MADS-MMS – Mathematics and Multivariate Statistics

Analytic Geometry

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Moodle (WiSe 24/25)

Agenda

Outline

Motivation

- one heavily exploited feature in machine learning are geometric relationships between instances

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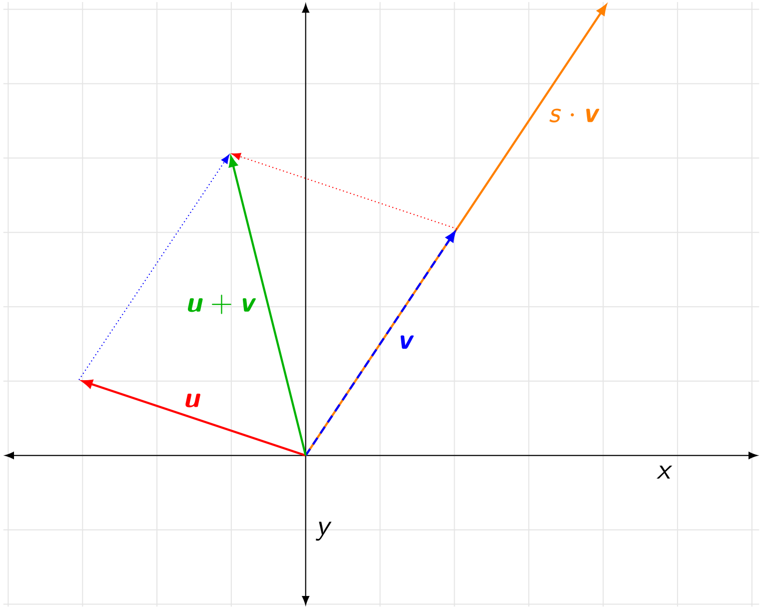
- kNN exploits distances between instances
- SVMs measure distances between planes and instances
- k-means groups instances with short distances between each other
- text-mining uses the angle between long vectors as similarity measure

Example 1 – $\mathbb{R}^2$ – Geometric Interpretation



Example 1 – $\mathbb{R}^2$ – Geometric Interpretation

- the geometric interpretation works similarly in $\mathbb{R}^n$ with $n > 2$
- it allows computing various geometric entities, like planes, volumes, distances, angles, ...

Chapter Goals

- mathematical foundations of geometry

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- distance functions (e.g. for clustering)
- geometric figures (e.g. for SVMs)

Outline

Motivation

Inner Products

Norms and Distances

Angles

Lines, Planes, Hyperplanes

Inner Product

Definition 1 (Inner Product)

Let V be a real-valued vector space. Then a function $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$ is called an **inner product**, if for all $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in V$ and $r, s \in \mathbb{R}$ holds

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1. $\langle r\boldsymbol{u} + s\boldsymbol{v}, \boldsymbol{w} \rangle = r\langle \boldsymbol{u}, \boldsymbol{w} \rangle + s\langle \boldsymbol{v}, \boldsymbol{w} \rangle$ and
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2. $\langle \boldsymbol{u}, \boldsymbol{v} \rangle = \langle \boldsymbol{v}, \boldsymbol{u} \rangle$ (**symmetric**)
3. $\langle \boldsymbol{v}, \boldsymbol{v} \rangle > 0$ for $\boldsymbol{v} \neq 0$ and $\langle 0, 0 \rangle = 0$ (**positive definite**)

Example in $\mathbb{R}^2$:

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle = u_1 v_1 - (u_1 v_2 + u_2 v_1) + 2 u_2 v_2$$

The Dot Product

- In the vector space $\mathbb{R}^n$, the dot product or scalar product

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- $\mathbb{R}^n$ together with the dot product is called a **Euclidean vector space**.

Outline

Vector Norm

Definition 2

A **norm** on a vector space is a function $\|\cdot\| : V \to \mathbb{R}$, such that for all $\boldsymbol{u}, \boldsymbol{v} \in V$ and $r \in \mathbb{R}$ holds

1. $\|r\boldsymbol{v}\| = |r| \cdot \|v\|$
2. $\|\boldsymbol{u} + \boldsymbol{v}\| \leq \|\boldsymbol{u}\| + \|\boldsymbol{v}\|$ (**triangle inequality**)
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The norm of a vector can be understood as its length.

Example: Manhattan Norm

$$\|\boldsymbol{v}\|_1 = \sum_{i=1}^{n} |v_i|$$

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Observation:

$$\|\boldsymbol{v}\|_2 = \sqrt{\langle \boldsymbol{v}, \boldsymbol{v} \rangle}$$

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- Not each norm is an induced norm (e.g. Manhattan norm).

Unit Vectors

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Proof: $\left\|\frac{1}{\|v\|}\boldsymbol{v}\right\| = \frac{1}{\|v\|}\|\boldsymbol{v}\| = 1.$

Distance Function

Definition 3

Let O be a set of objects. A **distance function** is a function $d : O \times O \to \mathbb{R}_{\geq 0}$ such that

1. $d(o_1, o_2) = d(o_2, o_1)$
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A distance function d is called a metric, if for all o_1, o_2, o_3 the triangle inequality holds:

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The general definition of distance allows for various inclusions and combinations of an objects features.

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The different inner products and their distance function properties are the key ingredient in SVMs using the kernel trick.

Distance functions: Minkowski-Metrics

Definition 5 (Minkowski-Metric)

Let $\boldsymbol{u} = (u_1, \ldots, u_n)$ and $\boldsymbol{v} = (v_1, \ldots, v_n)$ be real-valued vectors and $p \in \mathbb{R}_{>0}$. For $p \geq 1$, the Minkowski-Metric (L_p-metric) is defined as:

$$d_p(\boldsymbol{u}, \boldsymbol{v}) := \sqrt[p]{\sum_{i=1}^{n} |u_i - v_i|^p}$$

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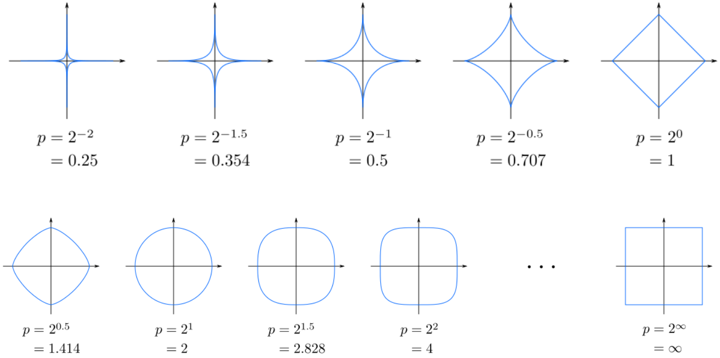
- Maximum ($p = \infty$): $d_\infty(\boldsymbol{u}, \boldsymbol{v}) = \max_{i=1}^{n} |u_i - v_i|$

Weighted Minkowski-Metric

- Sometimes we want to emphasize particularly important dimensions.
- The Minkowski-Metrics can be extended using weights ω_k:

$$d_p^{\omega}(\boldsymbol{u}, \boldsymbol{v}) = \sqrt[p]{\sum_{i=1}^{n} \omega_i |u_i - v_i|^p}$$

Unit Circles in Different Minkowski-Metrics



Source: https://commons.wikimedia.org/wiki/User:Waldir

Other Distance Functions

- For categorical attributes, the Hamming-Distance:

$$d(\boldsymbol{u}, \boldsymbol{v}) = \sum_{i=1}^{n} \delta(u_i, v_i) \quad \text{with} \quad \delta(u_i, v_i) = \begin{cases} 0 & \text{if } u_i = v_i \\ 1 & \text{otherwise} \end{cases}$$

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- many more, see e.g. implementations of `sklearn.neighbors.DistanceMetric`

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Exercises 1–3

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The Cosine of Two Vectors

- Let V be a vector space with inner product $\langle \cdot, \cdot \rangle$, then for two vectors $\boldsymbol{u}, \boldsymbol{v} \neq 0$

$$\cos \alpha = \frac{\langle \boldsymbol{u}, \boldsymbol{v} \rangle}{\|\boldsymbol{u}\| \cdot \|\boldsymbol{v}\|}$$

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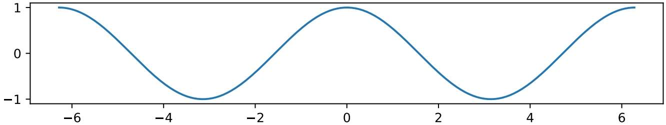
- With the dot product (thus Euclidean norm), the angles correspond to our usual intuition of angles

Recap Cosine



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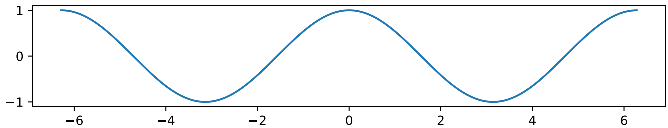

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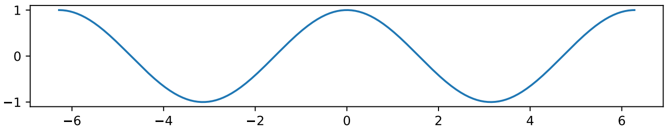

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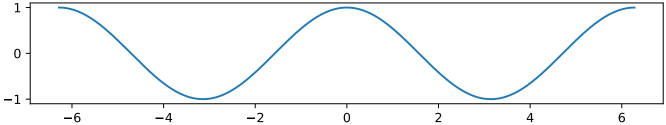

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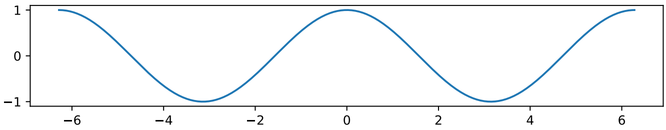

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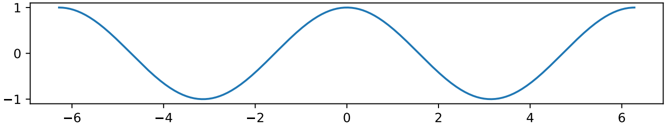

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- $\cos(\pi) = -1 \qquad (180^\circ)$

Orthogonal Vectors

Two vectors are orthogonal (angle 90°) if their inner product is zero.

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- 1 means identical orientation
- -1 means inverse orientation
- $1 - d(\boldsymbol{u}, \boldsymbol{v})$ is often used as distance measure, however not a proper metric (triangle inequality)

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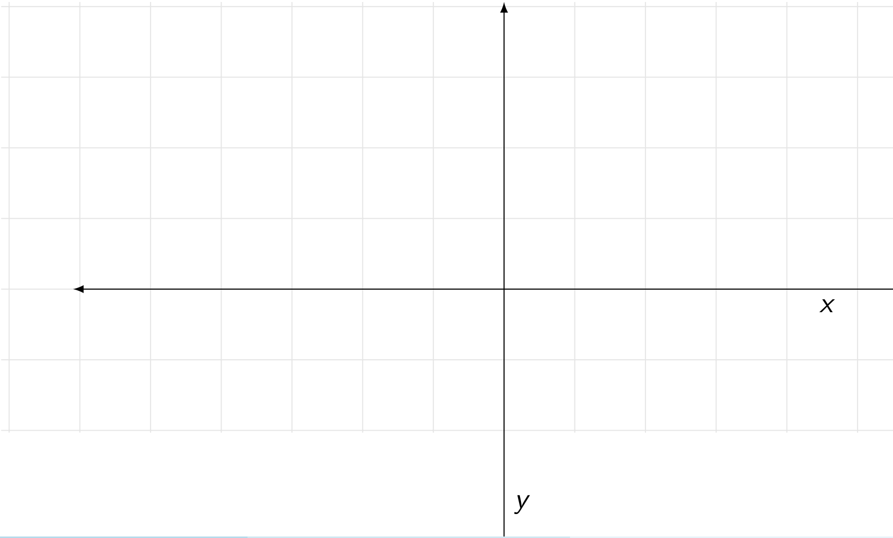
- cosine similarity works well with texts of different length
- a text and the same text appended to itself have cosine distance 0 but would have high values with many other distance functions (e.g. Euclidean)

Outline

A Line in $\mathbb{R}^2$

Let's consider $\mathbb{R}^2$. How can we describe a line?



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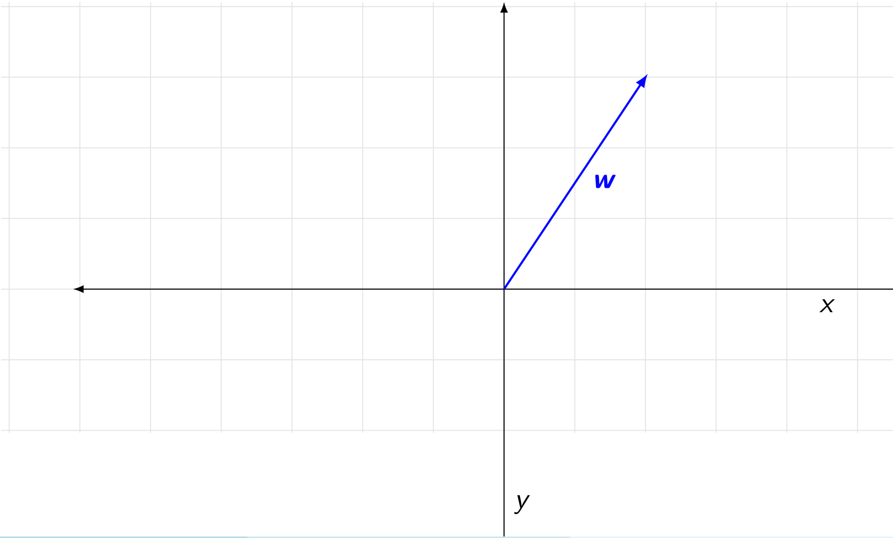

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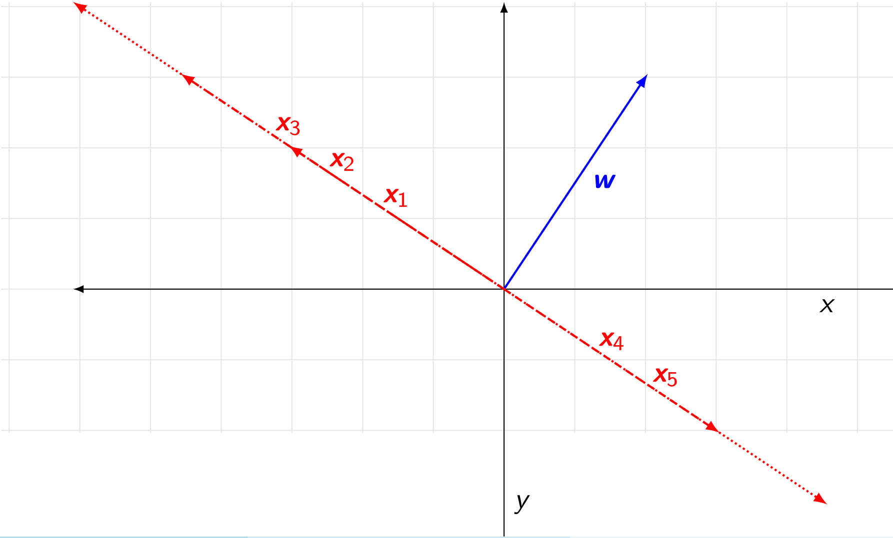

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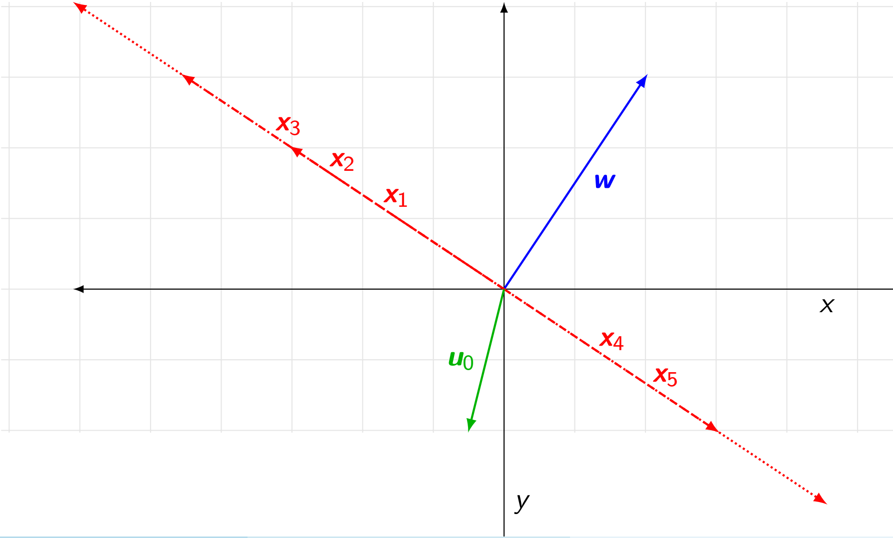

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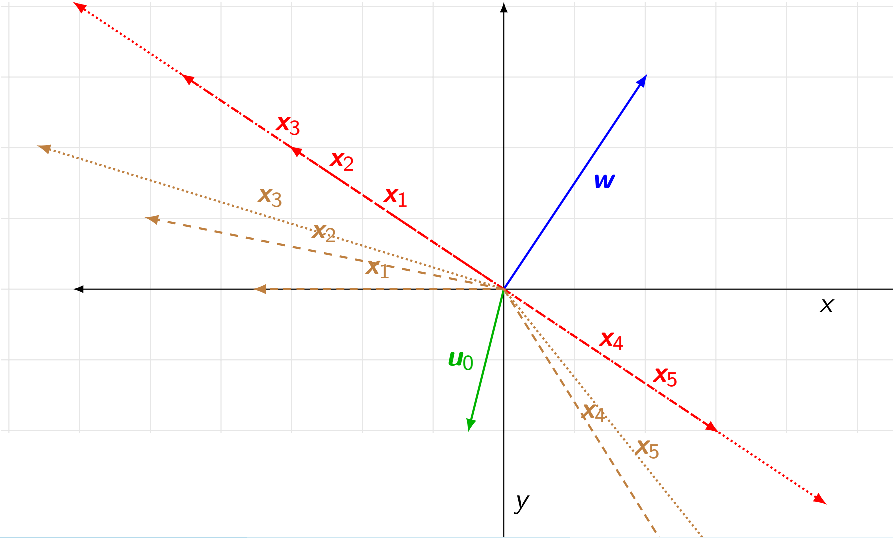

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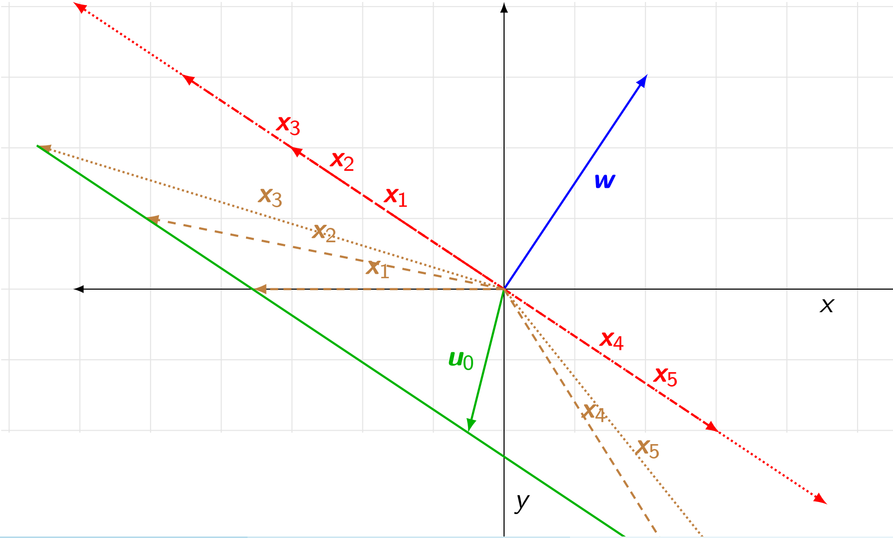

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- In this model: $\boldsymbol{w}$ and u_0 are fix parameters that determine the line.

Alternative Line Descriptions in $\mathbb{R}^2$

$$\langle \boldsymbol{x} - \boldsymbol{u}_0, \boldsymbol{w} \rangle = 0 \quad \text{with } \boldsymbol{w}, u_0 \in \mathbb{R}^2$$

$$\langle \boldsymbol{x}, \boldsymbol{w} \rangle + b = 0 \quad \text{with } \boldsymbol{w} \in \mathbb{R}^2, b \in \mathbb{R}$$

$$x_2 = mx_1 + n \quad \text{with } \boldsymbol{x} = (x_1, x_2), m, n \in \mathbb{R}$$

With $\langle \cdot, \cdot \rangle$ being the dot product, the first two are equivalent. The third is the linear function description of a line. It is however not fully equivalent to the other two.

Exercises Homework: Prove 1 $\iff$ 2, Here: Prove 2 $\iff$ 3.

Hyperplane

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- n=1 → point
- n=2 → line
- n=3 → (regular) plane

The construction of hyperplanes is exactly analogous to the hyperplanes in $\mathbb{R}^2$ (lines).

Distance between Point and Hyperplane

Given a hyperplane in $\mathbb{R}^n$ as $\langle \boldsymbol{x}, \boldsymbol{w} \rangle + b = 0$ and a vector $\boldsymbol{v} \in \mathbb{R}^n$. Assuming $\boldsymbol{w} \neq 0$, what is the distance between $\boldsymbol{v}$ and the hyperplane?

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- to $\boldsymbol{v}$, add a vector $\boldsymbol{z}$ that is orthogonal to the hyperplane, such that the sum is on the hyperplane:

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Exercises 4–6