Metodi Numerici dell'Informatica

Orthogonality and QR decomposition

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Motivation

Column space

For any $\mathbf{A} \in \mathbb{R}^{n \times m}$, the linear problem:

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

can be seen as:

"write $\mathbf{b}$ as a linear combination of the columns of $\mathbf{A}$ with coefficients stored in $\mathbf{x}$".

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Numerical instability

Consider the following situation:

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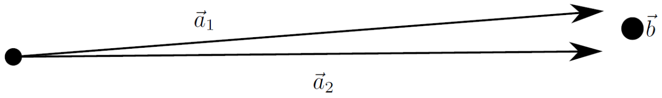
The columns are almost linearly dependent:



This problem is poorly conditioned, since we can write either:

$$\mathbf{b} \approx x_1\mathbf{a}_1 + x_2\mathbf{a}_2$$

$$\mathbf{b} \approx x_2\mathbf{a}_1 + x_1\mathbf{a}_2$$

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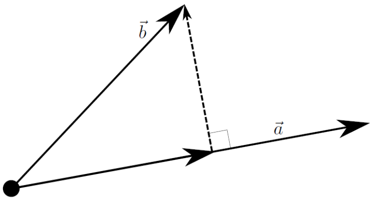
Can we find a simpler representation for the column space?

Can we deal with numerical instability explicitly?

Orthogonality

Projections

Consider two vectors $\mathbf{a}$ and $\mathbf{b}$. Which multiple of $\mathbf{a}$ is closest to $\mathbf{b}$?



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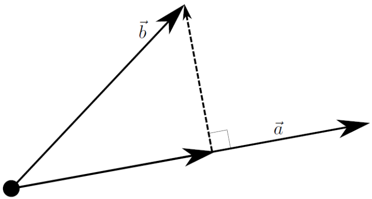

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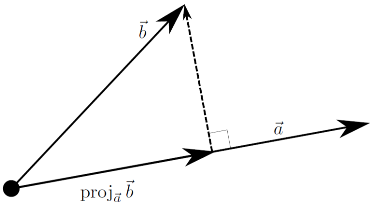

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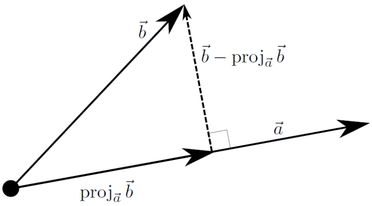

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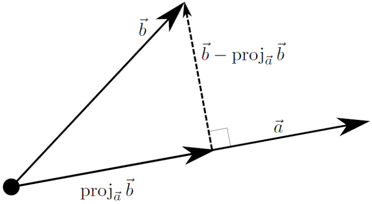

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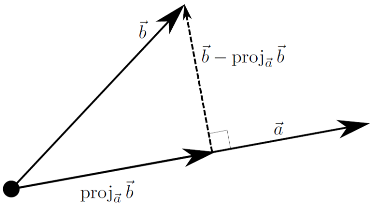

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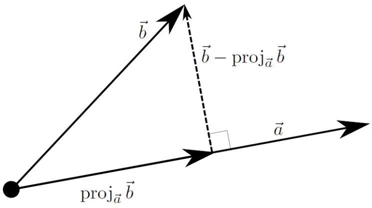

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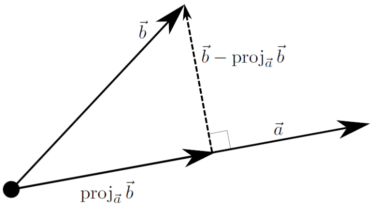

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Therefore:

$$\mathrm{proj}_{\mathbf{a}}\mathbf{b} = \frac{\mathbf{a}^\top \mathbf{b}}{\|\mathbf{a}\|_2^2}\mathbf{a}$$

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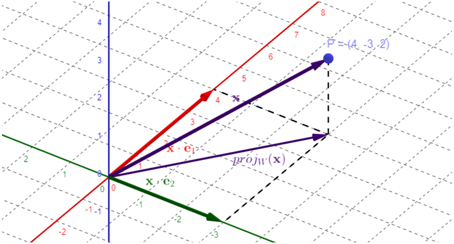

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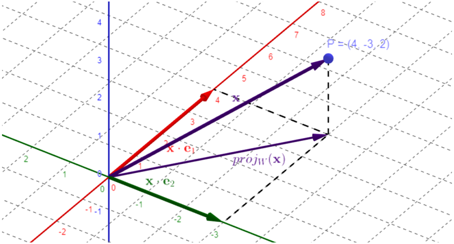

The projection is: $\mathrm{proj}_{\mathrm{span}(\mathbf{a}_1,\ldots,\mathbf{a}_k)}\mathbf{b} = (\mathbf{a}_1^\top\mathbf{b})\mathbf{a}_1 + \cdots + (\mathbf{a}_k^\top\mathbf{b})\mathbf{a}_k$

Orthogonal matrices

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In the lucky case where $\mathbf{A}^\top \mathbf{A} = \mathbf{I}$ (i.e. matrix $\mathbf{A}$ is orthogonal), we boil down to the trivial case. Further, this implies that $\mathbf{A}^{-1} = \mathbf{A}^\top$.

Let's analyze this more carefully.

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For clarity, let us call $\mathbf{Q}$ the orthogonal matrices.

The product $\mathbf{Q}^\top \mathbf{Q}$ has the structure:

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- The identity matrix $\mathbf{I}$ is orthogonal
- Any permutation matrix is orthogonal

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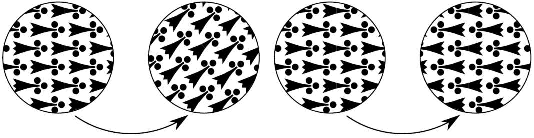
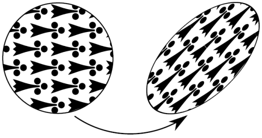


(a) Isometric



(b) Not isometric

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Then, the operation

$$\mathbf{A}\mathbf{R}^{-1} = \mathbf{Q}$$

can be seen as transforming the columns of $\mathbf{A}$ to make them orthogonal.

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$$\text{col } \mathbf{A}\mathbf{R}^{-1} = \text{col } \mathbf{A}$$

i.e., orthogonalization does not change the column space of $\mathbf{A}$.

QR decomposition

It turns out that any matrix $\mathbf{A}$ admits the factorization:

$$\mathbf{A} = \mathbf{QR}$$

which means that we can always "orthogonalize" the columns of any $\mathbf{A}$.

Further, it can be shown that

$$\text{col } \mathbf{AR}^{-1} = \text{col } \mathbf{A}$$

i.e., orthogonalization does not change the column space of $\mathbf{A}$.

Since $\mathbf{Q} = \mathbf{AR}^{-1}$, then

$$\text{col } \mathbf{Q} = \text{col } \mathbf{A}$$

means that the columns of $\mathbf{Q}$ are an orthonormal basis for $\text{col } \mathbf{A}$.

Better conditioning

How does this help us?

Recall the "almost parallel" numerical issue we encountered before:

$$\mathbf{A} = \begin{pmatrix} | & | & \\ \mathbf{a}_1 & \mathbf{a}_2 & \cdots \\ | & | & \end{pmatrix} = \begin{pmatrix} 0 & 0.0001 & \\ \vdots & \vdots & \dots \\ 1 & 1.0001 & \end{pmatrix}$$

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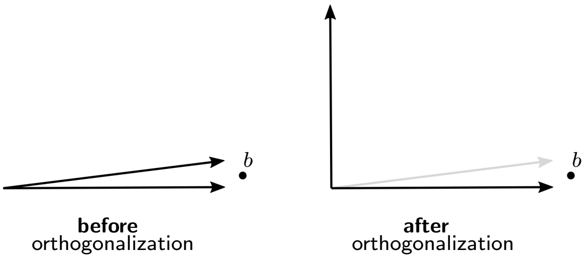
With orthogonalization, we make the problem better conditioned by simply applying invertible transformations to the columns of $\mathbf{A}$.



QR for least squares

Using QR factorization, the normal equations:

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

become:

$$(\mathbf{Q}\mathbf{R})^\top \mathbf{Q}\mathbf{R}\mathbf{x} = (\mathbf{Q}\mathbf{R})^\top \mathbf{b}$$

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And since $\mathbf{R}$ is invertible:

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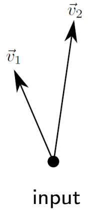
One additional property of matrix $\mathbf{R}$ in QR decomposition, is that it is upper triangular.

$$U = \begin{bmatrix} u_{1,1} & u_{1,2} & u_{1,3} & \dots & u_{1,n} \\ & u_{2,2} & u_{2,3} & \dots & u_{2,n} \\ & & \ddots & \ddots & \vdots \\ & & & \ddots & u_{n-1,n} \\ 0 & & & & u_{n,n} \end{bmatrix}$$

This makes the system immediate to solve by back-substitution.

Gram-Schmidt algorithm



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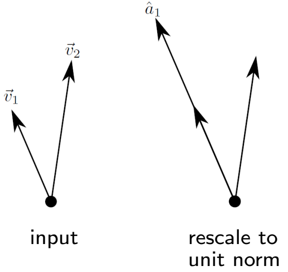

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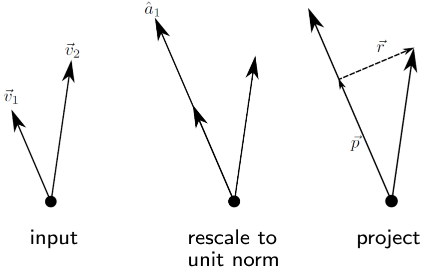

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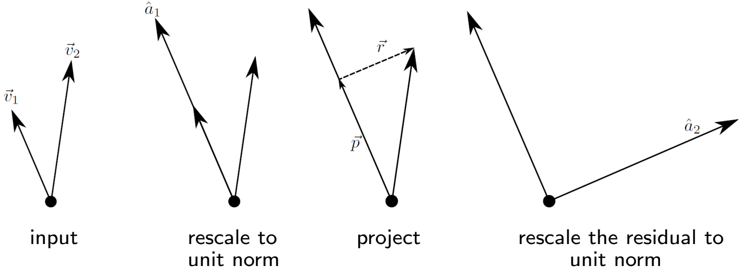

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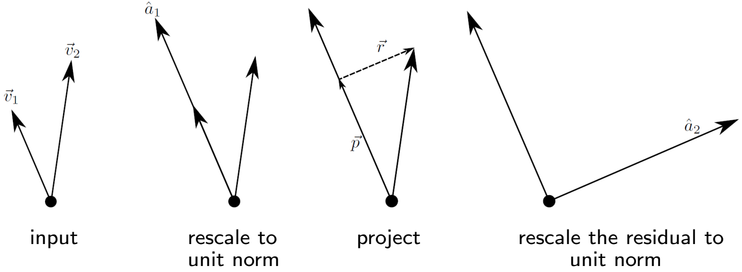

Observe the following:

- The orthogonalized vectors span the same space of $\mathbf{v}_1, \mathbf{v}_2$

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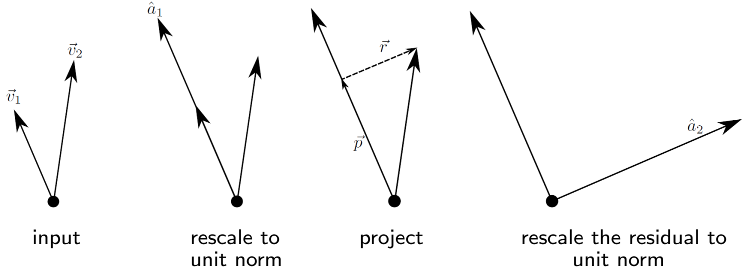

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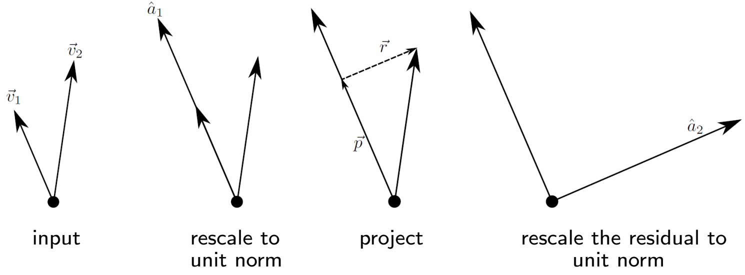

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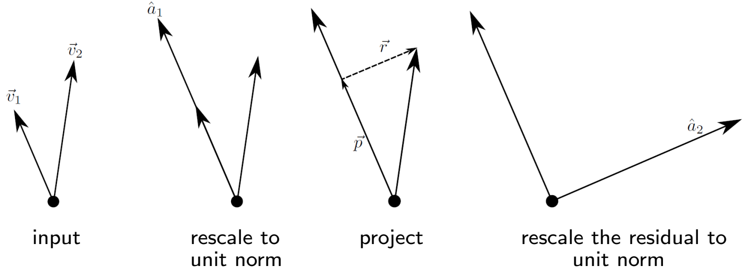

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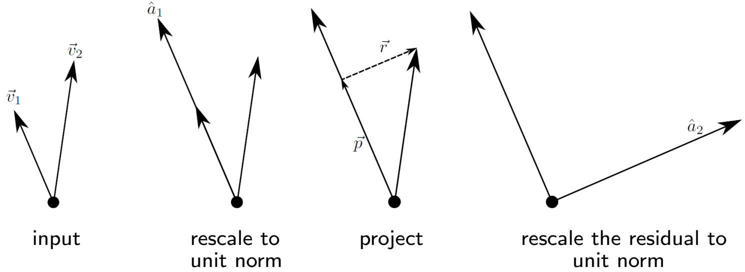
- The orthogonalized vectors span the same space of $\mathbf{v}_1, \mathbf{v}_2$
- We can introduce more input vectors one at a time, and orthogonalize them with respect to the previous ones
- If the input vectors are columns of $\mathbf{A}$, the orthogonalized vectors are the columns of $\mathbf{Q}$. Further, we can compute $\mathbf{R} = \mathbf{Q}^\top \mathbf{A}$.

Gram-Schmidt algorithm



function GRAM-SCHMIDT($\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_k$)
  ▷ Computes an orthonormal basis $\hat{a}_1, \ldots, \hat{a}_k$ for span $\{\vec{v}_1, \ldots, \vec{v}_k\}$
  ▷ Assumes $\vec{v}_1, \ldots, \vec{v}_k$ are linearly independent.

```
â₁ ← v₁/‖v₁‖₂                         ▷ Nothing to project out of the first vector
for i ← 2, 3, ..., k
    p ← 0                              ▷ Projection of vᵢ onto span {â₁, ..., âᵢ₋₁}
    for j ← 1, 2, ..., i − 1
        p ← p + (vᵢ · âⱼ)âⱼ            ▷ Projecting onto orthonormal basis
    r ← vᵢ − p                         ▷ Residual is orthogonal to current basis
    âᵢ ← r/‖r‖₂                        ▷ Normalize this residual and add it to the basis
return {â₁, ..., âₖ}
```

$\hat{a}_1 \leftarrow \vec{v}_1/\|\vec{v}_1\|_2$ ▷ Nothing to project out of the first vector
for $i \leftarrow 2, 3, \ldots, k$
  $\vec{p} \leftarrow \vec{0}$ ▷ Projection of $\vec{v}_i$ onto span $\{\hat{a}_1, \ldots, \hat{a}_{i-1}\}$
  for $j \leftarrow 1, 2, \ldots, i-1$
    $\vec{p} \leftarrow \vec{p} + (\vec{v}_i \cdot \hat{a}_j)\hat{a}_j$ ▷ Projecting onto orthonormal basis
  $\vec{r} \leftarrow \vec{v}_i - \vec{p}$ ▷ Residual is orthogonal to current basis
  $\hat{a}_i \leftarrow \vec{r}/\|\vec{r}\|_2$ ▷ Normalize this residual and add it to the basis
return $\{\hat{a}_1, \ldots, \hat{a}_k\}$

Reduced QR

Let us take a closer look at the dimensions:

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

In general, $\mathbf{A}$ will be tall with size $m \times n$.

Reduced QR

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$$\underbrace{\mathbf{A}}_{m\times n} = \underbrace{\mathbf{Q}}_{m\times n}\underbrace{\mathbf{R}}_{n\times n}$$

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- $\mathbf{A}$ has $k \leq n$ linearly independent columns...
- ...therefore, we can discard the last $n - k$ columns of $\mathbf{Q}$

Suggested reading

Read Sections 5.1 – 5.4 of the book:

J. Solomon, "Numerical Algorithms"