Scuola Interdipartimentale delle **Scienze**, dell'**Ingegneria** e della **Salute**

UNIVERSITÀ PARTHENOPE — DiST — Dipartimento di Scienze e Tecnologie

L. Magistrale in IA (ML&BD)

Scientific Computing (part 2 – 6 credits)

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- **Gram-Schmidt Orthonormalization (GSO).**

Orthogonal and orthonormal vector systems

The set of non-zero vectors $\{\varphi_1, \varphi_2, \ldots, \varphi_n\}$, in a normed linear space, is said

- an **orthogonal system** if the vectors are mutually orthogonal

$$\langle \varphi_k, \varphi_j \rangle = \begin{cases} = 0 & k \neq j \\ \neq 0 & k = j \end{cases}$$

- an **orthonormal system** if, in addition, they have unit norm

$$\langle \varphi_k, \varphi_j \rangle = \begin{cases} = 0 & k \neq j \\ = 1 & k = j \end{cases} \quad \Leftrightarrow \quad \|\varphi_k\| = 1$$

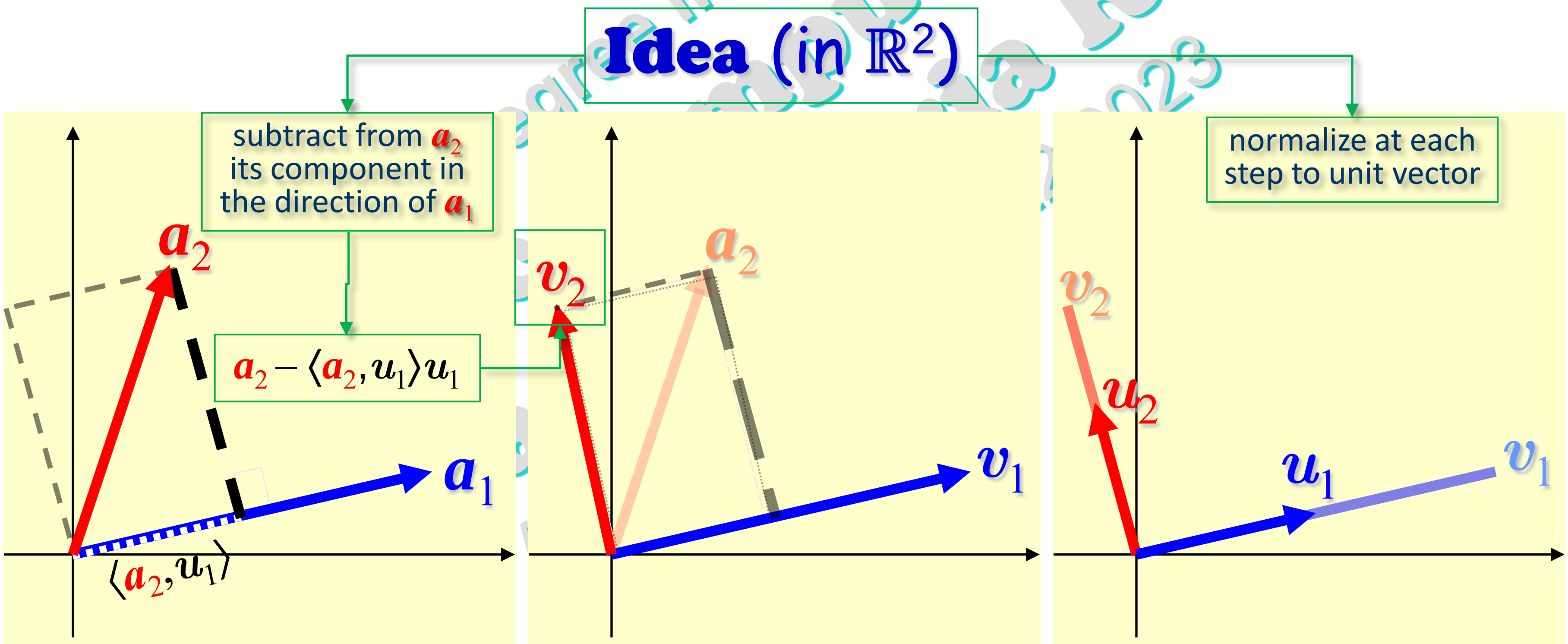
An orthogonal basis corresponds to introduce a Coordinate Reference System with orthogonal axes.
An orthonormal basis corresponds to a Coordinate Reference System with orthogonal axes, all measured in the same unit of length (monometric orthogonal reference system).

Gram-Schmidt orthonormalization in $\mathbb{R}^n$

This algorithm transforms any subspace basis into an orthonormal basis

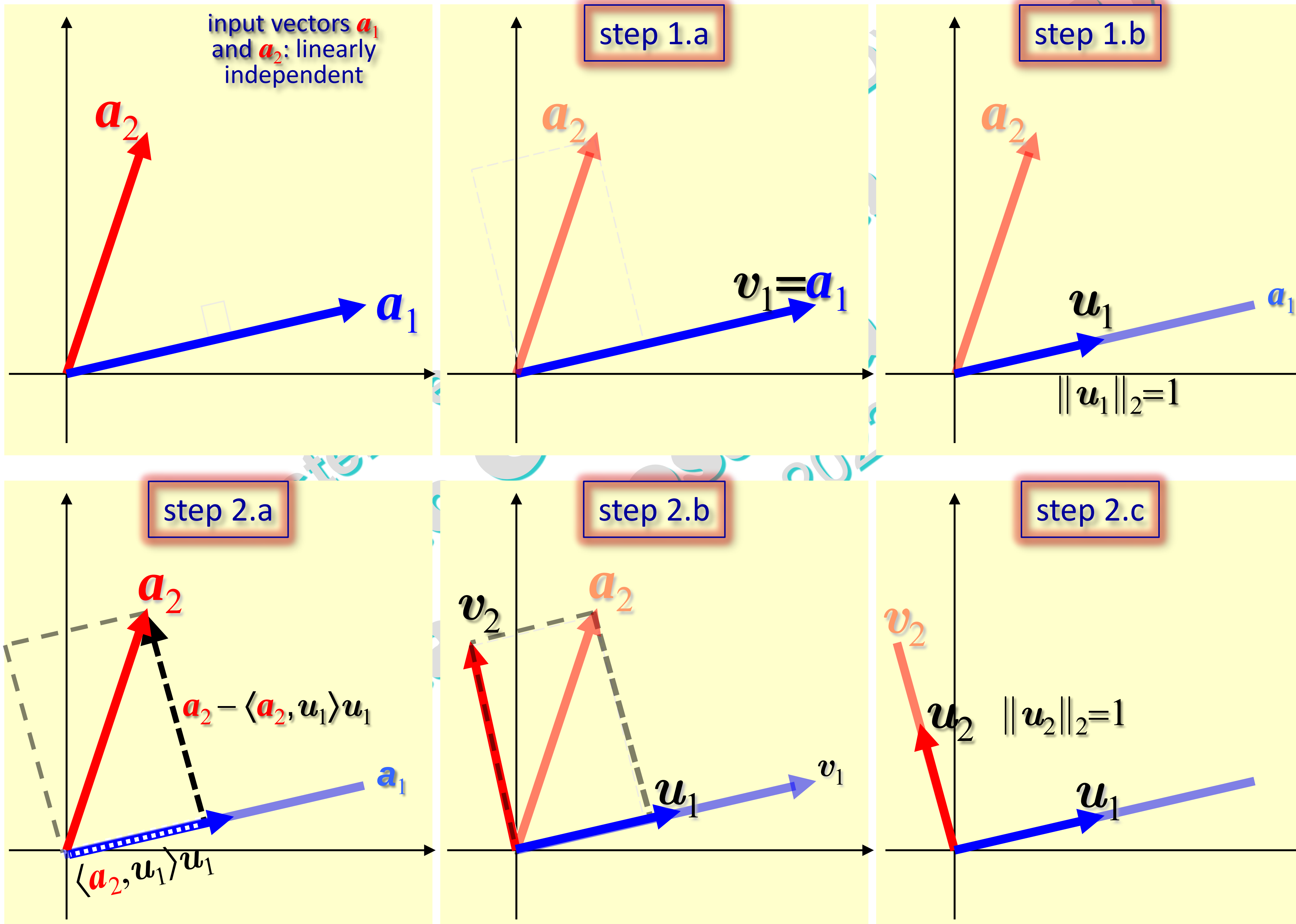
input: n linearly independent vectors $\{a_i\}$

output: n orthogonal vectors $\{v_i\}$ and n orthonormal vectors $\{u_i\}$



Linearly independent vector system $\{a_1, a_2\}$ ⇒ Orthogonal vector system ⇒ Orthonormal vector system

Gram-Schmidt Orthonormalization algorithm: steps



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Gram-Schmidt Orthonormalization algorithm (GSO)

step 1.a

step 1.b

$$v_1 = a_1; \quad u_1 = \frac{v_1}{\|v_1\|}$$

the 1st vector is only normalized to a unit vector

step k.a

$$v_k = a_k - \sum_{j=1}^{k-1} \langle a_k, u_j \rangle u_j$$

step k.c

$$u_k = \frac{v_k}{\|v_k\|}$$

for $k = 2, 3, \ldots, n$

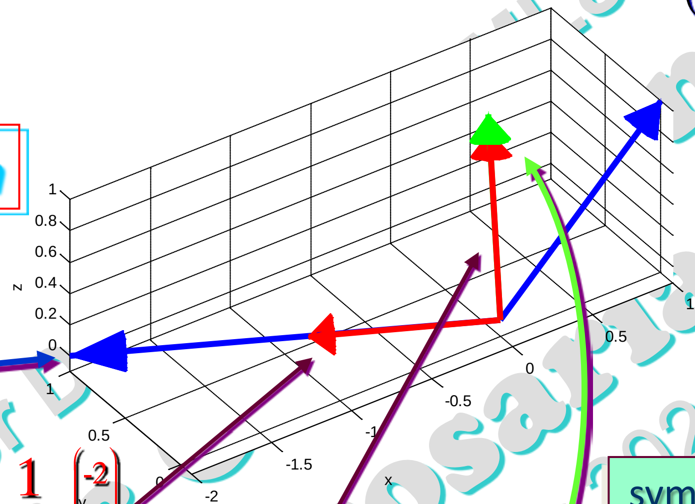
Idea: subtract, from each input vector, its components along the already orthonormalized vectors

Lab.: compute an orthonormal basis

parametric eq. of the plane π $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \alpha \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \forall \alpha, \beta \in \mathbb{R}$

non-orthonormal basis

GSO algorithm



orthonormal basis

$$v_1 = \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix}$$

$$u_1 = \frac{v_1}{\|v_1\|} = \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix}$$

$$v_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} - \left\langle \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix} \right\rangle \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/5 \\ 2/5 \\ 1 \end{pmatrix}$$

$$u_2 = \frac{v_2}{\|v_2\|} = \frac{1}{\sqrt{30}} \begin{pmatrix} 1 \\ 2 \\ 5 \end{pmatrix}$$

numerical MATLAB

```
A=[-2 1 0; 1 0 1]';
disp(orth(A))
  -0.9129   -0.0000
   0.3651   -0.4472
  -0.1826   -0.8944
```

symbolic GSO algorithm

```
a1=sym([-2 1 0]'); a2=sym([1 0 1]');
v1=a1; u1=v1/norm(v1);
v2=a2-a2'*u1*u1; u2=v2/norm(v2);
disp([u1 u2])
[   -(2*5^(1/2))/5, (5^(1/2)*6^(1/2))/30]
[        5^(1/2)/5, (5^(1/2)*6^(1/2))/15]
[                0,  (5^(1/2)*6^(1/2))/6]
disp(double([u1 u2]))
  -0.8944    0.1826
   0.4472    0.3651
   0         0.9129
```

```
disp(orth([a1 a2]))
```

$$\pi = \mathrm{span}\left\{ \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \right\} = \mathrm{span}\left\{ \frac{1}{\sqrt{5}} \begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{30}} \begin{pmatrix} 1 \\ 2 \\ 5 \end{pmatrix} \right\}$$

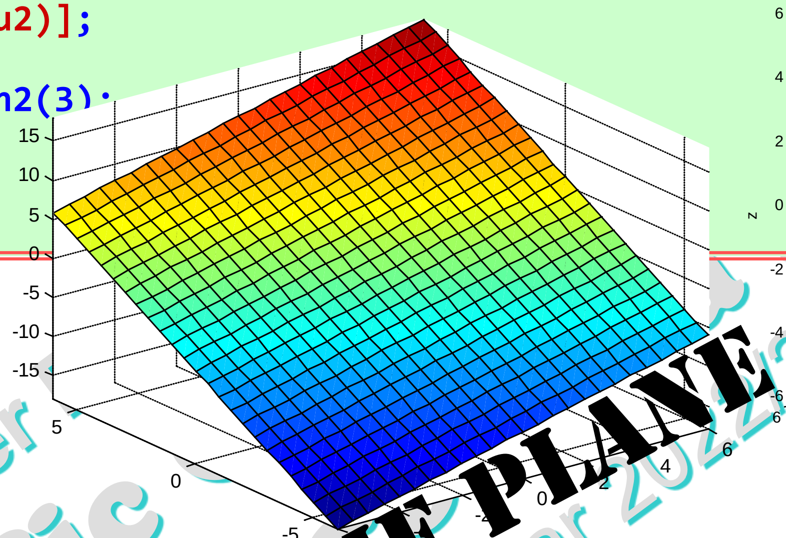
check

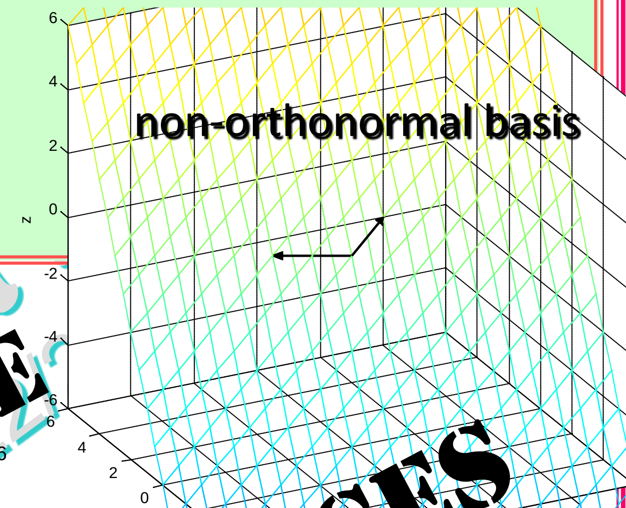
```
disp(rank([orth(A) double([u1 u2])]))
     2
```

the same subspace

Lab (contd)

```
... [x,y]=meshgrid(linspace(-6,6,25)); A=[-2 1 0;1 0 1]'; n1=null(A');
P1=(-n1(1)*x-n1(2)*y)/n1(3); % cartesian eq.
subplot(2,2,1); surf(x,y,P1); axis('tight'); subplot(2,2,2); mesh(x,y,P1); hidden off
hold on; axis equal; quiver3([0 0],[0 0],[0 0],A(1,:),A(2,:),A(3,:),1)
view([n1(1),n1(2),n1(3)])
A2=[double(u1) double(u2)];
n2=null(A2');
P2=(-n2(1)*x-n2(2)*y)/n2(3);
subplot(2,2,3);
surf(x,y,P2);...
...
```



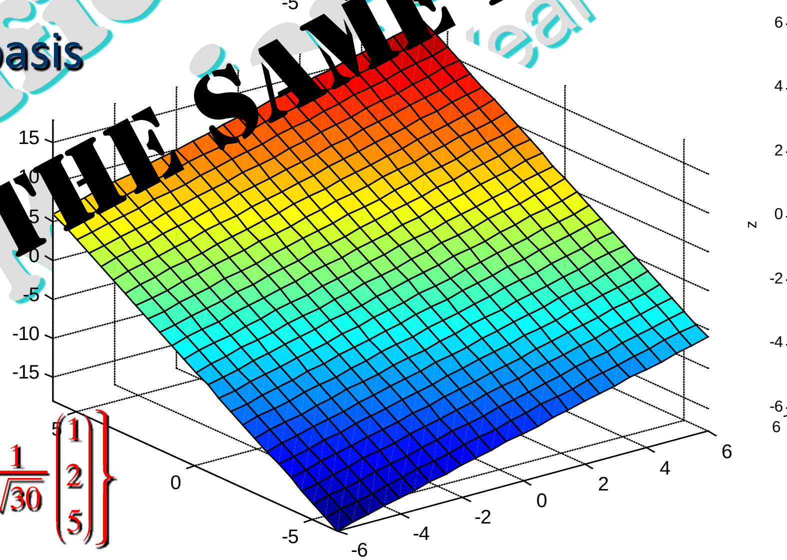


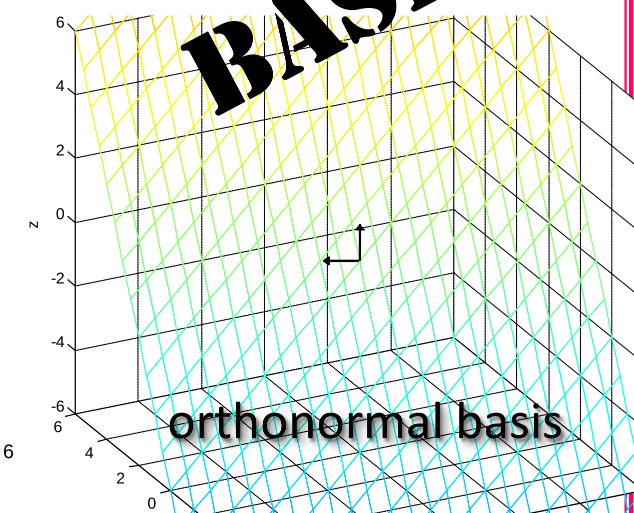
$$\pi = \text{span}\left\{\begin{pmatrix}-2\\1\\0\end{pmatrix}, \begin{pmatrix}1\\0\\1\end{pmatrix}\right\}$$

non-orthonormal basis

THE SAME PLANE

BASES





orthonormal basis

$$\pi = \text{span}\left\{\frac{1}{\sqrt{5}}\begin{pmatrix}-2\\1\\0\end{pmatrix}, \quad \frac{1}{\sqrt{30}}\begin{pmatrix}1\\2\\5\end{pmatrix}\right\}$$

Matrix with orthonormal columns

A real matrix **Q**, of size (m×n), with **orthonormal columns**, satisfies the following equation: $\mathbf{Q}^T\mathbf{Q}=I$ ($\mathbf{Q}^T$: *left inverse*) but, in general, $\mathbf{Q}\mathbf{Q}^T=I$ **does not hold**. $\mathbf{Q}^T\mathbf{Q}$ is known as "Gram matrix" of **Q**.

If Q has **orthonormal columns** then it

- preserves **std scalar products**: $\langle \mathbf{Qx},\mathbf{Qy}\rangle = \langle \mathbf{x},\mathbf{y}\rangle$
- leaves **vector lengths unchanged**: $\|\mathbf{Qx}\|_2 = \|\mathbf{x}\|_2$
- preserves **distances**: $\|\mathbf{Qx} - \mathbf{Qy}\|_2 = \|\mathbf{x} - \mathbf{y}\|_2$
- and preserves **angles between vectors**:

$$\cos(\mathbf{Qx}\angle\mathbf{Qy})=\langle \mathbf{Qx},\mathbf{Qy}\rangle/(\|\mathbf{Qx}\|_2\,\|\mathbf{Qy}\|_2)=\langle \mathbf{x},\mathbf{y}\rangle/(\|\mathbf{x}\|_2\,\|\mathbf{y}\|_2)=\cos(\mathbf{x}\angle\mathbf{y})$$

If **Q** is a real square matrix, and $\mathbf{Q}^T\mathbf{Q}=I=\mathbf{Q}\mathbf{Q}^T \Leftrightarrow \mathbf{Q}^T=\mathbf{Q}^{-1}$ i.e., the transpose matrix is its inverse, then **Q** is called an **orthogonal matrix**.

If **Q** is a complex square matrix, and $\mathbf{Q}^H\mathbf{Q}=I=\mathbf{Q}\mathbf{Q}^H \Leftrightarrow \mathbf{Q}^H=\mathbf{Q}^{-1}$ i.e., the transpose and conjugate matrix is its inverse, then **Q** is called a **unitary matrix**.

Examples of orthogonal matrices: Permutations, Rotations, Reflections.
Do you know what they are?

... later

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Gram-Schmidt Orthonormalization (GSO)

It can be applied to any kind of vectors

Example 1 compute an orthonormal basis, with respect to the standard dot product in $[-1,1]$, in the subspace Π_1 containing the real algebraic polynomials of degree at most 1.

standard dot product in $[-1,1]$: $\langle f,g\rangle = \int_{-1}^{1} f(x)g(x)dx$

$$P_1(x) = b + ax$$

$$\Pi_1 = \textbf{span}\{1, x\}$$ ← orthogonal, but non-orthonormal, basis

GSO Alg. → orthonormal basis → $\left\{\frac{1}{\sqrt{2}}, x\sqrt{\frac{3}{2}}\right\}$

$$u_1 = \frac{\varphi_1}{\|\varphi_1\|_2} = \frac{1}{\sqrt{2}} \quad \text{since} \quad \|\varphi_1\|_2 = \sqrt{\int_{-1}^{1} 1dx}$$

$$v_2 = \varphi_2 - \langle\varphi_2, u_1\rangle u_1 = x \quad \text{since} \quad \langle\varphi_2, u_1\rangle = \int_{-1}^{1} x\frac{1}{\sqrt{2}}dx = 0$$

$$u_2 = \frac{v_2}{\|v_2\|_2} = x\sqrt{\frac{3}{2}} \quad \text{since} \quad \|v_2\|_2 = \sqrt{\int_{-1}^{1} x^2dx} = \sqrt{\frac{2}{3}}$$

GSO: Example 1 in MATLAB

outer product of two vectors = Kronecker product of vectors

subspace Π_1

$$\Pi_1 = \{ax + b, \quad a, b \in \mathbb{R}\}$$

MATLAB Symbolic Math Toolbox

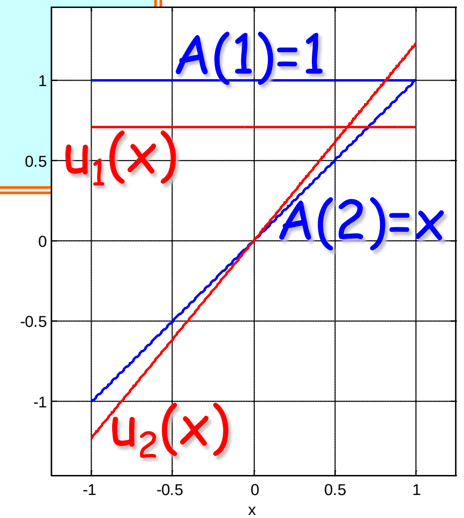
```
disp(A'*A)
[1,    x]
[x, x^2]
disp(kron(A',A))
[1,    x]
[x, x^2]
```

```
disp(int(A'*A,-1,1))
[   2,   0]   orthogonal
[   0, 2/3]
disp(int(v'*v,-1,1))
[ 2,   0]     orthogonal
[ 0, 2/3]
disp(int(u'*u,-1,1))
[ 1,   0]     orthonormal
[ 0,   1]
```

```
dotProd = @(f,g) int(f*g,-1,1);

syms x real;    A=[sym(1) x] % basis for Π1
A =
[ 1, x]
v(1)=A(1);
u(1)=v(1)/sqrt(dotProd(v(1),v(1)));
v(2)=A(2) - dotProd(A(2),u(1))*u(1);
u(2)=v(2)/sqrt(dotProd(v(2),v(2)));

disp(v)    v orthogonal system
[   1, x]

disp(u)    u orthonormal system
[   2^(1/2)/2, (2^(1/2)*3^(1/2)*x)/2]
```

$$\langle f, g \rangle = \int_{-1}^{1} f(x) g(x)\, dx$$

$$\|f(x)\| = \sqrt{\int_{-1}^{1} [f(x)]^2\, dx}$$



Function plots do not represent the vectors of Π_1; to think about them as vectors of a linear subspace, we have to consider the vectors in $\mathbb{R}^2$, the real plane.

GSO Algorithm

It can be applied to any kind of vectors

Example 2 compute an orthonormal basis, with respect to the standard dot product in $[-1,1]$, in the subspace Π_2 containing the real algebraic polynomials of degree at most 2.

$P_2(x) = c + bx + ax^2$

standard dot product in $[-1,1]$: $\langle f,g\rangle = \int_{-1}^{1} f(x)g(x)\,dx$

$\Pi_2 = \mathrm{span}\{1,x,x^2\}$ ← orthogonal, but non-orthonormal, basis

GSO Alg. ⇒ orthonormal basis → $\left\{\frac{1}{\sqrt{2}},\ x\sqrt{\frac{3}{2}},\ \frac{3}{2}\left(x^2-\frac{1}{3}\right)\sqrt{\frac{5}{2}}\right\}$

$v_1 = \varphi_1 \quad u_1 = \frac{v_1}{\|v_1\|_2} = \frac{1}{\sqrt{2}}$ since $\|v_1\|_2 = \sqrt{\int_{-1}^{1} 1\,dx}$

$v_2 = \varphi_2 - \langle\varphi_2,u_1\rangle u_1 = x$ since $\langle\varphi_2,u_1\rangle = \int_{-1}^{1} x\frac{1}{\sqrt{2}}\,dx = 0$

$u_2 = \frac{v_2}{\|v_2\|_2} = x\sqrt{\frac{3}{2}}$ since $\|v_2\|_2 = \sqrt{\int_{-1}^{1} x^2\,dx} = \sqrt{\frac{2}{3}}$

$v_3 = \varphi_3 - \langle\varphi_3,u_1\rangle u_1 - \langle\varphi_3,u_2\rangle u_2$

$u_3 = \frac{v_3}{\|v_3\|_2}$

GSO: Example 2 in MATLAB

outer product of two vectors = Kronecker product of vectors

subspace $\Pi_2 = \{ax^2 + bx + c, \quad a,b,c \in \mathbb{R}\}$

MATLAB Symbolic Math Toolbox

$$\langle f,g\rangle = \int_{-1}^{1} f(x)g(x)dx$$

$$\|f(x)\| = \sqrt{\int_{-1}^{1}[f(x)]^2 dx}$$

```
dotProd = @(f,g) int(f*g,-1,1);

syms x real;  A=[sym(1) x x^2] % base per Π2
A =
[ 1, x, x^2]
v(1)=A(1);
u(1)=v(1)/sqrt(dotProd(v(1),v(1)));
v(2)=A(2) - dotProd(A(2),u(1))*u(1);
u(2)=v(2)/sqrt(dotProd(v(2),v(2)));
v(3)=A(3)-dotProd(A(3),u(1))*u(1)-dotProd(A(3),u(2))*u(2);
u(3)=v(3)/sqrt(dotProd(v(3),v(3)));
disp(v)
[   1,  x,  x^2 - 1/3]
u=simplify(u)
u =
[2^(1/2)/2, (6^(1/2)*x)/2, (3*2^(1/2)*5^(1/2)*(x^2 - 1/3))/4]
```

v: orthogonal system

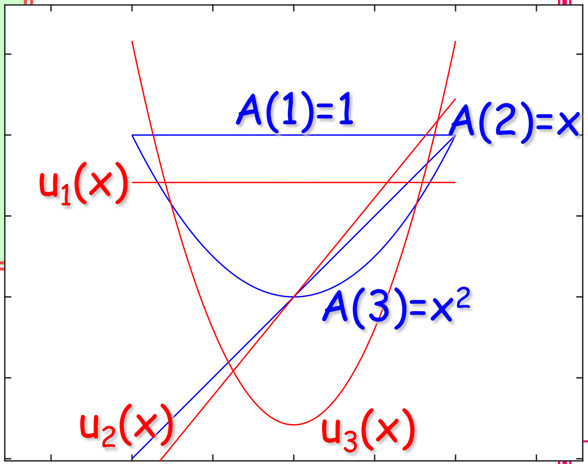
u: orthonormal system

```
disp(int(A'*A, -1,1))
[   2,   0, 2/3]
[   0, 2/3,   0]
[ 2/3,   0, 2/5]
disp(int(v'*v, -1,1))
[ 2,   0,    0]
[ 0, 2/3,    0]
[ 0,   0, 8/45]
disp(int(u'*u, -1,1))
[ 1,   0,    0]
[ 0,   1,    0]
[ 0,   0,    1]
```

non-orthogonal

orthogonal

orthonormal



Function plots do not represent the vectors of Π_1; to think of them as vectors of a linear subspace, we have to consider the vectors in $\mathbb{R}^3$, the real space.