Week 7: Clustering and Dimensionality Reduction

Matthew Caldwell

COMP0088 Introduction to Machine Learning • UCL Computer Science • Autumn 2024

Admin

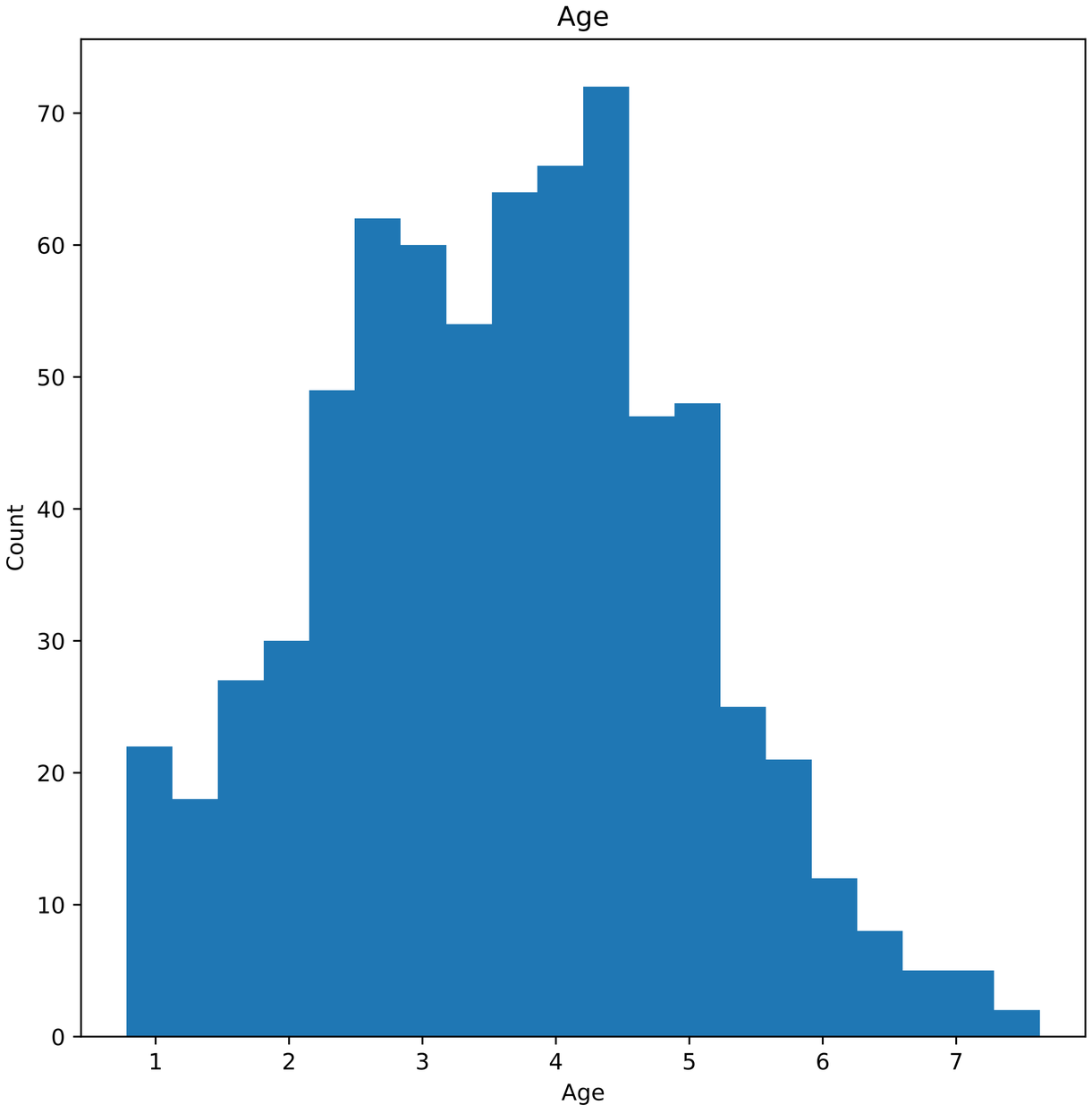
- Pulse surveys feedback

Week 7 Recap

Groundhog Day

groundhogs

	Age	Weight	Height	Length	Tail	Whiskers	Incisors	E
0	2.2	3.8	14.3	14.7	5.5	4.5	1.4	
1	4.9	2.6	11.8	13.3	8.3	0.9	2.2	
2	2.6	5.2	12.6	15.9	9.9	1.9	3.6	
3	7.5	4.3	7.0	15.2	9.3	0.5	1.8	
4	2.2	3.1	11.4	15.0	12.0	1.8	2.6	
5	5.2	6.1	13.2	15.7	5.6	3.3	3.3	
6	3.5	3.1	7.7	20.2	7.4	0.7	2.9	
7	3.7	1.7	2.8	15.3	12.7	3.2	3.8	
8	2.5	2.4	9.6	14.1	7.2	1.5	2.0	
9	4.4	6.6	5.4	20.9	8.8	2.6	4.0	
10	3.3	5.7	9.1	18.2	3.6	1.7	3.6	
11	4.3	4.7	9.4	19.6	7.1	3.5	-0.4	
12	7.3	5.8	12.3	12.9	10.1	3.8	2.4	
	[illegible]	4.7	6.5	16.4	[illegible]	[illegible]	4.6	


Age
Count
Age
0
10
20
30
40
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70
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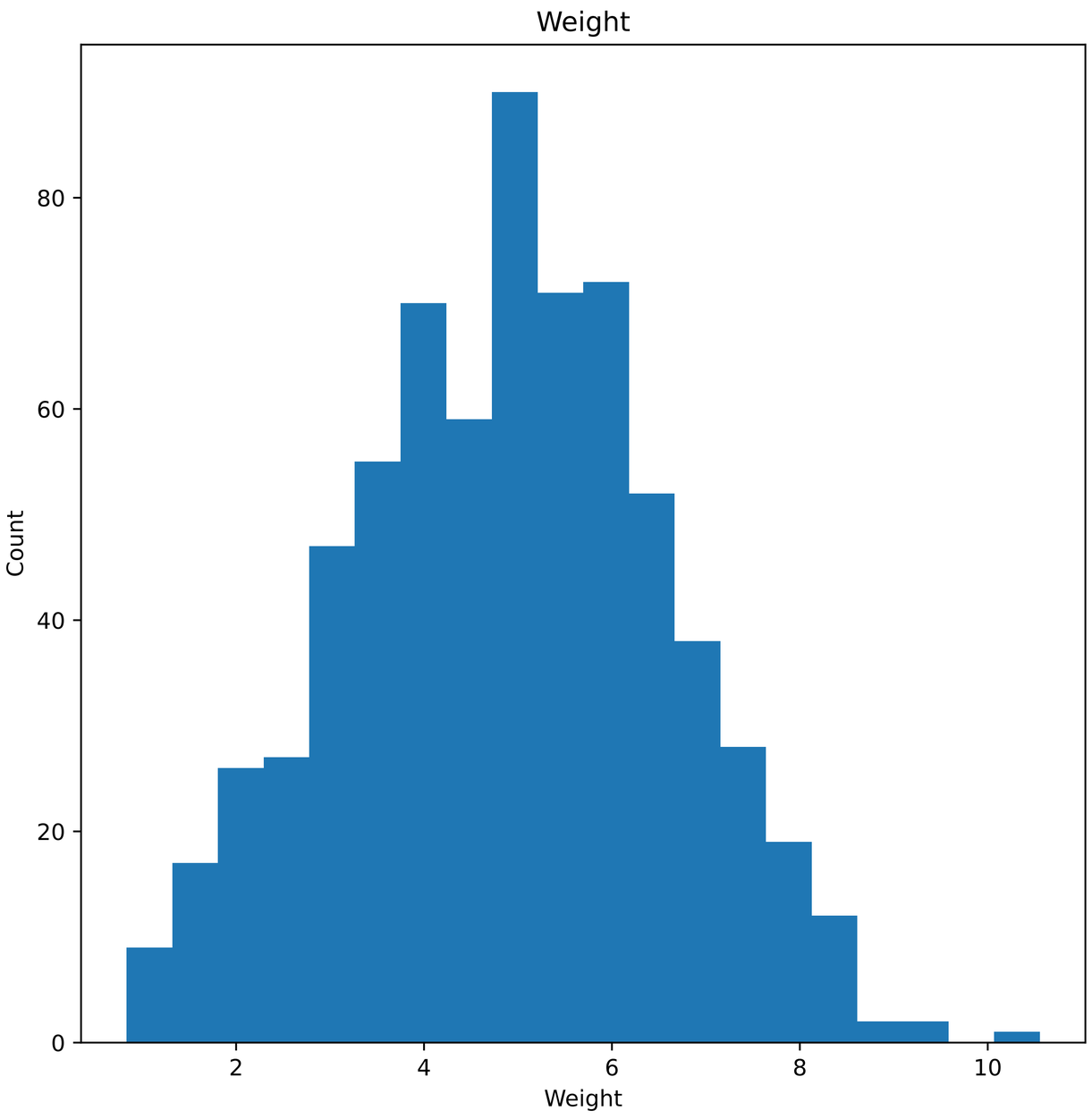
7


Weight
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0
20
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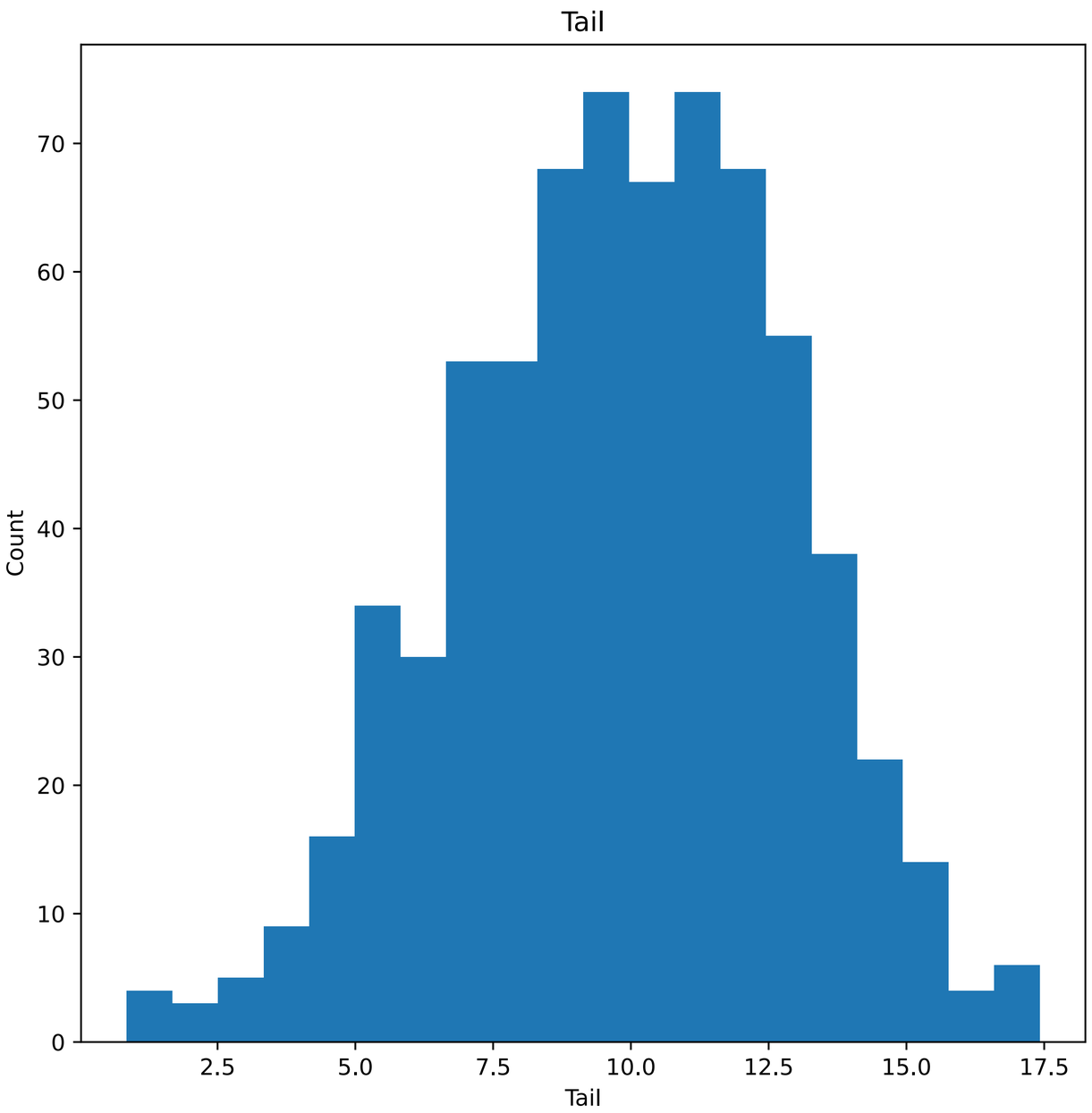
Weight


Tail
Count
0
10
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2.5
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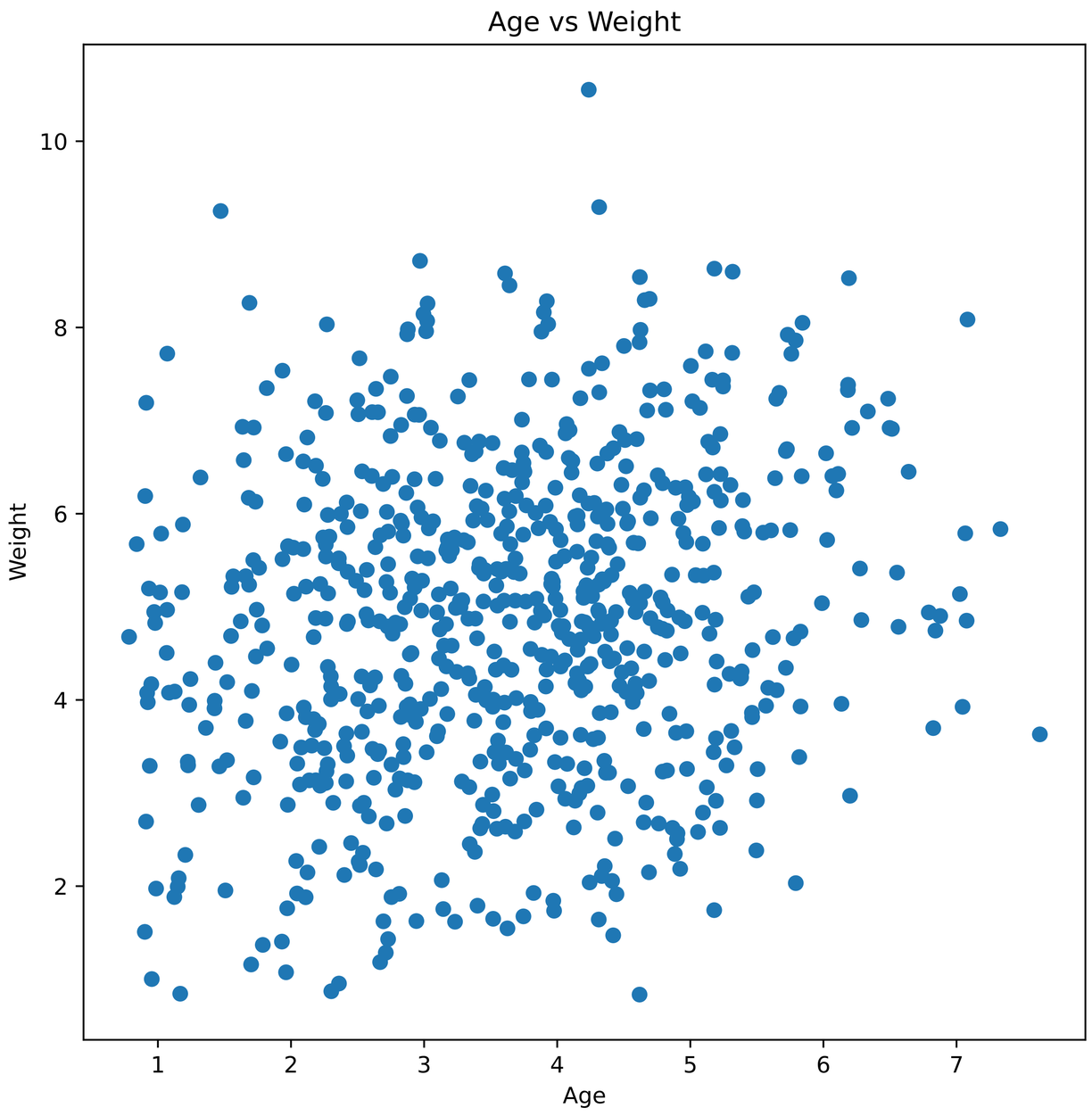
17.5
Tail


Age vs Weight
Weight
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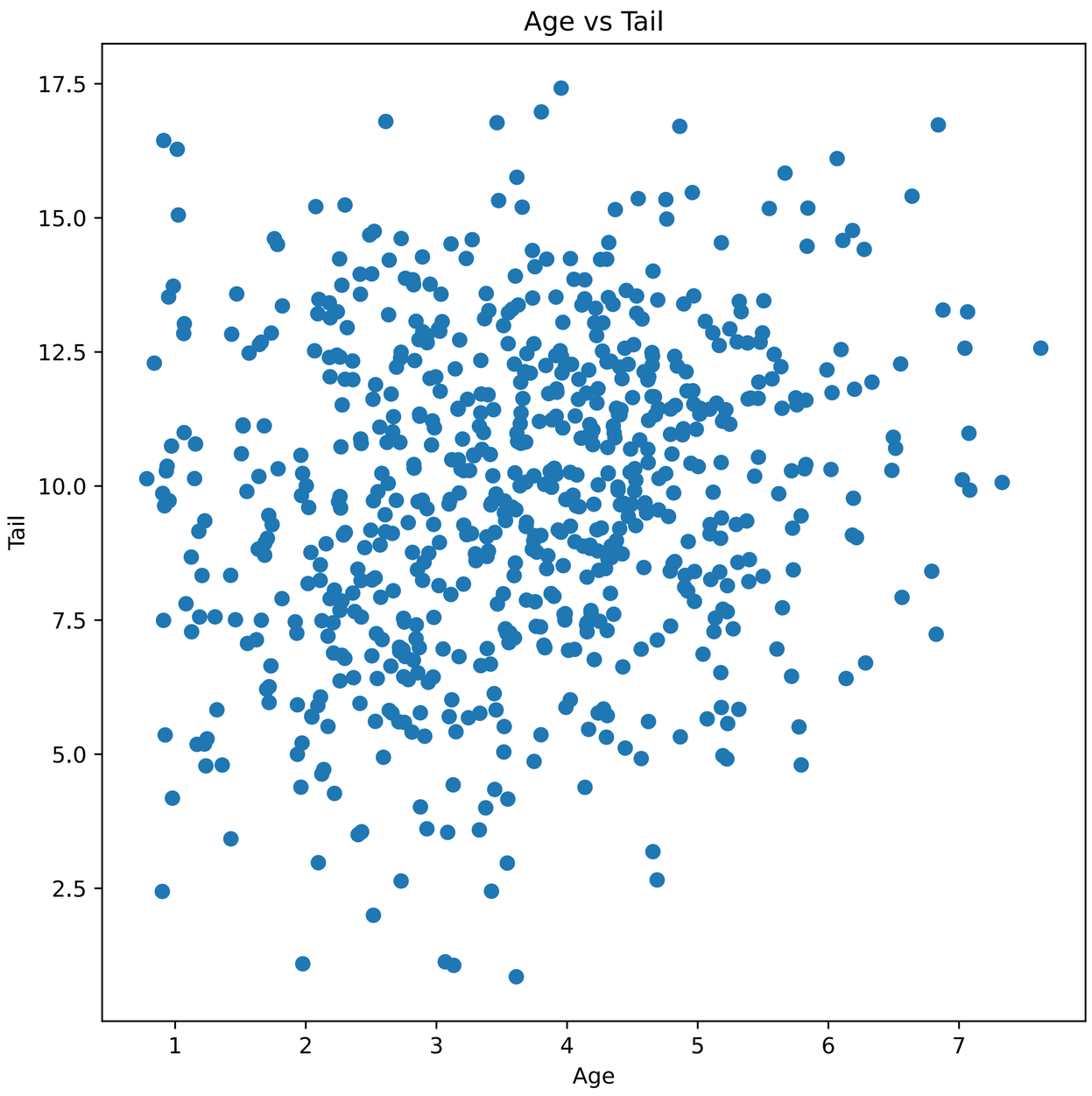
Age vs Tail
17.5
15.0
12.5
10.0
7.5
5.0
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Tail
1
2
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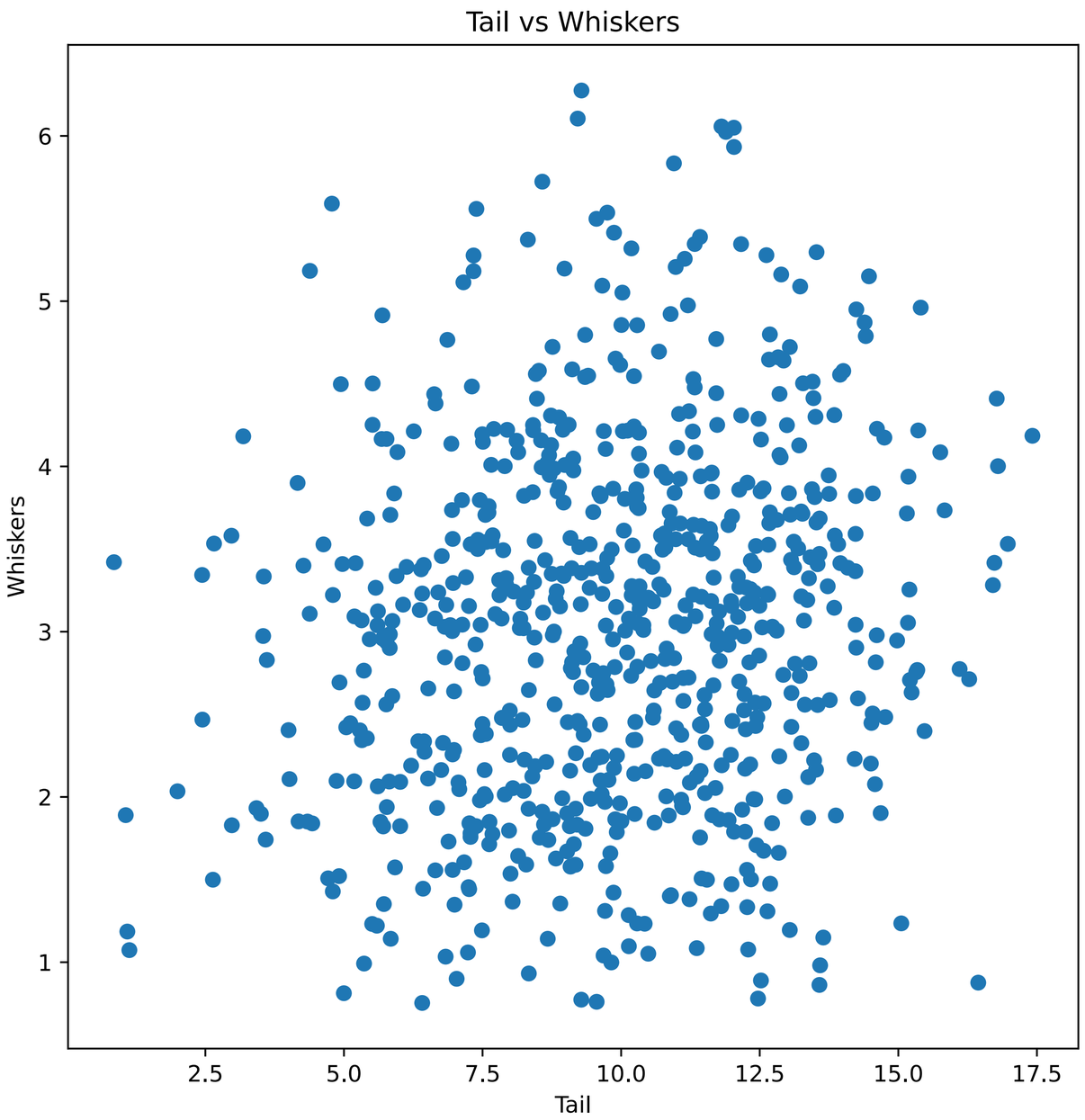
5
6
7
Age


Tail vs Whiskers
Whiskers
Tail
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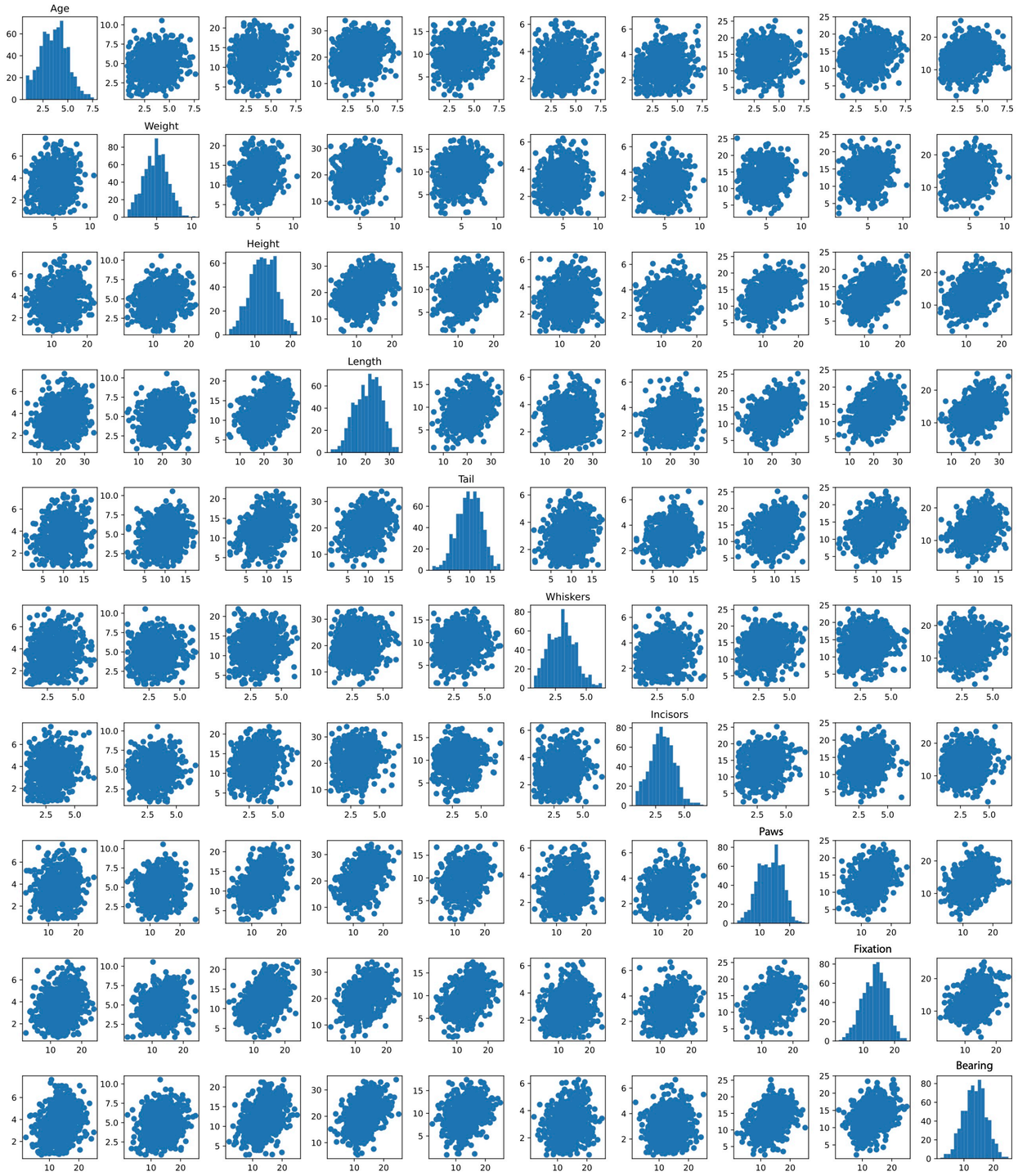
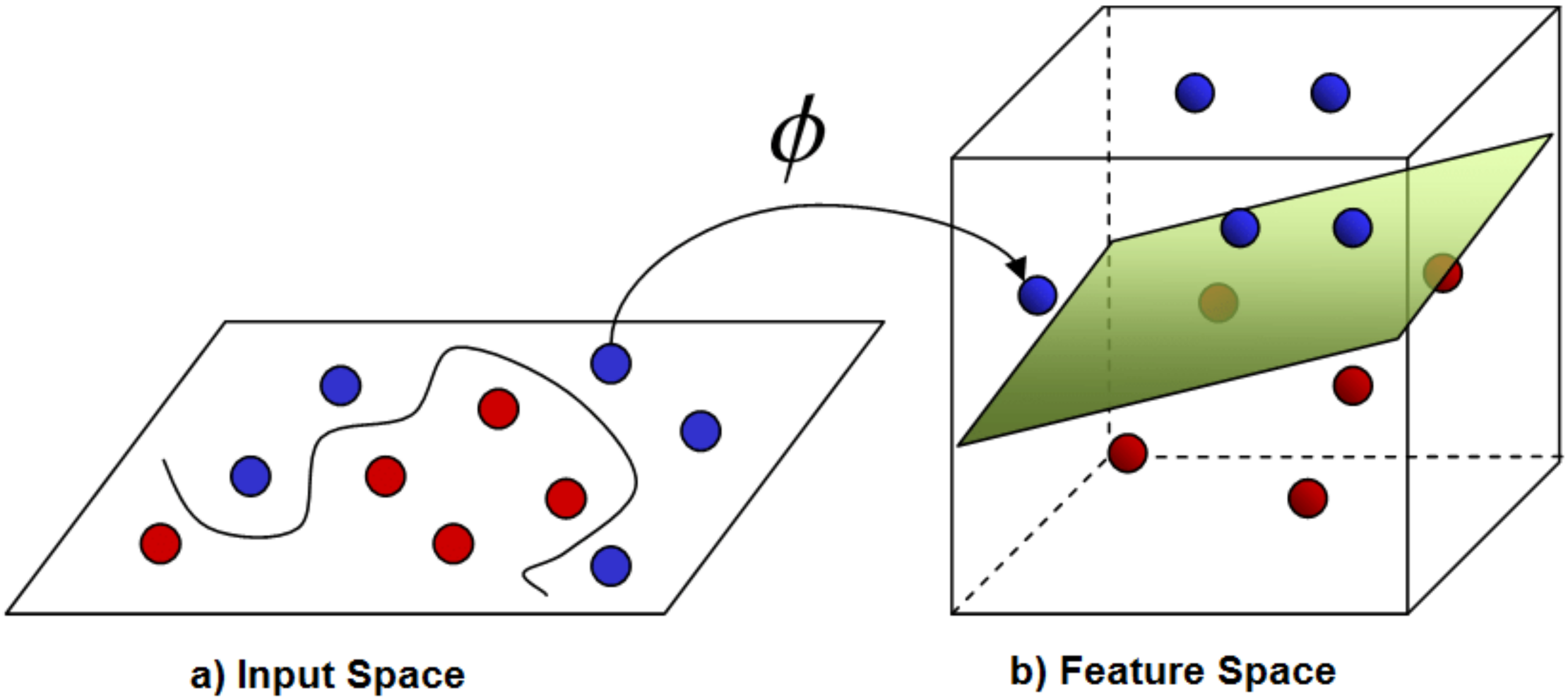
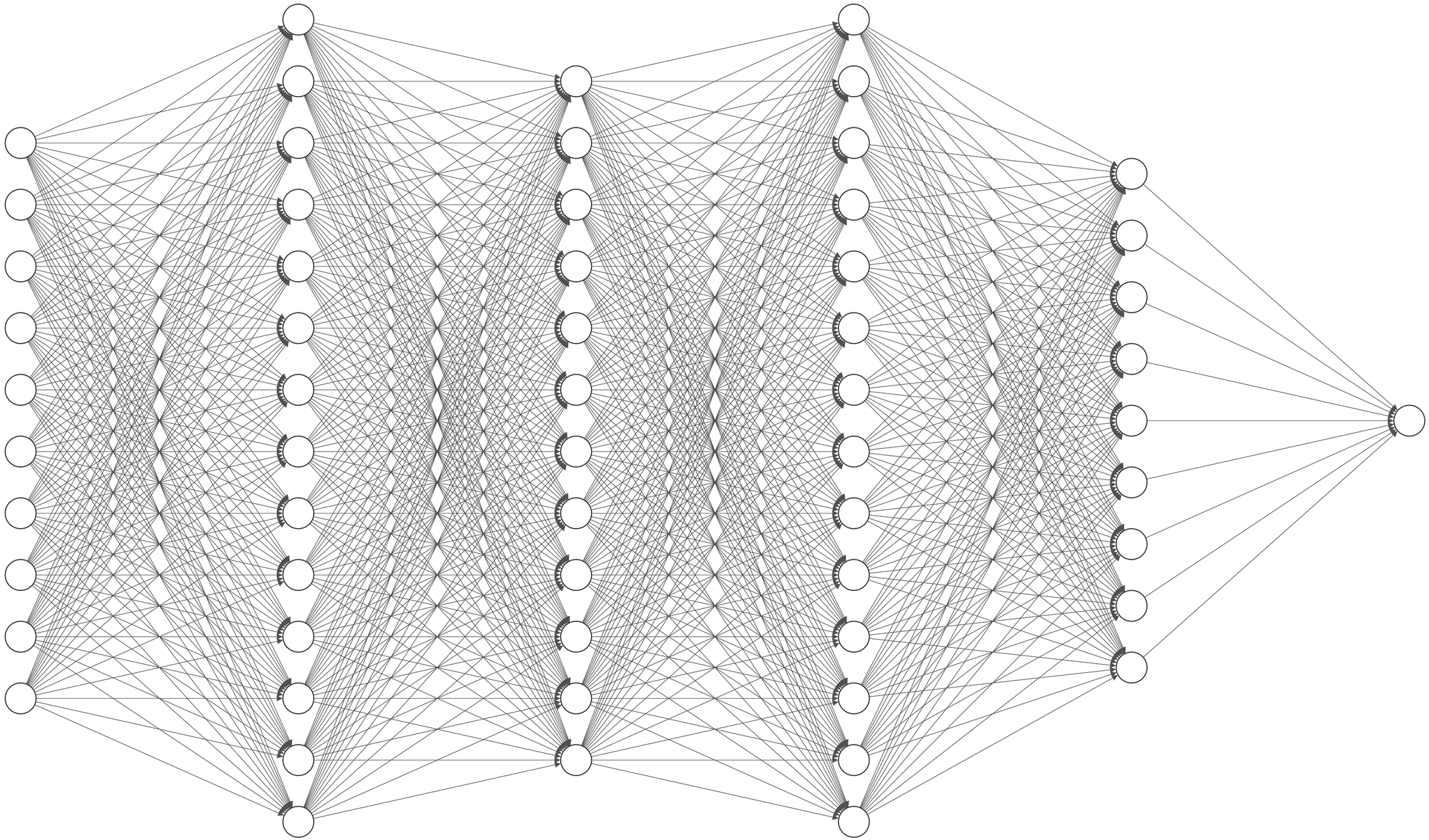
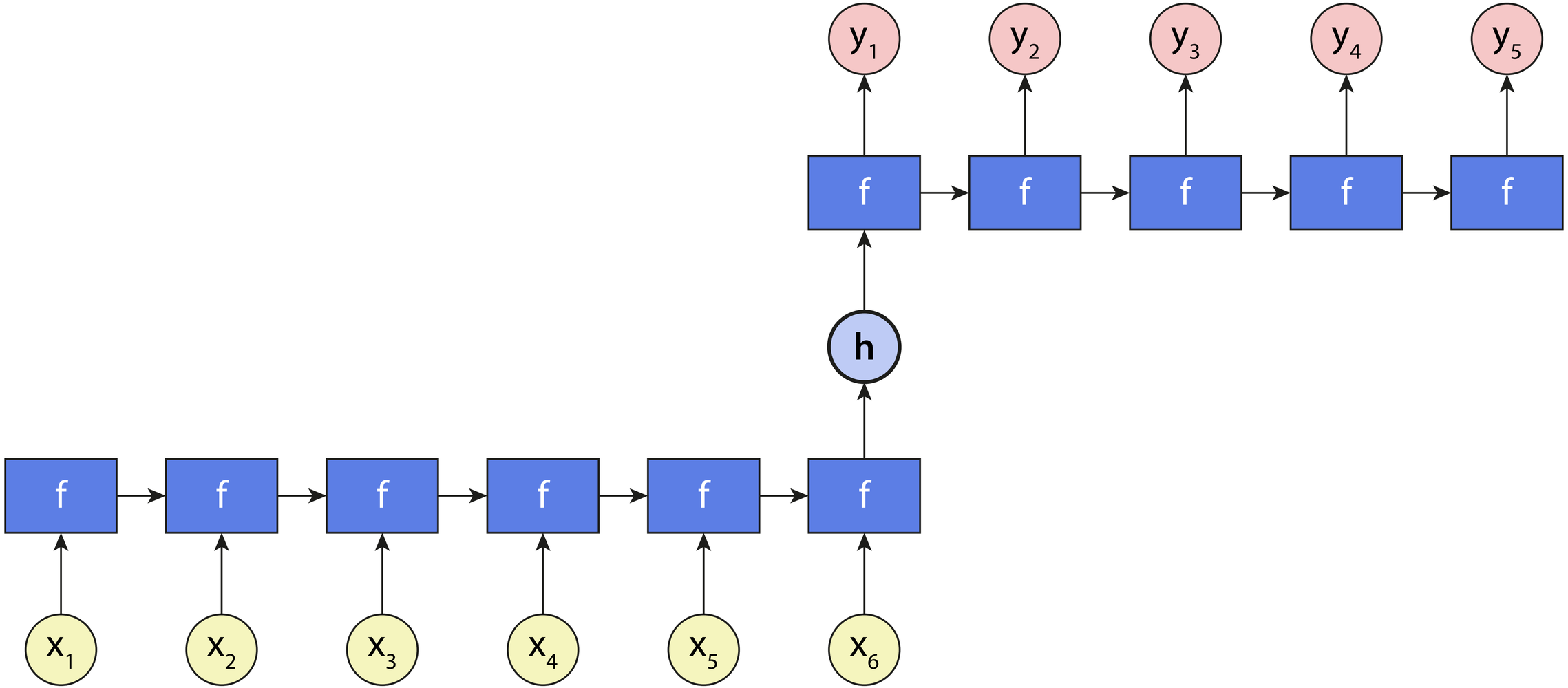

Age
Weight
Height
Length
Tail
Whiskers
Incisors
Paws
Fixation
Bearing

Mayer

embeddings


ϕ
a) Input Space
b) Feature Space




y1
y2
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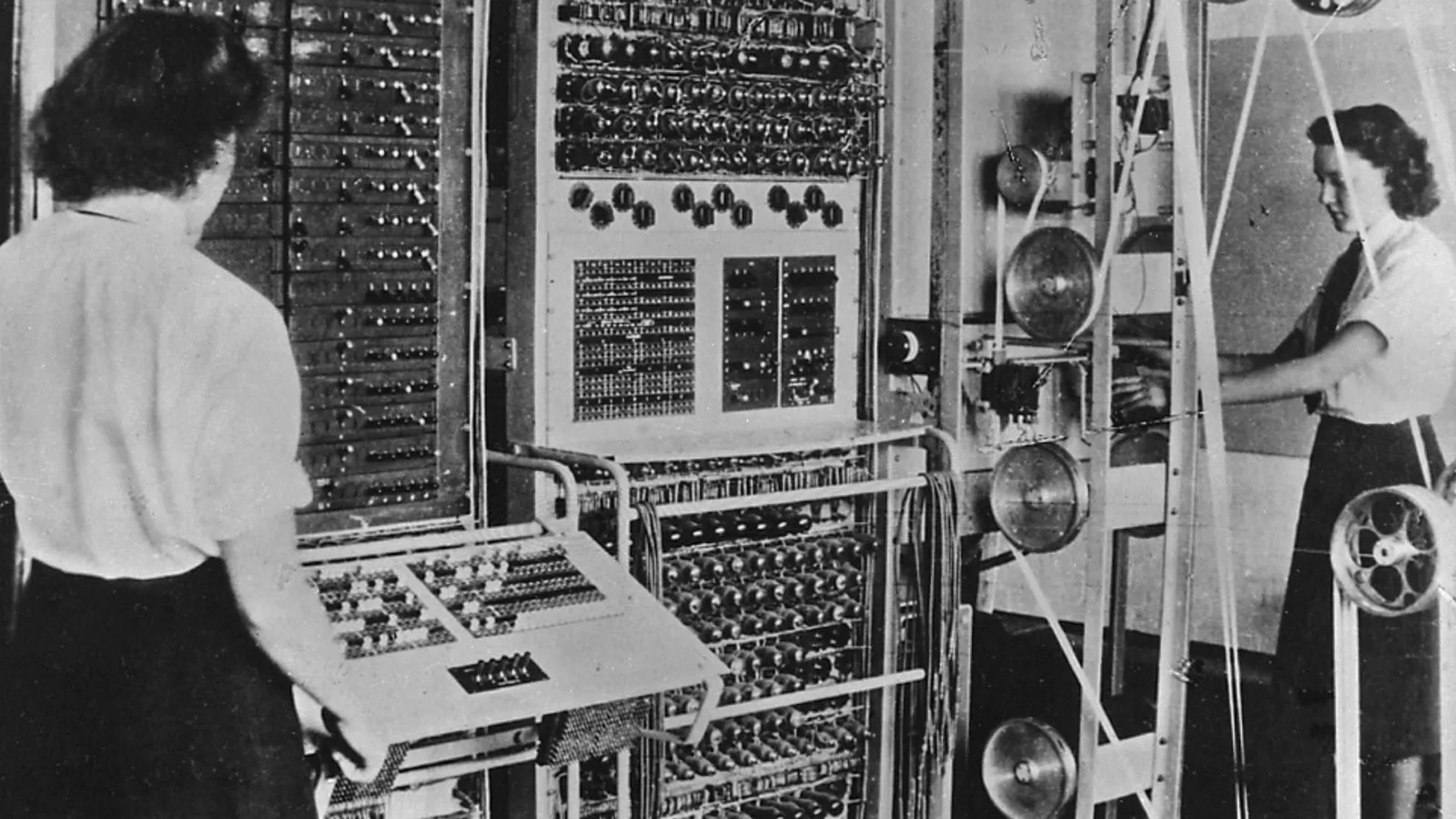
x6



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effect
effort
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election
else
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end
energy
enjoy
enough
husband
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very
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view
violence
visit
voice
vote
wait
walk
wall
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water
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weight

$\mathbf{x}^T$

(one-hot)

$$\mathbf{x}^\mathsf{T} \longrightarrow \tilde{\mathbf{x}}^\mathsf{T}$$

(one-hot) (embedding)

$\mathbf{x}^\top$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^\top$

(embedding)

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

	e_1	e_2	e_3
vampire	0.99	0.64	0.15
groundhogs	0.45	0.03	0.88
cast	0.02	0.46	0.6
no	0.73	0.89	0.9
shadow	0.83	0.75	0.44

$\tilde{\mathbf{x}}^T$

(embedding)

$\mathbf{x}^T$

(one-hot)

[0, 1, 0, 0, 0]

$\mathbf{W}$

	e_1	e_2	e_3
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$\tilde{\mathbf{x}}^T$

(embedding)

$\mathbf{x}^T$

(one-hot)

$[\ 0, 1, 0, 0, 0\ ] \quad \times$

$\mathbf{W}$

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$\tilde{\mathbf{x}}^T$

(embedding)

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^T$

(embedding)

$[\ 0, 1, 0, 0, 0\ ] \times$

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$= [\qquad\qquad\qquad

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^T$

(embedding)

$[\ 0, 1, 0, 0, 0\ ] \times$

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$= [\qquad\qquad\qquad

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^T$

(embedding)

$[\,0, 1, 0, 0, 0\,] \times$

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$= [\,0.45 \qquad\qquad\qquad\

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^T$

(embedding)

$[\,0, 1, 0, 0, 0\,] \times$

	e_1	e_2	e_3
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$= [\,0.45 \qquad\qquad\qquad\

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^T$

(embedding)

$[\,0, 1, 0, 0, 0\,] \times$

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$= [\,0.45, 0.03\,]$

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^T$

(embedding)

$[\,0, 1, 0, 0, 0\,] \times$

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no	0.73	0.89	0.9
shadow	0.83	0.75	0.44

$= [\,0.45, 0.03 \quad\quad\quad\

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^T$

(embedding)

$[\ 0, 1, 0, 0, 0\ ] \times$

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shadow	0.83	0.75	0.44

$= [\ 0.45, 0.03, 0.88\ ]$

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^T$

(embedding)

$[\ 0, 1, 0, 0, 0\ ] \times$

	e_1	e_2	e_3
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$= [\ 0.45, 0.03, 0.88\ ]$

$\mathbf{x}^T$

(one-hot)

$\mathbf{W}$

$\tilde{\mathbf{x}}^T$

(embedding)

$[\ 0, 1, 0, 0, 0\ ] \times$

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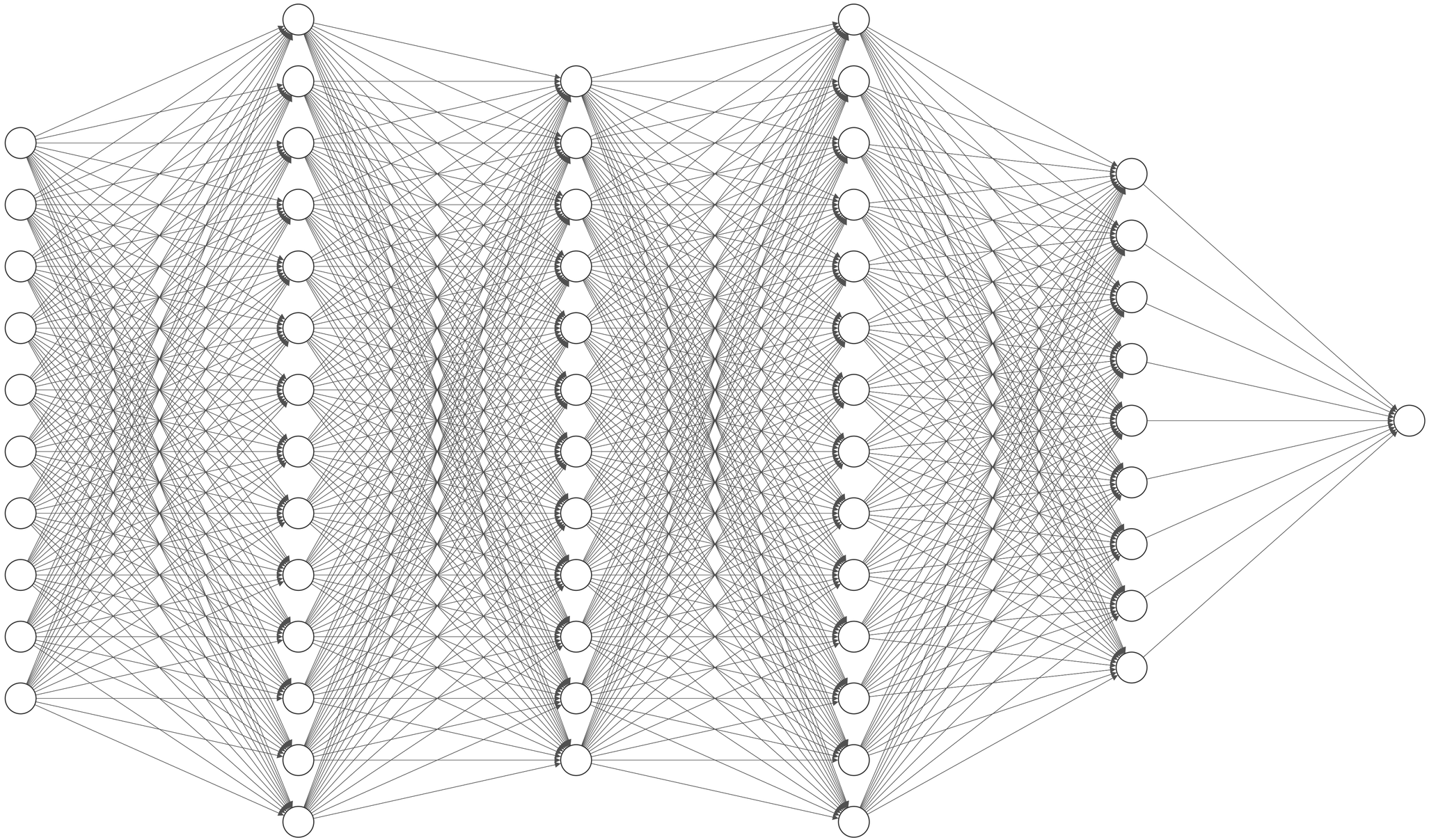
$= [\ 0.45, 0.03, 0.88\ ]$



In the population of Transylvania there are four distinct nationalities: Saxons in the South, and mixed with them the Wallachs, who are the descendants of the Dacians; Magyars in the West, and Szekelys in the East and North. I am going among the latter, who claim to be descended from Attila and the Huns. This may be so, for when the Magyars conquered the country in the eleventh century they found the Huns settled in it. I read that every known superstition in the world is gathered into the horseshoe of the Carpathians, as if it were the centre of some sort of imaginative whirlpool; if so my stay may be very interesting. (*Mem.*, I must ask the Count all about them.)

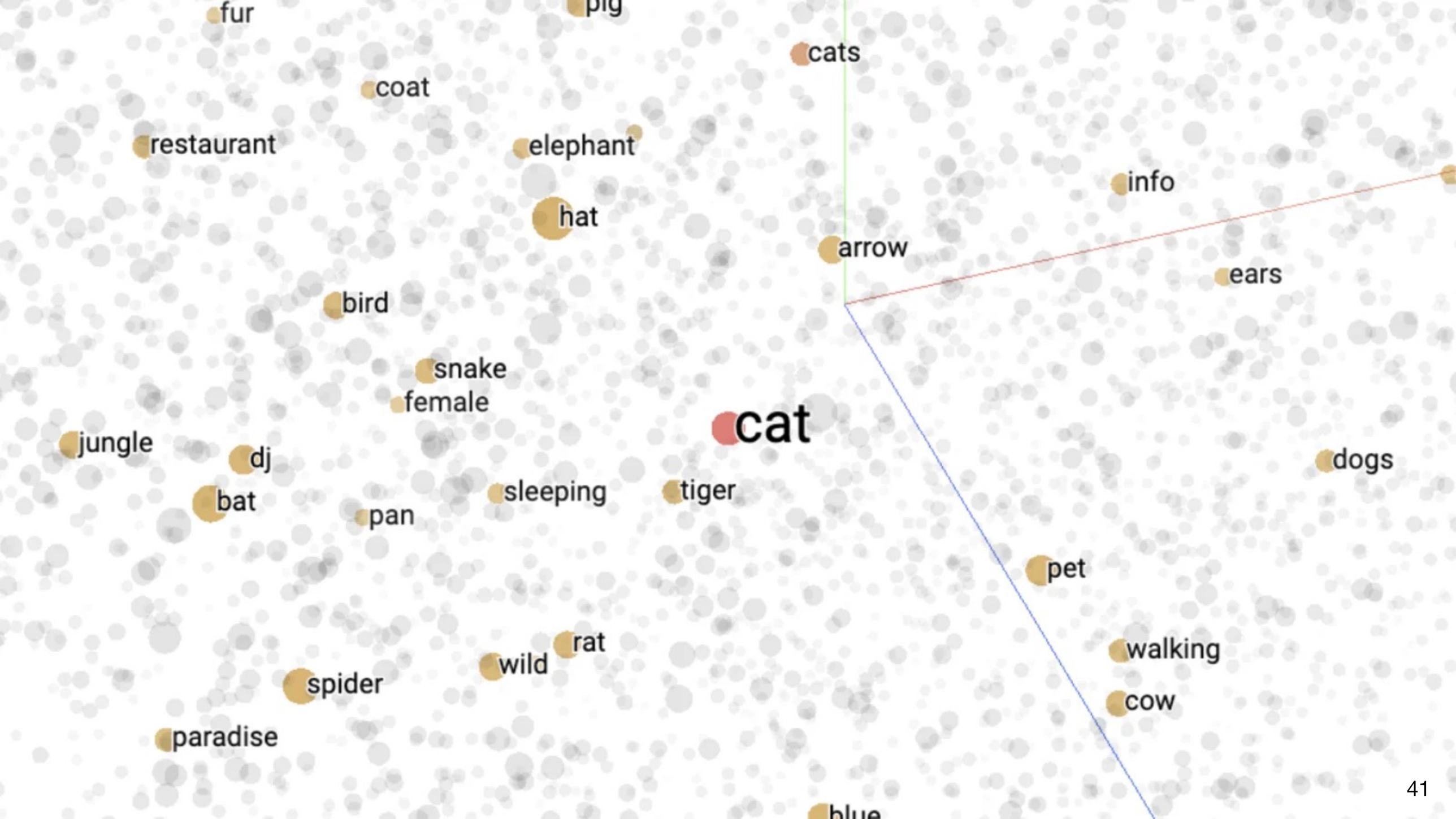
I did not sleep well, though my bed was comfortable enough, for I had all sorts of queer dreams. There was a dog howling all night under my window, which may have had something to do with it; or it may have been the paprika, for I had to drink up all the water in my carafe, and was still thirsty. Towards morning I slept and was wakened by the continuous knocking at my door, so I guess I must have been sleeping soundly then. I had for breakfast more paprika, and a sort of porridge of maize flour which they said was "mamaliga," and egg-plant stuffed with forcemeat, a very excellent dish, which they call "impletata." (*Mem.*, get recipe for this also.) I had to hurry breakfast, for the train started a little before eight, or rather it ought to have done so, for after rushing to the station at 7:30 I had to sit in the carriage for more than an hour before we began to move. It seems to me that the further east you go the more unpunctual are the trains. What ought they to be in China?

All day long we seemed to dawdle through a country which was full of beauty of every kind. Sometimes we saw little towns or castles on the top of steep hills such as we see in old missals; sometimes we ran by rivers and streams which seemed from the wide stony margin on each side of them to be subject to great floods. It takes a lot of water, and running strong, to sweep the outside edge of a river clear. At every station there were groups of people, sometimes crowds, and in all sorts of attire. Some of them were just like the peasants at home or those I saw coming through France and Germany, with short jackets and round hats and home-made trousers; but others were very picturesque. The women looked pretty, except when you got near them, but they were very clumsy about the waist. They had all full white sleeves of some kind or other, and most of them had big belts with a lot of strips of something fluttering from them like the dresses in a ballet, but of course there were petticoats under them. The strangest figures we saw were the Slovaks, who were more barbarian than the rest, with their big cow-boy hats, great baggy dirty-white trousers, white linen shirts, and enormous heavy leather belts, nearly a foot wide, all studded over with brass nails. They wore high boots, with their trousers tucked into them, and had long black hair and heavy black moustaches. They are very picturesque, but do not look prepossessing. On the stage they would be set down at once as some old Oriental band of brigands. They are, however, I am told, very harmless and rather wanting in natural self-assertion.

It was on the dark side of twilight when we got to Bistritz, which is a very interesting old place. Being practically on the frontier—for the Borgo Pass leads from it into Bukovina—it has had a very stormy existence, and it certainly shows marks of it. Fifty years ago a series of great fires took place, which made terrible havoc on five separate occasions. At the very beginning of the seventeenth century it underwent a siege of three weeks and lost 13,000 people, the casualties of war proper being assisted by famine and disease.

Count Dracula had directed me to go to the Golden Krone Hotel, which I found, to my great delight, to be thoroughly old-fashioned, for of course I wanted to see all I could of the ways of the country. I was evidently expected, for when I got near the door I faced a cheery-looking elderly woman in the usual peasant dress—white undergarment with long double apron, front, and back, of coloured stuff fitting almost too tight for modesty. When I came close she bowed and said, "The Herr Englishman?" "Yes," I said, "Jonathan Harker." She smiled, and gave some message to an elderly man in white shirt-sleeves, who had followed her to the door. He went, but immediately returned with a letter:—

"My Friend.—Welcome to the Carpathians. I am anxiously expecting you. Sleep well to-night. At three to-morrow the diligence will start for Bukovina; a place on it is kept for you. At the Borgo Pass my carriage will await you and will bring you to me. I trust that your journey from London has been a happy one, and that you will enjoy your stay in my beautiful land.


fur
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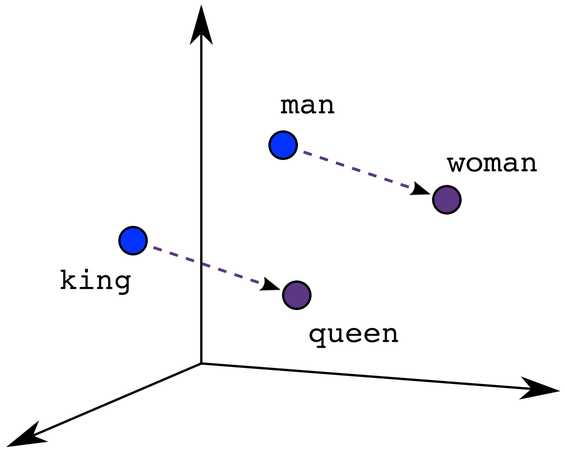
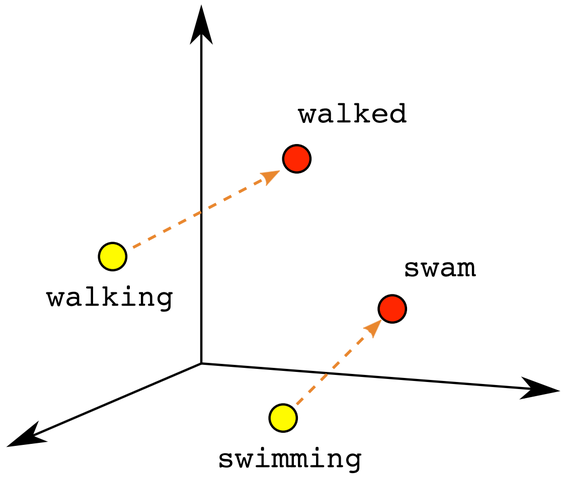
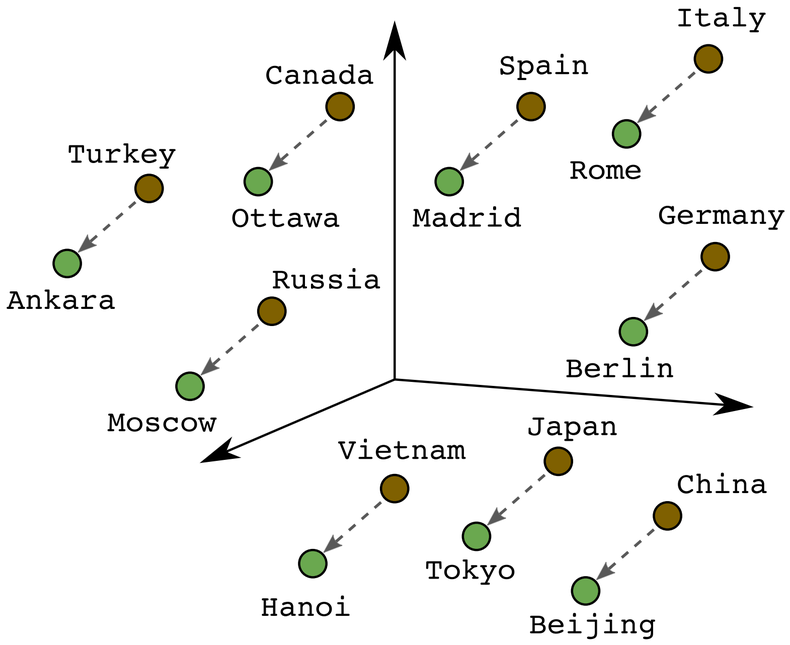


Male-Female



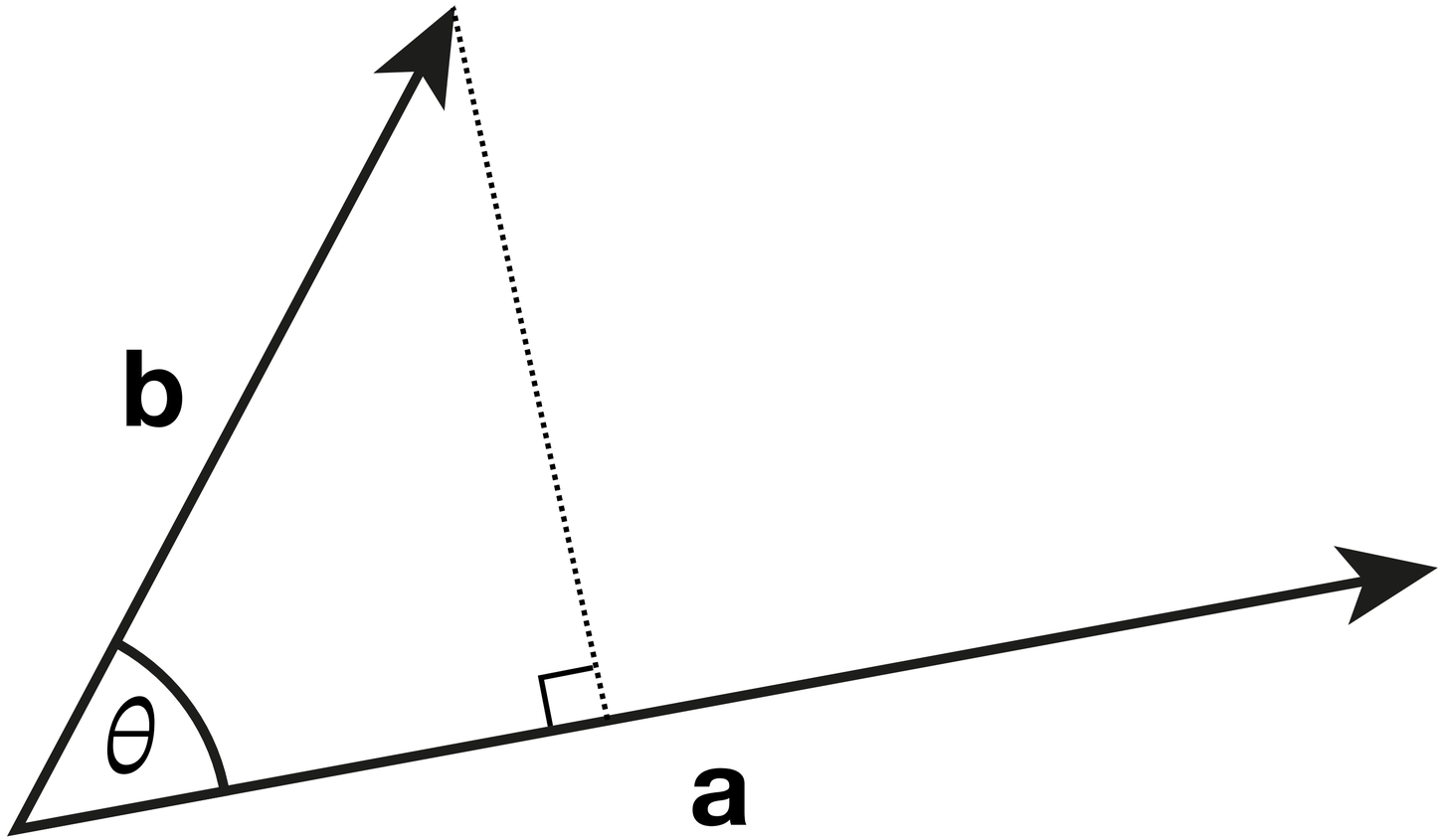
Verb Tense

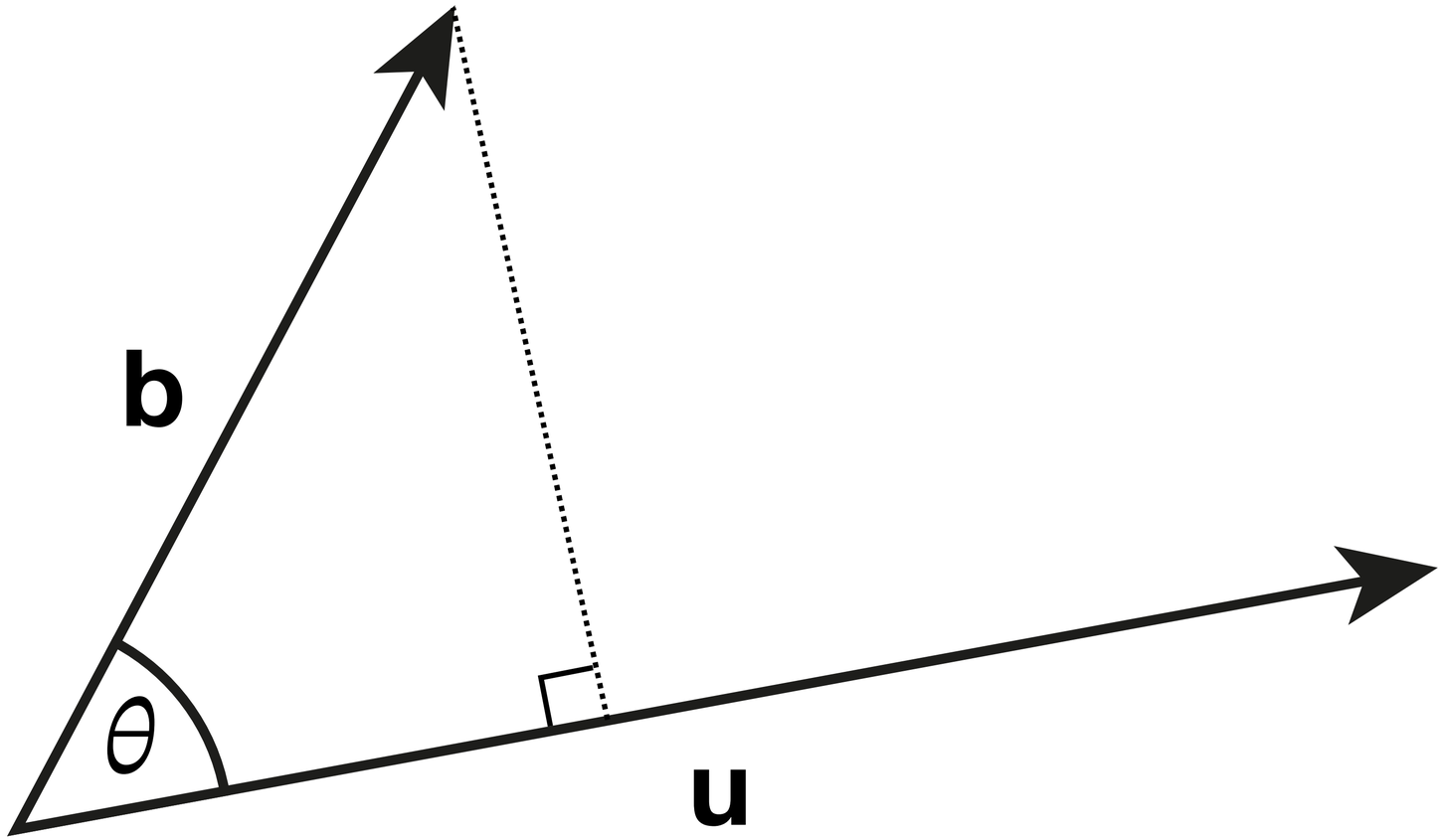


Country-Capital

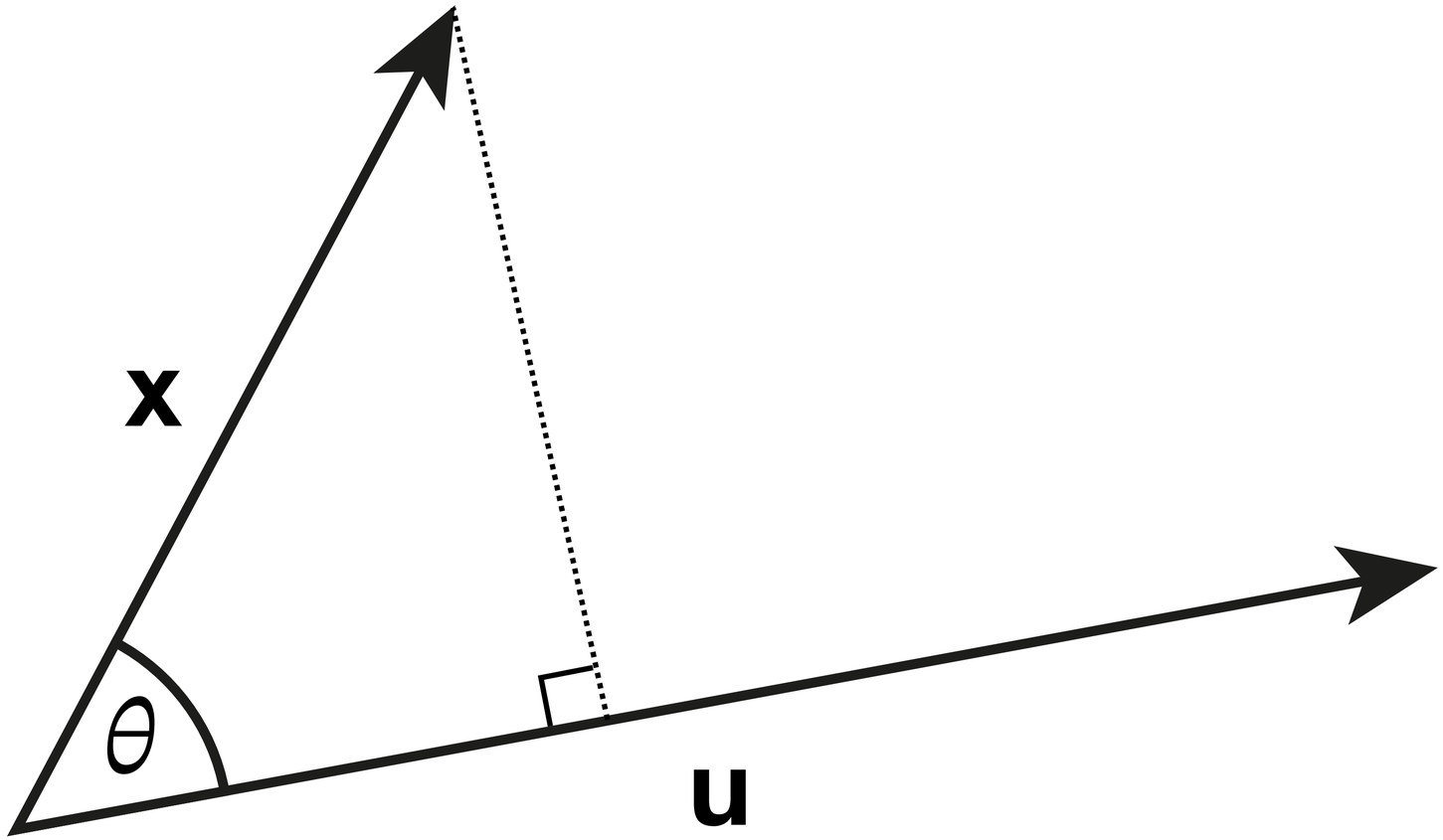
PCA

$$\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}||\mathbf{b}| \cos \theta$$


b
θ
a



$$|\mathbf{u}| = 1$$



$$|\mathbf{u}| = 1$$

$$\mathbf{x} \cdot \mathbf{u} = |\mathbf{x}| \cos \theta$$

$$\mathbf{x} \cdot \mathbf{u}_1 = |\mathbf{x}| \cos \theta_1 = \tilde{x}_1$$

$$\mathbf{x} \cdot \mathbf{u}_1 = |\mathbf{x}| \cos\theta_1 = \tilde{x}_1$$

$$\mathbf{x} \cdot \mathbf{u}_2 = |\mathbf{x}| \cos\theta_2 = \tilde{x}_2$$

$$\mathbf{x} \cdot \mathbf{u}_1 = |\mathbf{x}| \cos\theta_1 = \tilde{x}_1$$

$$\mathbf{x} \cdot \mathbf{u}_2 = |\mathbf{x}| \cos\theta_2 = \tilde{x}_2$$

$$\vdots$$

$$\mathbf{x} \cdot \mathbf{u}_p = |\mathbf{x}| \cos\theta_p = \tilde{x}_p$$

$$\mathbf{x}^\top \mathbf{U} = \tilde{\mathbf{x}}$$

$$\mathbf{XU} = \tilde{\mathbf{X}}$$

$$\mathbf{X} \in \mathbb{R}^{n \times d}$$

$$\mathbf{X} \in \mathbb{R}^{n \times d}$$

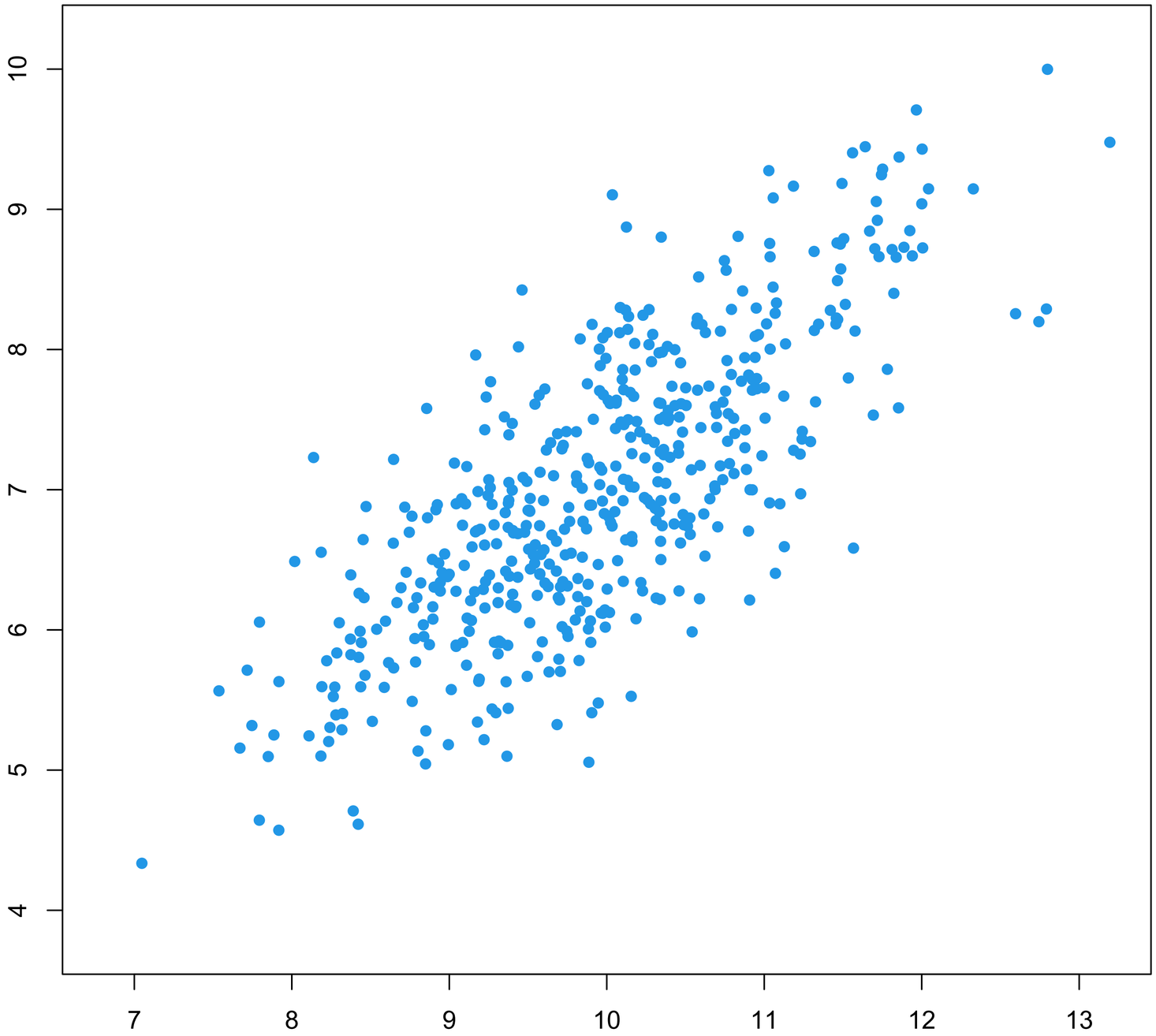
$$\mathbf{U} \in \mathbb{R}^{d \times p}$$

$$\mathbf{X} \in \mathbb{R}^{n \times d}$$

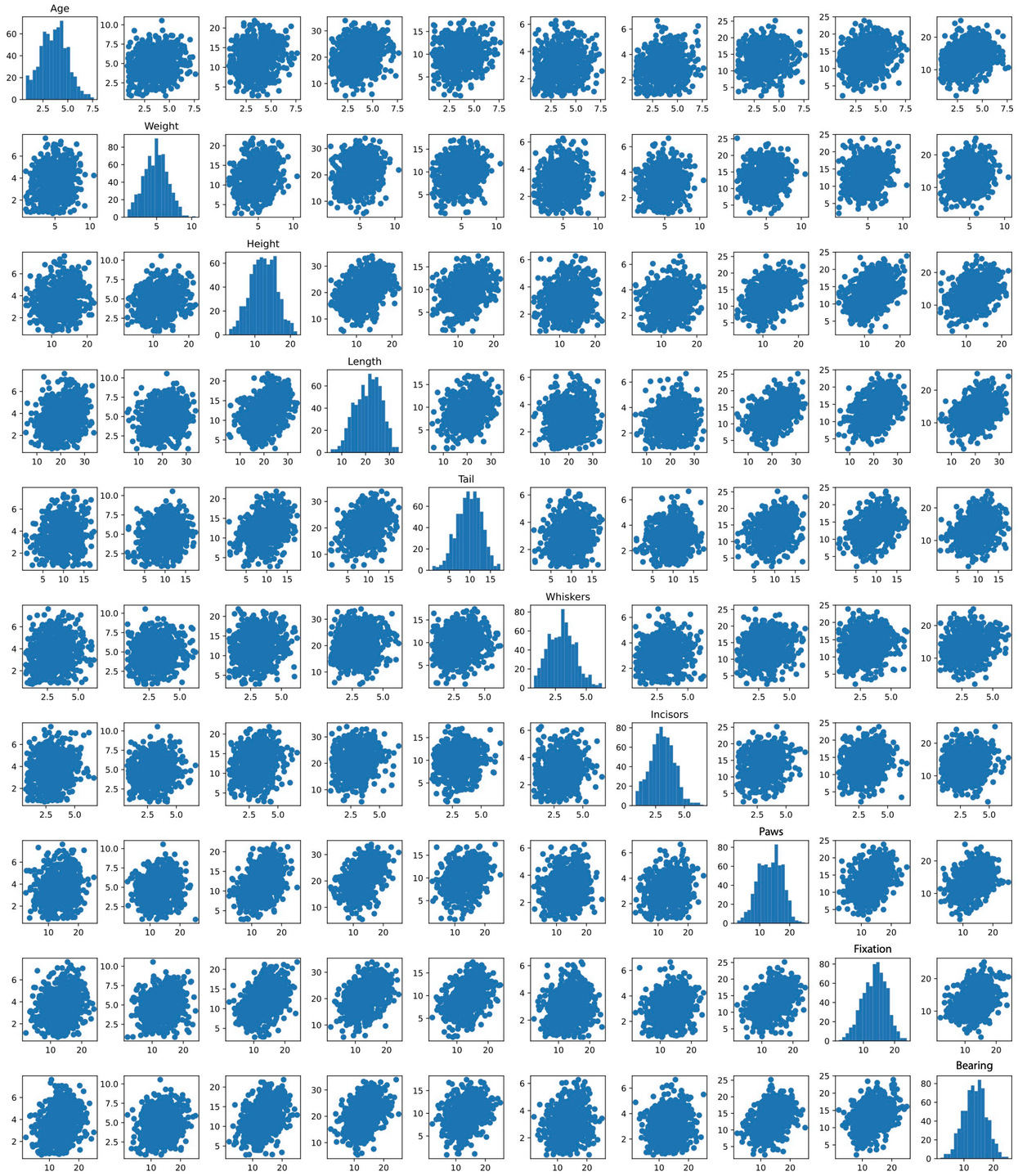
$$\mathbf{U} \in \mathbb{R}^{d \times p}$$

$$\tilde{\mathbf{X}} = \mathbf{X}\mathbf{U} \in \mathbb{R}^{n \times p}$$

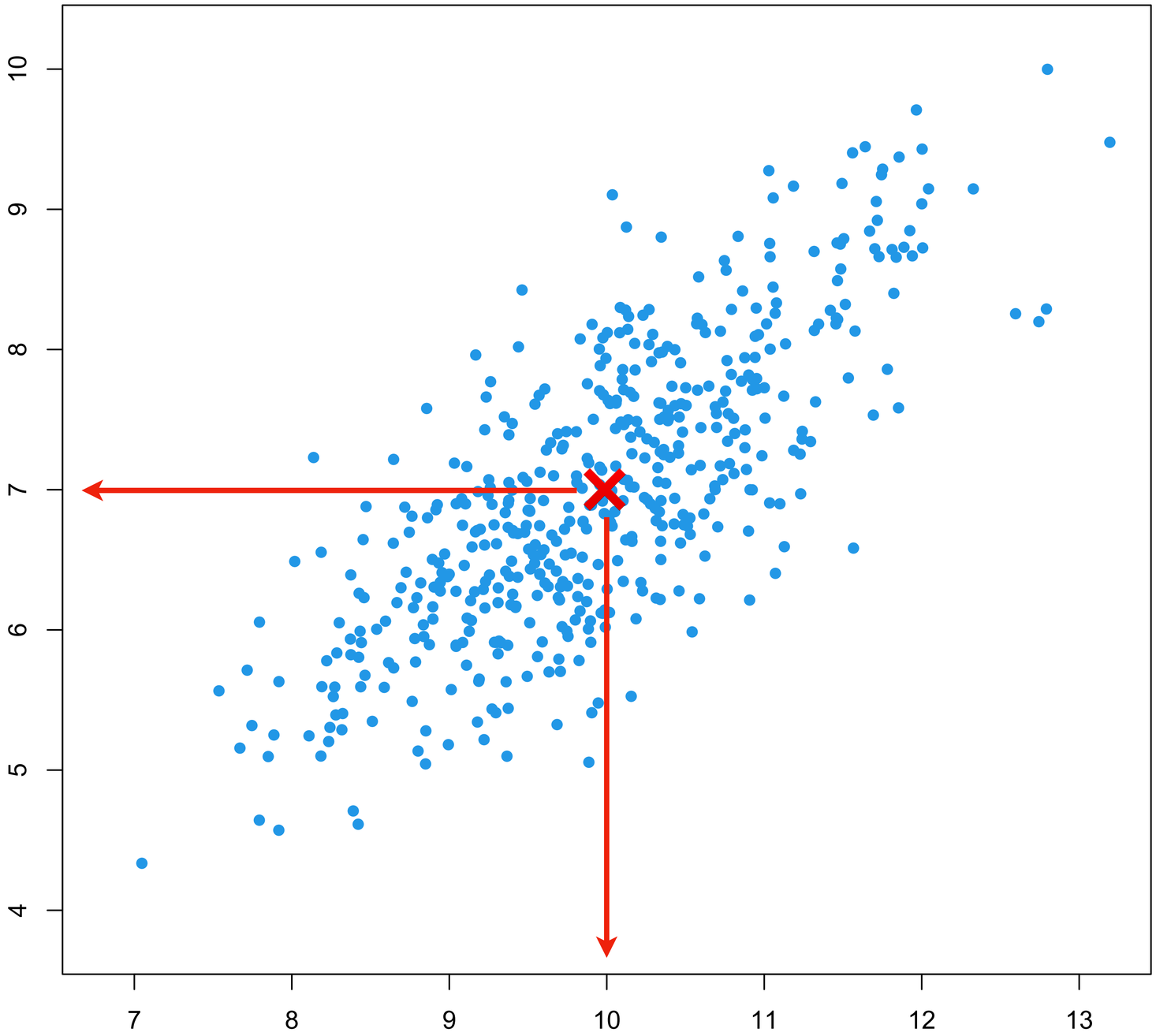
$$\tilde{\mathbf{X}} = \mathbf{X}\mathbf{U}$$

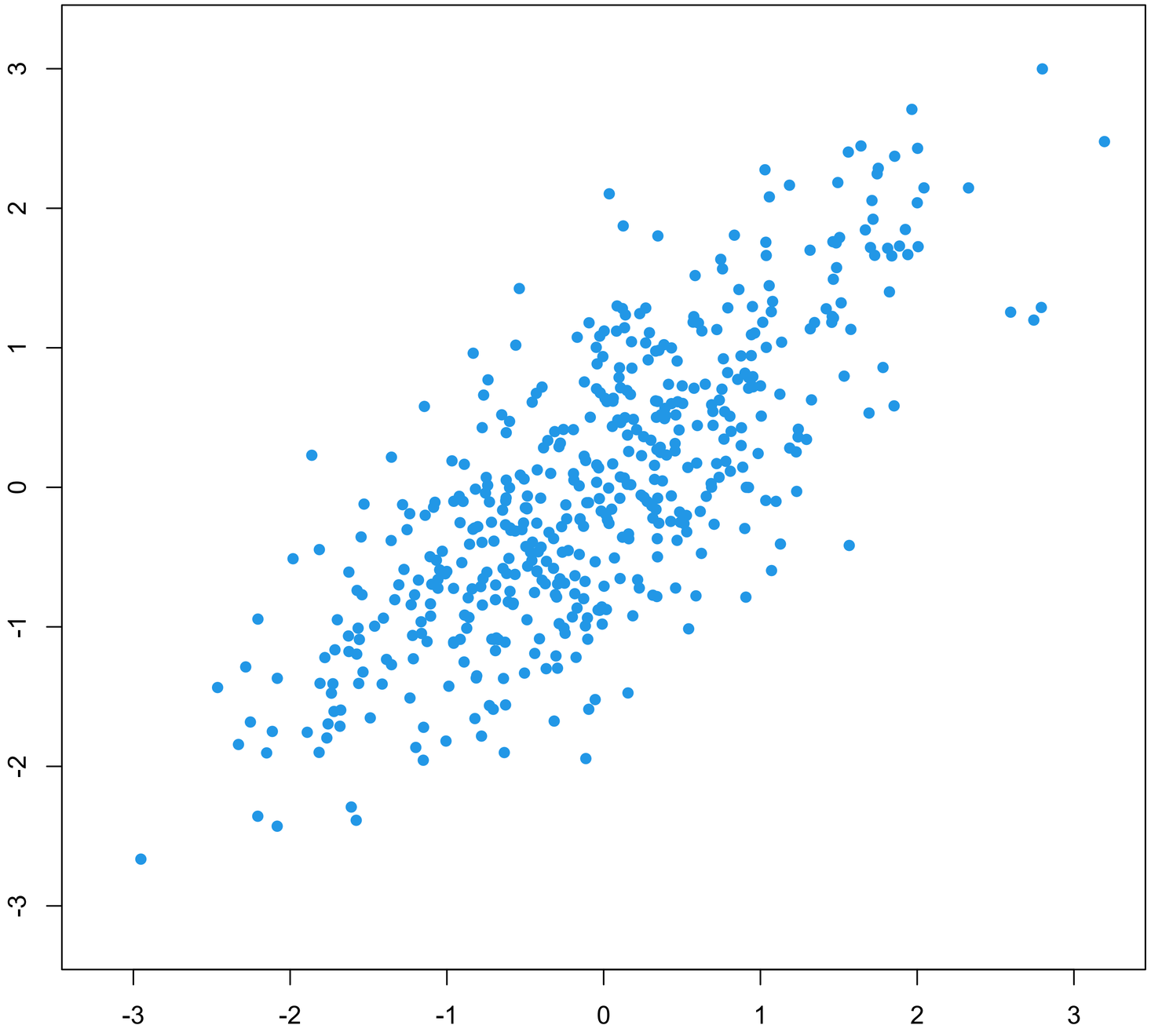

10
9
8
7
6
5
4
7
8
9
10
11
12
13

$$\Sigma = \begin{bmatrix} \mathrm{var}(\mathbf{x}_{|1}) & \mathrm{covar}(\mathbf{x}_{|1}, \mathbf{x}_{|2}) & \cdots & \mathrm{covar}(\mathbf{x}_{|1}, \mathbf{x}_{|d}) \\ \mathrm{covar}(\mathbf{x}_{|2}, \mathbf{x}_{|1}) & \mathrm{var}(\mathbf{x}_{|2}) & \cdots & \mathrm{covar}(\mathbf{x}_{|2}, \mathbf{x}_{|d}) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{covar}(\mathbf{x}_{|d}, \mathbf{x}_{|1}) & \mathrm{covar}(\mathbf{x}_{|d}, \mathbf{x}_{|2}) & \cdots & \mathrm{var}(\mathbf{x}_{|d}) \end{bmatrix}$$

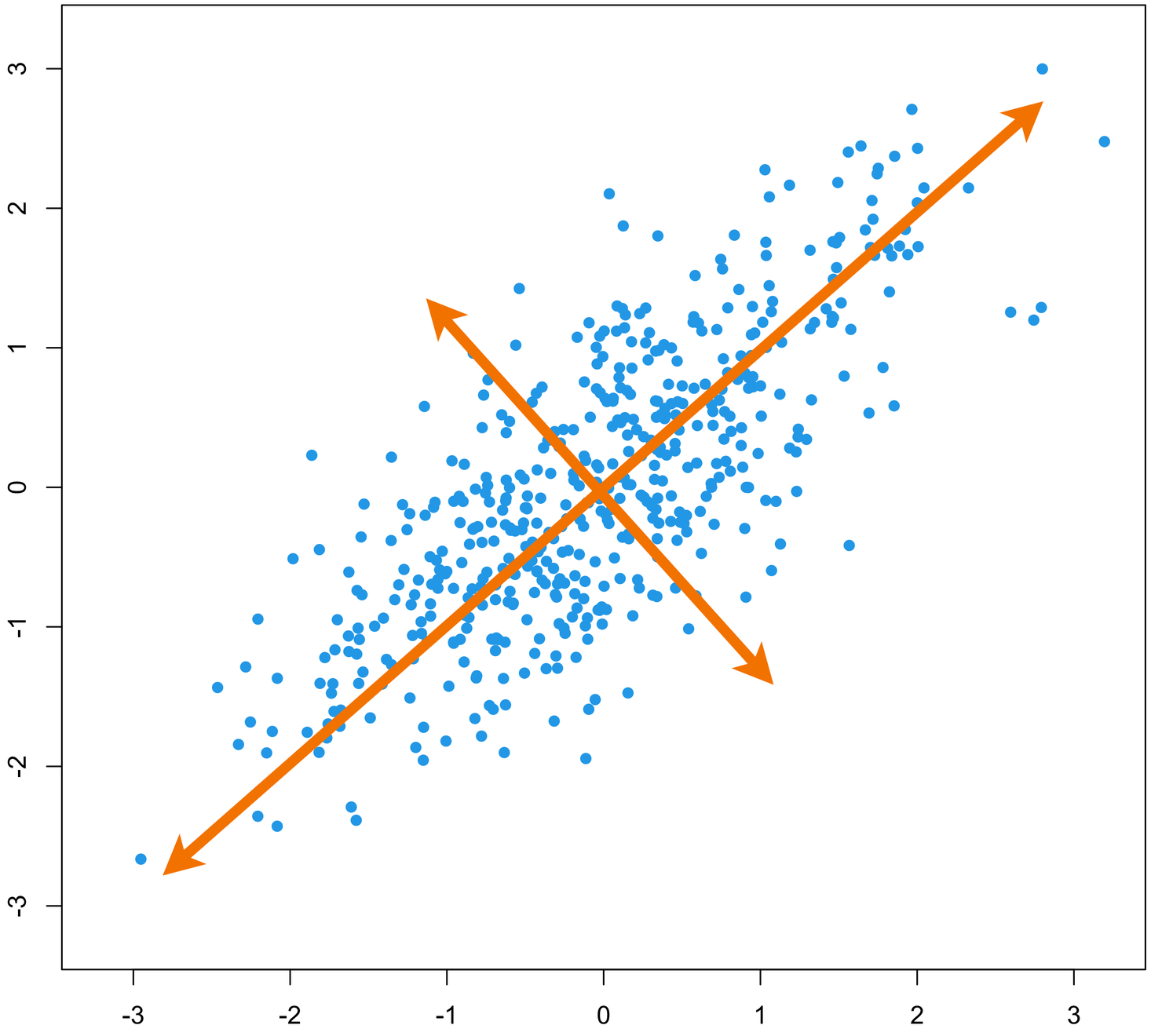

Age
Weight
Height
Length
Tail
Whiskers
Incisors
Paws
Fixation
Bearing

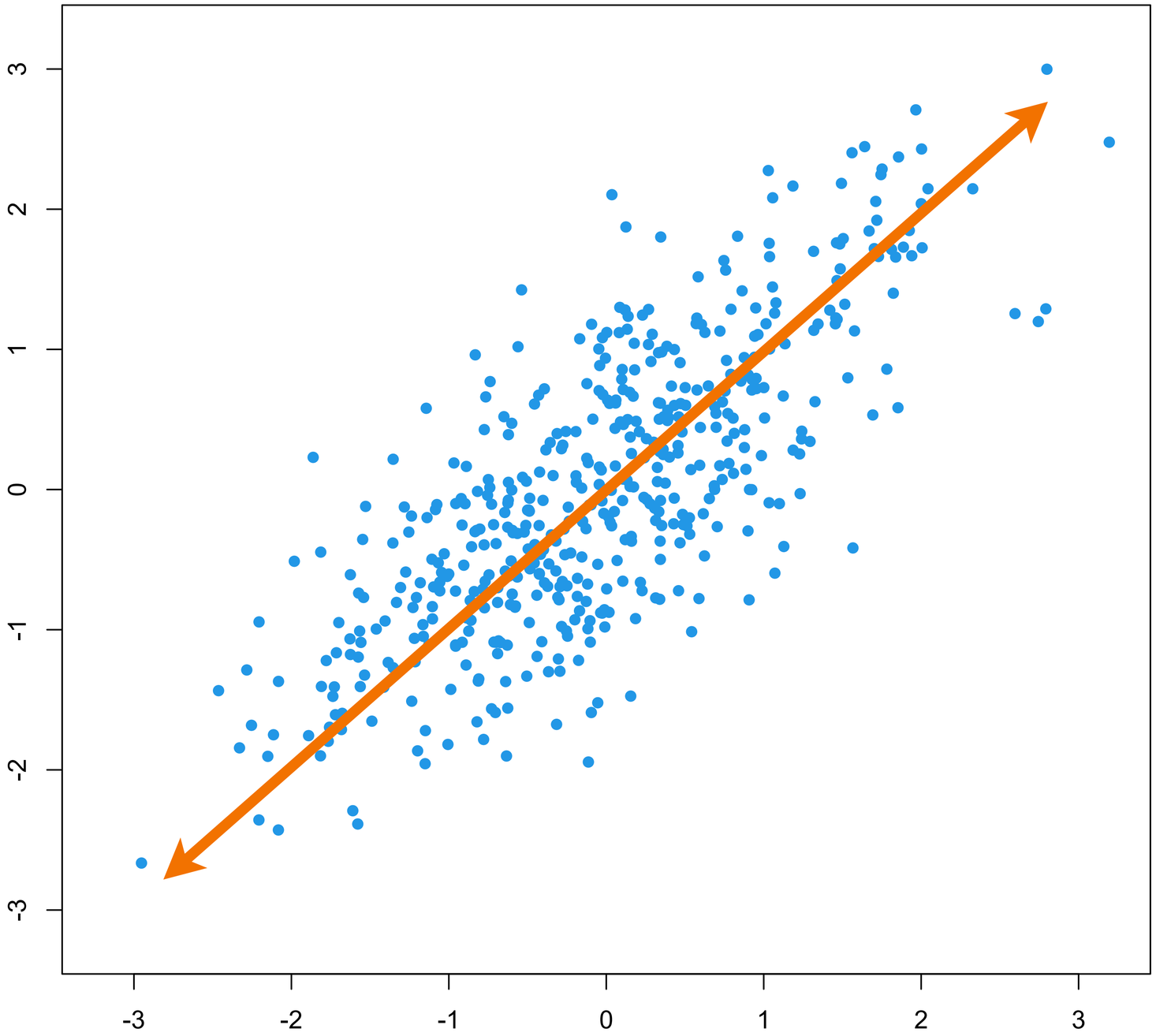
$$\Sigma = \frac{1}{n}\mathbf{X}^{\top}\mathbf{X}$$


10
9
8
7
6
5
4
7
8
9
10
11
12
13


3
2
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3

$$\mathbf{M}\mathbf{v} = \lambda\mathbf{v}$$


3
2
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3


3
2
1
0
-1
-2
-3
-3
-2
-1
0
1
2
3

$$\tilde{x}_i = \mathbf{u} \cdot \mathbf{x}_i$$

$$\tilde{\mathbf{x}}_i = \tilde{x}_i \mathbf{u} = \left(\mathbf{u} \cdot \mathbf{x}_i\right)\mathbf{u}$$

$$\mathrm{var}(\tilde{\mathbf{x}}) = \frac{1}{n} \sum_i \tilde{x}_i^2$$

$$
\begin{aligned}
\mathrm{var}(\tilde{\mathbf{X}}) &= \frac{1}{n}\sum_i \tilde{x}_i^2 \\
&= \frac{1}{n}\sum_i (\mathbf{u}\cdot\mathbf{x}_i)^2
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{var}(\tilde{\mathbf{X}}) &= \frac{1}{n}\sum_i \tilde{x}_i^2 \\
&= \frac{1}{n}\sum_i (\mathbf{u}\cdot\mathbf{x}_i)^2 \\
&= \frac{1}{n}\mathbf{u}^\top \mathbf{X}^\top \mathbf{X}\mathbf{u}
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{var}(\tilde{\mathbf{X}}) &= \frac{1}{n}\sum_i \tilde{x}_i^2 \\
&= \frac{1}{n}\sum_i (\mathbf{u}\cdot\mathbf{x}_i)^2 \\
&= \frac{1}{n}\mathbf{u}^\top \mathbf{X}^\top \mathbf{X}\mathbf{u} \\
&= \mathbf{u}^\top \boldsymbol{\Sigma}\mathbf{u}
\end{aligned}
$$

$$\underset{\mathbf{u}}{\text{maximise}} \quad \mathbf{u}^\top \boldsymbol{\Sigma} \mathbf{u}$$

$$\underset{\mathbf{u}}{\text{maximise}} \;\; \mathbf{u}^\top \boldsymbol{\Sigma} \mathbf{u}$$

$$\text{subject to: } \|\mathbf{u}\| = 1$$

$$\mathbf{u}^\top \boldsymbol{\Sigma} \mathbf{u} + \lambda(1 - \mathbf{u}^\top \mathbf{u})$$

$$\mathbf{u}^\top \boldsymbol{\Sigma} \mathbf{u} + \lambda(1 - \mathbf{u}^\top \mathbf{u})$$

$$2\boldsymbol{\Sigma}\mathbf{u} - 2\lambda\mathbf{u}$$

$$\mathbf{u}^\top \boldsymbol{\Sigma} \mathbf{u} + \lambda(1 - \mathbf{u}^\top \mathbf{u})$$

$$2\boldsymbol{\Sigma}\mathbf{u} - 2\lambda\mathbf{u} = 0$$

$$\mathbf{u}^\top \boldsymbol{\Sigma} \mathbf{u} + \lambda(1 - \mathbf{u}^\top \mathbf{u})$$

$$2\boldsymbol{\Sigma}\mathbf{u} - 2\lambda\mathbf{u} = 0$$

$$\boldsymbol{\Sigma}\mathbf{u} = \lambda\mathbf{u}$$

$$\mathbf{u}^\top \boldsymbol{\Sigma} \mathbf{u} = \lambda \mathbf{u}^\top \mathbf{u}$$

$$\mathbf{u}^\top \boldsymbol{\Sigma} \mathbf{u} = \lambda \mathbf{u}^\top \mathbf{u} = \lambda$$

$\mathbf{U} \in \mathbb{R}^{d \times d}$ cols eigenvectors of $\mathbf{X}^\top \mathbf{X}$

$$\mathbf{X} = \mathbf{V}\mathbf{D}\mathbf{U}^\top$$

$\mathbf{X} \in \mathbb{R}^{n \times d}$ original data

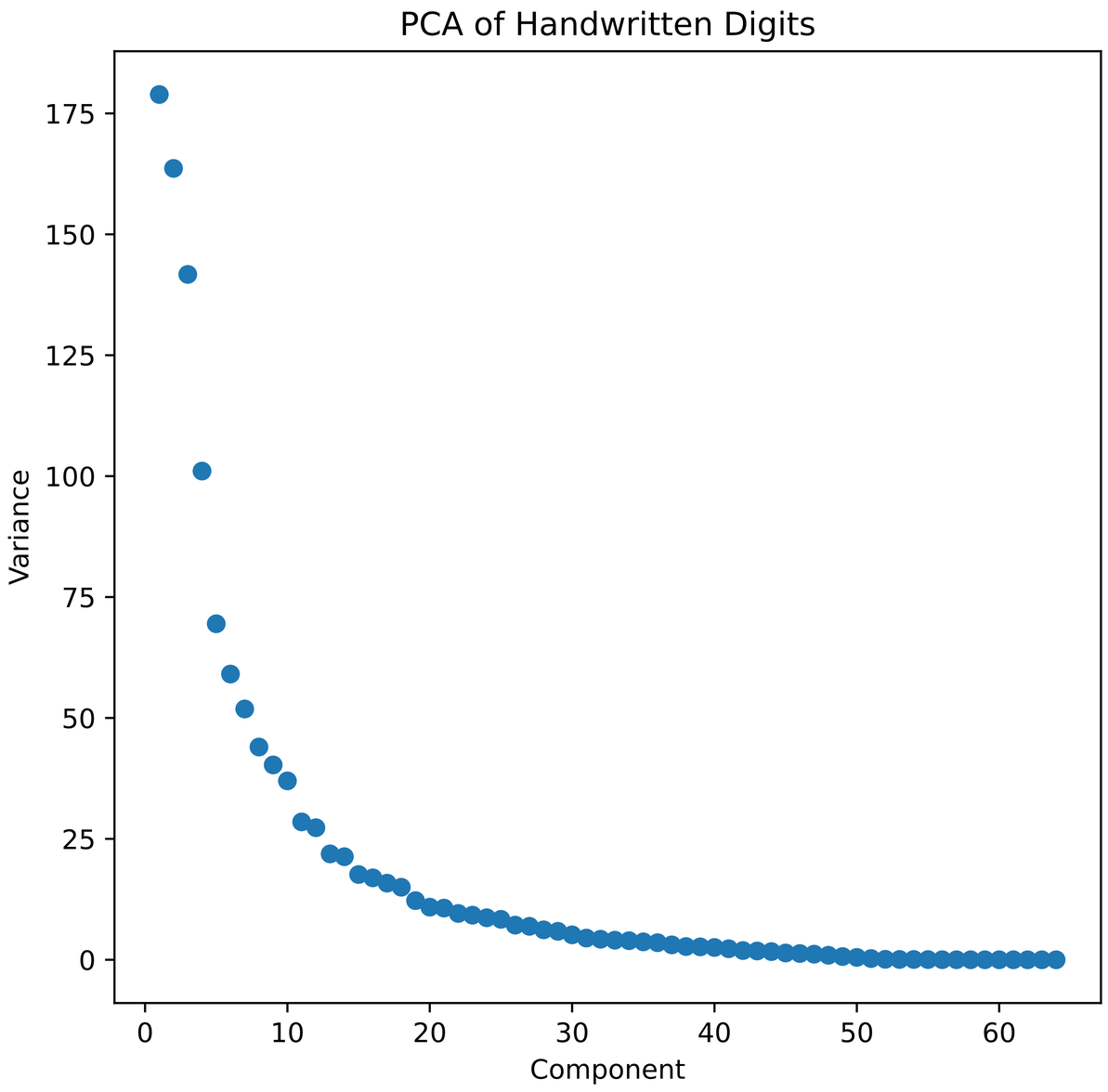
$\mathbf{V} \in \mathbb{R}^{n \times n}$ cols are eigenvectors of $\mathbf{X}\mathbf{X}^\top$

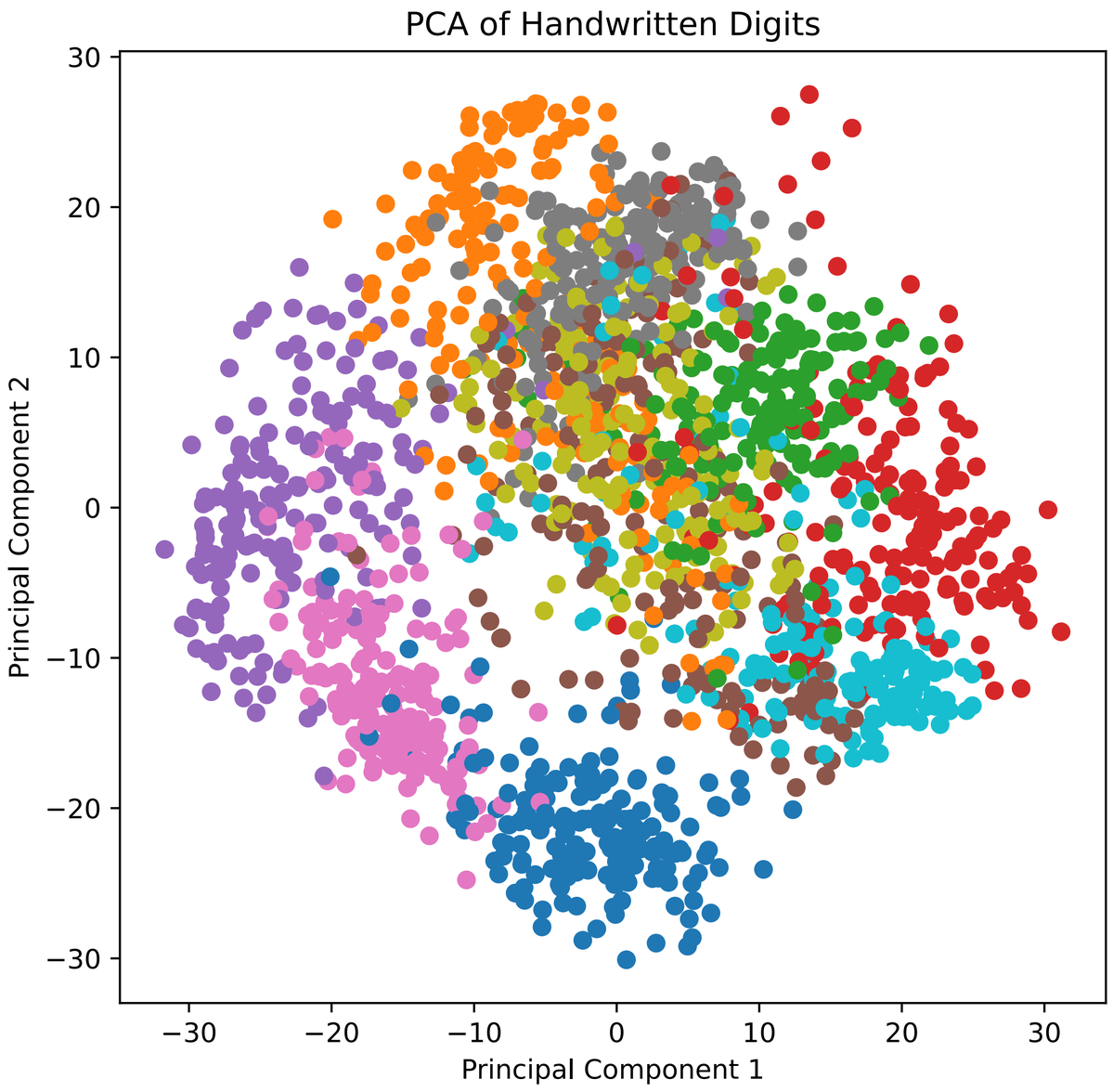
$\mathbf{D} \in \mathbb{R}^{n \times d}$ $\sqrt{\mathrm{diag}(\mathrm{eig}(\mathbf{X}\mathbf{X}^\top))}$

$\mathbf{U} \in \mathbb{R}^{d \times d}$ cols eigenvectors of $\mathbf{X}^\top\mathbf{X}$

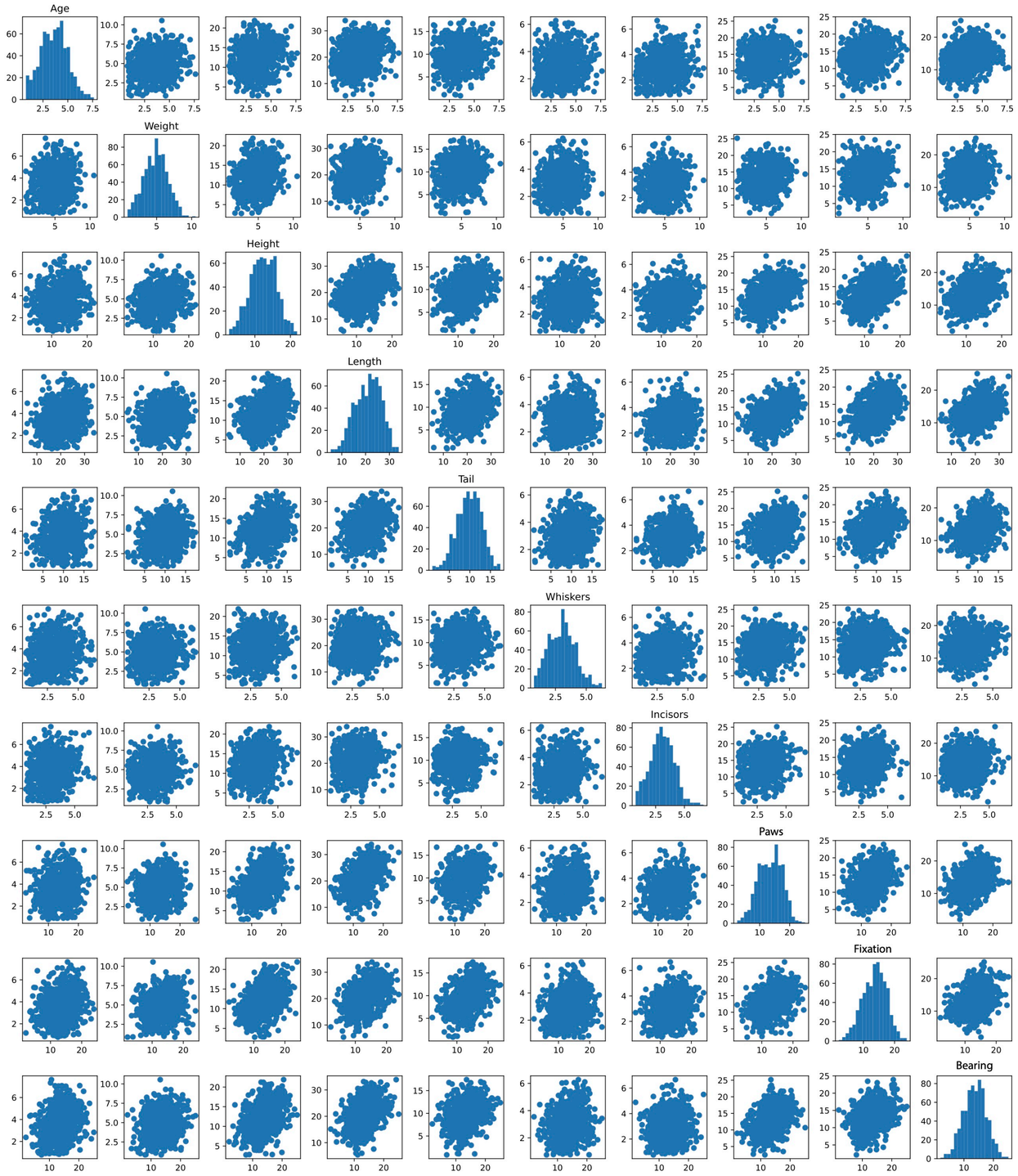
$$\mathbf{X} = \mathbf{V}\mathbf{D}\mathbf{U}^\top$$

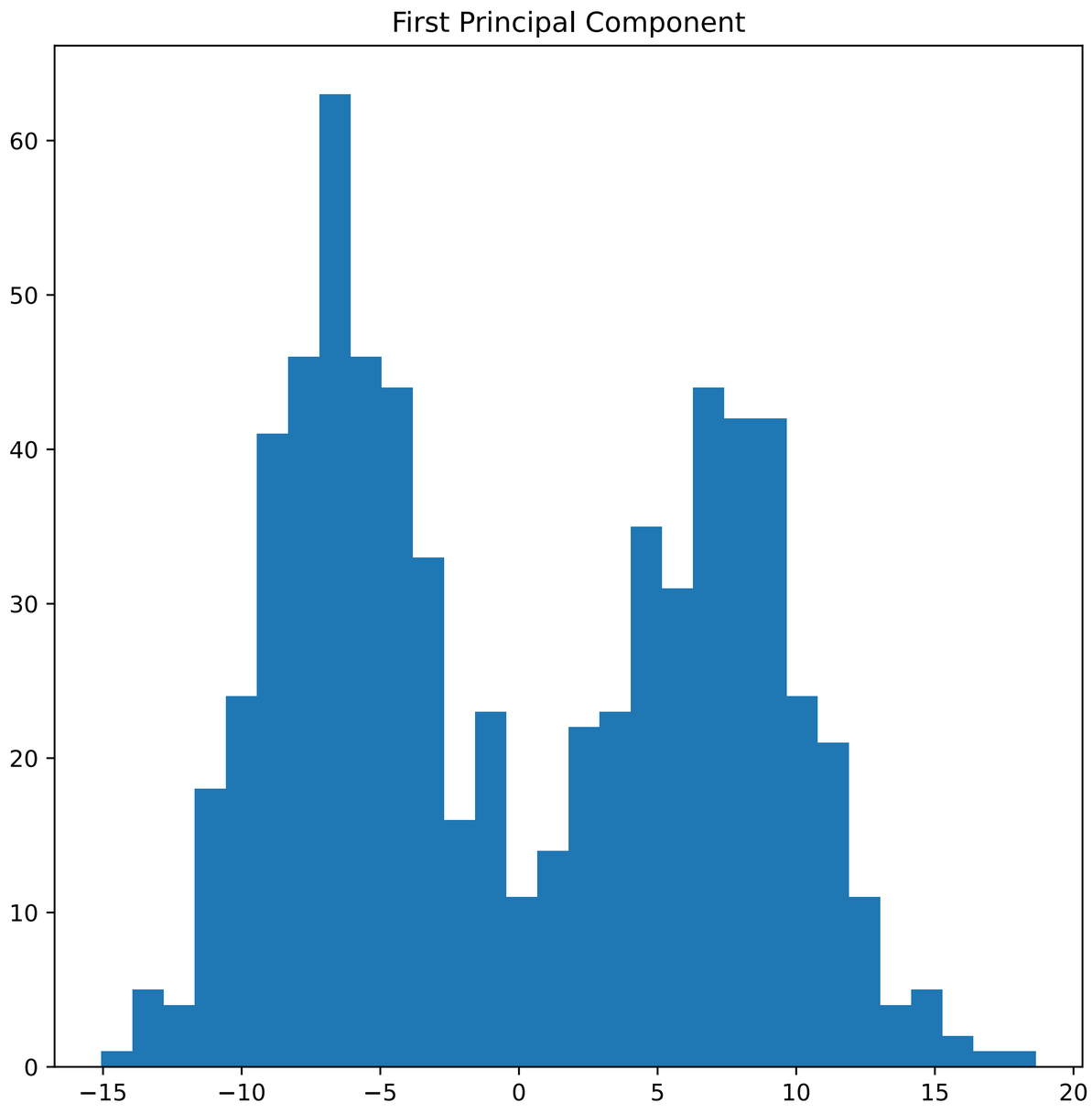
$$\begin{aligned}\tilde{\mathbf{X}} &= \mathbf{X}\mathbf{U} \\ &= \mathbf{V}\mathbf{D}\mathbf{U}^\top\mathbf{U} \\ &= \mathbf{V}\mathbf{D}\end{aligned}$$

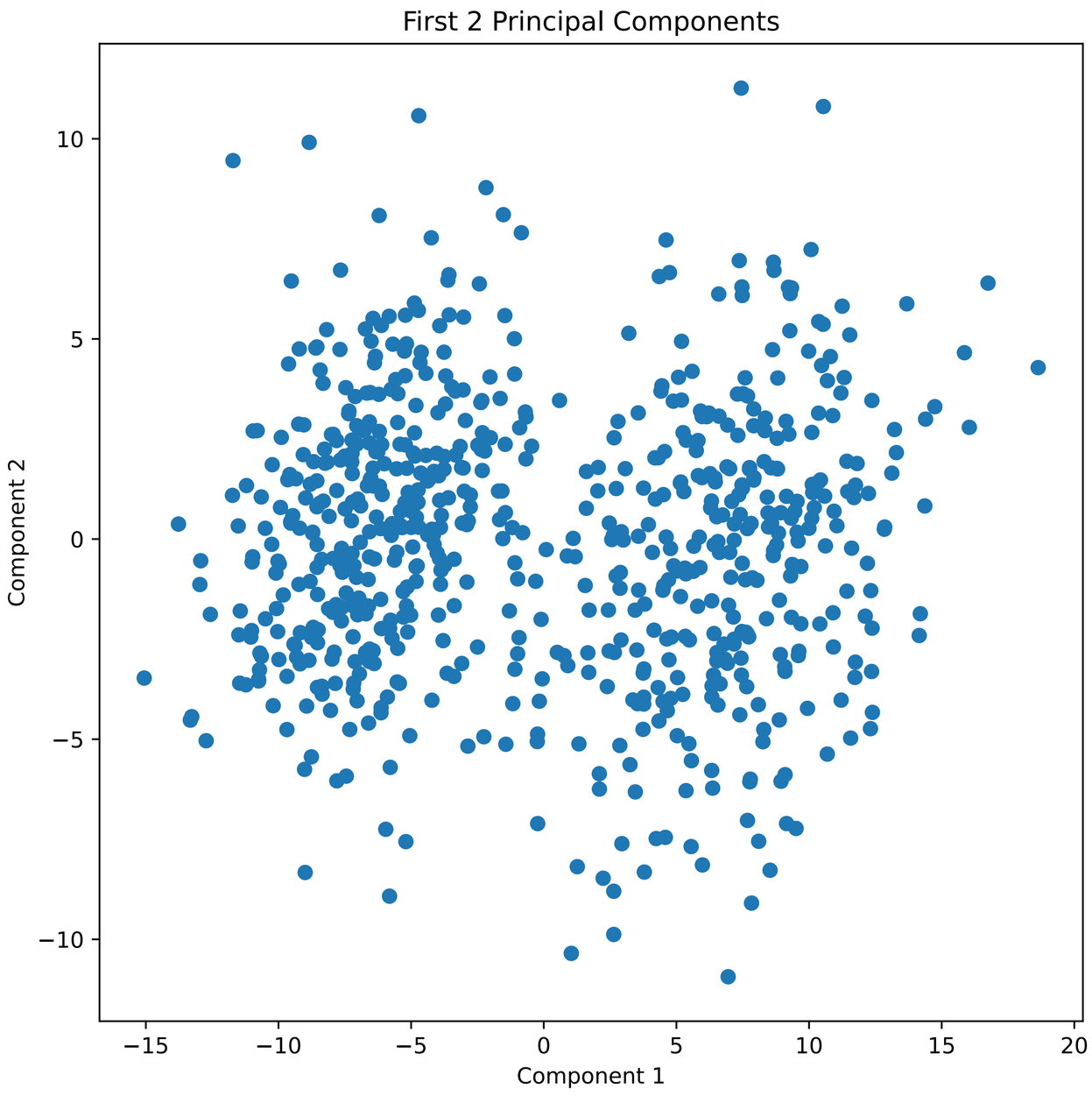

PCA of Handwritten Digits
Variance
Component
0
25
50
75
100
125
150
175
0
10
20
30
40
50
60


PCA of Handwritten Digits
Principal Component 2
Principal Component 1
30
20
10
0
−10
−20
−30
−30
−20
−10
0
10
20
30

Original Images
Mean Only
1 Component
2 Components
3 Components
4 Components
5 Components
6 Components
7 Components
8 Components
9 Components
10 Components
11 Components
12 Components
13 Components
14 Components
15 Components
16 Components
17 Components
18 Components
19 Components
20 Components
21 Components
22 Components


Age
Weight
Height
Length
Tail
Whiskers
Incisors
Paws
Fixation
Bearing


First Principal Component
60
50
40
30
20
10
0
−15
−10
−5
0
5
10
15
20


First 2 Principal Components
Component 2
Component 1
10
5
0
−5
−10
−15
−10
−5
0
5
10
15
20

clustering

$$\mathbf{C} = \{\mathbf{c}_1, \mathbf{c}_2, ..., \mathbf{c}_k\} \quad \text{cluster centroids} \in \mathbb{R}^d$$

$$\mathbf{a} = \{a_1, a_2, ..., a_n\} \quad \text{cluster assignments} \ \in \{1, 2, ..., k\}$$

$$\hat{\mathbf{C}}, \hat{\mathbf{a}} = \underset{\mathbf{C},\mathbf{a}}{\operatorname{argmin}} \sum_{i}^{n} \|\mathbf{x}_i - \mathbf{c}_{a_i}\|^2$$

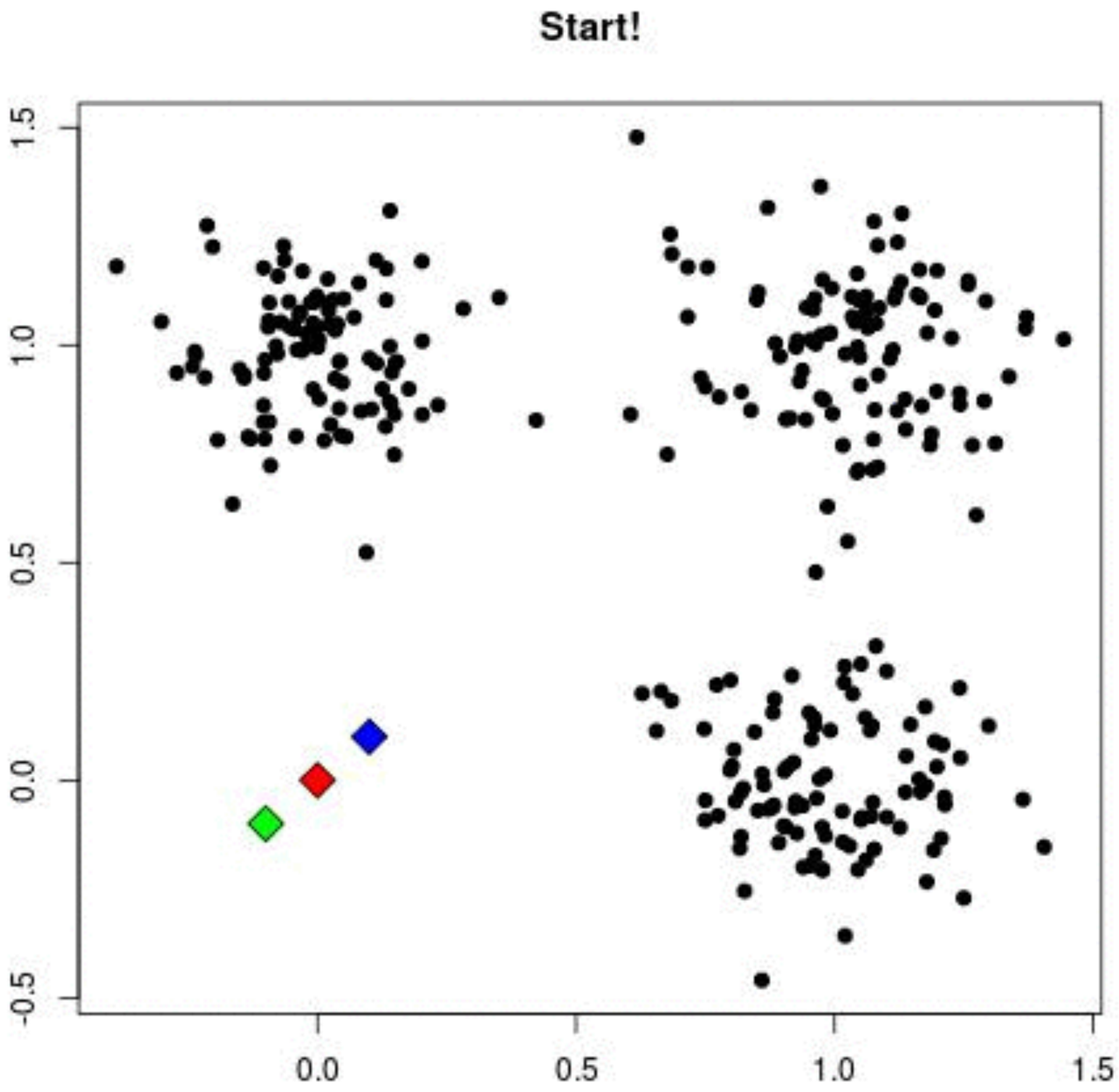
Initialise **c** somehow

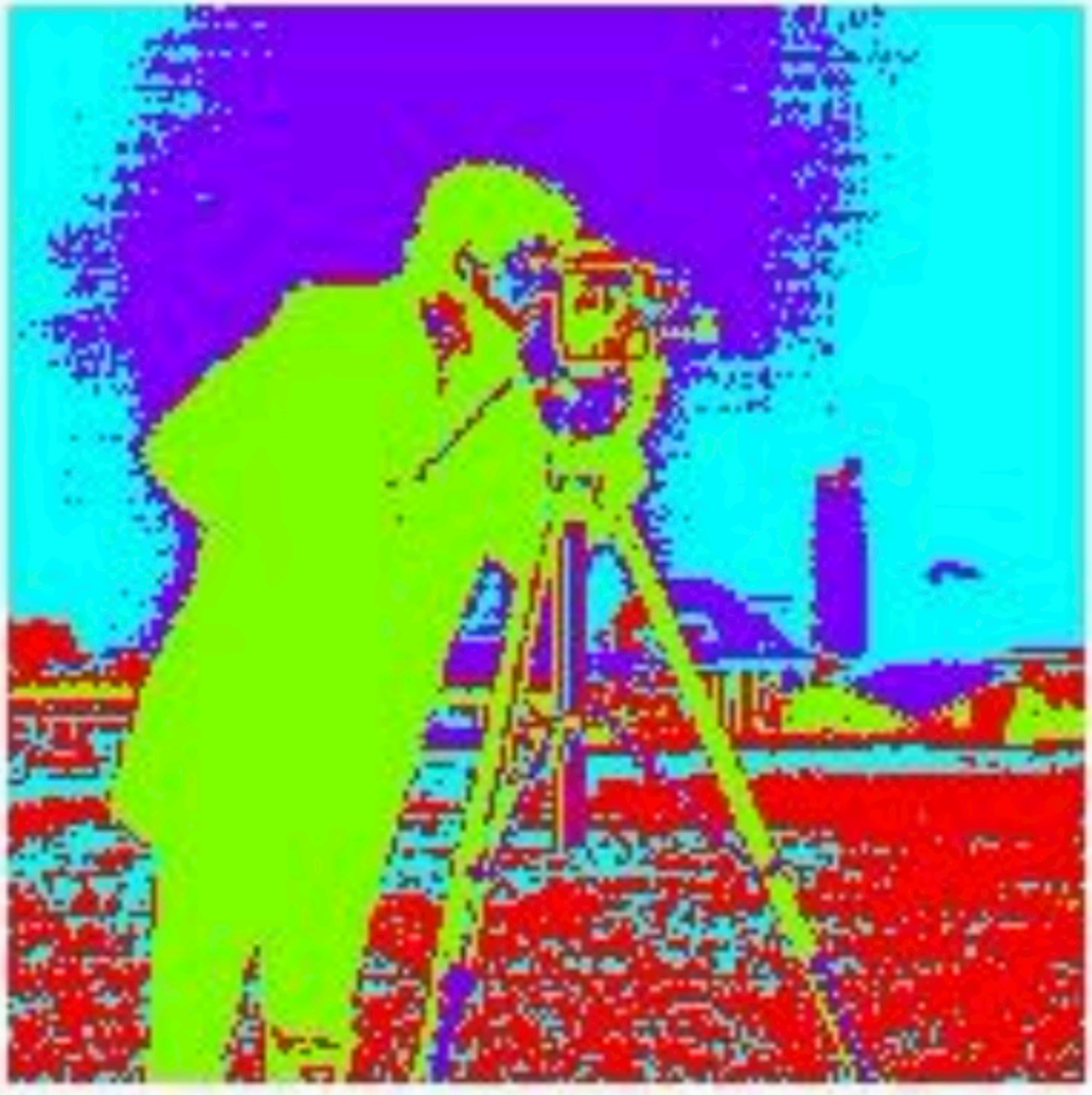
Repeat

  Assign each **x** to its nearest **c**

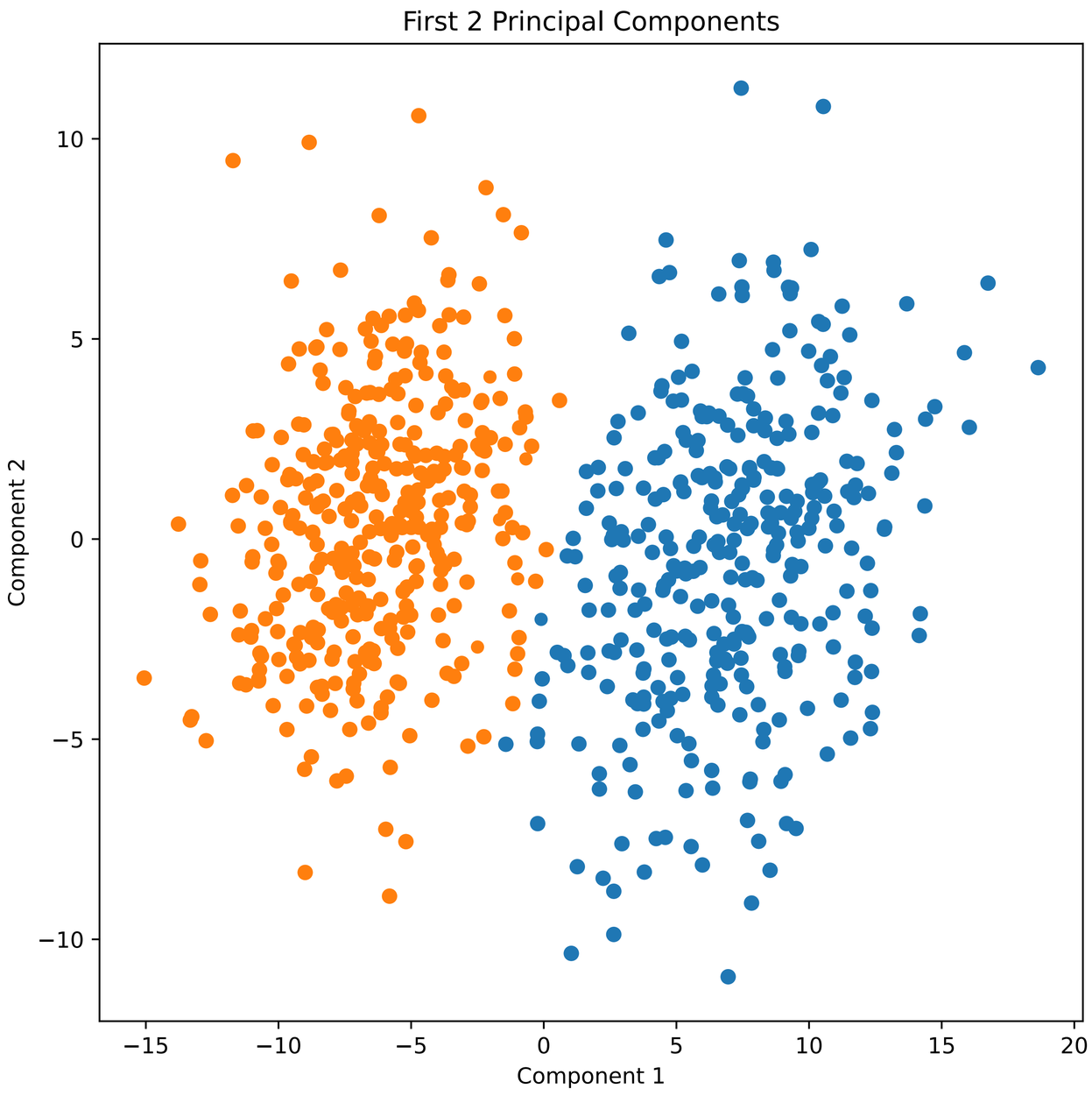
  Update each **c** to be the mean of all **x** assigned to it

Until nothing changes


Start!
1.5
1.0
0.5
0.0
-0.5
0.0
0.5
1.0
1.5



Agglomerative
Divisive


First 2 Principal Components
Component 2
Component 1
10
5
0
−5
−10
−15
−10
−5
0
5
10
15
20

Questions?

Next: Expectation Maximisation