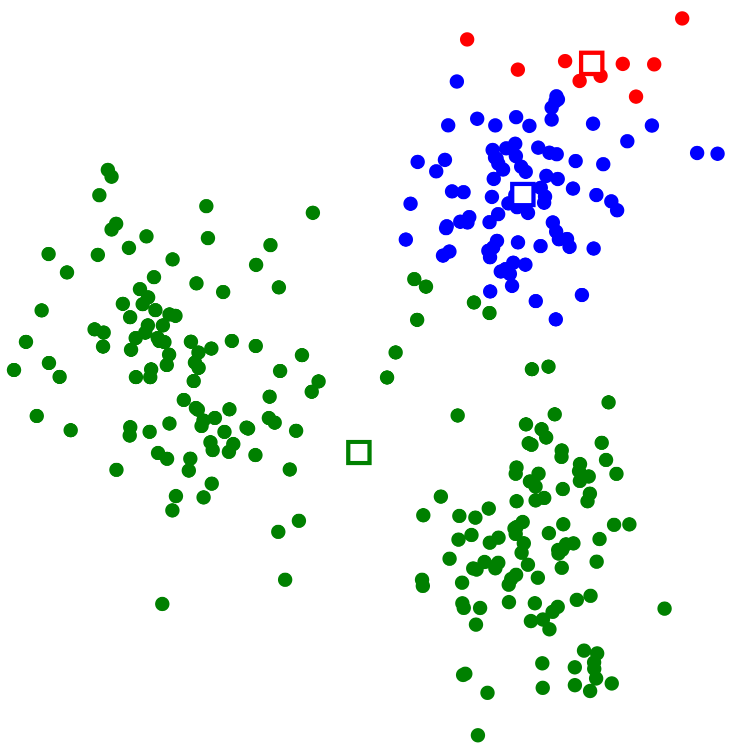


updated representatives

Iteration 2

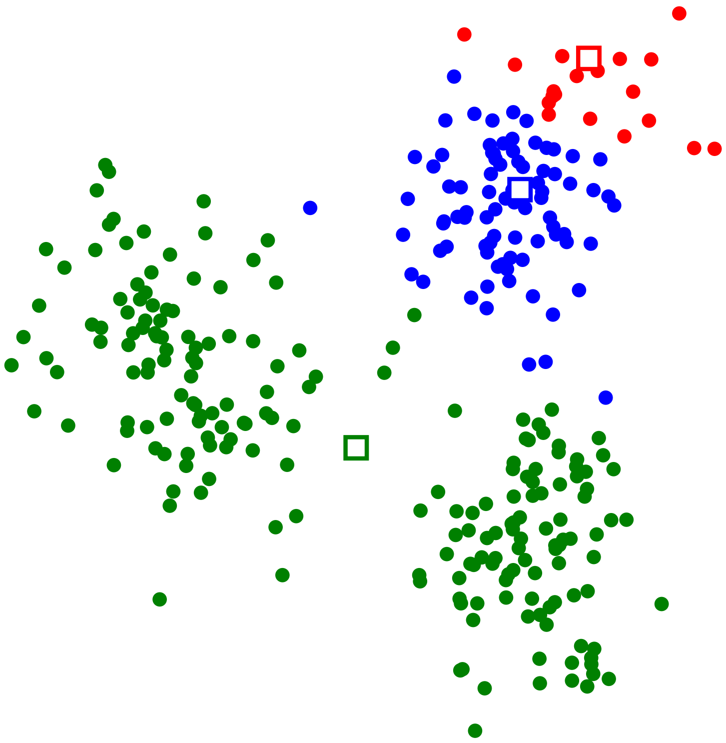


assignment to groups

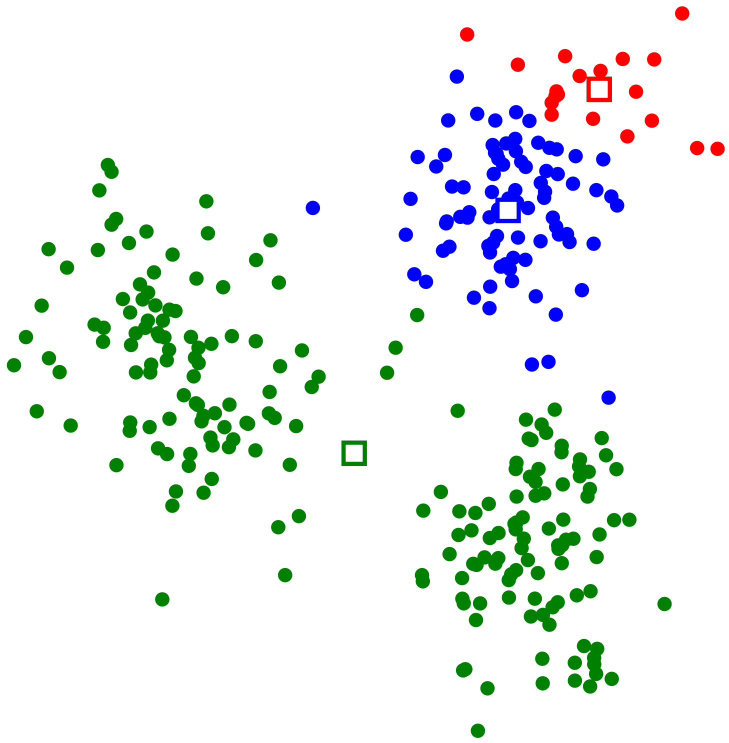


updated representatives

Iteration 3

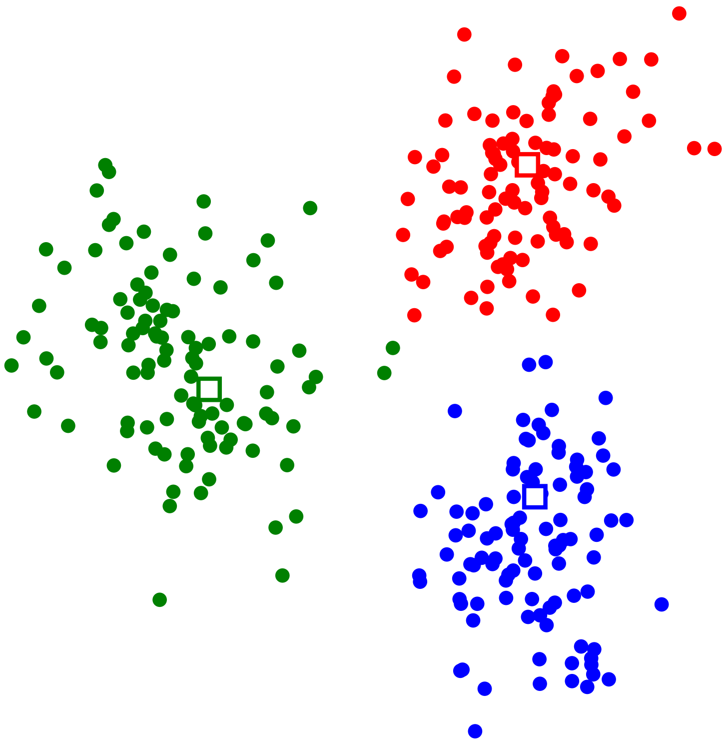


assignment to groups

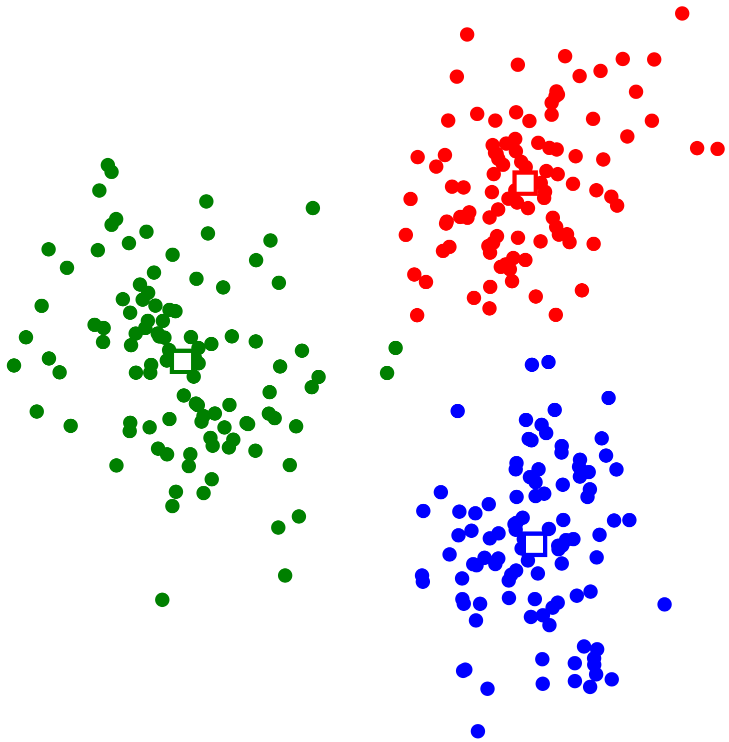


updated representatives

Iteration 11

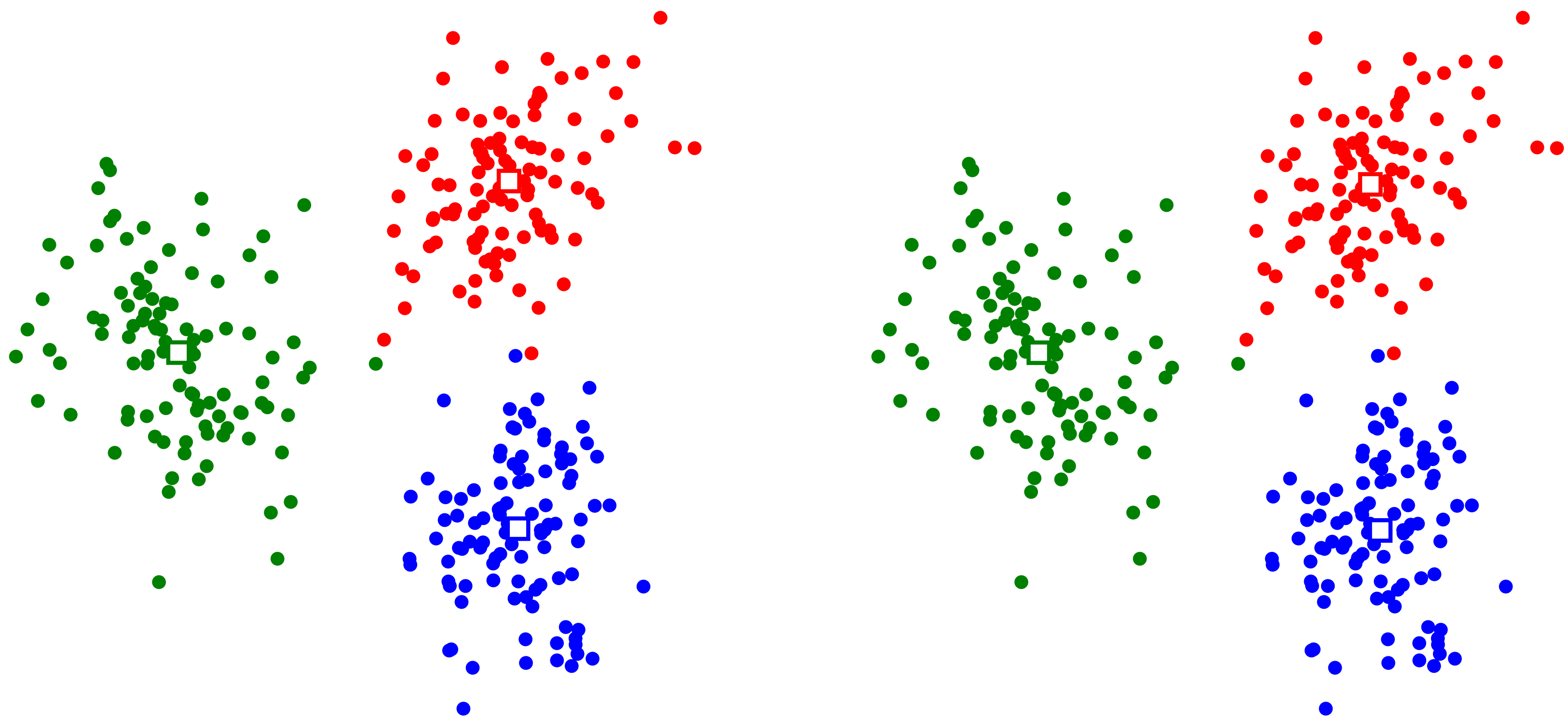


assignment to groups



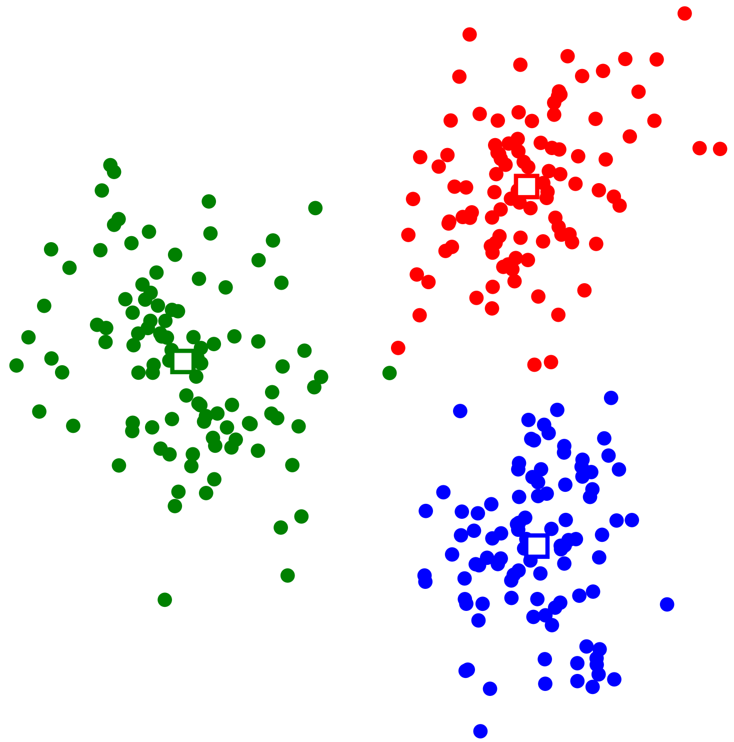
updated representatives

Iteration 12

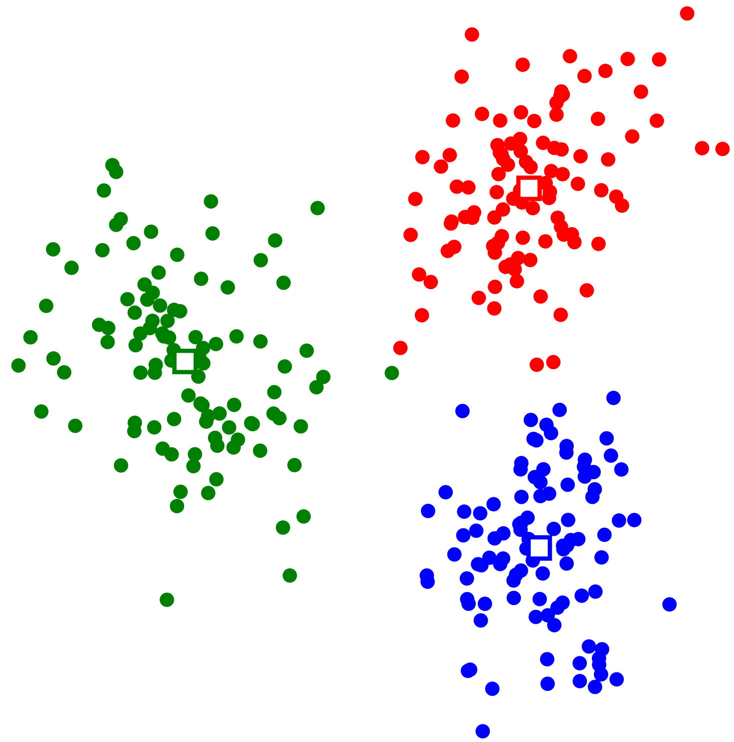


assignment to groups | updated representatives

Iteration 13

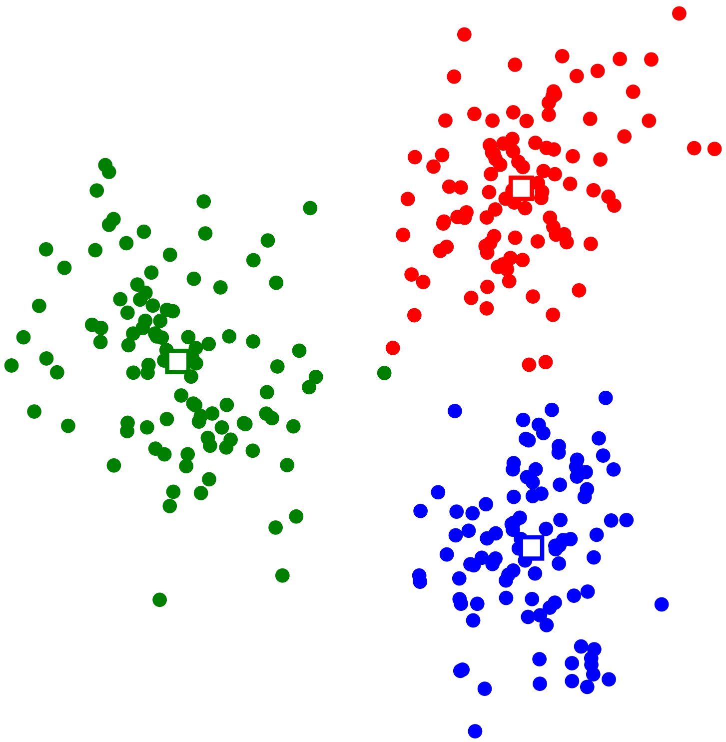


assignment to groups

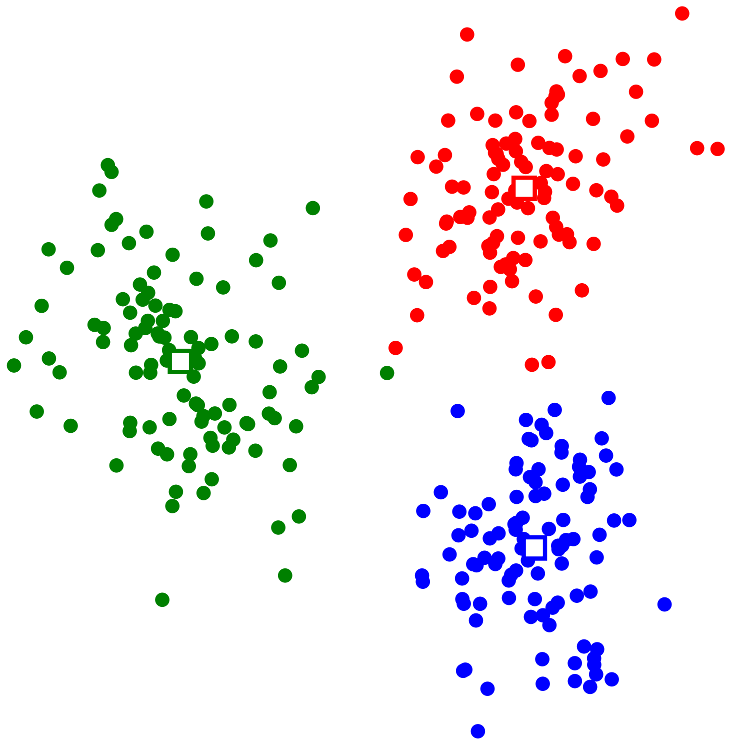


updated representatives

Iteration 14



assignment to groups



updated representatives

Final clustering

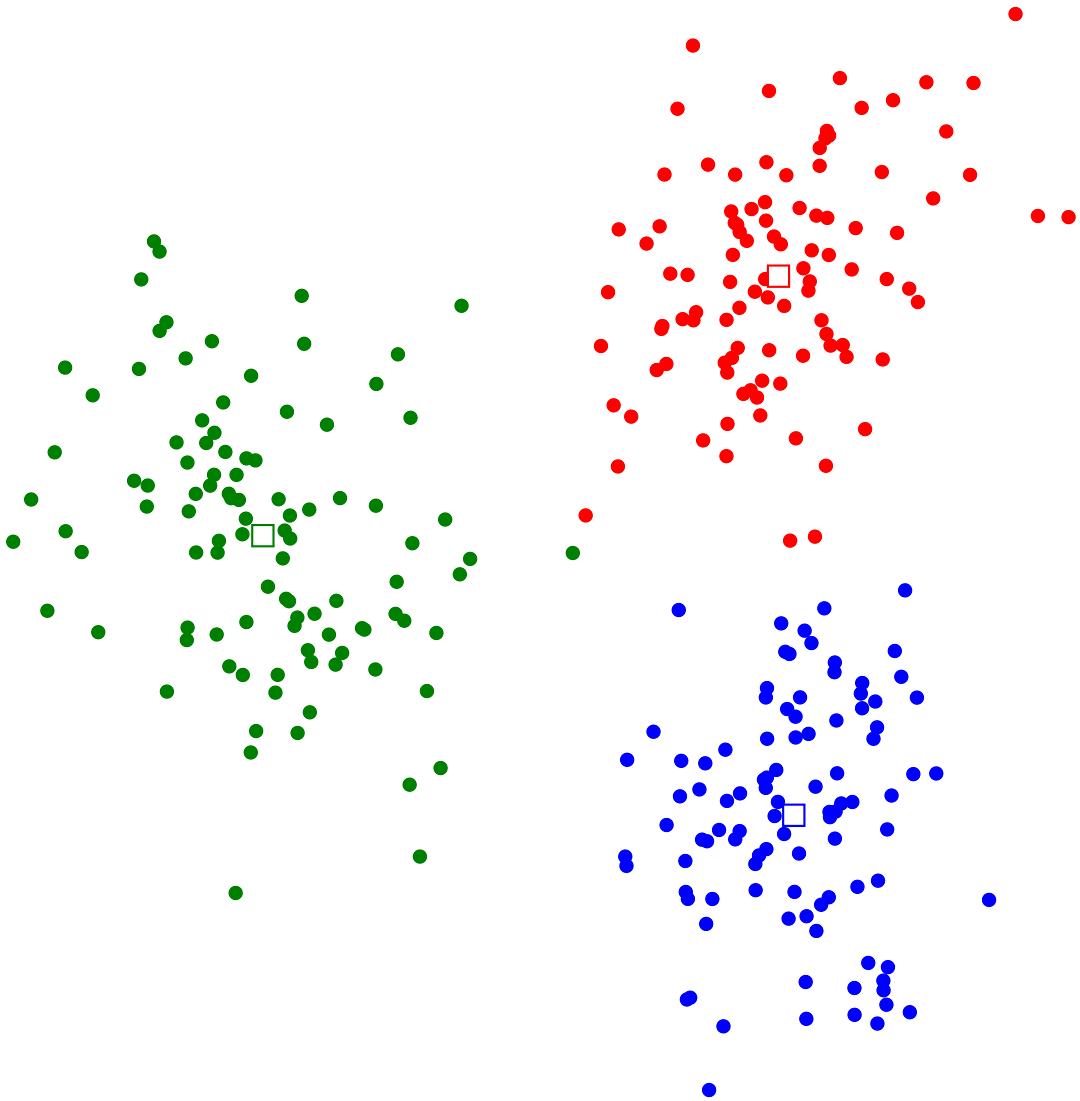
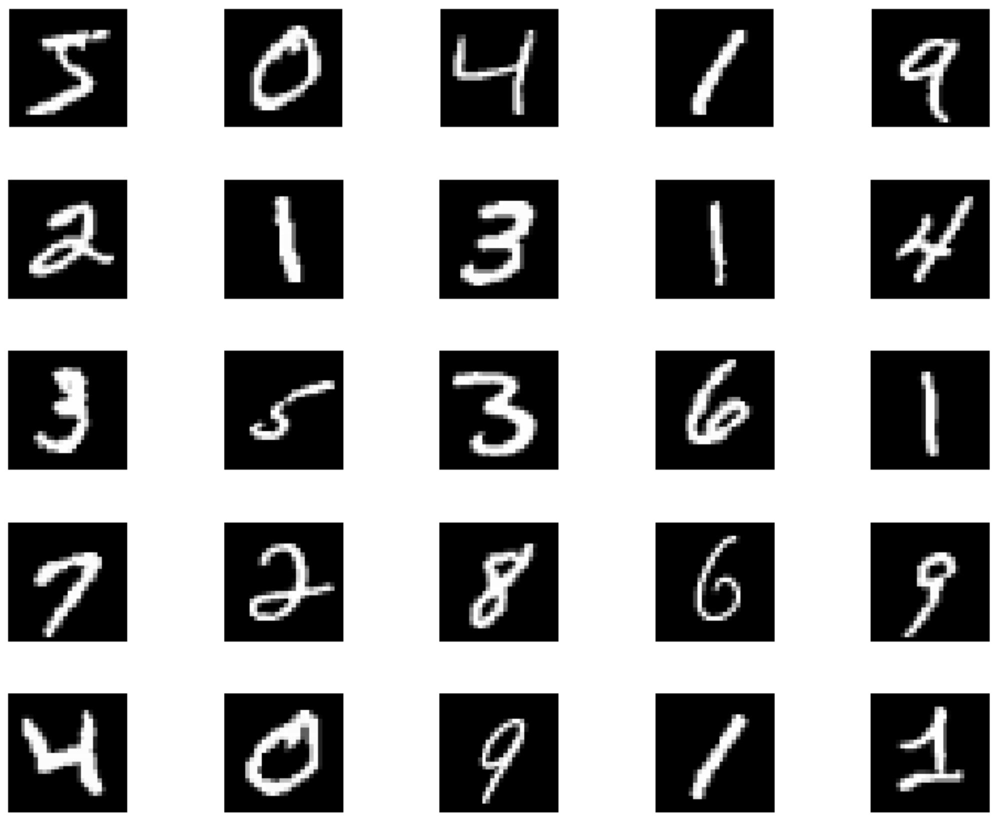


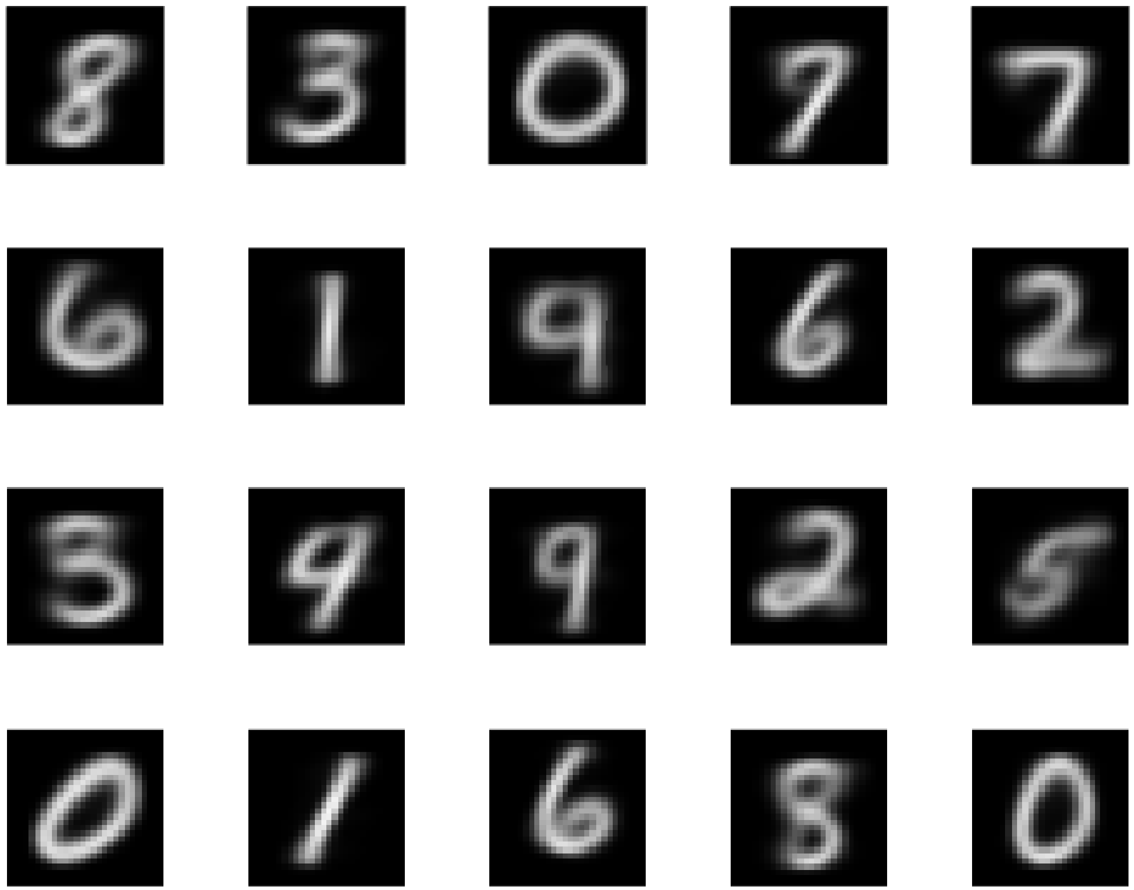
Image clustering

- MNIST dataset of handwritten digits
- $N = 60000$ grayscale images of size 28×28 (vectors x_i of size $28^2 = 784$)
- 25 examples:



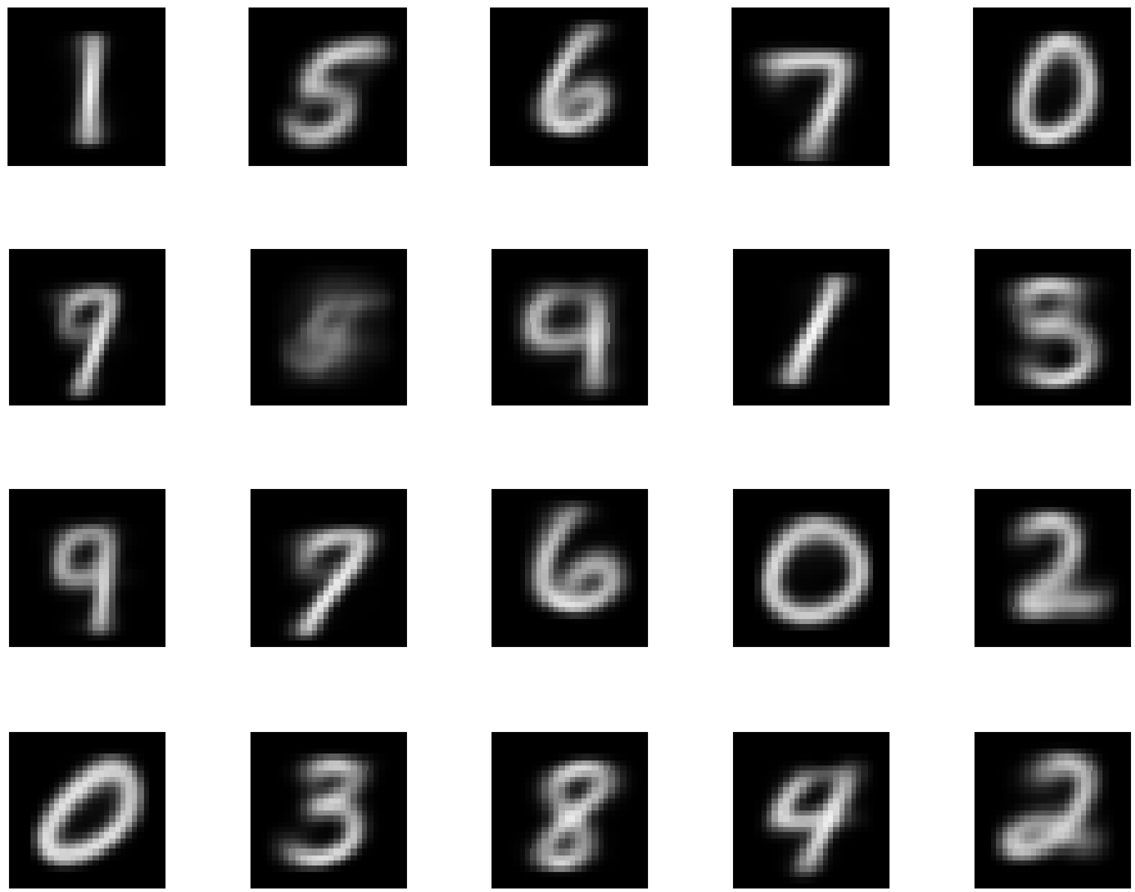
Group representatives ($k = 20$)

- k-means algorithm, with $k = 20$ and randomly chosen initial partition
- 20 group representatives



Group representatives ($k = 20$)

result for another initial partition



Document topic discovery

- $N = 500$ Wikipedia articles, from weekly most popular lists (9/2015–6/2016)
- dictionary of 4423 words
- each article represented by a word histogram vector of size 4423
- result of k-means algorithm with $k = 9$ and randomly chosen initial partition

Cluster 1

- largest coefficients in cluster representative z_1

word	fight	win	event	champion	fighter	...
coefficient	0.038	0.022	0.019	0.015	0.015	...

- documents in cluster 1 closest to representative

  "Floyd Mayweather, Jr", "Kimbo Slice", "Ronda Rousey", "José Aldo", "Joe Frazier", ...

Cluster 2

- largest coefficients in cluster representative z_2

word	holiday	celebrate	festival	celebration	calendar	...
coefficient	0.012	0.009	0.007	0.006	0.006	...

- documents in cluster 2 closest to representative

  "Halloween", "Guy Fawkes Night", "Diwali", "Hannukah", "Groundhog Day", ...

Cluster 3

- largest coefficients in cluster representative z_3

word	united	family	party	president	government	...
coefficient	0.004	0.003	0.003	0.003	0.003	...

- documents in cluster 3 closest to representative

  "Mahatma Gandhi", "Sigmund Freund", "Carly Fiorina", "Frederick Douglass", "Marco Rubio", ...

Cluster 4

- largest coefficients in cluster representative z_4

word	album	release	song	music	single	...
coefficient	0.031	0.016	0.015	0.014	0.011	...

- documents in cluster 4 closest to representative

  "David Bowie", "Kanye West", "Celine Dion", "Kesha", "Ariana Grande", ...

Cluster 5

- largest coefficients in cluster representative z_5

word	game	season	team	win	player	...
coefficient	0.023	0.020	0.018	0.017	0.014	...

- documents in cluster 5 closest to representative

  "Kobe Bryant", "Lamar Odom", "Johan Cruyff", "Yogi Berra", "José Mourinho", ...

Cluster 6

- largest coefficients in representative z_6

word	series	season	episode	character	film	...
coefficient	0.029	0.027	0.013	0.011	0.008	...

- documents in cluster 6 closest to cluster representative

  "The X-Files", "Game of Thrones", "House of Cards", "Daredevil", "Supergirl", ...

Cluster 7

- largest coefficients in representative z_7

word	match	win	championship	team	event	...
coefficient	0.065	0.018	0.016	0.015	0.015	...

- documents in cluster 7 closest to cluster representative

  "Wrestlemania 32", "Payback (2016)", "Survivor Series (2015)", "Royal Rumble (2016)", "Night of Champions (2015)", ...

Cluster 8

- largest coefficients in representative z_8

word	film	star	role	play	series	...
coefficient	0.036	0.014	0.014	0.010	0.009	...

- documents in cluster 8 closest to cluster representative

  "Ben Affleck", "Johnny Depp", "Maureen O'Hara", "Kate Beckinsale", "Leonardo DiCaprio", ...

Cluster 9

- largest coefficients in representative z_9

word	film	million	release	star	character	...
coefficient	0.061	0.019	0.013	0.010	0.006	...

- documents in cluster 9 closest to cluster representative

  "Star Wars: The Force Awakens", "Star Wars Episode I: The Phantom Menace", "The Martian (film)", "The Revenant (2015 film)", "The Hateful Eight", ...

Outline

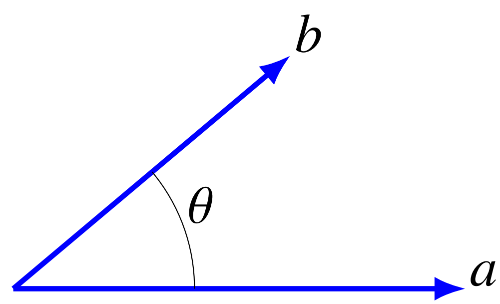
- norm
- distance
- k-means algorithm
- **angle**
- complex vectors

Angle between vectors

the angle between nonzero real vectors a, b is defined as

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

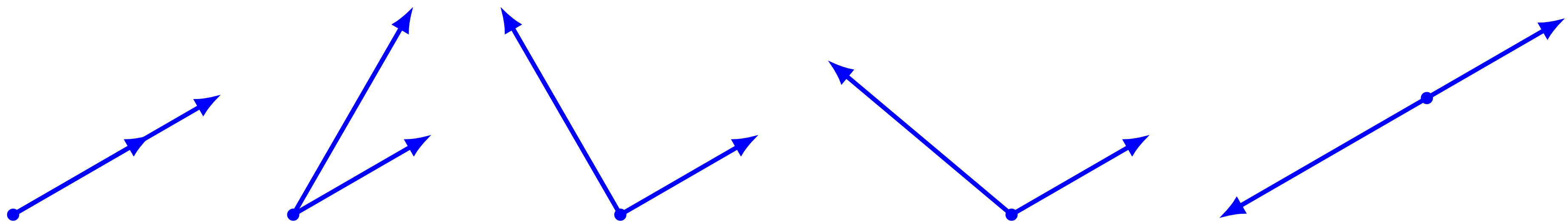
- this is the unique value of $\theta \in [0, \pi]$ that satisfies $a^T b = \|a\|\|b\|\cos\theta$



- Cauchy–Schwarz inequality guarantees that

$$-1 \leq \frac{a^T b}{\|a\|\,\|b\|} \leq 1$$

Terminology



$\theta = 0$	$a^T b = \|a\|\|b\|$	vectors are aligned or parallel
$0 \leq \theta < \pi/2$	$a^T b > 0$	vectors make an acute angle
$\theta = \pi/2$	$a^T b = 0$	vectors are orthogonal ($a \perp b$)
$\pi/2 < \theta \leq \pi$	$a^T b < 0$	vectors make an obtuse angle
$\theta = \pi$	$a^T b = -\|a\|\|b\|$	vectors are anti-aligned or opposed

Correlation coefficient

the *correlation coefficient* between non-constant vectors a, b is

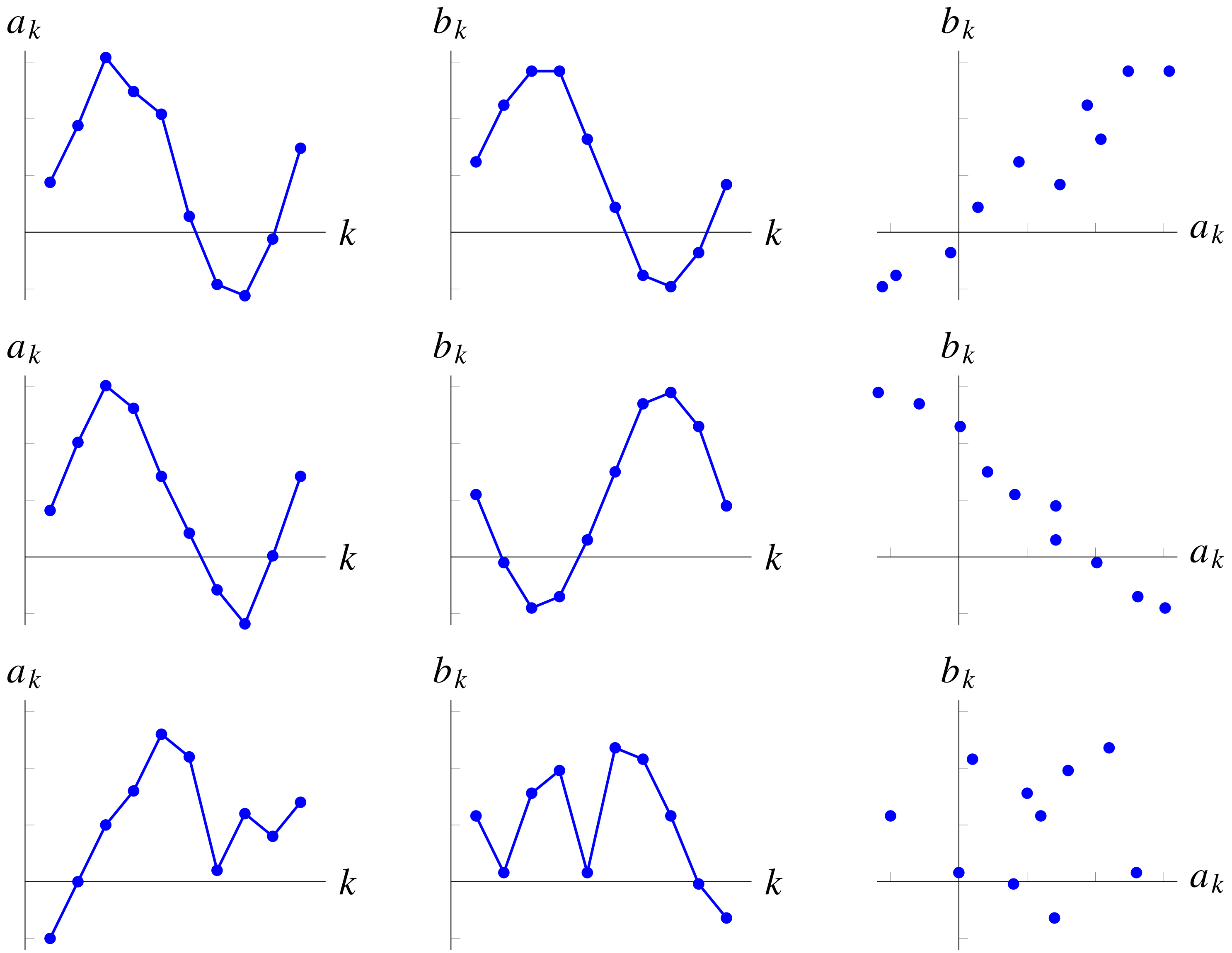
$$\rho_{ab} = \frac{\tilde{a}^T \tilde{b}}{\|\tilde{a}\| \, \|\tilde{b}\|}$$

where $\tilde{a} = a - \mathbf{avg}(a)\mathbf{1}$ and $\tilde{b} = b - \mathbf{avg}(b)\mathbf{1}$ are the de-meaned vectors

- only defined when a and b are not constant ($\tilde{a} \neq 0$ and $\tilde{b} \neq 0$)
- ρ_{ab} is the cosine of the angle between the de-meaned vectors
- a number between -1 and 1
- ρ_{ab} is the average product of the deviations from the mean in standard units

$$\rho_{ab} = \frac{1}{n} \sum_{i=1}^{n} \frac{(a_i - \mathbf{avg}(a))}{\mathbf{std}(a)} \frac{(b_i - \mathbf{avg}(b))}{\mathbf{std}(b)}$$

Examples



$\rho_{ab} = 0.968$

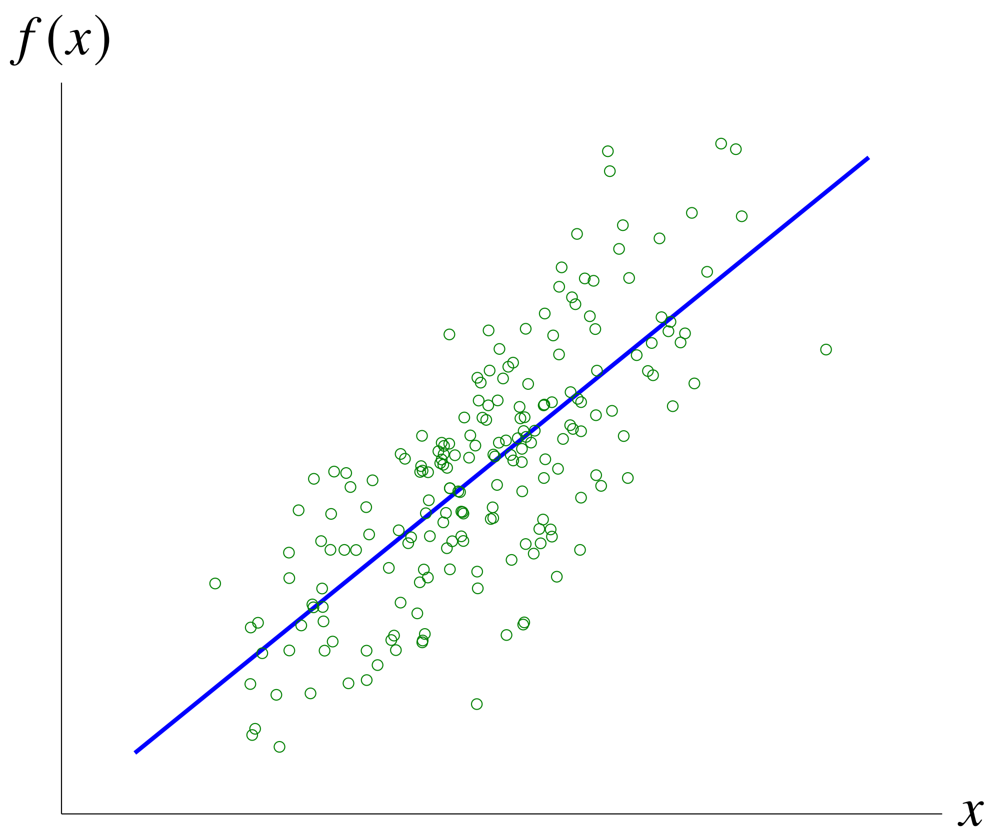
$\rho_{ab} = -0.988$

$\rho_{ab} = 0.004$

Regression line

- scatter plot shows two n-vectors a, b as n points (a_k, b_k)
- straight line shows affine function $f(x) = c_1 + c_2 x$ with

$$f(a_k) \approx b_k, \quad k = 1, \ldots, n$$



Least squares regression

use coefficients c_1, c_2 that minimize $J = \dfrac{1}{n}\sum_{k=1}^{n}(f(a_k) - b_k)^2$

- J is a quadratic function of c_1 and c_2:

$$
\begin{aligned}
J &= \frac{1}{n}\sum_{k=1}^{n}(c_1 + c_2 a_k - b_k)^2 \\
&= \left(nc_1^2 + 2n\,\mathbf{avg}(a)c_1c_2 + \|a\|^2c_2^2 - 2n\,\mathbf{avg}(b)c_1 - 2a^Tbc_2 + \|b\|^2\right)/n
\end{aligned}
$$

- to minimize J, set derivatives with respect to c_1, c_2 to zero:

$$
c_1 + \mathbf{avg}(a)c_2 = \mathbf{avg}(b), \qquad n\,\mathbf{avg}(a)c_1 + \|a\|^2c_2 = a^Tb
$$

- solution is

$$
c_2 = \frac{a^Tb - n\,\mathbf{avg}(a)\,\mathbf{avg}(b)}{\|a\|^2 - n\,\mathbf{avg}(a)^2}, \qquad c_1 = \mathbf{avg}(b) - \mathbf{avg}(a)c_2
$$

Interpretation

slope c_2 can be written in terms of correlation coefficient of a and b:

$$c_2 = \frac{(a - \mathbf{avg}(a)\mathbf{1})^T(b - \mathbf{avg}(b)\mathbf{1})}{\|a - \mathbf{avg}(a)\mathbf{1}\|^2} = \rho_{ab}\,\frac{\mathbf{std}(b)}{\mathbf{std}(a)}$$

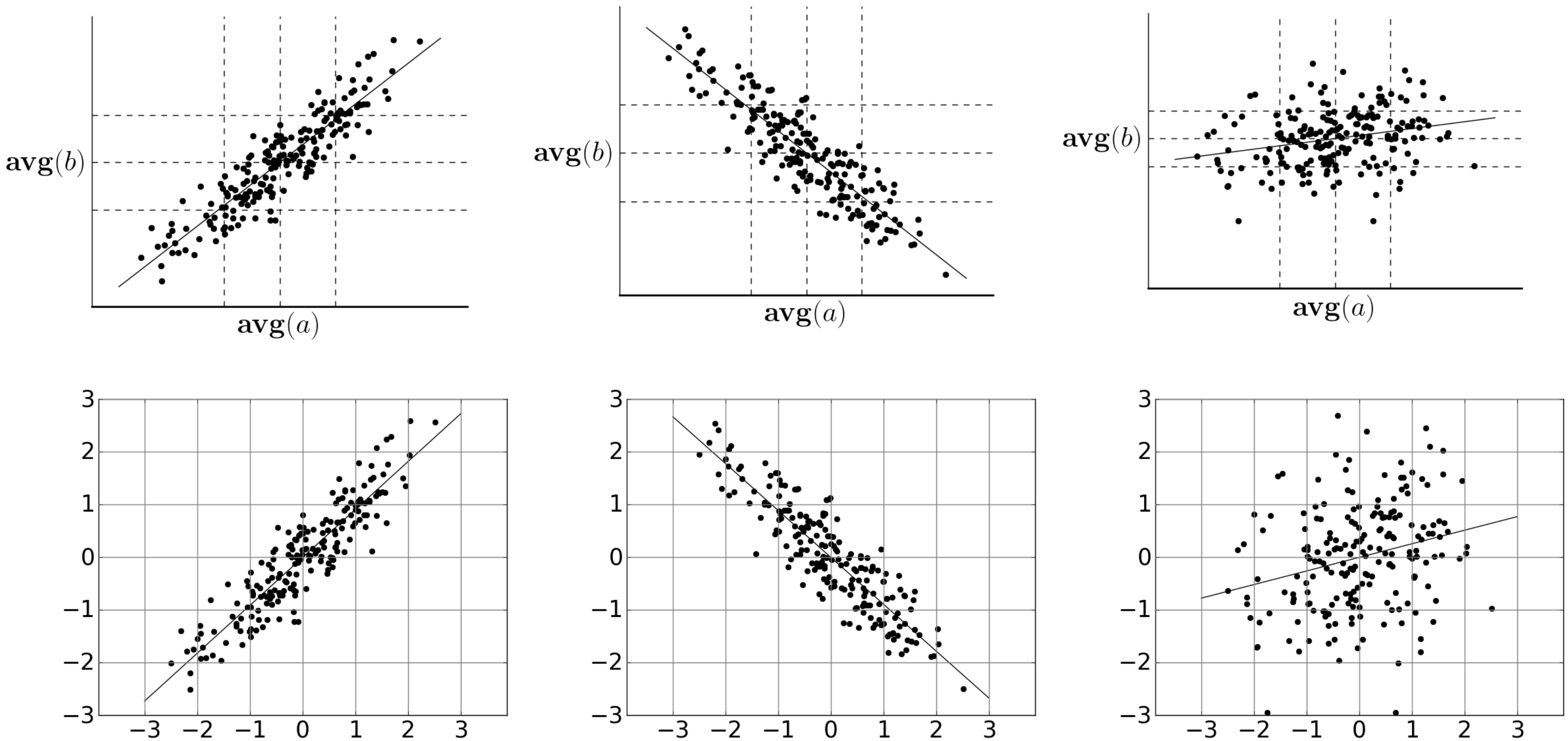
- hence, expression for regression line can be written as

$$f(x) = \mathbf{avg}(b) + \frac{\rho_{ab}\,\mathbf{std}(b)}{\mathbf{std}(a)}(x - \mathbf{avg}(a))$$

- correlation coefficient ρ_{ab} is the slope after converting to standard units:

$$\frac{f(x) - \mathbf{avg}(b)}{\mathbf{std}(b)} = \rho_{ab}\,\frac{x - \mathbf{avg}(a)}{\mathbf{std}(a)}$$

Examples



$\rho_{ab} = 0.91$ $\rho_{ab} = -0.89$ $\rho_{ab} = 0.25$

- dashed lines in top row show average ± standard deviation
- bottom row shows scatter plots of top row in standard units

Outline

- norm
- distance
- k-means algorithm
- angle
- **complex vectors**

Norm

norm of vector $a \in \mathbf{C}^n$:

$$\begin{aligned} \|a\| &= \sqrt{|a_1|^2 + |a_2|^2 + \cdots + |a_n|^2} \\ &= \sqrt{a^H a} \end{aligned}$$

- positive definite:

$$\|a\| \geq 0 \quad \text{for all } a, \qquad \|a\| = 0 \quad \text{only if } a = 0$$

- homogeneous:

$$\|\beta a\| = |\beta| \|a\| \quad \text{for all vectors } a, \text{ complex scalars } \beta$$

- triangle inequality:

$$\|a + b\| \leq \|a\| + \|b\| \quad \text{for all vectors } a, b \text{ of equal size}$$

Cauchy–Schwarz inequality for complex vectors

$$|a^H b| \leq \|a\| \|b\| \quad \text{for all } a, b \in \mathbf{C}^n$$

moreover, equality $|a^H b| = \|a\| \|b\|$ holds if:

- $a = 0$ or $b = 0$
- $a \neq 0$ and $b \neq 0$, and $b = \gamma a$ for some (complex) scalar γ

- exercise: generalize proof for real vectors on page 2.4
- we say a and b are *orthogonal* if $a^H b = 0$
- we will not need definition of angle, correlation coefficient, ... in $\mathbf{C}^n$