Mathematics for Artificial Intelligence

Transformation and Applications

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Outline

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Going further than solving $Ax = y$

We can go further

We can think on the matrix A as a function!!!

- It is easy to find the range $\mathbb{R}^m$

Going further than solving $A\boldsymbol{x} = \boldsymbol{y}$

We can go further

We can think on the matrix A as a function!!!

In general

A function f whose domain $\mathbb{R}^n$ and defines a rule that associate $\boldsymbol{x} \in \mathbb{R}^n$ to a vector $\boldsymbol{y} \in \mathbb{R}^m$

$$\boldsymbol{y} = f(\boldsymbol{x}) \text{ equivalently } f : \mathbb{R}^n \longrightarrow \mathbb{R}^m$$

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We like the second expression because

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Examples

$f : \mathbb{R} \to \mathbb{R}^3$

$$f\left(t\right) = \begin{pmatrix} x\left(t\right) \\ y\left(t\right) \\ z\left(t\right) \end{pmatrix} = \begin{pmatrix} t \\ 3t^2 + 1 \\ sin\left(t\right) \end{pmatrix}$$

This are called parametric functions

- Depending on the context, it could represent the position or the velocity of a mass point.

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A Classic Example

We have

if A is a $m \times n$, we can use A to define a function.

We will call them

$$f_A : \mathbb{R}^n \to \mathbb{R}^m$$

In other words

$$f_A(\boldsymbol{x}) = Ax$$

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Example

Let

$$A_{2\times 3} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

This allows to define

$$f_A\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x + 2y + z \\ 4x + 5y + 6z \end{pmatrix}$$

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- For each vector $x \in \mathbb{R}^3$ to the vector $Ax \in \mathbb{R}^2$

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Definition

A function $f : \mathbb{R}^n \to \mathbb{R}^m$ is said to be linear if

1. $f\left(\boldsymbol{x}_1 + \boldsymbol{x}_2\right) = f\left(\boldsymbol{x}_1\right) + f\left(\boldsymbol{x}_2\right)$
2. $f\left(c\boldsymbol{x}\right) = cf\left(\boldsymbol{x}\right)$

for all $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{R}^n$ and for all the scalars c.

Thus

A linear function f is also known as a linear transformation.

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$$f\left(c_1 \boldsymbol{x}_1 + c_2 \boldsymbol{x}_2\right) = c_1 f\left(\boldsymbol{x}_1\right) + c_2 f\left(\boldsymbol{x}_2\right)$$

Proof

Any idea?

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Proof

If $A_{m\times n}$ is a matrix, f_A is a linear transformation

How?

First

$$f_A(x_1 + x_2) = A(x_1 + x_2) = Ax_1 + Ax_2 = f_A(x_1) + f_A(x_2)$$

Second

What about $f_A(cx_1)$?

Proof

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What about $f_A\left(c\boldsymbol{x}_1\right)$?

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Definition (Actually related the null-space)

If $f : \mathbb{R}^n \to \mathbb{R}^m$ is linear, the kernel of f is defined by

$$Ker\left(f\right) = \left\{\boldsymbol{v} \in \mathbb{R}^n | f\left(\boldsymbol{v}\right) = 0\right\}$$

Definition

If $f : \mathbb{R}^n \to \mathbb{R}^m$ is linear, the range of f is defined by

$$Range\left(f\right) = \left\{y \in \mathbb{R}^m | y = f\left(x\right) \text{ for somer } x \in \mathbb{R}^n\right\}$$

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We have also the following Spaces

Row Space

We have that the span of the row vectors of A form a subspace.

Column Space

We have that the span of the column vectors of A, also, form a subspace.

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From This

It can be shown that

$Ker\left(f\right)$ is a subspace of $\mathbb{R}^n$

Also

$Range\left(f\right)$ is a subspace of $\mathbb{R}^m$

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Outline

Assume the following

Let

$$\boldsymbol{e}_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{n\times 1}, \boldsymbol{e}_3 = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}_{n\times 1}, ..., \boldsymbol{e}_n = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}_{n\times 1}$$

Then any vector $x \in \mathbb{R}^n$

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = x_1 e_1 + x_2 e_2 + \dots + x_n e_n$$

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Then

Applying f

$$f(\boldsymbol{x}) = x_1 f(\boldsymbol{e}_1) + x_2 f(\boldsymbol{e}_2) + ... + x_n f(\boldsymbol{e}_n)$$

A linear combination of elements

$$\{f(\boldsymbol{e}_1), f(\boldsymbol{e}_2), ..., f(\boldsymbol{e}_n)\}$$

They are column vectors in $\mathbb{R}^m$

$$A = (f(\boldsymbol{e}_1) | f(\boldsymbol{e}_2) | ... | f(\boldsymbol{e}_n))_{m \times n}$$

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Thus, we have

Finally, we have

$$f(\boldsymbol{x}) = (f(\boldsymbol{e}_1)\,|f(\boldsymbol{e}_2)\,|...|f(\boldsymbol{e}_n))\,\boldsymbol{x} = A\boldsymbol{x}$$

Definition

- The matrix A defined above for the function f is called the matrix of f in the standard basis.

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Given an $m \times n$ matrix A

The set of all solutions to the homogeneous equation $A\boldsymbol{x}$

- It is a subspace V of $\mathbb{R}^n$.

$$A\boldsymbol{x} = 0$$

Remember how to prove the subspaces...

$$\boldsymbol{x}_2 + \boldsymbol{x}_2 \in V \text{ and } c\boldsymbol{x} \in V$$

- Do you remember?

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- This important subspace is called the null space of A, and is denoted $Null(A)$

It is also known as

$$x_H = \{x | Ax = 0\}$$

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Knowing that Range(f) and Ker(f) are sub-spaces

Which ones they are?

Any Idea?

Range(f)

The column space of the matrix A.

Ker(f)

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We have a nice theorem

Dimension Theorem

Let $f:\mathbb{R}^n \to \mathbb{R}^m$ be linear. Then

$$dim\left(domain\left(f\right)\right) = dim\left(Range\left(f\right)\right) + dim\left(Ker\left(f\right)\right)$$

Where

The dimension of V, written $dim(V)$, is the number of elements in any basis of V.

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Rank and Nullity of a Matrix

Definition

- The rank of the matrix A is the dimension of the row space of A, and is denoted $R(A)$.

Example

- The rank of $I_{n \times n}$ is n.

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Theorem

The rank of a matrix in Gauss-Jordan form is equal to the number of leading variables.

Proof

- In the G form of a matrix, every non-zero row has a leading 1, which is the only non-zero entry in its column.

Then

- No elementary row operation can zero out a leading 1, so these non-zero rows are linearly independent.

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Thus

We have

- Since all the other rows are zero, the dimension of the row space of the Gauss-Jordan form is equal to the number of leading 1's.

Finally

- This is the same as the number of leading variables. Q.E.D.

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About the Nullity of the Matrix

Definition

- The nullity of the matrix A is the dimension of the null space of A, and is denoted by $dim\left[N(A)\right]$.

Example

- The nullity of I is 0.

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Number of Free Variables

Theorem

The nullity of a matrix in Gauss-Jordan form is equal to the number of free variables.

Proof

- Suppose A is $m \times n$, and that the Gauss-Jordan form has j leading variables and k free variables:

$$j + k = n$$

Proof

Then, when computing the solution to the homogeneous equation

- We solve for the first j (leading) variables in terms of the remaining k free variables:

$$s_1, s_2, s_3, \ldots, s_k$$

Then

- Then the general solution to the homogeneous equation are:

$$s_1 v_1 + s_2 v_2 + s_3 v_3 + \cdots + s_k v_k$$

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Where

The vectors are the Canonical Ones

- Here, a trick!!!

Meaning in v_1, we have 1, after many 0

- It appears at position $j+1$, with zeros afterwards, and so on.

Therefore the vectors are linearly independents

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Therefore

They are a basis for the null space of A

And there are k of them, the same as the number of free variables.

Now

Definition

The matrix B is said to be row equivalent to A ($B \sim A$) if B can be obtained from A by a finite sequence of elementary row operations.

In matrix terms

$B \sim A \Leftrightarrow$ There exist elementary matrices such that

$$B = E_k E_{k-1} E_{k-1} \cdots E_1 A$$

If we write $C = E_k E_{k-1} E_{k-1} \cdots E_1$

B is row equivalent to A if $B = CA$ with C invertible.

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Then, we have

Theorem

If $B \sim A$, then $Null(B) = Null(A)$.

Theorem

If $B \sim A$, then the row space of B is identical to that of A.

Summarizing

Row operations change neither the row space nor the null space of A.

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Corollaries

Corollary 1

- If R is the Gauss-Jordan form of A, then R has the same null space and row space as A.

Corollary 2

- If $B \sim A$, then $R(B) = R(A)$, and $N(B) = N(A)$.

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Theorem

- The number of linearly independent rows of the matrix A is equal to the number of linearly independent columns of A.

Thus

- In particular, the rank of A is also equal to the number of linearly independent columns, and hence to the dimension of the column space of A.

Therefore

- The number of linearly independent columns of A is then just the number of leading entries in the Gauss-Jordan form of A which is, as we know, the same as the rank of A.

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Proof of the theorem (Dimension Theorem)

First

- The rank of A is the same as the rank of the Gauss-Jordan form of A which is equal to the number of leading entries in the Gauss-Jordan form.

Additionally

- The dimension of the null space is equal to the number of free variables in the reduced echelon (Gauss-Jordan) form of A.

Then

We know further that the number of free variables plus the number of leading entries is exactly the number of columns.

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Many Times

We want to obtain a maximum or a minimum of a cost function expressed in terms of matrices....

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Thus, this discussion is useful in Machine Learning.

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Basic Definition

Let $\psi(\boldsymbol{x}) = \boldsymbol{y}$

Where $\boldsymbol{y}$ is an m-element vector, and $\boldsymbol{x}$ is an n-element vector

Then, we define the derivative with respect to a vector

$$\frac{\partial y}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \frac{\partial y_m}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$

Basic Definition

Let $\psi(\boldsymbol{x}) = \boldsymbol{y}$

Where $\boldsymbol{y}$ is an m-element vector, and $\boldsymbol{x}$ is an n-element vector

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What is this

The Matrix denotes the $m \times n$ matrix of first order partial derivatives

- Such a matrix is called the Jacobian matrix of the transformation $\psi(\boldsymbol{x})$.

Then, we can get our first ideas on derivatives

- For Linear Transformations.

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Outline

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Derivative of $\boldsymbol{y} = A\boldsymbol{x}$

Theorem

- Let $\boldsymbol{y} = A\boldsymbol{x}$ where $\boldsymbol{y}$ is a $m \times 1$, $\boldsymbol{x}$ is a $n \times 1$, A is a $m \times n$ and A does not depend on $\boldsymbol{x}$, then

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} = A$$

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Proof

Each i^{th} element of $\boldsymbol{y}$ is given by

$$y_i = \sum_{k=1}^{N} a_{ik} x_k$$

We have that

$$\frac{\partial y_i}{\partial x_j} = a_{ij}$$

for all $i = 1, 2, ..., m$ and $j = 1, 2, ..., n$

Hence

$$\frac{\partial y}{\partial x} = A$$

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Outline

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Derivative of $\boldsymbol{y}^T A\boldsymbol{x}$

Theorem

- Let the scalar α be defined by

$$\alpha = \boldsymbol{y}^T A\boldsymbol{x}$$

where

$\boldsymbol{y}$ is a $m \times 1$, $\boldsymbol{x}$ is a $n \times 1$, A is a $m \times n$ and A does not depend on $\boldsymbol{x}$ and $\boldsymbol{y}$, then

$$\frac{\partial \alpha}{\partial \boldsymbol{x}} = \boldsymbol{y}^T A \text{ and } \frac{\partial \alpha}{\partial \boldsymbol{y}} = \boldsymbol{x}^T A^T$$

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Proof

Define

$$\boldsymbol{w}^T = \boldsymbol{y}^T A$$

Note

$$\alpha = \boldsymbol{w}^T \boldsymbol{x}$$

By the previous theorem

$$\frac{\partial \alpha}{\partial \boldsymbol{x}} = \boldsymbol{w}^T = \boldsymbol{y}^T A$$

In a similar way, you can prove the other statement.

Proof

Define

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$$\frac{\partial \alpha}{\partial x} = w^T = y^T A$$

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In a similar way, you can prove the other statement.

Outline

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What is it?

First than anything, we have a parametric model!!!

Here, we have an hyperplane as a model:

$$g(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + w_0 \tag{1}$$

Note: $\boldsymbol{w}^T \boldsymbol{x}$ is also know as dot product

In the case of $\mathbb{R}^2$

We have:

$$g(\boldsymbol{x}) = (w_1, w_2) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + w_0 = w_1 x_1 + w_2 x_2 + w_0 \tag{2}$$

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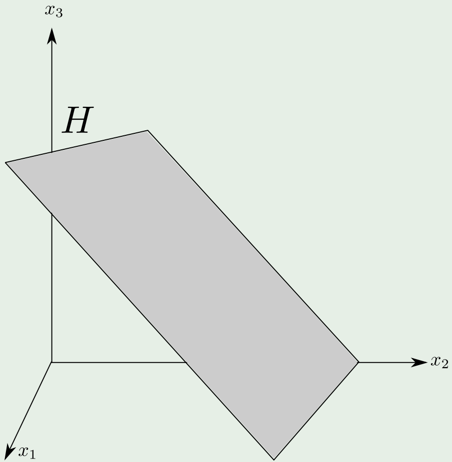
Example

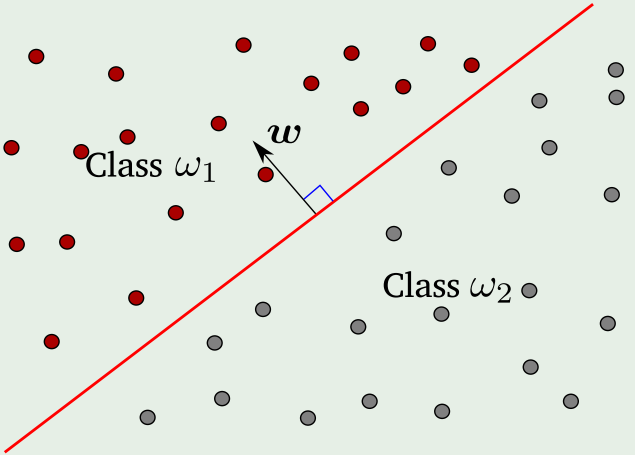
Hyperplane in $\mathbb{R}^3$



Outline

Splitting The Space $\mathbb{R}^2$

Using a simple straight line (Hyperplane)



Splitting the Space?

For example, assume the following vector $\boldsymbol{w}$ and constant w_0

$$\boldsymbol{w} = (-1, 2)^T \text{ and } w_0 = 0$$

Hyperplane

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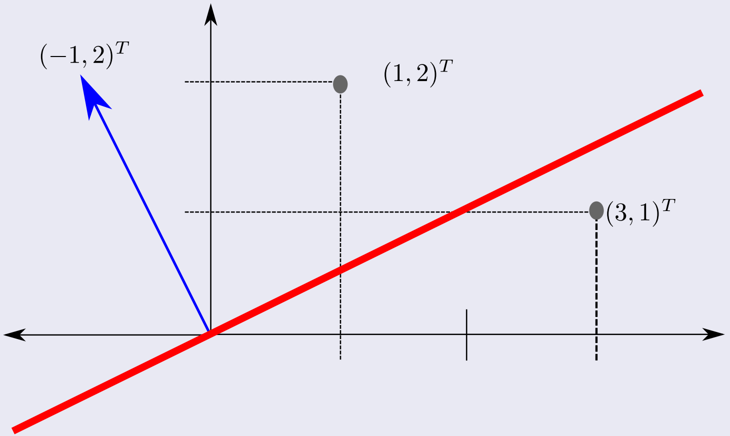

Then, we have

The following results

$$g\left(\left(\begin{array}{c}1\\2\end{array}\right)\right) = (-1,2)\left(\begin{array}{c}1\\2\end{array}\right) = -1\times 1 + 2\times 2 = 3$$

$$g\left(\left(\begin{array}{c}3\\1\end{array}\right)\right) = (-1,2)\left(\begin{array}{c}3\\1\end{array}\right) = -1\times 3 + 2\times 1 = -1$$

YES!!! We have a positive side and a negative side!!!

Outline

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The Decision Surface

The equation $g(x) = 0$ defines a decision surface

Separating the elements in classes, ω_1 and ω_2.

When $g(x)$ is linear the decision surface is an hyperplane

Now assume x_1 and x_2 are both on the decision surface

$$w^T x_1 + w_0 = 0$$
$$w^T x_2 + w_0 = 0$$

Thus

$$w^T x_1 + w_0 = w^T x_2 + w_0 \quad (3)$$

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Defining a Decision Surface

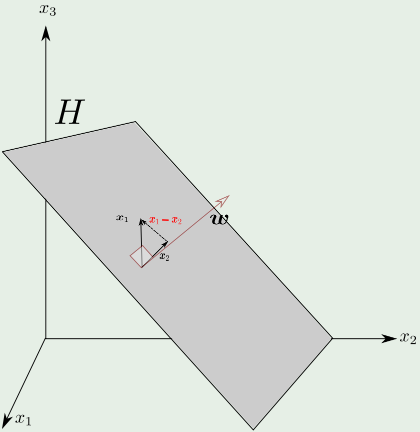
Then

$$\boldsymbol{w}^T \left(\boldsymbol{x}_1 - \boldsymbol{x}_2\right) = 0 \tag{4}$$

Therefore

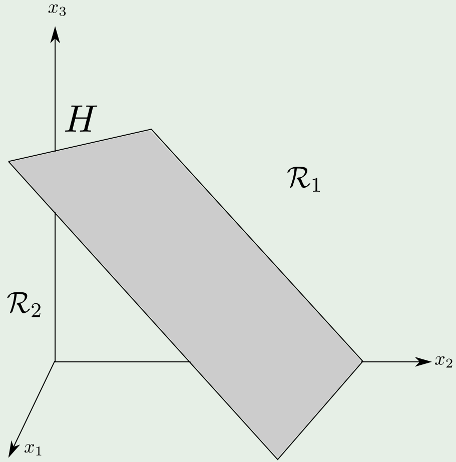
$\boldsymbol{x}_1 - \boldsymbol{x}_2$ lives in the hyperplane i.e. it is perpendicular to $\boldsymbol{w}^T$

- Remark: any vector in the hyperplane is a linear combination of elements in a basis
- **Therefore any vector in the plane is perpendicular to w^T**



Therefore

The space is split in two regions (Example in $\mathbb{R}^3$) by the hyperplane H



Outline

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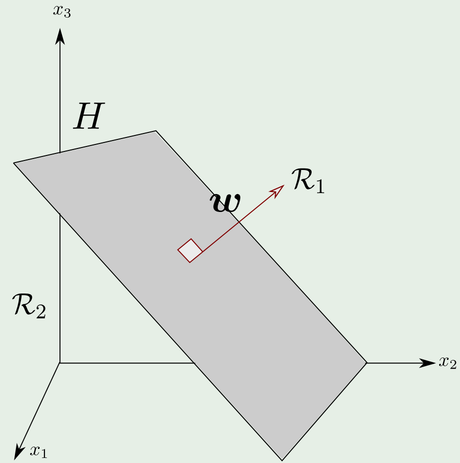
Some Properties of the Hyperplane

Given that $g(\boldsymbol{x}) > 0$ if $\boldsymbol{x} \in \mathcal{R}_1$



It is more

We can say the following

- Any $\boldsymbol{x} \in \mathcal{R}_1$ is on the positive side of H.
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In addition, $g(\boldsymbol{x})$ can give us a way to obtain the distance from $\boldsymbol{x}$ to the hyperplane H

First, we express any $\boldsymbol{x}$ as follows

$$\boldsymbol{x} = \boldsymbol{x}_p + r\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|}$$

- r is the desired distance
  - Positive, if $\boldsymbol{x}$ is in the positive side
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We have something like this

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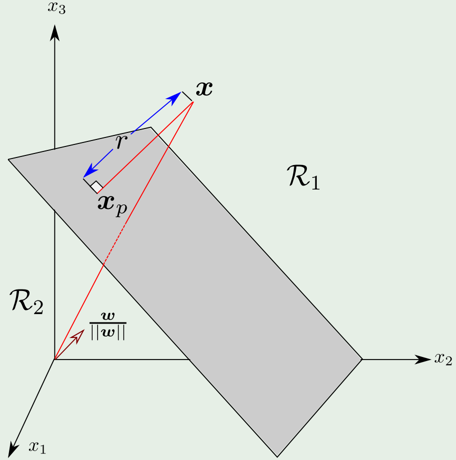

Now

Since $g(\boldsymbol{x}_p) = 0$

We have that

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g(\boldsymbol{x}) &= g\left(\boldsymbol{x}_p + r\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|}\right)\\
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&= \boldsymbol{w}^T\boldsymbol{x}_p + w_0 + r\frac{\boldsymbol{w}^T\boldsymbol{w}}{\|\boldsymbol{w}\|}\\
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In particular

The distance from the origin to H

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Remarks

- If $w_0 > 0$, the origin is on the positive side of H.
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- If $w_0 = 0$, the hyperplane has the homogeneous form $w^T x$ and hyperplane passes through the origin.

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Outline

We want to solve the independence of w_0

We would like w_0 as part of the dot product by making $x_0 = 1$

$$g(\boldsymbol{x}) = w_0 \times 1 + \sum_{i=1}^{d} w_i x_i = w_0 \times x_0 + \sum_{i=1}^{d} w_i x_i = \sum_{i=0}^{d} w_i x_i \quad (7)$$

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By making

$$x_{aug} = \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{pmatrix} = \begin{pmatrix} 1 \\ \boldsymbol{x} \end{pmatrix}$$

x_{aug} is called an augmented feature vector.

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In a similar way

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- The addition of a constant component to $\boldsymbol{x}$ preserves all the distance relationship between samples.
- The resulting x_{aug} vectors, all lie in a d-dimensional subspace which is the x-space itself.

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More Remarks

In addition

The hyperplane decision surface $\widehat{H}$ defined by

$$\boldsymbol{w}_{aug}^{T}\boldsymbol{x}_{aug} = 0$$

passes through the origin in $\boldsymbol{x}_{aug}$-space.

Even Though

The corresponding hyperplane H can be in any position of the x-space.

More Remarks

In addition

The hyperplane decision surface $\widehat{H}$ defined by

$$\boldsymbol{w}_{aug}^T \boldsymbol{x}_{aug} = 0$$

passes through the origin in $\boldsymbol{x}_{aug}$-space.

Even Though

The corresponding hyperplane H can be in any position of the $\boldsymbol{x}$-space.

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In addition

The distance from $\boldsymbol{y}$ to $\widehat{H}$ is:

$$\frac{\left|\boldsymbol{w}_{aug}^{T}\boldsymbol{x}_{aug}\right|}{\left\|\boldsymbol{w}_{aug}\right\|} = \frac{\left|g\left(\boldsymbol{x}_{aug}\right)\right|}{\left\|\boldsymbol{w}_{aug}\right\|}$$

Now

Is $\|\boldsymbol{w}\| \leq \|\boldsymbol{w}_{aug}\|$

- Ideas?

$$\sqrt{\sum_{i=1}^{d} w_i^2} \leq \sqrt{\sum_{i=1}^{d} w_i^2 + w_0^2}$$

This mapping is quite useful

Because we only need to find a weight vector w_{aug} instead of finding the weight vector w and the threshold w_0.

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Outline

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Initial Supposition

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n samples $\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n$ some labeled ω_1 and some labeled ω_2.

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A Simple Solution For Our Quandary

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Now, What?

Assume true function f is given by

$$y_{noise} = g_{noise}(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + w_0 + e \quad (8)$$

Where the e

It has a $e \sim N(\mu, \sigma^2)$

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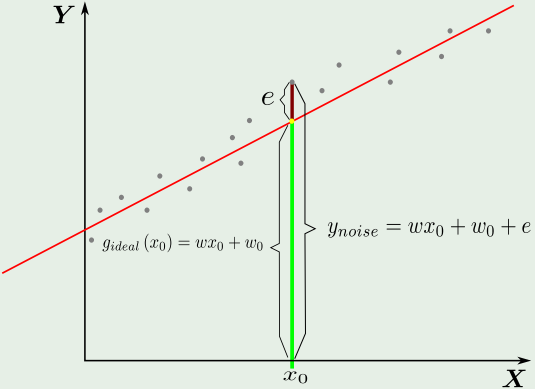

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A TRICK... Quite a good one!!! Instead of using y_{noise}

$$e = y_{noise} - g_{ideal}(\boldsymbol{x}) \tag{11}$$

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Outline

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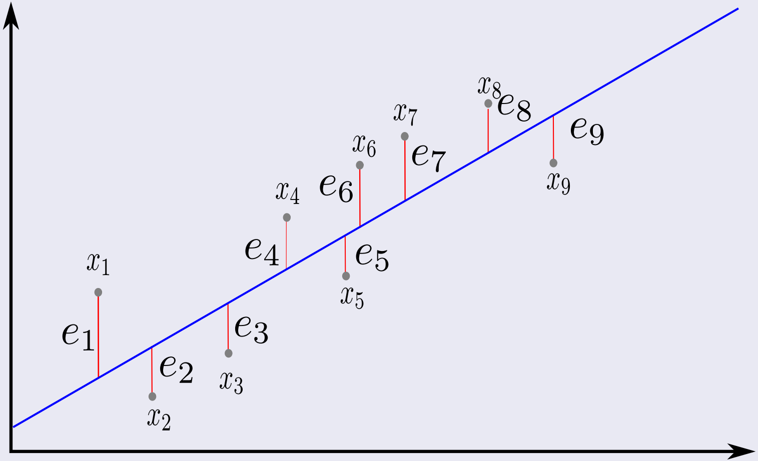
Here, we have multiple errors

What can we do?



Sum Over All the Errors

We can do the following

$$J(\boldsymbol{w}) = \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} \left(y_i - g_{ideal}(\boldsymbol{x}_i)\right)^2 \tag{13}$$

Remark: This is know as the Least Squared Error cost function

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We can use a trick

The following function

$$g_{ideal}\left(\boldsymbol{x}\right) = \begin{pmatrix} 1 & x_1 & x_2 & \dots & x_d \end{pmatrix} \begin{pmatrix} w_0 \\ w_2 \\ w_3 \\ \vdots \\ w_d \end{pmatrix} = \boldsymbol{x}^T \boldsymbol{w}$$

We can rewrite the error equation as

$$J\left(\boldsymbol{w}\right) = \sum_{i=1}^{N} \left(y_i - g_{ideal}\left(\boldsymbol{x}_i\right)\right)^2 = \sum_{i=1}^{N} \left(y_i - \boldsymbol{x}_i^T \boldsymbol{w}\right)^2 \quad (14)$$

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Furthermore

Then stacking all the possible estimations into the product Data Matrix and weight vector

$$\boldsymbol{X}\boldsymbol{w} = \begin{pmatrix} 1 & (\boldsymbol{x}_1)_1 & \cdots & (\boldsymbol{x}_1)_j & \cdots & (\boldsymbol{x}_1)_d \\ \vdots & & & \vdots & & \vdots \\ 1 & (\boldsymbol{x}_i)_1 & & (\boldsymbol{x}_i)_j & & (\boldsymbol{x}_i)_d \\ \vdots & & & \vdots & & \vdots \\ 1 & (\boldsymbol{x}_N)_1 & \cdots & (\boldsymbol{x}_N)_j & \cdots & (\boldsymbol{x}_N)_d \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_{d+1} \end{pmatrix}$$

Note about other representations

We could have $\boldsymbol{x}^T = (x_1, x_2, ..., x_d, 1)$ thus

$$\boldsymbol{X} = \begin{pmatrix} (\boldsymbol{x}_1)_1 & \cdots & (\boldsymbol{x}_1)_j & \cdots & (\boldsymbol{x}_1)_d & 1 \\ & & \vdots & & \vdots & \vdots \\ (\boldsymbol{x}_i)_1 & & (\boldsymbol{x}_i)_j & & (\boldsymbol{x}_i)_d & 1 \\ & & \vdots & & \vdots & \vdots \\ (\boldsymbol{x}_N)_1 & \cdots & (\boldsymbol{x}_N)_j & \cdots & (\boldsymbol{x}_N)_d & 1 \end{pmatrix} \quad (15)$$

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Then, we have the following trick with $\boldsymbol{X}$

With the Data Matrix

$$\boldsymbol{X}w = \begin{pmatrix} \boldsymbol{x}_1^T \boldsymbol{w} \\ \boldsymbol{x}_2^T \boldsymbol{w} \\ \boldsymbol{x}_3^T \boldsymbol{w} \\ \vdots \\ \boldsymbol{x}_N^T \boldsymbol{w} \end{pmatrix} \quad (16)$$

Therefore

We have that

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_4 \end{pmatrix} - \begin{pmatrix} \boldsymbol{x}_1^T \boldsymbol{w} \\ \boldsymbol{x}_2^T \boldsymbol{w} \\ \boldsymbol{x}_3^T \boldsymbol{w} \\ \vdots \\ \boldsymbol{x}_N^T \boldsymbol{w} \end{pmatrix} = \begin{pmatrix} y_1 - \boldsymbol{x}_1^T \boldsymbol{w} \\ y_2 - \boldsymbol{x}_2^T \boldsymbol{w} \\ y_3 - \boldsymbol{x}_3^T \boldsymbol{w} \\ \vdots \\ y_4 - \boldsymbol{x}_N^T \boldsymbol{w} \end{pmatrix}$$

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The following equality

$$\sum_{i=1}^{N}\left(y_i - \boldsymbol{x}_i^T\boldsymbol{w}\right)^2 = (\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w})^T(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w}) = \|\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w}\|_2^2 \tag{17}$$

We can expand our quadratic formula!!!

Thus

$$\left(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w}\right)^{T}\left(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{w}\right)=\boldsymbol{y}^{T}\boldsymbol{y}-\boldsymbol{y}^{T}\boldsymbol{X}\boldsymbol{w}-\boldsymbol{w}^{T}\boldsymbol{X}^{T}y+\boldsymbol{w}^{T}\boldsymbol{X}^{T}\boldsymbol{X}\boldsymbol{w} \quad (18)$$

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- Derive with respect to $\boldsymbol{w}$
- Assume that $X^{T}X$ is invertible

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Therefore

We have the following equivalences

$$\frac{d\boldsymbol{w}^T A\boldsymbol{w}}{d\boldsymbol{w}} = \boldsymbol{w}^T\left(A + A^T\right),\ \frac{d\boldsymbol{w}^T A}{d\boldsymbol{w}} = A^T \tag{19}$$

Now given that the transpose of a number is the number itself

$$y^T X w = \left[y^T X w\right]^T = w^T X^T y$$

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Then, when we derive by $\boldsymbol{w}$

We have then

$$\frac{d\left(\boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{w}^T\boldsymbol{X}^T y + \boldsymbol{w}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w}\right)}{d\boldsymbol{w}} = -2\boldsymbol{y}^T\boldsymbol{X} + \boldsymbol{w}^T\left(\boldsymbol{X}^T\boldsymbol{X} + \left(\boldsymbol{X}^T\boldsymbol{X}\right)\right)$$

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Making this equal to the zero row vector

$$-2y^T X + 2w^T\left(X^T X\right) = 0$$

$$\left[-2y^T X + 2w^T\left(X^T X\right)\right]^T$$

$$-2X^T y + 2\left(X^T X\right) w$$

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Solving for $\boldsymbol{w}$

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$$\boldsymbol{w} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y} \tag{20}$$

Note: $\boldsymbol{X}^T\boldsymbol{X}$ is always positive semi-definite. If it is also invertible, it is positive definite.

Thus, How we get the discriminant function?

Any Ideas?

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The Final Discriminant Function

Very Simple!!!

$$g(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{w} = \boldsymbol{x}^T \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{y} \tag{21}$$

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Outline

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Also Known as Karhunen-Loeve Transform

Setup

- Consider a data set of observations $\{\boldsymbol{x}_n\}$ with $n = 1, 2, ..., N$ and $\boldsymbol{x_n} \in R^d$.

Goal

Project data onto space with dimensionality $m < d$ (We assume m is given)

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Dimensional Variance

Remember the Variance Sample in $\mathbb{R}$

$$VAR(X) = \frac{\sum_{i=1}^{N} (x_i - \overline{x})^2}{N-1} \quad (22)$$

You can do the same in the case of two variables X and Y

$$COV(x, y) = \frac{\sum_{i=1}^{N} (x_i - \overline{x})(y_i - \overline{y})}{N-1} \quad (23)$$

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Now, Define

Given the data

$$\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_N \tag{24}$$

where $\boldsymbol{x}_i$ is a column vector

Construct the sample mean

$$\overline{\boldsymbol{x}} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x}_i \tag{25}$$

Center data

$$\boldsymbol{x}_1 - \overline{\boldsymbol{x}}, \boldsymbol{x}_2 - \overline{\boldsymbol{x}}, ..., \boldsymbol{x}_N - \overline{\boldsymbol{x}} \tag{26}$$

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Build the Sample Mean

The Covariance Matrix

$$S=\frac{1}{N-1}\sum_{i=1}^{N}\left(\boldsymbol{x}_i-\overline{\boldsymbol{x}}\right)\left(\boldsymbol{x}_i-\overline{\boldsymbol{x}}\right)^T \tag{27}$$

Properties

1. The ijth value of S is equivalent to σ_{ij}^2.
2. The iith value of S is equivalent to σ_{ii}^2.

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The Covariance Matrix

$$S=\frac{1}{N-1}\sum_{i=1}^{N}\left(\boldsymbol{x}_i-\overline{\boldsymbol{x}}\right)\left(\boldsymbol{x}_i-\overline{\boldsymbol{x}}\right)^T \tag{27}$$

Properties

1. The ijth value of S is equivalent to σ_{ij}^2.
2. The iith value of S is equivalent to σ_{ii}^2.

Outline

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Using S to Project Data

For this we use a u_1

- with $u_1^T u_1 = 1$, an orthonormal vector

Question

- What is the Sample Variance of the Projected Data?

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Thus we have

Variance of the projected data

$$\frac{1}{N-1}\sum_{i=1}^{N}\left[\boldsymbol{u}_1\boldsymbol{x}_i-\boldsymbol{u}_1\overline{\boldsymbol{x}}\right]=\boldsymbol{u}_1^T S\boldsymbol{u}_1 \tag{28}$$

Use Lagrange Multipliers to Maximize

$$\boldsymbol{u}_1^T S\boldsymbol{u}_1+\lambda_1\left(1-\boldsymbol{u}_1^T\boldsymbol{u}_1\right) \tag{29}$$

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Derive by $\boldsymbol{u}_1$

We get

$$S\boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1 \tag{30}$$

Then

$\boldsymbol{u}_1$ is an eigenvector of S.

If we left-multiply by $\boldsymbol{u}_1$

$$\boldsymbol{u}_1^T S \boldsymbol{u}_1 = \lambda_1 \tag{31}$$

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What about the second eigenvector $\boldsymbol{u}_2$

We have the following optimization problem

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\begin{aligned}
\max \quad & \boldsymbol{u}_2^T S \boldsymbol{u}_2 \\
\text{s.t.} \quad & \boldsymbol{u}_2^T \boldsymbol{u}_2 = 1 \\
& \boldsymbol{u}_2^T \boldsymbol{u}_1 = 0
\end{aligned}
$$

Lagrangian

$$
L\left(\boldsymbol{u}_2, \lambda_1, \lambda_2\right) = \boldsymbol{u}_2^T S \boldsymbol{u}_2 - \lambda_1 \left(\boldsymbol{u}_2^T \boldsymbol{u}_2 - 1\right) - \lambda_2 \left(\boldsymbol{u}_2^T \boldsymbol{u}_1 - 0\right)
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Explanation

First the constrained minimization

- We want to to maximize $\boldsymbol{u}_2^T S \boldsymbol{u}_2$

Given that the second eigenvector is orthonormal

- We have then $\boldsymbol{u}_2^T \boldsymbol{u}_2 = 1$

Under orthonormal vectors

- The covariance goes to zero
  $cov(\boldsymbol{u}_1, \boldsymbol{u}_2) = \boldsymbol{u}_2^T S \boldsymbol{u}_1 = \boldsymbol{u}_2 \lambda_1 \boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1^T \boldsymbol{u}_2 = 0$

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Meaning

The PCA's are perpendicular

$$L\left(\boldsymbol{u}_2, \lambda_1, \lambda_2\right) = \boldsymbol{u}_2^T S \boldsymbol{u}_2 - \lambda_1 \left(\boldsymbol{u}_2^T \boldsymbol{u}_2 - 1\right) - \lambda_2 \left(\boldsymbol{u}_2^T \boldsymbol{u}_1 - 0\right)$$

The the derivative with respect to $\boldsymbol{u}_2$

$$\frac{\partial L\left(\boldsymbol{u}_2, \lambda_1, \lambda_2\right)}{\partial \boldsymbol{u}_2} = S\boldsymbol{u}_2 - \lambda_1 \boldsymbol{u}_2 - \lambda_2 \boldsymbol{u}_1 = 0$$

Then, we left multiply $\boldsymbol{u}_1$

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Then, we have that

Something Notable

$$0 - 0 - \lambda_2 = 0$$

We have

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Implying

- $\boldsymbol{u}_2$ is the eigenvector of S with second largest eigenvalue λ_2.

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Thus

Variance will be the maximum when

$$u_1^T S u_1 = \lambda_1 \quad (32)$$

is set to the largest eigenvalue. Also know as the First Principal Component

By Induction

It is possible for M-dimensional space to define M eigenvectors $u_1, u_2, ..., u_M$ of the data covariance S corresponding to $\lambda_1, \lambda_2, ..., \lambda_M$ that maximize the variance of the projected data.

Computational Cost

1. Full eigenvector decomposition $O\left(d^3\right)$
2. Power Method $O\left(Md^2\right)$ "Golub and Van Loan, 1996)"
3. Use the Expectation Maximization Algorithm

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We have the following steps

Determine covariance matrix

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Generate the decomposition

$$S = U\Sigma U^T$$

With

- Eigenvalues in Σ and eigenvectors in the columns of U.

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Then

Project samples $\boldsymbol{x}_i$ into subspaces dim$=k$

$$z_i = U_K^T \boldsymbol{x}_i$$

- With U_k is a matrix with k columns

Outline

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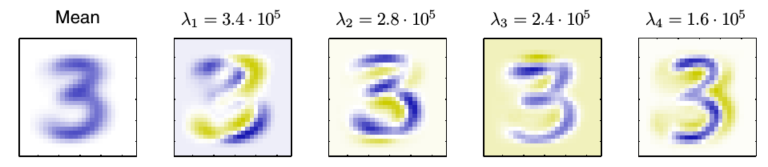
Example

From Bishop



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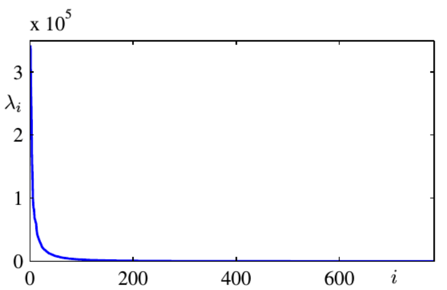

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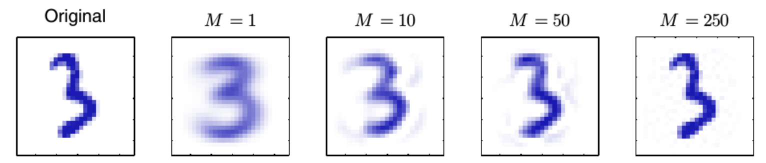

Outline

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What happened with no-square matrices

We can still diagonalize it

Thus, we can obtain certain properties.

We want to avoid the problems with

$$S^{-1}AS$$

The eigenvectors in S have three big problems

1. They are usually not orthogonal.
2. There are not always enough eigenvectors.
3. $Ax = \lambda x$ requires A to be square.

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Therefore, we can look at the following problem

We have a series of vectors

$$\{\boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_d\}$$

Then imagine a set of projection vectors and differences

$$\{\beta_1, \beta_2, ..., \beta_d\} \text{ and } \{\alpha_1, \alpha_2, ..., \alpha_d\}$$

We want to know a little bit of the relations between them

- After all, we are looking at the possibility of using them for our problem

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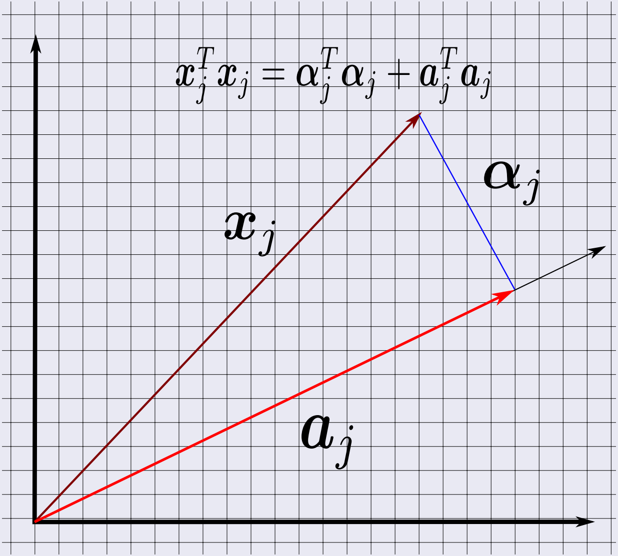
Using the Hypotenuse

A little bit of Geometry, we get



Therefore

We have two possible quantities for each j

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Then, we can minimize and maximize given that $x_j^T x_j$ is a constant

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\min \sum_{j=1}^{n} \alpha_j^T \alpha_j
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$$\max \sum_{j=1}^{n} \boldsymbol{a}_j^T \boldsymbol{a}_j$$

Actually this is know as the dual problem (Weak Duality)

An example of this

$$\begin{aligned} \min \ & \boldsymbol{w}^T\boldsymbol{x} \\ s.t \mathsf{A}\boldsymbol{x} \leq & \boldsymbol{b} \\ \boldsymbol{x} \geq & 0 \end{aligned}$$

Then, using what is know as slack variables

$$Ax + A'x = b$$

Each row lives in the column space, but the y_i lives in the column space

$$\left(Ax + A'x\right)_i \to y_i \text{ and } x' \geq 0$$

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Example

$$\begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Element in the column space of dimensionality have three dimensions

- But in the row space their dimension is 2

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Properties

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Stack such vectors that in the d-dimensional space

- In a matrix A of $n \times d$

$$A = \begin{bmatrix} \boldsymbol{a}_1^T \\ \boldsymbol{a}_2^T \\ \vdots \\ \boldsymbol{a}_n^T \end{bmatrix}$$

The matrix works as a Projection Matrix

- We are looking for a unit vector v such that length of the projection is maximized.

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The matrix works as a Projection Matrix

- We are looking for a unit vector $\boldsymbol{v}$ such that length of the projection is maximized.

Why? Do you remember the Projection to a single vector $\boldsymbol{p}$?

Definition of the projection under unitary vector

$$\boldsymbol{p} = \frac{\boldsymbol{v}^T \boldsymbol{a}_i}{\boldsymbol{v}^T \boldsymbol{v}} \boldsymbol{v} = \left[\boldsymbol{v}^T \boldsymbol{a}_i \right] \boldsymbol{v}$$

Therefore the length of the projected vector is

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Then

It is possible to ask to maximize the longitude of such vector (Singular Vector)

$$\boldsymbol{v}_1 = \arg \max_{\|\boldsymbol{v}\|=1} \|A\boldsymbol{v}\|$$

Then, we can define the following singular value

$$\sigma_1(A) = \|A\boldsymbol{v}_1\|$$

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Definition

- The **best-fit line problem** describes the problem of finding the best line for a set of data points, where the quality of the line is measured by the sum of squared (perpendicular) distances of the points to the line.
  - Remember, we are looking at the dual problem....

Generalization

- This can be transferred to higher dimensions: One can find the best-fit d-dimensional subspace, so the subspace which minimizes the sum of the squared distances of the points to the subspace

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Then, in a Greedy Fashion

The second singular vector $\boldsymbol{v}_2$

$$\boldsymbol{v}_2 = \arg \max_{\boldsymbol{v} \perp \boldsymbol{v}_1, \|\boldsymbol{v}\|=1} \|A\boldsymbol{v}\|$$

Them you go through this process

- Stop when we have found all the following vectors:

$$\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_r$$

As singular vectors and

$$\arg \max_{\substack{\boldsymbol{v} \perp \boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_r \\ \|\boldsymbol{v}\| = 1}} \|A\boldsymbol{v}\|$$

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Proving that the strategy is good

Theorem

- Let A be an $n \times d$ matrix where $\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_r$ are the singular vectors defined above. For $1 \leq k \leq r$, let V_k be the subspace spanned by $\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_k$. Then for each k, V_k is the best-fit k-dimensional subspace for A.

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Proof

For $k = 1$

- What about $k = 2$? Let W be a best-fit 2- dimensional subspace for A.

For any basis w_1, w_2 of W

- $|Aw_1|^2 + |Aw_2|^2$ is the sum of the squared lengths of the projections of the rows of A to W.

Now, choose a basis w_1, w_2 so that w_2 is perpendicular to v_1

- This can be a unit vector perpendicular to v_1 projection in W.

Proof

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- This can be a unit vector perpendicular to $\boldsymbol{v}_1$ projection in W.

Proof

For $k = 1$

- What about $k = 2$? Let W be a best-fit 2- dimensional subspace for A.

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Cinvestav

Do you remember $\boldsymbol{v}_1 = \arg\max_{\|\boldsymbol{v}\|=1} \|A\boldsymbol{v}\|$?

Therefore

$$|A\boldsymbol{w}_1|^2 \leq |A\boldsymbol{v}_1|^2 \text{ and } |A\boldsymbol{w}_2|^2 \leq |A\boldsymbol{v}_2|^2$$

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In a similar way for $k > 2$

- V_k is at least as good as W and hence is optimal.

Cinvestav

Do you remember $v_1 = \arg\max_{\|v\|=1} \|Av\|$?

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$$|Aw_1|^2 \leq |Av_1|^2 \text{ and } |Aw_2|^2 \leq |Av_2|^2$$

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Remarks

Every Matrix has a singular value decomposition

$$A = U\Sigma V^T$$

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Properties of the Singular Value Decomposition

First

The eigenvalues of the symmetric matrix $A^T A$ are equal to the square of the singular values of A

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Outline

Singular Value Decomposition as Sums

The singular value decomposition can be viewed as a sum of rank 1 matrices

$$A = A_1 + A_2 + ... + A_R \tag{34}$$

Why?

$$u_1 A = U \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_R \end{pmatrix} V^T = \begin{pmatrix} \boldsymbol{u}_1 & \boldsymbol{u}_2 & \cdots & \boldsymbol{u}_R \end{pmatrix} \begin{pmatrix} \sigma_1 \boldsymbol{v}_1^T \\ \sigma_2 \boldsymbol{v}_2^T \\ \vdots \\ \sigma_R \boldsymbol{v}_R^T \end{pmatrix}$$

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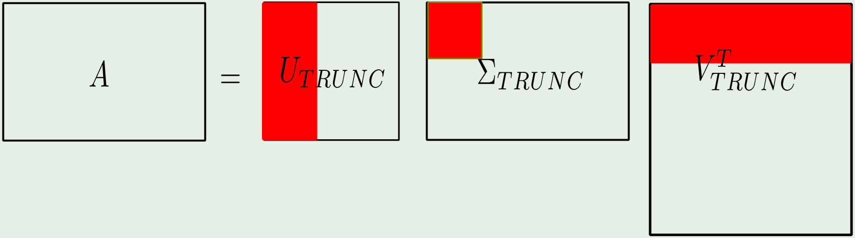
Truncating

Truncating the singular value decomposition allows us to represent the matrix with less parameters



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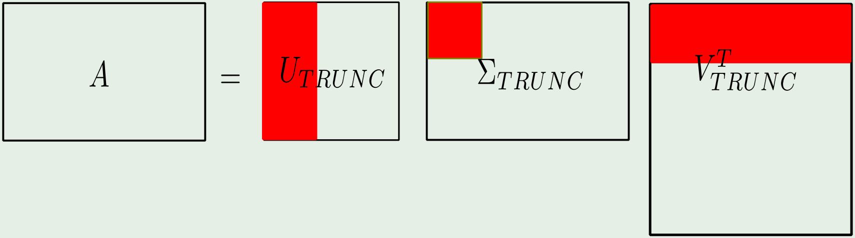

For a 512×512

- Full Representation $512 \times 512 = 262,144$
- Rank 10 approximation $512{\times}10 + 10 + 10 \times 512 = 10,250$
- Rank 40 approximation $512{\times}40 + 40 + 40 \times 512 = 41,000$
- Rank 80 approximation $512{\times}80 + 80 + 80 \times 512 = 82,000$

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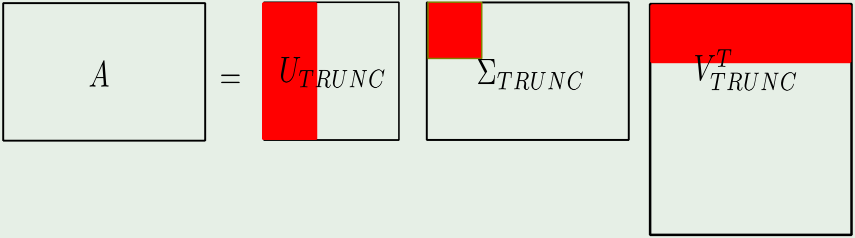

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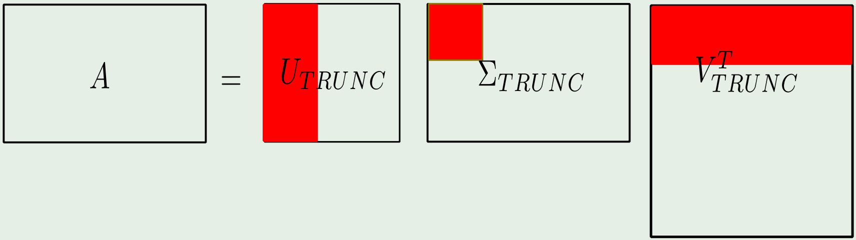

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