Chapter 7. Orthogonality and least squares

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Biomedical Engineering

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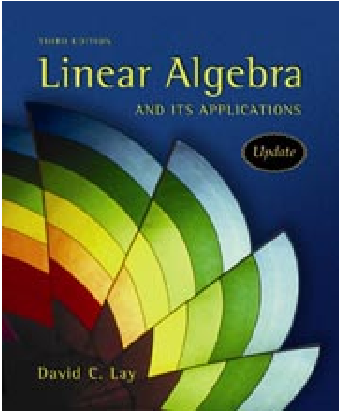
Outline

7. Orthogonality and least squares
   - Inner product, length and orthogonality (a)
   - Orthogonal sets, bases and matrices (a)
   - Orthogonal projections (b)
   - Gram-Schmidt orthogonalization (b)
   - Least squares (c)
   - Least-squares linear regression (c)
   - Inner product spaces (d)
   - Applications of inner product spaces (d)

References



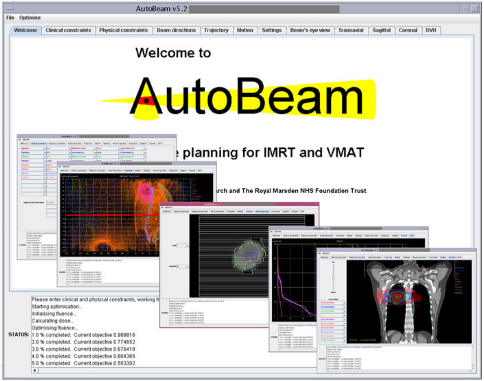
D. Lay. Linear algebra and its applications (3rd ed). Pearson (2006). Chapter 6.

A little bit of history

Least squares was first used to solve problems in geodesy (Andrien-Marie Legendre, 1805) and astronomy (Carl Friedrich Gauss, 1809). Gauss made the connection of this method to the distribution of measurement errors. Currently it is one of the best understood and most widely spread methods.


Applications

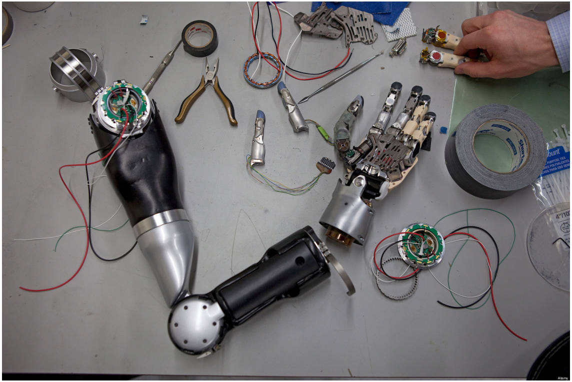
In this example Least Squares are used to plan a radiation therapy.



Bedford, J. L. *Sinogram analysis of aperture optimization by iterative least-squares in volumetric modulated arc therapy*. Physics in Medicine and Biology, **2013**, 58, 1235-1250

Applications

Traditionally, control applications were formulated in a least-squares setup. Currently, they have found more sophisticated goal functions that can be regarded as evolved versions of least squares.



Outline

7 Orthogonality and least squares

Inner product

Definition 1.1 (Inner product or dot product)

Let $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$ *be two vectors. The* ***inner product*** *or* ***dot product*** *between these two vectors is defined as*

$$\mathbf{u} \cdot \mathbf{v} = \langle \mathbf{u}, \mathbf{v} \rangle \triangleq \sum_{i=1}^{n} u_i v_i$$

Theorem 1.1

If we considered $\mathbf{u}$ *and* $\mathbf{v}$ *to be column vectors* ($\in \mathcal{M}_{n\times 1}$)*, then*

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^T \mathbf{v}$$

Example

Let $\mathbf{u} = (2, -5, -1)$ and $\mathbf{v} = (3, 2, -3)$.

$$\mathbf{u} \cdot \mathbf{v} = 2 \cdot 3 + (-5) \cdot 2 + 1 \cdot (-3) = -1$$

Inner product

Theorem 1.2

For any three vectors $\mathbf{u}, \mathbf{v}, \mathbf{w} \in \mathbb{R}^n$ *and any scalar* $r \in \mathbb{R}$ *it is verified that*

1. $\mathbf{u} \cdot \mathbf{v} = \mathbf{v} \cdot \mathbf{u}$
2. $(\mathbf{u} + \mathbf{v}) \cdot \mathbf{w} = \mathbf{u} \cdot \mathbf{w} + \mathbf{v} \cdot \mathbf{w}$
3. $(r\mathbf{u}) \cdot \mathbf{v} = r(\mathbf{u} \cdot \mathbf{v}) = \mathbf{u} \cdot (r\mathbf{v})$
4. $\mathbf{u} \cdot \mathbf{u} \geq 0$
5. $\mathbf{u} \cdot \mathbf{u} = 0 \Leftrightarrow \mathbf{u} = \mathbf{0}$

Corollary

$$(r_1\mathbf{u}_1 + r_2\mathbf{u}_2 + ... + r_p\mathbf{u}_p) \cdot \mathbf{v} = r_1(\mathbf{u}_1 \cdot \mathbf{v}) + r_2(\mathbf{u}_2 \cdot \mathbf{v}) + ... + r_p(\mathbf{u}_p \cdot \mathbf{v})$$

Length

Definition 1.2 (Length of a vector)

Given any vector $\mathbf{v}$*, its length is defined as*

$$\|\mathbf{v}\| \triangleq \sqrt{\mathbf{v} \cdot \mathbf{v}}$$

Theorem 1.3

Given any vector $\mathbf{v} \in \mathbb{R}^n$

$$\|\mathbf{v}\| = \sqrt{v_1^2 + v_2^2 + ... + v_n^2}$$

Example

The length of $\mathbf{v} = (1, -2, 2, 0)$ is

$$\|\mathbf{v}\| = \sqrt{1^2 + (-2)^2 + 2^2 + 0^2} = 3$$

Length

Theorem 1.4

For any vector $\mathbf{v}$ *and any scalar* r *it is verified that*

$$\|r\mathbf{v}\| = |r|\|\mathbf{v}\|$$

Proof
It will be given only for $\mathbf{v} \in \mathbb{R}^n$*:*

$$\begin{aligned} \|r\mathbf{v}\| &= \sqrt{(rv_1)^2 + (rv_2)^2 + \ldots + (rv_n)^2} = \sqrt{r^2(v_1^2 + v_2^2 + \ldots + v_n^2)} \\ &= \sqrt{r^2}\sqrt{v_1^2 + v_2^2 + \ldots + v_n^2} = |r|\|\mathbf{v}\| \end{aligned} \quad \textit{(q.e.d.)}$$

Example (continued)

Find a vector of unit length that has the same direction as $\mathbf{v} = (1, -2, 2, 0)$.
Solution

$$\mathbf{u}_{\mathbf{v}} = \frac{\mathbf{v}}{\|\mathbf{v}\|} = \left(\frac{1}{3}, -\frac{2}{3}, \frac{2}{3}, 0\right) \Rightarrow \|\mathbf{u}_{\mathbf{v}}\| = \sqrt{\frac{1}{9} + \frac{4}{9} + \frac{4}{9} + 0} = 1$$

Distance

Definition 1.3 (Distance in $\mathbb{R}$)

The distance between any two numbers $a, b \in \mathbb{R}$ can be defined as

$$d(a, b) = |a - b|$$

Example

Calculate the distance between 2 and 8 as well as between -3 and 4.

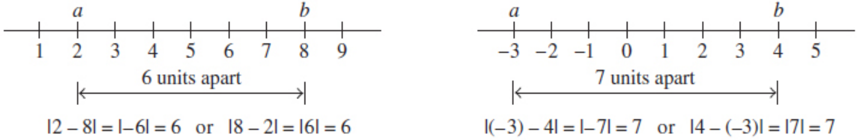


FIGURE 3 Distances in $\mathbb{R}$.

Distance

Definition 1.4 (Distance in $\mathbb{R}^n$)

The distance between any two vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$ *can be defined as*

$$d(\mathbf{u}, \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\|$$

Example

Calculate the distance between $\mathbf{u} = (7, 1)$ and $\mathbf{v} = (3, 2)$

$$d(\mathbf{u}, \mathbf{v}) = \|(7, 1) - (3, 2)\| = \|(4, -1)\| = \sqrt{4^2 + 1^2} = \sqrt{17}$$

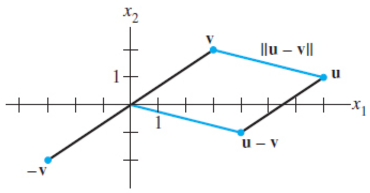


FIGURE 4 The distance between $\mathbf{u}$ and $\mathbf{v}$ is the length of $\mathbf{u} - \mathbf{v}$.

Distance

Example

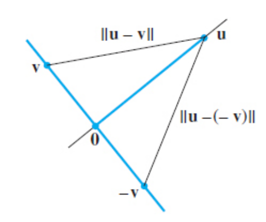
For any two vectors in $\mathbb{R}^3$, **u** and **v**, the distance can be calculated through

$$d(\mathbf{u},\mathbf{v}) = \|\mathbf{u}-\mathbf{v}\| = \|(u_1-v_1, u_2-v_2, u_3-v_3)\| = \sqrt{(u_1-v_1)^2+(u_2-v_2)^2+(u_3-v_3)^2}$$

Orthogonality

Example

Any two vectors in $\mathbb{R}^2$, $\mathbf{u}$ and $\mathbf{v}$, are orthogonal if $d(\mathbf{u},\mathbf{v}) = d(\mathbf{u},-\mathbf{v})$



$$d^2(\mathbf{u},\mathbf{v}) = \|\mathbf{u}-\mathbf{v}\|^2 = (\mathbf{u}-\mathbf{v})\cdot(\mathbf{u}-\mathbf{v}) = \mathbf{u}\cdot\mathbf{u}+\mathbf{v}\cdot\mathbf{v}-2\mathbf{u}\cdot\mathbf{v} = \|\mathbf{u}\|^2+\|\mathbf{v}\|^2-2\mathbf{u}\cdot\mathbf{v}$$
$$d^2(\mathbf{u},-\mathbf{v}) = \|\mathbf{u}+\mathbf{v}\|^2 = (\mathbf{u}+\mathbf{v})\cdot(\mathbf{u}+\mathbf{v}) = \mathbf{u}\cdot\mathbf{u}+\mathbf{v}\cdot\mathbf{v}+2\mathbf{u}\cdot\mathbf{v} = \|\mathbf{u}\|^2+\|\mathbf{v}\|^2+2\mathbf{u}\cdot\mathbf{v}$$

$$d^2(\mathbf{u},\mathbf{v}) = d^2(\mathbf{u},-\mathbf{v}) \Rightarrow -2\mathbf{u}\cdot\mathbf{v} = 2\mathbf{u}\cdot\mathbf{v} \Rightarrow \mathbf{u}\cdot\mathbf{v} = 0$$

Orthogonality

Definition 1.5 (Orthogonality between two vectors)

Any two different vectors, $\mathbf{u}$ *and* $\mathbf{v}$*, in a vector space* V *are* ***orthogonal*** *iff*

$$\mathbf{u} \cdot \mathbf{v} = 0$$

Corollary

$\mathbf{0}$ is orthogonal to any other vector.

Theorem 1.5 (Pythagorean theorem)

Any two vectors, $\mathbf{u}$ *and* $\mathbf{v}$*, in a vector space* V *are orthogonal iff*

$$\|\mathbf{u} + \mathbf{v}\|^2 = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2$$

Orthogonality

Definition 1.6 (Orthogonality between vector and vector space)

Let $\mathbf{u}$ *be a vector in a vector space* V *and* W *a vector subspace of* V*.* $\mathbf{u}$ *is* ***orthogonal*** *to* W *if* $\mathbf{u}$ *is orthogonal to all vectors in* W*. The set of all vectors orthogonal to* W *is denoted as* $W^{\perp}$ *(the* ***orthogonal complement*** *of* W*).*

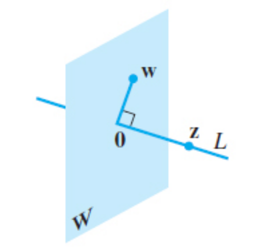
Example

Let W be a plane in $\mathbb{R}^3$ passing through the origin and L be a line, passing through the origin and perpendicular to W. For any vector $\mathbf{w} \in W$ and any vector $\mathbf{z} \in L$ we have

$$\mathbf{w} \cdot \mathbf{z} = 0$$

Therefore,

$$L = W^{\perp} \Leftrightarrow W = L^{\perp}$$



Orthogonality

Theorem 1.6

Let W be a vector subspace of a vector space V.

1. $\mathbf{x} \in W^{\perp}$ *iff* $\mathbf{x}$ *is orthogonal to every vector in a set that spans W.*
2. $W^{\perp}$ *is a vector subspace of V.*

Theorem 1.7

Let $A \in \mathcal{M}_{m\times n}$, then

1. $(\mathrm{Row}\{A\})^{\perp} = \mathrm{Nul}\{A\}$
2. $(\mathrm{Col}\{A\})^{\perp} = \mathrm{Nul}\{A^T\}$

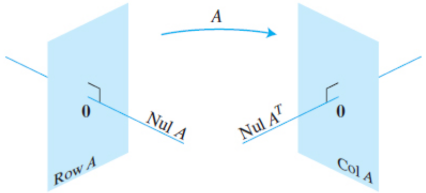


FIGURE 8 The fundamental subspaces determined by an $m \times n$ matrix A.

Orthogonality

Proof $\mathrm{Nul}\{A\} \subseteq (\mathrm{Row}\{A\})^{\perp}$

Consider the rows of A, $\mathbf{a}_i$ ($i = 1, 2, ..., m$) as column vectors, then for any vector $\mathbf{x} \in \mathrm{Nul}\{A\}$ we know

$$A\mathbf{x} = \mathbf{0} \Rightarrow \begin{pmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \dots \\ \mathbf{a}_m^T \end{pmatrix} \mathbf{x} = \begin{pmatrix} \mathbf{a}_1^T\mathbf{x} \\ \mathbf{a}_2^T\mathbf{x} \\ \dots \\ \mathbf{a}_m^T\mathbf{x} \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \cdot \mathbf{x} \\ \mathbf{a}_2 \cdot \mathbf{x} \\ \dots \\ \mathbf{a}_m \cdot \mathbf{x} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \dots \\ 0 \end{pmatrix}$$

Consequently, $\mathbf{x}$ is orthogonal to all the rows of A, which span $\mathrm{Row}\{A\}$ and by the previous theorem, $\mathbf{x} \in (\mathrm{Row}\{A\})^{\perp}$

Proof $\mathrm{Nul}\{A\} \supseteq (\mathrm{Row}\{A\})^{\perp}$

Conversely, let $\mathbf{x} \in (\mathrm{Row}\{A\})^{\perp}$, then by the previous theorem we know that

$$\mathbf{a}_i \cdot \mathbf{x} \quad \text{for } i = 1, 2, ..., m \Rightarrow A\mathbf{x} = \mathbf{0}$$

So, $\mathbf{x} \in \mathrm{Nul}\{A\}$

Orthogonality

Proof $(\mathrm{Col}\{A\})^{\perp} = \mathrm{Nul}\{A^T\}$

Let's define $B = A^T$. By the first part of this theorem, we know

$$(\mathrm{Row}\{B\})^{\perp} = \mathrm{Nul}\{B\} \Rightarrow (\mathrm{Row}\{A^T\})^{\perp} = \mathrm{Nul}\{A^T\} \Rightarrow (\mathrm{Col}\{A\})^{\perp} = \mathrm{Nul}\{A^T\}$$

Theorem 1.8

For any two vectors $\mathbf{u}$ *and* $\mathbf{v}$ *in a vector space* V*, the angle between the two can be measured through the dot product:*

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

Exercises

Exercises

From Lay (3rd ed.), Chapter 6, Section 1:

- 6.1.15
- 6.1.22
- 6.1.24
- 6.1.26
- 6.1.28
- 6.1.30
- 6.1.32 (computer)

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   - Inner product spaces (d)
   - Applications of inner product spaces (d)

Orthogonal sets

Definition 2.1 (Orthogonal set)

Let $S = \{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_p\}$ *be a set of vectors.* S *is an orthogonal set iff*

$$\mathbf{u}_i \cdot \mathbf{u}_j = 0 \quad \forall i, j \in \{1, 2, ..., p\} \; i \neq j$$

Example

Let $\mathbf{u}_1 = (3, 1, 1)$, $\mathbf{u}_2 = (-1, 2, 1)$, $\mathbf{u}_3 = (-\frac{1}{2}, -2, \frac{7}{2})$. Check whether the set $S = \{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$ is orthogonal.

Solution

$$\begin{aligned} \mathbf{u}_1 \cdot \mathbf{u}_2 &= 3 \cdot (-1) + 1 \cdot 2 + 1 \cdot 1 = 0 \\ \mathbf{u}_1 \cdot \mathbf{u}_3 &= 3 \cdot (-\tfrac{1}{2}) + 1 \cdot (-2) + 1 \cdot (\tfrac{7}{2}) = 0 \\ \mathbf{u}_2 \cdot \mathbf{u}_3 &= (-1) \cdot (-\tfrac{1}{2}) + 2 \cdot (-2) + 1 \cdot (\tfrac{7}{2}) = 0 \end{aligned}$$

Orthogonal sets

Theorem 2.1

If S is an orthogonal set of non-null vectors, then S is linearly independent and, consequently, it is a basis of the subspace spanned by S.

Proof

Let $\mathbf{u}_i$ $(i = 1, 2, ..., p)$ be the elements of S. Let us assume that S is linearly dependent. Then, there exists coefficients c_1, c_2, ..., c_p not all of them null such that

$$\mathbf{0} = c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + ... + c_p\mathbf{u}_p$$

Now, we compute the inner product with $\mathbf{u}_1$

$$\begin{gathered}\mathbf{0} \cdot \mathbf{u}_1 = (c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + ... + c_p\mathbf{u}_p) \cdot \mathbf{u}_1 \\ 0 = c_1(\mathbf{u}_1 \cdot \mathbf{u}_1) + c_2(\mathbf{u}_2 \cdot \mathbf{u}_1) + ... + c_p(\mathbf{u}_p \cdot \mathbf{u}_1) = c_1\|\mathbf{u}_1\|^2 \Rightarrow c_1 = 0\end{gathered}$$

Multiplying by $\mathbf{u}_i$ $(i = 2, 3, ..., p)$ we can show that all c_i's are 0, and, therefore, the set S is linearly independent.

Orthogonal basis

Definition 2.2 (Orthogonal basis)

A set of vectors B is an ortohogonal basis of a vector space V if it is an ortohogonal set and it is a basis of V.

Theorem 2.2

Let $\{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_p\}$ be an orthogonal basis for a vector space V, for each $\mathbf{x} \in V$ we have

$$\mathbf{x} = \frac{\mathbf{x} \cdot \mathbf{u_1}}{\|\mathbf{u}_1\|^2}\mathbf{u}_1 + \frac{\mathbf{x} \cdot \mathbf{u_2}}{\|\mathbf{u}_2\|^2}\mathbf{u}_2 + ... + \frac{\mathbf{x} \cdot \mathbf{u_p}}{\|\mathbf{u}_p\|^2}\mathbf{u}_p$$

Proof

If $\mathbf{x}$ is in V, then it can be expressed as a linear combination of the vectors in a basis of V

$$\mathbf{x} = c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + ... + c_p\mathbf{u}_p$$

Now, we calculate the dot product with $\mathbf{u}_1$

$$\mathbf{x} \cdot \mathbf{u}_1 = (c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + ... + c_p\mathbf{u}_p) \cdot \mathbf{u}_1 = c_1\|\mathbf{u}_1\|^2 \Rightarrow c_1 = \frac{\mathbf{x} \cdot \mathbf{u_1}}{\|\mathbf{u}_1\|^2}$$

Orthogonal basis

Example

Let $\mathbf{u}_1 = (3, 1, 1)$, $\mathbf{u}_2 = (-1, 2, 1)$, $\mathbf{u}_3 = (-\frac{1}{2}, -2, \frac{7}{2})$, and $B = \{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$ be an orthogonal basis of $\mathbb{R}^3$. Let $\mathbf{x} = (6, 1, -8)$. The coordinates of $\mathbf{x}$ in B are given by

$$\begin{array}{ccc} \mathbf{x} \cdot \mathbf{u}_1 = 11 & \mathbf{x} \cdot \mathbf{u}_2 = -12 & \mathbf{x} \cdot \mathbf{u}_1 = -33 \\ \|\mathbf{u}_1\|^2 = 11 & \|\mathbf{u}_2\|^2 = 6 & \|\mathbf{u}_3\|^2 = \frac{33}{2} \end{array}$$

$$\begin{aligned} \mathbf{x} &= \frac{11}{11}\mathbf{u}_1 + \frac{-12}{6}\mathbf{u}_2 + \frac{-33}{\frac{33}{2}}\mathbf{u}_3 \\ &= \mathbf{u}_1 - 2\mathbf{u}_2 - 2\mathbf{u}_3 \end{aligned}$$

The coordinates of $\mathbf{x}$ in the basis B are

$$[\mathbf{x}]_B = (1, -2, -2)$$

Orthogonal projections

Orthogonal projection onto a vector

Consider a vector $\mathbf{y}$ and another one $\mathbf{u}$. Let us assume we want to decompose $\mathbf{y}$ as the sum of two orthogonal vectors $\hat{\mathbf{y}}$ (along the direction of $\mathbf{u}$) and another vector $\mathbf{z}$ (orthogonal to $\mathbf{u}$):

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z} = \alpha\mathbf{u} + \mathbf{z} \Rightarrow$$
$$\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}$$

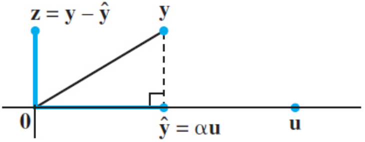


FIGURE 2

Finding α to make $\mathbf{y} - \hat{\mathbf{y}}$ orthogonal to $\mathbf{u}$.

We need to find α that makes $\mathbf{u}$ and $\mathbf{z}$ orthogonal.

$$0 = \mathbf{z} \cdot \mathbf{u} = (\mathbf{y} - \alpha\mathbf{u}) \cdot \mathbf{u} = \mathbf{y} \cdot \mathbf{u} - \alpha\|\mathbf{u}\|^2 \Rightarrow \alpha = \frac{\mathbf{y}\cdot\mathbf{u}}{\|\mathbf{u}\|^2}$$

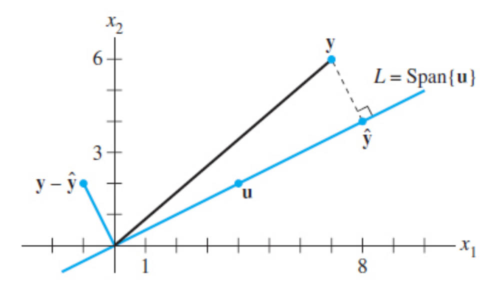
$\hat{\mathbf{y}}$ is the **orthogonal projection** of $\mathbf{y}$ onto $\mathbf{u}$.

Orthogonal projections

Example

Let $\mathbf{y} = (7, 6)$ and $\mathbf{u} = (4, 2)$. Then,

$$\left.\begin{array}{r} \mathbf{y} \cdot \mathbf{u} = 40 \\ \|\mathbf{u}\|^2 = 20 \end{array}\right\} \Rightarrow \quad \begin{array}{c} \hat{\mathbf{y}} = \frac{\mathbf{y} \cdot \mathbf{u}}{\|\mathbf{u}\|^2}\mathbf{u} = \frac{40}{20}\mathbf{u} = 2\mathbf{u} = \begin{pmatrix} 8 \\ 4 \end{pmatrix} \\ \mathbf{z} = \mathbf{y} - \hat{\mathbf{y}} = \begin{pmatrix} 7 \\ 6 \end{pmatrix} - \begin{pmatrix} 8 \\ 4 \end{pmatrix} = \begin{pmatrix} -1 \\ 2 \end{pmatrix} \\ d(\mathbf{y}, \hat{\mathbf{y}}) = \|\mathbf{y} - \hat{\mathbf{y}}\| = \|\mathbf{z}\| = \sqrt{(-1)^2 + 2^2} = \sqrt{5} \end{array}$$



Orthonormal set

Definition 2.3 (Orthonormal set)

$\{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_p\}$ *is an* ***orthonormal set*** *if it is an orthogonal set and all* $\mathbf{u}_i$ *vectors have unit length.*

Example

Show that the set $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$ is orthonormal, with

$$\mathbf{u}_1 = \frac{1}{\sqrt{11}}\begin{pmatrix}3\\1\\1\end{pmatrix} \quad \mathbf{u}_2 = \frac{1}{\sqrt{6}}\begin{pmatrix}-1\\2\\1\end{pmatrix} \quad \mathbf{u}_3 = \frac{1}{\sqrt{66}}\begin{pmatrix}-1\\-4\\7\end{pmatrix}$$

Solution

Let's check that they are orthogonal:

$$\begin{aligned}
\mathbf{u}_1 \cdot \mathbf{u}_2 &= \frac{1}{\sqrt{11}}\frac{1}{\sqrt{6}}(3\cdot(-1) + 1\cdot 2 + 1\cdot 1) = 0\\
\mathbf{u}_1 \cdot \mathbf{u}_3 &= \frac{1}{\sqrt{11}}\frac{1}{\sqrt{66}}(3\cdot(-1) + 1\cdot(-4) + 1\cdot 7) = 0\\
\mathbf{u}_2 \cdot \mathbf{u}_3 &= \frac{1}{\sqrt{6}}\frac{1}{\sqrt{66}}((-1)\cdot(-1) + (2)\cdot(-4) + (1)\cdot 7) = 0
\end{aligned}$$

Orthonormal set

Example (continued)

Now, let's check that they have unit length:

$$\|\mathbf{u}_1\| = \sqrt{\left(\frac{1}{\sqrt{11}}\right)^2 (3^2 + 1^2 + 1^2)} = \sqrt{\frac{9+1+1}{11}} = 1$$

$$\|\mathbf{u}_2\| = \sqrt{\left(\frac{1}{\sqrt{6}}\right)^2 ((-1)^2 + 2^2 + 1^2)} = \sqrt{\frac{1+4+1}{6}} = 1$$

$$\|\mathbf{u}_3\| = \sqrt{\left(\frac{1}{\sqrt{66}}\right)^2 ((-1)^2 + (-4)^2 + 7^2)} = \sqrt{\frac{1+16+49}{66}} = 1$$

Theorem 2.3

If $S = \{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n\}$ *is an orthonormal set, then it is an orthonormal basis of* $\mathrm{Span}\{S\}$.

Example

$\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\}$ is an orthonormal basis of $\mathbb{R}^n$.

Orthonormal basis

Theorem 2.4

Let $S = \{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_n\}$ *is an orthogonal set of vectors, then the set* $S' = \{\mathbf{u}'_1, \mathbf{u}'_2, ..., \mathbf{u}'_n\}$ *where*

$$\mathbf{u}'_i = \frac{\mathbf{u}_i}{\|\mathbf{u}_i\|}$$

is a orthonormal set (this operation is called ***vector normalization****).*

Proof

Let's check that the $\mathbf{u}'_i$ *vectors are orthogonal:*

$$\mathbf{u}'_i \cdot \mathbf{u}'_j = \frac{\mathbf{u}_i}{\|\mathbf{u}_i\|} \cdot \frac{\mathbf{u}_j}{\|\mathbf{u}_j\|} = \frac{1}{\|\mathbf{u}_i\|\|\mathbf{u}_j\|}\mathbf{u}_i \cdot \mathbf{u}_j$$

But this product is obviusly 0 because the $\mathbf{u}_i$ *vectors are orthogonal. Let's check now that the* $\mathbf{u}'_i$ *vectors have unit length:*

$$\|\mathbf{u}'_i\| = \left\| \frac{\mathbf{u}_i}{\|\mathbf{u}_i\|} \right\| = \frac{\|\mathbf{u}_i\|}{\|\mathbf{u}_i\|} = 1$$

Orthonormal matrix

Theorem 2.5

Let $U \in \mathcal{M}_{m\times n}$ be a square matrix. The columns of U form an orthonormal set iff

$$U^T U = I_n$$

*It is said that U is an **orthonormal matrix**.*

Proof

Let's consider the columns of U

$$U = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_n \end{pmatrix}$$

Let's calculate now $U^T U$

$$U^T U = \begin{pmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \dots \\ \mathbf{u}_n^T \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_n \end{pmatrix} = \begin{pmatrix} \mathbf{u}_1^T\mathbf{u}_1 & \mathbf{u}_1^T\mathbf{u}_2 & \dots & \mathbf{u}_1^T\mathbf{u}_n \\ \mathbf{u}_2^T\mathbf{u}_1 & \mathbf{u}_2^T\mathbf{u}_2 & \dots & \mathbf{u}_2^T\mathbf{u}_n \\ \dots & \dots & \dots & \dots \\ \mathbf{u}_n^T\mathbf{u}_1 & \mathbf{u}_n^T\mathbf{u}_2 & \dots & \mathbf{u}_n^T\mathbf{u}_n \end{pmatrix}$$

The condition $U^T U = I_n$ simply states $\left\{ \begin{array}{ll} \mathbf{u}_i^T\mathbf{u}_j = 0 & i \neq j \\ \mathbf{u}_i^T\mathbf{u}_j = 1 & i = j \end{array} \right.$, which is the definition of an orthonormal set.

Orthonormal matrix

Theorem 2.6

Let $U \in \mathcal{M}_{n\times n}$ *be an orthonormal matrix and* $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, *then*

1. $\|U\mathbf{x}\| = \|\mathbf{x}\|$
2. $(U\mathbf{x}) \cdot (U\mathbf{y}) = \mathbf{x} \cdot \mathbf{y}$
3. $(U\mathbf{x}) \cdot (U\mathbf{y}) = 0 \Leftrightarrow \mathbf{x} \cdot \mathbf{y} = 0$

Example

Let $U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{2}{3} \\ \frac{1}{\sqrt{2}} & -\frac{2}{3} \\ 0 & \frac{1}{3} \end{pmatrix}$ and $\mathbf{x} = \begin{pmatrix} \sqrt{2} \\ 3 \end{pmatrix}$.

U is an orthonormal matrix because

$$U^T U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{2}{3} & -\frac{2}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{2}{3} \\ \frac{1}{\sqrt{2}} & -\frac{2}{3} \\ 0 & \frac{1}{3} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Orthonormal matrix

Example (continued)

Let's calculate now $U\mathbf{x}$

$$U\mathbf{x} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{2}{3} \\ \frac{1}{\sqrt{2}} & -\frac{2}{3} \\ 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} \sqrt{2} \\ 3 \end{pmatrix} = \begin{pmatrix} 3 \\ -1 \\ 1 \end{pmatrix}$$

Let's check now that $\|U\mathbf{x}\| = \|\mathbf{x}\|$

$$\|U\mathbf{x}\| = \|(3,-1,1)\| = \sqrt{3^2 + (-1)^2 + 1^2} = \sqrt{11}$$
$$\|\mathbf{x}\| = \left\|(\sqrt{2},3)\right\| = \sqrt{(\sqrt{2})^2 + 3^2} = \sqrt{11}$$

Theorem 2.7

Let U be an orthonormal and square matrix. Then,

1. $U^{-1} = U^T$
2. U^T *is also an orthonormal matrix (i.e., the rows of U also form an orthonormal set of vectors).*

Exercises

Exercises

From Lay (3rd ed.), Chapter 6, Section 2:

- 6.2.1
- 6.2.10
- 6.2.15
- 6.2.25
- 6.2.26
- 6.2.29
- 6.2.35 (computer)

Outline

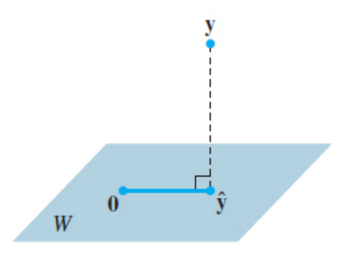
7. Orthogonality and least squares
   - Inner product, length and orthogonality (a)
   - Orthogonal sets, bases and matrices (a)
   - Orthogonal projections (b)
   - Gram-Schmidt orthogonalization (b)
   - Least squares (c)
   - Least-squares linear regression (c)
   - Inner product spaces (d)
   - Applications of inner product spaces (d)

Orthogonal projections

Definition 3.1 (Orthogonal projection)

The orthogonal projection of a point $\mathbf{y}$ *onto a vector subspace* W *is a point* $\hat{\mathbf{y}} \in W$ *such that*

$$\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}$$
$$\mathbf{z} \perp W$$



Orthogonal projections

Example

Let $\{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_5\}$ be an orthogonal basis of $\mathbb{R}^5$. Consider the subspace $W = \text{Span}\{\mathbf{u}_1, \mathbf{u}_2\}$. Given any vector $\mathbf{y} \in \mathbb{R}^5$, we can decompose it as the sum of a vector in W and a vector perpendicular to W

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z}$$

Solution

If $\{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_5\}$ is a basis of $\mathbb{R}^5$, then any vector $\mathbf{y} \in \mathbb{R}^5$ can be written as

$$\mathbf{y} = c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + ... + c_5\mathbf{u}_5$$

We may decompose this sum as

$$\hat{\mathbf{y}} = c_1\mathbf{u}_1 + c_2\mathbf{u}_2$$
$$\mathbf{z} = c_3\mathbf{u}_3 + c_4\mathbf{u}_4 + c_5\mathbf{u}_5$$

Orthogonal projections

Example (continued)

It is obvious that $\hat{\mathbf{y}} \in W$. Now we need to show that $\mathbf{z} \in W^{\perp}$. For doing so, we will show that

$$\begin{aligned} \mathbf{z} \cdot \mathbf{u}_1 = 0 \\ \mathbf{z} \cdot \mathbf{u}_2 = 0 \end{aligned}$$

To show the first equation we note that

$$\begin{aligned} \mathbf{z} \cdot \mathbf{u}_1 &= (c_3\mathbf{u}_3 + c_4\mathbf{u}_4 + c_5\mathbf{u}_5) \cdot \mathbf{u}_1 \\ &= c_3(\mathbf{u}_3 \cdot \mathbf{u}_1) + c_4(\mathbf{u}_4 \cdot \mathbf{u}_1) + c_5(\mathbf{u}_5 \cdot \mathbf{u}_1) \\ &= c_3 \cdot 0 + c_4 \cdot 0 + c_5 \cdot 0 \\ &= 0 \end{aligned}$$

We would proceed analogously for $\mathbf{z} \cdot \mathbf{u}_2 = 0$.

Orthogonal projections

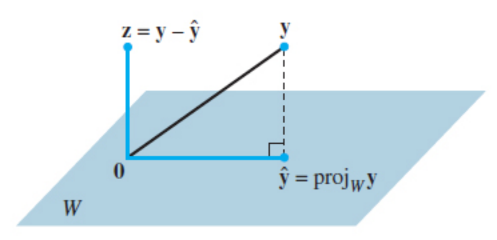
Theorem 3.1 (Orthogonal Decomposition Theorem)

Let W be a vector subspace of a vector space V. Then, any vector $\mathbf{y} \in V$ can be written uniquely as

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z}$$

with $\hat{\mathbf{y}} \in W$ and $\mathbf{z} \in W^{\perp}$. In fact, if $\{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_p\}$ is an orthogonal basis of W, then

$$\hat{\mathbf{y}} = \frac{\mathbf{y}\cdot\mathbf{u}_1}{\|\mathbf{u}_1\|^2}\mathbf{u}_1 + \frac{\mathbf{y}\cdot\mathbf{u}_2}{\|\mathbf{u}_2\|^2}\mathbf{u}_2 + ... + \frac{\mathbf{y}\cdot\mathbf{u}_p}{\|\mathbf{u}_p\|^2}\mathbf{u}_p$$



Orthogonal projections

Proof

$\hat{\mathbf{y}}$ is obviously in W since it has been written as a linear combination of vectors in a basis of W. $\mathbf{z}$ is perpendicular to W because

$$\begin{array}{rcl}
\mathbf{z}\cdot\mathbf{u}_1 & = & \left(\mathbf{y} - \left(\frac{\mathbf{y}\cdot\mathbf{u}_1}{\|\mathbf{u}_1\|^2}\mathbf{u}_1 + \frac{\mathbf{y}\cdot\mathbf{u}_2}{\|\mathbf{u}_2\|^2}\mathbf{u}_2 + \ldots + \frac{\mathbf{y}\cdot\mathbf{u}_p}{\|\mathbf{u}_p\|^2}\mathbf{u}_p\right)\right)\cdot\mathbf{u}_1 \\
& = & \mathbf{y}\cdot\mathbf{u}_1 - \frac{\mathbf{y}\cdot\mathbf{u}_1}{\|\mathbf{u}_1\|^2}(\mathbf{u}_1\cdot\mathbf{u}_1) - \frac{\mathbf{y}\cdot\mathbf{u}_2}{\|\mathbf{u}_2\|^2}(\mathbf{u}_2\cdot\mathbf{u}_1) - \ldots - \frac{\mathbf{y}\cdot\mathbf{u}_p}{\|\mathbf{u}_p\|^2}(\mathbf{u}_p\cdot\mathbf{u}_1) \\
& & [\{\mathbf{u}_i\} \text{ is an orthogonal set}] \\
& = & \mathbf{y}\cdot\mathbf{u}_1 - \frac{\mathbf{y}\cdot\mathbf{u}_1}{\|\mathbf{u}_1\|^2}(\mathbf{u}_1\cdot\mathbf{u}_1) \\
& = & \mathbf{y}\cdot\mathbf{u}_1 - \frac{\mathbf{y}\cdot\mathbf{u}_1}{\|\mathbf{u}_1\|^2}\|\mathbf{u}_1\|^2 \\
& = & \mathbf{y}\cdot\mathbf{u}_1 - \mathbf{y}\cdot\mathbf{u}_1 \\
& = & 0
\end{array}$$

We could proceed analogously for all elements in the basis of W.

Orthogonal projections

We need to show now that the decomposition is unique. Let us assume that it is not unique. Consequently, there exist different vectors such that

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z}$$
$$\mathbf{y} = \hat{\mathbf{y}}' + \mathbf{z}'$$

We subtract both equations

$$\mathbf{0} = (\hat{\mathbf{y}} - \hat{\mathbf{y}}') + (\mathbf{z} - \mathbf{z}') \Rightarrow \hat{\mathbf{y}} - \hat{\mathbf{y}}' = \mathbf{z}' - \mathbf{z}$$

Let $\mathbf{v} = \hat{\mathbf{y}} - \hat{\mathbf{y}}'$. It is obvious that $\mathbf{v} \in W$ because it is written as a linear combination of vectors in W. On the other side, $\mathbf{v} = \mathbf{z}' - \mathbf{z}$, i.e., it is a linear combination of vectors in $W^\perp$, so $\mathbf{v} \in W^\perp$. The only vector that belongs to W and $W^\perp$ at the same time is

$$\mathbf{v} = \mathbf{0} \Rightarrow \left\{ \begin{array}{l} \hat{\mathbf{y}} = \hat{\mathbf{y}}' \\ \mathbf{z} = \mathbf{z}' \end{array} \right. .$$

and consequently, the orthogonal decomposition is unique. Additionally, the uniqueness of the decomposition depends only on W and not on the particular basis chosen for W.

Orthogonal projections

Example

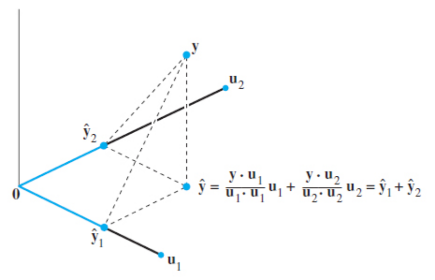
Let $\mathbf{u}_1 = (2, 5, -1)$ and $\mathbf{u}_2 = (-2, 1, 1)$. Let W be the subspace spanned by $\mathbf{u}_1$ and $\mathbf{u}_2$. Let $\mathbf{y} = (1, 2, 3) \in \mathbb{R}^3$. The orthogonal projection of $\mathbf{y}$ onto W is

$$\begin{aligned}
\hat{\mathbf{y}} &= \frac{\mathbf{y}\cdot\mathbf{u}_1}{\|\mathbf{u}_1\|^2}\mathbf{u}_1 + \frac{\mathbf{y}\cdot\mathbf{u}_2}{\|\mathbf{u}_2\|^2}\mathbf{u}_2 \\
&= \frac{1\cdot 2+2\cdot 5+3\cdot(-1)}{2^2+5^2+(-1)^2}\begin{pmatrix} 2 \\ 5 \\ -1 \end{pmatrix} + \frac{1\cdot(-2)+2\cdot 1+3\cdot 1}{(-2)^2+1^2+1^2}\begin{pmatrix} -2 \\ 1 \\ 1 \end{pmatrix} \\
&= \frac{9}{30}\begin{pmatrix} 2 \\ 5 \\ -1 \end{pmatrix} + \frac{15}{30}\begin{pmatrix} -2 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -\frac{2}{5} \\ 2 \\ \frac{1}{5} \end{pmatrix} \\
\mathbf{z} &= \mathbf{y} - \hat{\mathbf{y}} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} - \begin{pmatrix} -\frac{2}{5} \\ 2 \\ \frac{1}{5} \end{pmatrix} = \begin{pmatrix} \frac{7}{5} \\ 0 \\ \frac{14}{5} \end{pmatrix}
\end{aligned}$$

Orthogonal projections

Geometrical interpretation

$\hat{\mathbf{y}}$ can be understood as the sum of the orthogonal projection of $\mathbf{y}$ onto each one of the elements of the basis of W.



Theorem 3.2

If $\mathbf{y}$ belongs to W, then the orthogonal projection of $\mathbf{y}$ onto W is itself:

$$\hat{\mathbf{y}} = \mathbf{y}$$

Properties of orthogonal projections

Theorem 3.3 (Best approximation theorem)

The orthogonal projection of $\mathbf{y}$ *onto* W *is the point in* W *with minimum distance to* $\mathbf{y}$, *i.e.,*

$$\|\mathbf{y} - \hat{\mathbf{y}}\| \leq \|\mathbf{y} - \mathbf{v}\|$$

for all $\mathbf{v} \in W, \mathbf{v} \neq \hat{\mathbf{y}}$.

Proof

We know that $\mathbf{y} - \hat{\mathbf{y}}$ *is orthogonal to* W. *For any vector* $\mathbf{v} \in W, \mathbf{v} \neq \hat{\mathbf{y}}$, *we have that* $\hat{\mathbf{y}} - \mathbf{v}$ *is in* W. *Now consider the orthogonal decomposition of the vector* $\mathbf{y} - \mathbf{v}$

$$\mathbf{y} - \mathbf{v} = (\mathbf{y} - \hat{\mathbf{y}}) + (\hat{\mathbf{y}} - \mathbf{v})$$

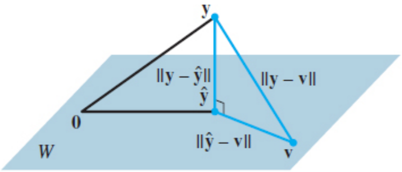


FIGURE 4 The orthogonal projection of $\mathbf{y}$ onto W is the closest point in W to $\mathbf{y}$.

Properties of orthogonal projections

Due to the orthogonal decomposition theorem (Theorem 3.1), this decomposition is unique and due to the Pythagorean theorem (Theorem 1.5) we have

$$\|\mathbf{y} - \mathbf{v}\|^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2 + \|\hat{\mathbf{y}} - \mathbf{v}\|^2$$

Since $\mathbf{v} \neq \hat{\mathbf{y}}$ we have $\|\hat{\mathbf{y}} - \mathbf{v}\|^2 > 0$ and consequently

$$\|\mathbf{y} - \mathbf{v}\|^2 > \|\mathbf{y} - \hat{\mathbf{y}}\|^2$$

Properties of orthogonal projections

Theorem 3.4

If $\{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_p\}$ is an orthonormal basis of W, then the orthogonal projection of $\mathbf{y}$ onto W is

$$\hat{\mathbf{y}} = \langle \mathbf{y}, \mathbf{u}_1 \rangle \mathbf{u}_1 + \langle \mathbf{y}, \mathbf{u}_2 \rangle \mathbf{u}_2 + ... + \langle \mathbf{y}, \mathbf{u}_p \rangle \mathbf{u}_p$$

If we construct the orthonormal matrix $U = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & ... & \mathbf{u}_p \end{pmatrix}$, then

$$\hat{\mathbf{y}} = UU^T\mathbf{y}$$

Proof

By Theorem 3.1 we know that for all orthogonal bases it is verified

$$\hat{\mathbf{y}} = \frac{\mathbf{y}\cdot\mathbf{u}_1}{\|\mathbf{u}_1\|^2}\mathbf{u}_1 + \frac{\mathbf{y}\cdot\mathbf{u}_2}{\|\mathbf{u}_2\|^2}\mathbf{u}_2 + ... + \frac{\mathbf{y}\cdot\mathbf{u}_p}{\|\mathbf{u}_p\|^2}\mathbf{u}_p$$

Since the basis is in this case orthonormal, then $\|\mathbf{u}\| = 1$ and consequently

$$\hat{\mathbf{y}} = \langle \mathbf{y}, \mathbf{u}_1 \rangle \mathbf{u}_1 + \langle \mathbf{y}, \mathbf{u}_2 \rangle \mathbf{u}_2 + ... + \langle \mathbf{y}, \mathbf{u}_p \rangle \mathbf{u}_p$$

Properties of orthogonal projections

On the other side we have

$$U^T\mathbf{y} = \begin{pmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \dots \\ \mathbf{u}_p^T \end{pmatrix} \mathbf{y} = \begin{pmatrix} \mathbf{u}_1^T\mathbf{y} \\ \mathbf{u}_2^T\mathbf{y} \\ \dots \\ \mathbf{u}_p^T\mathbf{y} \end{pmatrix} = \begin{pmatrix} \langle \mathbf{u}_1, \mathbf{y} \rangle \\ \langle \mathbf{u}_2, \mathbf{y} \rangle \\ \dots \\ \langle \mathbf{u}_p, \mathbf{y} \rangle \end{pmatrix}$$

Then,

$$UU^T\mathbf{y} = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_p \end{pmatrix} \begin{pmatrix} \langle \mathbf{u}_1, \mathbf{y} \rangle \\ \langle \mathbf{u}_2, \mathbf{y} \rangle \\ \dots \\ \langle \mathbf{u}_p, \mathbf{y} \rangle \end{pmatrix} = \langle \mathbf{y}, \mathbf{u}_1 \rangle \mathbf{u}_1 + \langle \mathbf{y}, \mathbf{u}_2 \rangle \mathbf{u}_2 + \dots + \langle \mathbf{y}, \mathbf{u}_p \rangle \mathbf{u}_p$$

(q.e.d.)

Properties of orthogonal projections

Corollary

Let $U = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \dots & \mathbf{u}_p \end{pmatrix}$ be a $n \times p$ matrix with orthonormal columns and $W = \mathrm{Col}\{U\}$ its column space. Then,

$$\begin{array}{lll} \forall \mathbf{x} \in \mathbb{R}^p & U^T U\mathbf{x} = \mathbf{x} & \text{No effect} \\ \forall \mathbf{y} \in \mathbb{R}^n & UU^T\mathbf{y} = \hat{\mathbf{y}} & \text{Orthogonal projection of } \mathbf{y} \text{ onto } W \end{array}$$

If U is a $n \times n$, then $W = \mathbb{R}^n$ and the projection has no effect

$$\forall \mathbf{y} \in \mathbb{R}^n \quad UU^T\mathbf{y} = \hat{\mathbf{y}} = \mathbf{y} \quad \text{No effect}$$

Exercises

Exercises

From Lay (3rd ed.), Chapter 6, Section 3:

- 6.3.1
- 6.3.7
- 6.3.15
- 6.3.23
- 6.3.24
- 6.3.25 (computer)

Outline

7. Orthogonality and least squares
   - Inner product, length and orthogonality (a)
   - Orthogonal sets, bases and matrices (a)
   - Orthogonal projections (b)
   - Gram-Schmidt orthogonalization (b)
   - Least squares (c)
   - Least-squares linear regression (c)
   - Inner product spaces (d)
   - Applications of inner product spaces (d)

Gram-Schmidt orthogonalization

Gram-Schmidt orthogonalization is a procedure aimed at producing an orthogonal basis of any subspace W.

Example

Let $W = \mathrm{Span}\{\mathbf{x}_1, \mathbf{x}_2\}$ with $\mathbf{x}_1 = (3, 6, 0)$ and $\mathbf{x}_2 = (1, 2, 2)$. Let's look for an orthogonal basis of W.

Solution

We may keep the first vector for the basis

$$\mathbf{v}_1 = \mathbf{x}_1 = (3, 6, 0)$$

For the second vector in the basis, we need to keep the component of $\mathbf{x}_2$ that is orthogonal to $\mathbf{x}_1$. For doing so we calculate the projection of $\mathbf{x}_2$ onto $\mathbf{x}_1$ ($\mathbf{p}$), and we decompose $\mathbf{x}_2$ as

$$\mathbf{x}_2 = \mathbf{p} + (\mathbf{x}_2 - \mathbf{p}) = (1, 2, 0) + (0, 0, 2)$$

We, then, keep the orthogonal part of $\mathbf{x}_2$

$$\mathbf{v}_2 = \mathbf{x}_2 - \mathbf{p} = (0, 0, 2)$$

Gram-Schmidt orthogonalization

Example (continued)

The set $\{\mathbf{v}_1, \mathbf{v}_2\}$ is an orthogonal basis of W.

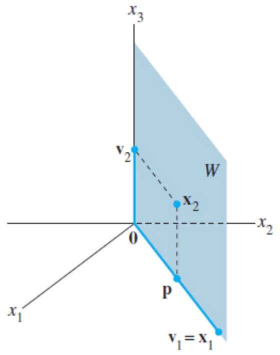


FIGURE 1

Construction of an orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2\}$.

Gram-Schmidt orthogonalization

Example

Let $W = \text{Span}\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ with $\mathbf{x}_1 = (1, 1, 1, 1)$, $\mathbf{x}_2 = (0, 1, 1, 1)$ and $\mathbf{x}_3 = (0, 0, 1, 1)$. Let's look for an orthogonal basis of W.

Solution

We may keep the first vector for the basis. Then we construct a subspace (W_1) with a single element in its basis

$$\mathbf{v}_1 = \mathbf{x}_1 = (1, 1, 1, 1) \quad W_1 = \text{Span}\{\mathbf{v}_1\}$$

For the second vector in the basis, we need to keep the component of $\mathbf{x}_2$ that is orthogonal to W_1. With the already computed basis vectors, we construct a new subspace (W_2) with two elements in its basis

$$\mathbf{v}_2 = \mathbf{x}_2 - \text{Proj}_{W_1}(\mathbf{x}_2) = (-\tfrac{3}{4}, \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}) \quad W_2 = \text{Span}\{\mathbf{v}_1, \mathbf{v}_2\}$$

For the third vector in the basis, we repeat the same procedure

$$\mathbf{v}_3 = \mathbf{x}_3 - \text{Proj}_{W_2}(\mathbf{x}_3) = (0, -\tfrac{2}{3}, \tfrac{1}{3}, \tfrac{1}{3}) \quad W_3 = \text{Span}\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$$

Gram-Schmidt orthogonalization

Theorem 4.1 (Gram-Schmidt orthogonalization)

Given a basis $\{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_p\}$ *for a vector subspace* W*. Define*

$$\begin{aligned} \mathbf{v}_1 &= \mathbf{x}_1 & W_1 &= \mathrm{Span}\{\mathbf{v}_1\} \\ \mathbf{v}_2 &= \mathbf{x}_2 - \mathrm{Proj}_{W_1}(\mathbf{x}_2) & W_2 &= \mathrm{Span}\{\mathbf{v}_1, \mathbf{v}_2\} \\ &... & & \\ \mathbf{v}_p &= \mathbf{x}_p - \mathrm{Proj}_{W_{p-1}}(\mathbf{x}_p) & W_p &= \mathrm{Span}\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_p\} = W \end{aligned}$$

Then $\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_p\}$ *is an orthogonal basis of* W*.*

Gram-Schmidt orthogonalization

Proof

Consider $W_k = \mathrm{Span}\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_k\}$ and let us assume that $\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_k\}$ is a basis of W_k. Now we construct

$$\mathbf{v}_{k+1} = \mathbf{x}_{k+1} - \mathrm{Proj}_{W_k}(\mathbf{x}_{k+1}) \quad W_{k+1} = \mathrm{Span}\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_{k+1}\}$$

By the orthogonal decomposition theorem (Theorem 3.1), we know that $\mathbf{v}_{k+1}$ is orthogonal to W_k. Because $\mathbf{x}_{k+1}$ is an element of a basis, we know that $\mathbf{x}_{k+1} \notin W_k$. Therefore, $\mathbf{v}_{k+1}$ is not null and $\mathbf{x}_{k+1} \in W_{k+1}$. Finally, the set $\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_{k+1}\}$ is a set of orthogonal, non-null vectors in the $(k+1)$-dimensional space W_{k+1}. Consequently, by Theorem 9.4 in Chapter 5, it must be a basis of W_{k+1}. This process can be iterated till $k = p$.

Gram-Schmidt orthogonalization

Orthonormal basis

Once we have an orthogonal basis, we simply have to normalize each vector to have an orthonormal basis.

Example

Let $W = \mathrm{Span}\{\mathbf{x}_1, \mathbf{x}_2\}$ with $\mathbf{x}_1 = (3, 6, 0)$ and $\mathbf{x}_2 = (1, 2, 2)$. Let's look for an orthonormal basis of W.

Solution

In Slide 52 we learned that an orthogonal basis was given by

$$\begin{aligned} \mathbf{v}_1 &= (3, 6, 0) \\ \mathbf{v}_2 &= (0, 0, 2) \end{aligned}$$

Now, we normalize these two vectors to obtain an orthonormal basis

$$\begin{aligned} \mathbf{v}'_1 &= \frac{\mathbf{v}_1}{\|\mathbf{v}_1\|} = \frac{1}{\sqrt{45}}(3, 6, 0) = (\frac{1}{\sqrt{5}}, \frac{2}{\sqrt{5}}, 0) \\ \mathbf{v}'_2 &= \frac{\mathbf{v}_2}{\|\mathbf{v}_2\|} = \frac{1}{2}(0, 0, 2) = (0, 0, 1) \end{aligned}$$

QR factorization of matrices

If we apply the Gram-Schmidt factorization to the columns of a matrix, we have the following factorization scheme. This factorization is used in practice to find eigenvalues and eigenvectors as well as to solve linear equation systems.

Theorem 4.2 (QR factorization)

Let $A \in \mathcal{M}_{m\times n}$ with linearly independent columns. Then, A can be factored as

$$A = QR$$

where $Q \in \mathcal{M}_{m\times n}$ is a matrix whose columns form an orthonormal basis of $\mathrm{Col}\{A\}$ and $R \in \mathcal{M}_{n\times n}$ is an upper triangular invertible matrix with positive entries on its diagonal.

Proof

Let's orthogonalize the columns of A following the Gram-Schmidt procedure and construct the orthonormal basis of $\mathrm{Col}\{A\}$. Let $\{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_n\}$ be such a basis. Let us construct the matrix

$$Q = \begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \ldots & \mathbf{u}_n \end{pmatrix}$$

QR factorization of matrices

Let us call $\mathbf{a}_i$ $(i = 1, 2, ..., n)$ to the columns of A. By the Gram-Schmidt orthogonalization, we know that for any k between 1 and n we have

$$\mathrm{Span}\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_k\} = \mathrm{Span}\{\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_k\}$$

Consequently, we can express each column of A in the orthonormal basis:

$$\mathbf{a}_k = r_{1k}\mathbf{u}_1 + r_{2k}\mathbf{u}_2 + ... + r_{kk}\mathbf{u}_k + 0 \cdot \mathbf{u}_{k+1} + ... + 0 \cdot \mathbf{u}_n$$

If r_{kk} is negative, we can multiply both r_{kk} and $\mathbf{u}_k$ by -1. We now collect all these coefficients in a vector $\mathbf{r}_k = (r_{1k}, r_{2k}, ..., r_{kk}, 0, 0, ..., 0)$ to have

$$\mathbf{a}_k = Q\mathbf{r}_k$$

By gathering all these vectors in a matrix, we have the triangular matrix R

$$R = \begin{pmatrix} \mathbf{r}_1 & \mathbf{r}_2 & ... & \mathbf{r}_n \end{pmatrix}$$

R is invertible because the columns of A are linearly independent.

QR factorization of matrices

Example

Let's calculate the QR factorization of $A = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$. From Slide 54 we know that the vectors

$$\begin{aligned} \mathbf{v}_1 &= (1,1,1,1) \\ \mathbf{v}_2 &= (-\tfrac{3}{4}, \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}) \\ \mathbf{v}_3 &= (0, -\tfrac{2}{3}, \tfrac{1}{3}, \tfrac{1}{3}) \end{aligned}$$

Is an orthogonal basis of the column space of A. We now normalize these vectors to obtain the orthonormal basis in Q

$$Q = \begin{pmatrix} \frac{1}{2} & -\frac{3}{\sqrt{12}} & 0 \\ \frac{1}{2} & \frac{1}{\sqrt{12}} & -\frac{2}{\sqrt{6}} \\ \frac{1}{2} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{6}} \\ \frac{1}{2} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{6}} \end{pmatrix}$$

QR factorization of matrices

Example (continued)

To find R we multiply on both sides of the factorization by Q^T

$$A = QR \Rightarrow Q^T A = Q^T QR = R$$

$$\begin{aligned} R = Q^T A &= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{3}{\sqrt{12}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{12}} \\ 0 & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 2 & \frac{3}{2} & 1 \\ 0 & \frac{3}{\sqrt{12}} & \frac{2}{\sqrt{12}} \\ 0 & 0 & \frac{1}{\sqrt{6}} \end{pmatrix} \end{aligned}$$

Exercises

Exercises

From Lay (3rd ed.), Chapter 6, Section 4:

- 6.4.7
- 6.4.13
- 6.4.19
- 6.4.22
- 6.4.24

Outline

Least squares

Let's assume we want to solve the equation system $A\mathbf{x} = \mathbf{b}$, but, due to noise, there is no solution. We may still look for a solution such that $A\mathbf{x} \approx \mathbf{b}$. In fact the goal will be to minimize $d(A\mathbf{x}, \mathbf{b})$.

Definition 5.1 (Least squares solution)

Let A be a $m \times n$ matrix and $\mathbf{b} \in \mathbb{R}^m$. $\hat{\mathbf{x}} \in \mathbb{R}^n$ is a ***least squares solution*** *of the equation system $A\mathbf{x} = \mathbf{b}$ iff*

$$\forall \mathbf{x} \in \mathbb{R}^n \quad \|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$$

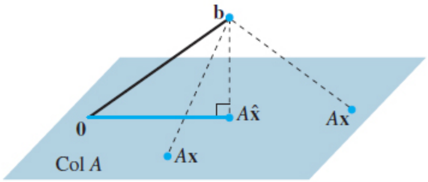


FIGURE 1 The vector **b** is closer to $A\hat{\mathbf{x}}$ than to $A\mathbf{x}$ for other **x**.

Least squares

Solution of the general least squares problem

Applying the Best Approximation Theorem (Theorem 3.3), we may project **b** onto the column space of A

$$\hat{\mathbf{b}} = \mathrm{Proj}_{\mathrm{Col}\{A\}}\{\mathbf{b}\}$$

Then, we solve the equation system

$$A\mathbf{x} = \hat{\mathbf{b}}$$

that has at least one solution.

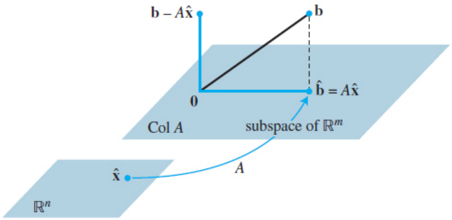


FIGURE 2 The least-squares solution $\hat{\mathbf{x}}$ is in $\mathbb{R}^n$.

Least squares

Theorem 5.1

The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ *is the same as the set of solutions of the normal equations*

$$A^T A\mathbf{x} = A^T\mathbf{b}$$

Proof: least-squares solutions $\subset$ *normal equations solutions*

Let us assume that $\hat{\mathbf{x}}$ *is a least-squares solution. Then,* $\mathbf{b} - A\hat{\mathbf{x}}$ *is orthogonal to* $\mathrm{Col}\{A\}$*, and in particular, to each one of the columns of* A *(*$\mathbf{a}_i$*,* $i = 1, 2, ..., n$*):*

$$\begin{gathered}\mathbf{a}_i \cdot (\mathbf{b} - A\hat{\mathbf{x}}) = 0 \quad \forall i \in \{1, 2, ..., n\} \Rightarrow \\ \mathbf{a}_i^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0 \quad \forall i \in \{1, 2, ..., n\} \Rightarrow \\ A^T(\mathbf{b} - A\hat{\mathbf{x}}) = \mathbf{0} \Rightarrow \\ A^T\mathbf{b} = A^T A\hat{\mathbf{x}}\end{gathered}$$

That is, every least-squares solution is also a solution of the normal equations.

Least squares

Proof: least-squares solutions $\supset$ normal equations solutions

Let us assume that $\hat{\mathbf{x}}$ is solution of the normal equations. Then,

$$A^T\mathbf{b} = A^T A\hat{\mathbf{x}} \Rightarrow$$
$$A^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0 \Rightarrow$$
$$\mathbf{a}_i^T(\mathbf{b} - A\hat{\mathbf{x}}) = 0 \quad \forall i \in \{1, 2, ..., n\}$$

That is, $\mathbf{b} - A\hat{\mathbf{x}}$ is orthogonal to the columns of A and, consequently, to $\mathrm{Col}\{A\}$. Hence, the equation

$$\mathbf{b} = A\hat{\mathbf{x}} + (\mathbf{b} - A\hat{\mathbf{x}})$$

is the orthogonal decomposition of $\mathbf{b}$ as a vector in $\mathrm{Col}\{A\}$ and a vector orthogonal to $\mathrm{Col}\{A\}$. By the uniqueness of the orthogonal decomposition, $A\hat{\mathbf{x}}$ must be the orthogonal projection of $\mathbf{b}$ onto $\mathrm{Col}\{A\}$ so that

$$A\hat{\mathbf{x}} = \hat{\mathbf{b}}$$

and, therefore, $\hat{\mathbf{x}}$ is a least-squares solution.

Least squares

Example

Find a least-squares solution to $A\mathbf{x} = \mathbf{b}$ with $A = \begin{pmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{pmatrix}$ and $\mathbf{b} = \begin{pmatrix} 2 \\ 0 \\ 11 \end{pmatrix}$.

Solution

Let's solve the normal equations $A^T A\hat{\mathbf{x}} = A^T\mathbf{b}$

$$A^T A = \begin{pmatrix} 17 & 1 \\ 1 & 5 \end{pmatrix} \quad A^T\mathbf{b} = \begin{pmatrix} 19 \\ 11 \end{pmatrix}$$

$$\begin{pmatrix} 17 & 1 \\ 1 & 5 \end{pmatrix}\hat{\mathbf{x}} = \begin{pmatrix} 19 \\ 11 \end{pmatrix} \Rightarrow \hat{\mathbf{x}} = \begin{pmatrix} 17 & 1 \\ 1 & 5 \end{pmatrix}^{-1}\begin{pmatrix} 19 \\ 11 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

Let's check that $\hat{\mathbf{x}}$ is not a solution of the original equation system but a least-squares solution

$$A\hat{\mathbf{x}} = \begin{pmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 4 \\ 4 \\ 3 \end{pmatrix} = \hat{\mathbf{b}} \neq \mathbf{b} = \begin{pmatrix} 2 \\ 0 \\ 11 \end{pmatrix}$$

Least squares

Definition 5.2 (Least-squares error)

The least-squares error is defined as

$$\sigma_\epsilon^2 \triangleq \|A\hat{\mathbf{x}} - \mathbf{b}\|^2 = \|\hat{\mathbf{b}} - \mathbf{b}\|^2$$

Example (continued)

In this case:

$$\sigma_\epsilon^2 = \|(4, 4, 3) - (2, 0, 11)\| = \|(2, 4, -8)\| \approx 9.165$$

Example

Unfortunately, the least-squares solution may not be unique as shown in the next example (arising in ANOVA). Find a least-squares solution to $A\mathbf{x} = \mathbf{b}$ with

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} -3 \\ -1 \\ 0 \\ 2 \\ 5 \\ 1 \end{pmatrix}.$$

Solution

$$A^T A = \begin{pmatrix} 6 & 2 & 2 & 2 \\ 2 & 2 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{pmatrix} \quad A^T \mathbf{b} = \begin{pmatrix} 4 \\ -4 \\ 2 \\ 6 \end{pmatrix}$$

Least squares

Example (continued)

The augmented matrix is

$$\left(\begin{array}{cccc|c} 6 & 2 & 2 & 2 & 4 \\ 2 & 2 & 0 & 0 & -4 \\ 2 & 0 & 2 & 0 & 2 \\ 2 & 0 & 0 & 2 & 6 \end{array}\right) \sim \left(\begin{array}{cccc|c} 1 & 0 & 0 & 1 & 3 \\ 0 & 1 & 0 & -1 & -5 \\ 0 & 0 & 1 & -1 & -2 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right)$$

Any point of the form

$$\hat{\mathbf{x}} = \begin{pmatrix} 3 \\ -5 \\ -2 \\ 0 \end{pmatrix} + x_4 \begin{pmatrix} -1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \quad \forall x_4 \in \mathbb{R}$$

is a least-squares solution of the problem.

Least squares

Theorem 5.2

The matrix $A^T A$ is invertible iff the columns of A are linearly independent. In this case, the equation system $A\mathbf{x} = \mathbf{b}$ has a unique least-squares solution given by

$$\hat{\mathbf{x}} = A^+\mathbf{b}$$

where A^+ is the ***Moore-Penrose pseudoinverse***

$$A^+ = (A^T A)^{-1} A^T$$

Least squares and QR decomposition

Sometimes $A^T A$ is ill-conditioned, this means that small perturbations in $\mathbf{b}$ translate into large perturbations in $\hat{\mathbf{x}}$. The QR decomposition offers a numerically more stable way of finding the least-squares solution.

Theorem 5.3

Let there be $A \in \mathcal{M}_{m\times n}$ with linearly independent columns. Consider its QR decomposition ($A = QR$). Then, for each $\mathbf{b} \in \mathbb{R}^m$ there is a unique least-squares solution of $A\mathbf{x} = \mathbf{b}$ given by

$$\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$$

Proof

If we substitute $\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$ into $A\mathbf{x}$ we have

$$A\hat{\mathbf{x}} = AR^{-1}Q^T\mathbf{b} = QRR^{-1}Q^T\mathbf{b} = QQ^T\mathbf{b}.$$

But Q is an orthonormal basis of $\mathrm{Col}\{A\}$ (Theorem 4.2 and Corollary in Slide 49) and consequently $QQ^T\mathbf{b}$ is the orthogonal projection of $\mathbf{b}$ onto $\mathrm{Col}\{A\}$, that is, $\hat{\mathbf{b}}$. So, $\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$ is a least-squares solution of $A\mathbf{x} = \mathbf{b}$. Additionally, since the columns of A are linearly independent, by Theorem 5.2, this solution is unique.

Least squares and QR decomposition

Remind that numerically it is easier to solve $R\hat{\mathbf{x}} = Q^T\mathbf{b}$ than $\hat{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$

L

et $A = \begin{pmatrix} 1 & 3 & 5 \\ 1 & 1 & 0 \\ 1 & 1 & 2 \\ 1 & 3 & 3 \end{pmatrix}$ and $\mathbf{b} = \begin{pmatrix} 3 \\ 5 \\ 7 \\ -3 \end{pmatrix}$. Its QR decomposition is

$$A = QR = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} 2 & 4 & 5 \\ 0 & 2 & 3 \\ 0 & 0 & 2 \end{pmatrix}$$

$$Q^T\mathbf{b} = \begin{pmatrix} 6 \\ -6 \\ 4 \end{pmatrix} \Rightarrow \begin{pmatrix} 2 & 4 & 5 \\ 0 & 2 & 3 \\ 0 & 0 & 2 \end{pmatrix} \hat{\mathbf{x}} = \begin{pmatrix} 6 \\ -6 \\ 4 \end{pmatrix} \Rightarrow \hat{\mathbf{x}} = \begin{pmatrix} 10 \\ -6 \\ 2 \end{pmatrix}$$

Exercises

Exercises

From Lay (3rd ed.), Chapter 6, Section 5:

- 6.5.1
- 6.5.19
- 6.5.20
- 6.5.21
- 6.5.24

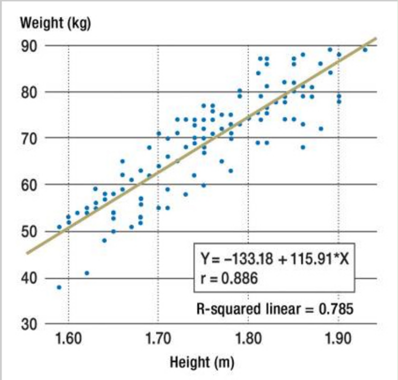
Outline

Least-squares linear regression

Example

In many scientific and engineering problems, it is needed to explain some observations **y** as a linear function of an independent variable **x**. For instance, we may try to explain the weight of a person as a linear function of its height

$$Weight = \beta_0 + \beta_1 Height$$



A. Schneider, G. Hommel, M. Blettner. *Linear Regression Analysis*. Dtsch Arztebl Int. **2010** November; 107(44): 776–782.

Least-squares linear regression

Example (continued)

For each observation we have an equation

Height (m.)	**Weight** (kg.)
1.70	57
1.53	43
1.90	94
...	...

$$57 = \beta_0 + 1.70\beta_1$$
$$43 = \beta_0 + 1.53\beta_1$$
$$94 = \beta_0 + 1.90\beta_1$$
$$\ldots$$

$$\begin{pmatrix} 1 & 1.70 \\ 1 & 1.53 \\ 1 & 1.90 \\ \ldots & \ldots \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} 57 \\ 43 \\ 94 \\ \ldots \end{pmatrix}$$

which is of the form

$$X\beta = \mathbf{y}$$

Least-squares linear regression

Least-squares regression

Each one of the observed **data points** (x_j, y_j) gives an equation. All together provide an equation system

$$X\beta = \mathbf{y}$$

that is an overdetermined, linear equation system of the form $A\mathbf{x} = \mathbf{b}$. The matrix X is called the **system matrix** and it is related to the **independent** (**predictor**) variables (the height in this case). The vector $\mathbf{y}$ is called the **observation vector** and collects the values of the **dependent** (**predicted**) variable (the weight in this case). The model

$$y = \beta_0 + \beta_1 x + \epsilon$$

is called the **linear regression of** y **on** x. β_0 and β_1 are called the **regression coefficients**. The difference between the predicted value and the observed value for a particular observation (ϵ) is called the **residual** of that observation.

Least-squares linear regression

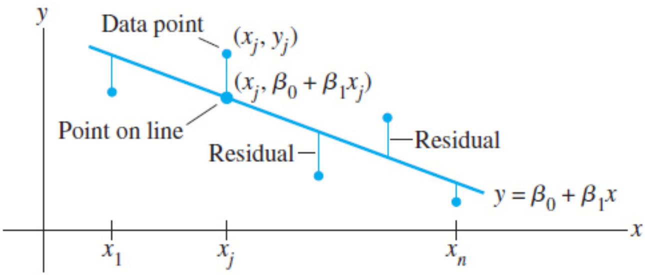


FIGURE 1 Fitting a line to experimental data.

The residual of the j-th observation is defined as

$$\epsilon_j = y_j - (\beta_0 + \beta_1 x_j)$$

Least-squares linear regression

The goal of least-squares regression is to minimize

$$\sum_{j=1}^{n} \epsilon_j^2 = \|\mathbf{y} - X\beta\|^2$$

Let's analyze this term

$$X\beta = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \dots & \dots \\ 1 & x_n \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} \beta_0 + \beta_1 x_1 \\ \beta_0 + \beta_2 x_2 \\ \dots \\ \beta_0 + \beta_n x_n \end{pmatrix} = \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \dots \\ \hat{y}_n \end{pmatrix}$$

Then

$$\|\mathbf{y} - X\beta\|^2 = \left\| \begin{pmatrix} y_1 - \hat{y}_1 \\ y_2 - \hat{y}_2 \\ \dots \\ y_n - \hat{y}_n \end{pmatrix} \right\|^2 = \sum_{j=1}^{n} (y_j - \hat{y}_j)^2 = \sum_{j=1}^{n} \epsilon_j^2$$

Least-squares linear regression

Example

Suppose we have observed the following values of height and weight (1.70,57), (1.53,43), (1.90,94). We construct the system matrix $X = \begin{pmatrix} 1 & 1.70 \\ 1 & 1.53 \\ 1 & 1.90 \end{pmatrix}$ and the observation vector $\mathbf{y} = \begin{pmatrix} 57 \\ 43 \\ 94 \end{pmatrix}$. Now we look the normal equations

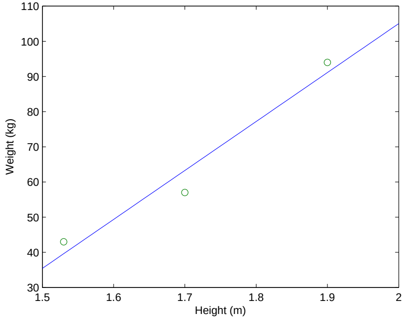
$$X\beta = \mathbf{y} \Rightarrow X^T X\beta = X^T\mathbf{y}$$

$$X^T X = \begin{pmatrix} 3.00 & 5.13 \\ 5.13 & 8.84 \end{pmatrix} \quad X^T\mathbf{y} = \begin{pmatrix} 194.00 \\ 341.29 \end{pmatrix} \quad \hat{\beta} = (X^T X)^{-1} X^T\mathbf{y} = \begin{pmatrix} -173.14 \\ 137.90 \end{pmatrix}$$

$$Weight = -173.39 + 139.21 Height$$

Least-squares linear regression

Example



MATLAB:

```
X=[1 1.70; 1 1.53; 1 1.90];
y=[57; 43; 94];
beta=inv(X'*X)*X'*y
x=1.5:0.01:2.00;
yp=beta(1)+beta(2)*x;
plot(x,yp,X(:,1),y,'o')
xlabel('Height (m)')
ylabel('Weight (kg)')
```

Least-squares linear regression

The general linear model

The linear model is not restricted to straight lines. We can use it to fit any kind of curves:

$$y = \beta_0 f_0(x) + \beta_1 f_1(x) + \beta_2 f_2(x) + \ldots$$

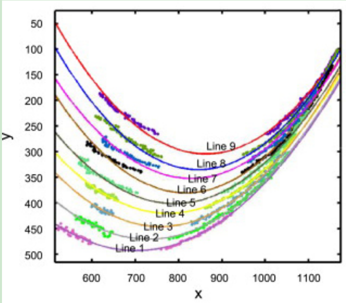
Fitting a parabola

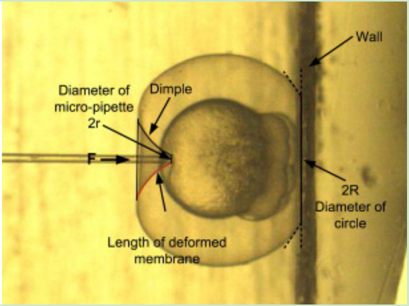
$$\begin{matrix} f_0(x) = 1 \\ f_1(x) = x \\ f_2(x) = x^2 \end{matrix} \quad \Rightarrow \quad \begin{matrix} y_1 = f_0(x_1) + \beta_1 f_1(x_1) + \beta_2 f_2(x_1) \\ y_2 = f_0(x_2) + \beta_1 f_1(x_2) + \beta_2 f_2(x_2) \\ \ldots \\ y_n = f_0(x_n) + \beta_1 f_1(x_n) + \beta_2 f_2(x_n) \end{matrix}$$

$$\begin{pmatrix} y_1 \\ y_2 \\ \ldots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \ldots & \ldots & \ldots \\ 1 & x_n & x_n^2 \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \ldots \\ \epsilon_n \end{pmatrix} \quad \Rightarrow \mathbf{y} = X\beta + \epsilon$$

Fitting a parabola

In this example they model the deformation of the wall of the zebra fish embryo as a function of strain.





Z. Lua, P. C.Y. Chen, H. Luo, J. Nam, R. Ge, W. Lin. *Models of maximum stress and strain of zebrafish embryos under indentation*. J. Biomechanics 42 (5): 620–625 (**2009**)

Least-squares linear regression

Multivariate linear regression

The linear model is not restricted to one variable. By fitting several variables we may fit surfaces and hypersurfaces

$$y = \beta_0 f_0(x_1, x_2) + \beta_1 f_1(x_1, x_2) + \beta_2 f_2(x_1, x_2) + \ldots$$

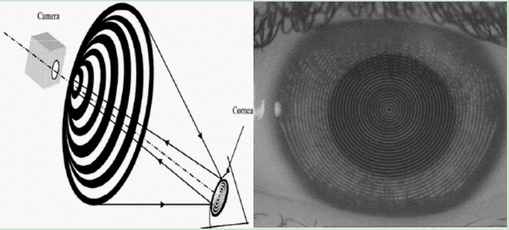
Fitting a parabolic surface

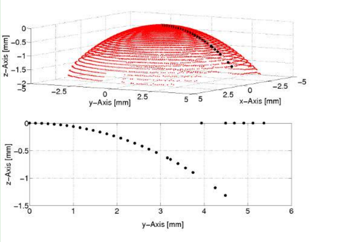
$$\begin{array}{l} f_0(x_1, x_2) = 1 \\ f_1(x_1, x_2) = x_1 \\ f_2(x_1, x_2) = x_2 \\ f_3(x_1, x_2) = x_1^2 \\ f_4(x_1, x_2) = x_2^2 \\ f_5(x_1, x_2) = x_1 x_2 \end{array} \Rightarrow X = \begin{pmatrix} 1 & x_{11} & x_{12} & x_{11}^2 & x_{12}^2 & x_{11}x_{12} \\ 1 & x_{21} & x_{22} & x_{21}^2 & x_{22}^2 & x_{21}x_{22} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & x_{n1} & x_{n2} & x_{n1}^2 & x_{n2}^2 & x_{n1}x_{n2} \end{pmatrix}$$

Least-squares linear regression

Fitting a parabolic surface

In this example they model the shape of cornea using videokeratoscopic images.





Exercises

Exercises

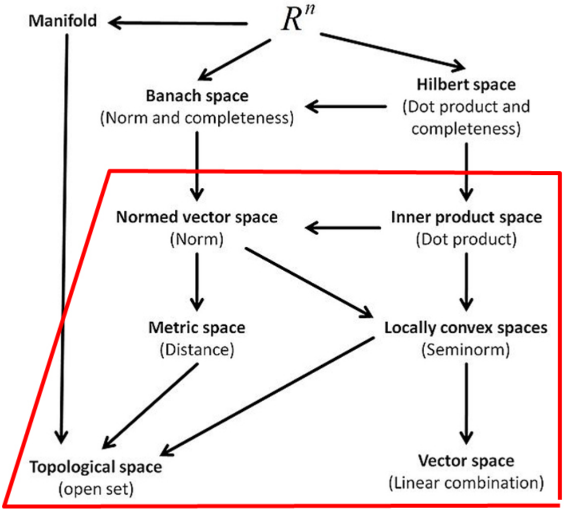
From Lay (3rd ed.), Chapter 6, Section 6:

- 6.6.1
- 6.6.5
- 6.6.9
- 6.6.12 (computer)

Outline

7. Orthogonality and least squares
   - Inner product, length and orthogonality (a)
   - Orthogonal sets, bases and matrices (a)
   - Orthogonal projections (b)
   - Gram-Schmidt orthogonalization (b)
   - Least squares (c)
   - Least-squares linear regression (c)
   - **Inner product spaces (d)**
   - Applications of inner product spaces (d)

Inner product spaces



Inner product spaces

Definition 7.1 (Inner product)

An inner product in a vector space V is a function that assigns a real number to every pair of vectors $\mathbf{u}$ *and* $\mathbf{v}$, $\langle \mathbf{u}, \mathbf{v} \rangle$ *and that satisfies the following axioms for all* $\mathbf{u}, \mathbf{v}, \mathbf{w} \in V$ *and all scalars* c*:*

1. $\langle \mathbf{u}, \mathbf{v} \rangle = \langle \mathbf{v}, \mathbf{u} \rangle$
2. $\langle \mathbf{u} + \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{u}, \mathbf{w} \rangle + \langle \mathbf{v}, \mathbf{w} \rangle$
3. $\langle c\mathbf{u}, \mathbf{v} \rangle = c \langle \mathbf{u}, \mathbf{v} \rangle$
4. $\langle \mathbf{u}, \mathbf{u} \rangle \geq 0$ *and* $\langle \mathbf{u}, \mathbf{u} \rangle = 0$ *iff* $\mathbf{u} = \mathbf{0}$.

Example

For instance in **Weighted Least Squares** (WLS) we may use an inner product in $\mathbb{R}^2$ defined as:

$$\langle \mathbf{u}, \mathbf{v} \rangle = 4u_1 v_1 + 5u_2 v_2$$

In this way we give less weight to distances in the first component with respect to distances in the second component.

Inner product spaces

Now we have to prove that this function is effectively an inner product:

1. $\langle \mathbf{u}, \mathbf{v} \rangle = \langle \mathbf{v}, \mathbf{u} \rangle$

$$\begin{aligned} \langle \mathbf{u}, \mathbf{v} \rangle &= 4u_1v_1 + 5u_2v_2 && \text{[by definition]} \\ &= 4v_1u_1 + 5v_2u_2 && \text{[commutativity of scalar multiplication]} \\ &= \langle \mathbf{v}, \mathbf{u} \rangle && \text{[by definition]} \end{aligned}$$

2. $\langle \mathbf{u} + \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{u}, \mathbf{w} \rangle + \langle \mathbf{v}, \mathbf{w} \rangle$

$$\begin{aligned} \langle \mathbf{u} + \mathbf{v}, \mathbf{w} \rangle &= 4(u_1 + v_1)w_1 + 5(u_2 + v_2)w_2 && \text{[by definition]} \\ &= 4u_1w_1 + 4v_1w_1 + 5u_2w_2 + 5v_2w_2 && \text{[distributivity of scalar]} \\ & && \text{[multiplication/addition]} \\ &= 4u_1w_1 + 5u_2w_2 + 4v_1w_1 + 5v_2w_2 && \text{[commutativity]} \\ & && \text{[of scalar addition]} \\ &= \langle \mathbf{u}, \mathbf{w} \rangle + \langle \mathbf{v}, \mathbf{w} \rangle && \text{[by definition]} \end{aligned}$$

Inner product spaces

3. $\langle c\mathbf{u}, \mathbf{v} \rangle = c \langle \mathbf{u}, \mathbf{v} \rangle$

$$\begin{aligned} \langle c\mathbf{u}, \mathbf{v} \rangle &= 4cu_1v_1 + 5cu_2v_2 && \text{[by definition]} \\ &= c4v_1u_1 + c5v_2u_2 && \text{[commutativity of scalar multiplication]} \\ &= c(4v_1u_1 + 5v_2u_2) && \text{[distributivity of scalar multiplication]} \\ &= c \langle \mathbf{u}, \mathbf{v} \rangle && \text{[by definition]} \end{aligned}$$

4. $\langle \mathbf{u}, \mathbf{u} \rangle \geq 0$ and $\langle \mathbf{u}, \mathbf{u} \rangle = 0$ iff $\mathbf{u} = \mathbf{0}$.
   1. $\langle \mathbf{u}, \mathbf{u} \rangle \geq 0$

      $$\langle \mathbf{u}, \mathbf{u} \rangle = 4u_1^2 + 5u_2^2 \qquad \text{[by definition]}$$

      which is obviously larger than 0.
   2. $\langle \mathbf{u}, \mathbf{u} \rangle = 0$ iff $\mathbf{u} = \mathbf{0}$.

      $$\langle \mathbf{u}, \mathbf{u} \rangle = 0 \Leftrightarrow 4u_1^2 + 5u_2^2 = 0 \Leftrightarrow u_1 = u_2 = 0$$

Inner product spaces

Example

Consider two vectors p and q the vector space of polynomials of degree n ($\mathbb{P}_n$). Let $t_0, t_1, ..., t_n$ be n distinct real numbers and K any scalar. The inner product between p and q is defined as

$$\langle p, q \rangle = K \left(p(t_0)q(t_0) + p(t_1)q(t_1) + ... + p(t_n)q(t_n) \right)$$

Axioms 1-3 are easy to check. Let's prove Axiom 4

4. $\langle p, p \rangle \geq 0$ and $\langle p, p \rangle = 0$ iff $p = 0$.
   1. $\langle p, p \rangle \geq 0$

      $$\langle p, p \rangle = K \left(p^2(t_0) + p^2(t_1) + ... + p^2(t_n) \right) \quad \text{[by definition]}$$

      which is obviously larger than 0.
   2. $\langle p, p \rangle = 0$ iff $p = 0$.

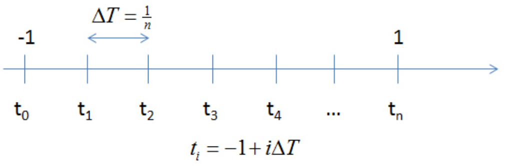
      $$\langle p, p \rangle = 0 \Leftrightarrow K \left(p^2(t_0) + p^2(t_1) + ... + p^2(t_n) \right) \Leftrightarrow$$
      $$p(t_0) = p(t_1) = ... = p(t_n) = 0$$

      But p is a polynomial of degree n so, at most, it can have n zeros. However, the previous condition requires the polynomial to vanish at $n + 1$ points. This is impossible unless $p = 0$.

Inner product spaces

Example

Consider two vectors p and q the vector space of polynomials of degree n ($\mathbb{P}_n$). Assume that we regularly space the $n+1$ points in the interval $[-1,1]$



and set $K = \Delta T$, then the inner product between the two polynomials becomes

$$\langle p, q \rangle = (p(t_0)q(t_0) + p(t_1)q(t_1) + \ldots + p(t_n)q(t_n))\,\Delta T = \sum_{i=0}^{n} p(t_i)q(t_i)\Delta T$$

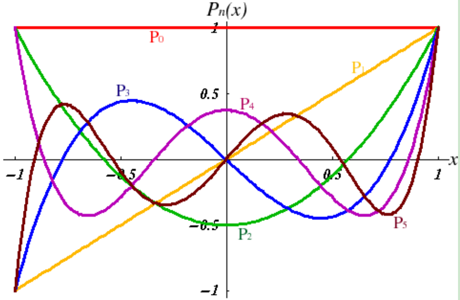
Making ΔT tend to 0, the inner product becomes

$$\langle p, q \rangle = \int_{-1}^{1} p(t)q(t)dt$$

Inner product spaces

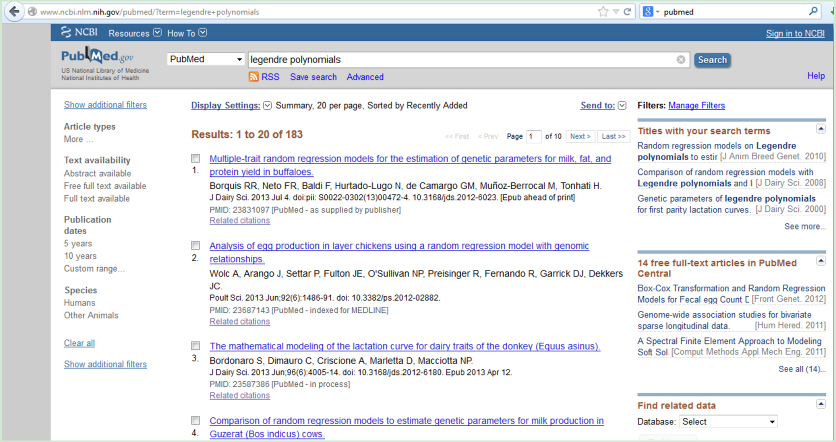
Legendre polynomials are orthogonal polynomials in the interval $[-1, 1]$

$$P_0(x) = 1$$
$$P_1(x) = x$$
$$P_2(x) = \tfrac{1}{2}(3x^2 - 1)$$
$$P_3(x) = \tfrac{1}{2}(5x^3 - 3x)$$
$$P_4(x) = \tfrac{1}{8}(35x^4 - 30x^2 + 3)$$
$$P_5(x) = \tfrac{1}{8}(63x^5 - 70x^3 + 15x)$$
$$P_6(x) = \tfrac{1}{16}(231x^6 - 315x^4 + 105x^2 - 5)$$
$$P_7(x) = \tfrac{1}{16}(429x^7 - 693x^5 + 315x^3 - 35x)$$



Legendre polynomials are very useful for regression of high-order polynomials as shown in next slide.

Inner product spaces



Length, distance and orthogonality

Length, distance and orthogonality

The **length** of a vector $\mathbf{u}$ in an inner product space is defined in the standard way

$$\|\mathbf{u}\| = \sqrt{\langle \mathbf{u}, \mathbf{u} \rangle}$$

Similarly, the **distance between two vectors u** and **v** is defined as

$$d(\mathbf{u}, \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\|$$

Finally, two vectors $\mathbf{u}$ and $\mathbf{v}$ are said to be **orthogonal** iff

$$\langle \mathbf{u}, \mathbf{v} \rangle = 0$$

Length, distance and orthogonality

Example

In the vector space of polynomials in the interval $[0,1]$, $\mathbb{P}[0,1]$, let's define the inner product

$$\langle p,q\rangle = \int_0^1 p(t)q(t)dt$$

What is the length of the vector $p(t) = 3t^2$?

Solution

$$\begin{aligned}\|p\| &= \sqrt{\langle p,p\rangle} = \sqrt{\int_0^1 p^2(t)dt} = \sqrt{\int_0^1 (3t^2)^2 dt} = \sqrt{\int_0^1 9t^4 dt} \\ &= \sqrt{9\frac{t^5}{5}\Big|_0^1} = \sqrt{9\left(\frac{1}{5}-0\right)} = \frac{3}{\sqrt{5}}\end{aligned}$$

Gram-Schmidt orthogonalization

Example

Gram-Schmidt is applied in the standard way. For instance, find an orthogonal basis of $\mathbb{P}_2[-1,1]$. A basis that spans this space is

$$\{1, t, t^2\}$$

Let's orthogonalize it

$$\begin{aligned}
p_0(t) &= 1 \\
p_1(t) &= t - \frac{\langle t, p_0(t)\rangle}{\|p_0\|^2} p_0(t) = t - \frac{\int_{-1}^{1} t dt}{\int_{-1}^{1} dt} 1 = t - \frac{0}{2} 1 = t \\
p_2(t) &= t^2 - \frac{\left\langle t^2, p_0(t)\right\rangle}{\|p_0\|^2} p_0(t) - \frac{\left\langle t^2, p_1(t)\right\rangle}{\|p_1\|^2} p_1(t) \\
&= t^2 - \frac{\int_{-1}^{1} t^2 dt}{\int_{-1}^{1} dt} - \frac{\int_{-1}^{1} t^2 t dt}{\int_{-1}^{1} t^2 dt} t = t^2 - \frac{\frac{2}{3}}{2} = t^2 - \frac{1}{3}
\end{aligned}$$

In Slide 97 we proposed the Legendre polynomial of degree 2 to be $P_2(t) = \frac{1}{2}(3t^2 - 1)$, we can easily show that $P_2(t) = \frac{3}{2} p_2(t)$. Consequently, if $p_2(t)$ is orthogonal to $p_0(t)$ and $p_1(t)$ so is $P_2(t)$.

Best approximation

Example

What is the best approximation in $\mathbb{P}_2[-1,1]$ of $p(t) = t^3$?

Solution

We know the answer is the orthogonal projection of $p(t)$ onto $\mathbb{P}_2[-1,1]$. An orthogonal basis of $\mathbb{P}_2[-1,1]$ is $\{1, t, t^2 - \frac{1}{3}\}$. Therefore, this projection can be calculated as

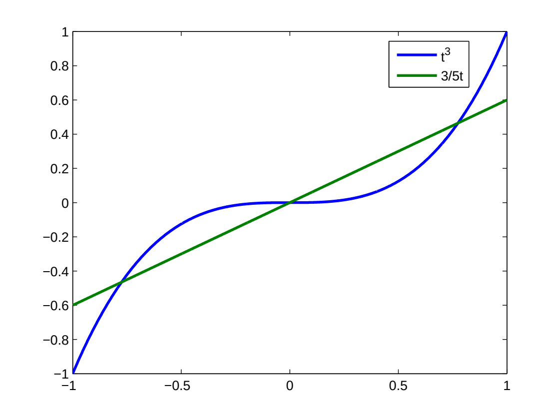
$$\hat{p}(t) = \mathrm{Proj}_{\mathbb{P}_2[-1,1]}\{p(t)\} = \frac{\langle p, p_0\rangle}{\|p_0\|^2} p_0(t) + \frac{\langle p, p_1\rangle}{\|p_1\|^2} p_1(t) + \frac{\langle p, p_2\rangle}{\|p_2\|^2} p_2(t)$$

Let's perform these calculations:

$$\begin{array}{l|l}
\langle p, p_0(t)\rangle = \int_{-1}^{1} t^3 dt = 0 & \|p_0\|^2 = \int_{-1}^{1} dt = 2 \\
\langle p, p_1(t)\rangle = \int_{-1}^{1} t^3 t dt = \frac{2}{5} & \|p_1\|^2 = \int_{-1}^{1} t^2 dt = \frac{2}{3} \\
\langle p, p_2(t)\rangle = \int_{-1}^{1} t^3 (t^2 - \frac{1}{3}) dt = 0 & \|p_2\|^2 = \int_{-1}^{1} (t^2 - \frac{1}{3})^2 dt = \frac{8}{45}
\end{array}$$

$$\hat{p}(t) = \frac{0}{2} + \frac{\frac{2}{5}}{\frac{2}{3}} t + \frac{0}{\frac{8}{45}}(t^2 - \frac{1}{3}) = \frac{3}{5} t$$

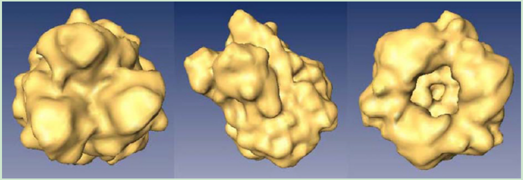
Best approximation



Best approximation

Example

In this example we exploited the best approximation property of orthogonal wavelets to speed-up and make more robust angular alignments of projections in 3D Electron Microscopy.



C.O.S.Sorzano, S. Jonic, C. El-Bez, J.M. Carazo, S. De Carlo, P. Thévenaz, M. Unser. *A multiresolution approach to orientation assignment in 3-D electron microscopy of single particles.* Journal of Structural Biology 146(3): 381-392 (**2004**, cover article)

Pythagorean theorem

Theorem 7.1 (Pythagorean theorem)

Given any vector $\mathbf{v}$ *in an inner product space* V *and a subspace of it* $W \subseteq V$ *we have*

$$\|\mathbf{v}\|^2 = \|\mathrm{Proj}_W\{\mathbf{v}\}\|^2 + \|\mathbf{v} - \mathrm{Proj}_W\{\mathbf{v}\}\|^2$$

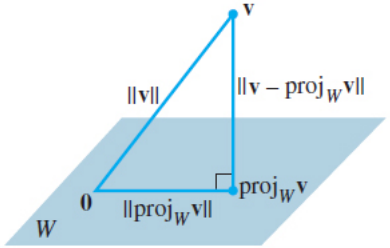


FIGURE 2

The hypotenuse is the longest side.

The Cauchy-Schwarz inequality

Theorem 7.2 (The Cauchy-Schwarz inequality)

For all $\mathbf{u}, \mathbf{v} \in V$ *it is verified*

$$|\langle \mathbf{u}, \mathbf{v} \rangle| \leq \|\mathbf{u}\| \|\mathbf{v}\|$$

Proof

If $\mathbf{u} = \mathbf{0}$, *then*

$$|\langle \mathbf{0}, \mathbf{v} \rangle| = 0 \quad \textit{and} \quad \|\mathbf{0}\| \|\mathbf{v}\| = 0 \|\mathbf{v}\| = 0$$

So the inequality becomes an equality.
If $\mathbf{u} \neq \mathbf{0}$, *then consider* $W = \mathrm{Span}\{\mathbf{u}\}$ *and*

$$\|\mathrm{Proj}_W\{\mathbf{v}\}\| = \left\| \frac{\langle \mathbf{v}, \mathbf{u} \rangle}{\|\mathbf{u}\|^2} \mathbf{u} \right\| = \frac{|\langle \mathbf{v}, \mathbf{u} \rangle|}{\|\mathbf{u}\|^2} \|\mathbf{u}\| = \frac{|\langle \mathbf{v}, \mathbf{u} \rangle|}{\|\mathbf{u}\|}$$

But by the Pythagorean Theorem (Theorem 7.1) we have $\|\mathrm{Proj}_W\{\mathbf{v}\}\| \leq \|\mathbf{v}\|$.
Consequently,

$$\frac{|\langle \mathbf{v}, \mathbf{u} \rangle|}{\|\mathbf{u}\|} \leq \|\mathbf{v}\| \Rightarrow |\langle \mathbf{v}, \mathbf{u} \rangle| \leq \|\mathbf{u}\| \|\mathbf{v}\| \textit{ (q.e.d.)}$$

The Triangle inequality

Theorem 7.3 (The Triangle inequality)

For all $\mathbf{u}, \mathbf{v} \in V$ *it is verified*

$$\|\mathbf{u} + \mathbf{v}\| \leq \|\mathbf{u}\| + \|\mathbf{v}\|$$

Proof

$$\begin{array}{rcll}
\|\mathbf{u} + \mathbf{v}\|^2 & = & \langle \mathbf{u} + \mathbf{v}, \mathbf{u} + \mathbf{v} \rangle & \textit{[By definition]} \\
 & = & \langle \mathbf{u}, \mathbf{u} \rangle + \langle \mathbf{v}, \mathbf{v} \rangle + 2 \langle \mathbf{u}, \mathbf{v} \rangle & \textit{[Properties of inner product]} \\
 & \leq & \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 + 2 |\langle \mathbf{u}, \mathbf{v} \rangle| & \langle \mathbf{u}, \mathbf{v} \rangle \leq |\langle \mathbf{u}, \mathbf{v} \rangle| \\
 & \leq & \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 + 2 \|\mathbf{u}\| \|\mathbf{v}\| & \textit{Cauchy-Schwarz} \\
 & = & (\|\mathbf{u}\| + \|\mathbf{v}\|)^2 & \\
 & \Rightarrow & & \\
\|\mathbf{u} + \mathbf{v}\| & \leq & \|\mathbf{u}\| + \|\mathbf{v}\| & \textit{[Taking square root]}
\end{array}$$

(q.e.d.)

Exercises

Exercises

From Lay (3rd ed.), Chapter 6, Section 7:

- 6.7.1
- 6.7.13
- 6.7.16
- 6.7.18

Outline

Weighted Least Squares

Weighted Least Squares

Let us assume we have a table of collected data and we want to fit a least squares model. However, we want to give more importance to some observations because we are more confident about them or they are more important. We encode the importance as a weight value (the larger the weight, the more importance the observation has)

X	**Y**	**W**
x_1	y_1	w_1
x_2	y_2	w_2
x_3	y_3	w_3
...	...	...

Let us call $\hat{y}_j$ the prediction of the model for the j-th observation and ϵ_j the committed error

$$y_j = \hat{y}_j + \epsilon_j$$

Weighted Least Squares

The goal is now to minimize the weighted sum of square errors

$$\sum_{j=1}^{n}(w_j\epsilon_j)^2 = \sum_{j=1}^{n}(w_j(y_j-\hat{y}_j))^2 = \sum_{j=1}^{n}(w_jy_j - w_j\hat{y}_j)^2$$

Let us collect all observed values into a vector $\mathbf{y}$ and do analogously with the predictions $\hat{\mathbf{y}}$. Let us define the diagonal matrix

$$W = \begin{pmatrix} w_1 & 0 & 0 & \ldots & 0 \\ 0 & w_2 & 0 & \ldots & 0 \\ 0 & 0 & w_3 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & w_n \end{pmatrix}$$

Then, the previous objective function becomes

$$\sum_{j=1}^{n}(w_jy_j - w_j\hat{y}_j)^2 = \|W\mathbf{y} - W\hat{\mathbf{y}}\|^2$$

Weighted Least Squares

Now, suppose that $\hat{\mathbf{y}}$ is calculated from the columns of a matrix A, that is, $\hat{\mathbf{y}} = A\mathbf{x}$. The objective function becomes

$$\sum_{j=1}^{n} (w_j y_j - w_j \hat{y}_j)^2 = \|W\mathbf{y} - WA\mathbf{x}\|^2$$

The minimum of this objective function is attained for $\hat{\mathbf{x}}$ that is the least-squares solution of the equation system

$$WA\mathbf{x} = W\mathbf{y}$$

The normal equations of the problem are

$$(WA)^T WA\mathbf{x} = (WA)^T W\mathbf{y}$$

Weighted Least Squares

Example

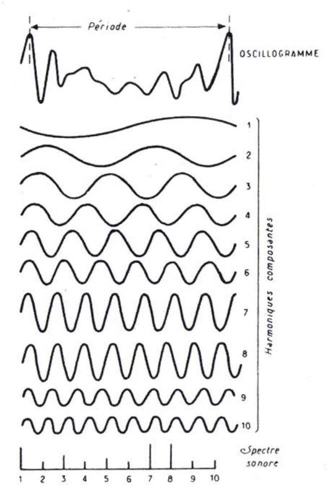
In this work they used Weighted Least Squares to calibrate a digital system to measure maximum respiratory pressures.

J.L. Ferreira, F.H. Vasconcelos, C.J. Tierra-Criollo. *A Case Study of Applying Weighted Least Squares to Calibrate a Digital Maximum Respiratory Pressures Measuring System*. Applied Biomedical Engineering, Chapter 18 (**2011**)

Fourier Series

Example

Fourier tools are, maybe, the most widespread tool to analyze signals and its frequency components. Fourier decomposition states that any signal can be obtained by summing sine waves of different amplitude, phase and frequency.



Fourier Series

Theorem 8.1

Consider the vector space of continuous functions in the interval $[0, 2\pi]$*,* $C[0, 2\pi]$*. The set*

$$S = \{1, \cos(t), \sin(t), \cos(2t), \sin(2t), ..., \cos(Nt), \sin(Nt)\}$$

is orthogonal with respect to the inner product defined as

$$\langle f(t), g(t)\rangle = \int_0^{2\pi} f(t)g(t)dt$$

Proof

$$\begin{array}{rcl} \langle \cos(nt), \cos(mt)\rangle & = & \int_0^{2\pi} \cos(nt)\cos(mt)dt \\ & = & \int_0^{2\pi} \frac{1}{2}(\cos((n+m)t) + \cos((n-m)t))dt \\ & = & \frac{1}{2}\left(\frac{\sin((n+m)t)}{n+m} + \frac{\sin((n-m)t)}{n-m}\right)\Big|_0^{2*\pi} \\ & = & 0 \end{array}$$

where we have used $\cos(A)\cos(B) = \frac{1}{2}(\cos(A+B) + \cos(A-B))$*.*

Fourier Series

Analogously we could prove that

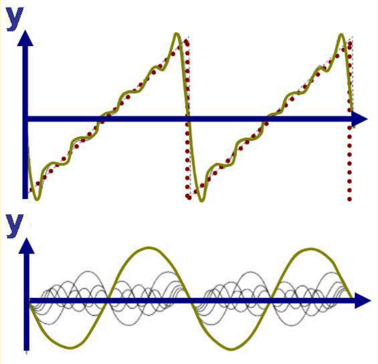
$$\begin{aligned}
\langle \cos(nt), \sin(mt) \rangle &= 0 \\
\langle \cos(nt), 1 \rangle &= 0 \\
\langle \sin(nt), 1 \rangle &= 0 \\
\| \cos(nt) \|^2 &= \pi \\
\| \sin(nt) \|^2 &= \pi \\
\| 1 \|^2 &= 2\pi
\end{aligned}$$

Fourier Series

Theorem 8.2 (Fourier series)

Given any function $f(t) \in C[0, 2\pi]$, $f(t)$ can be approximated as closely as desired by a sum of the form simply by orthogonally projecting it onto $W = \mathrm{Span}\{S\}$

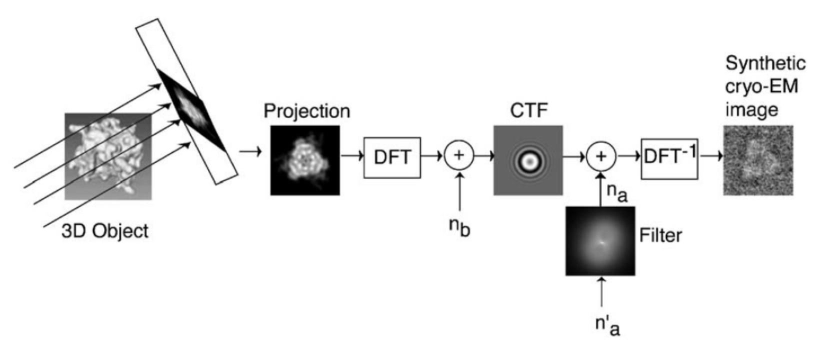
$$f(t) \approx \mathrm{Proj}_W\{f(t)\} = \frac{\langle f(t), 1\rangle}{\|1\|^2} + \sum_{n=1}^{N} \left(\frac{\langle f(t), \cos(nt)\rangle}{\|\cos(nt)\|^2} \cos(nt) + \frac{\langle f(t), \sin(nt)\rangle}{\|\sin(nt)\|^2} \sin(nt) \right)$$



Fourier Series

Example

In this work we used Fourier space to simulate and to align electron microscopy images



S. Jonic, C.O.S.Sorzano, P. Thévenaz, C. El-Bez, S. De Carlo, M. Unser. *Spline-Based image-to-volume registration for three-dimensional electron microscopy*. Ultramicroscopy, 103: 303-317 (**2005**)

Exercises

Exercises

From Lay (3rd ed.), Chapter 6, Section 8:

- 6.8.1
- 6.8.6
- 6.8.8
- 6.8.11

Outline

7. Orthogonality and least squares
   - Inner product, length and orthogonality (a)
   - Orthogonal sets, bases and matrices (a)
   - Orthogonal projections (b)
   - Gram-Schmidt orthogonalization (b)
   - Least squares (c)
   - Least-squares linear regression (c)
   - Inner product spaces (d)
   - Applications of inner product spaces (d)