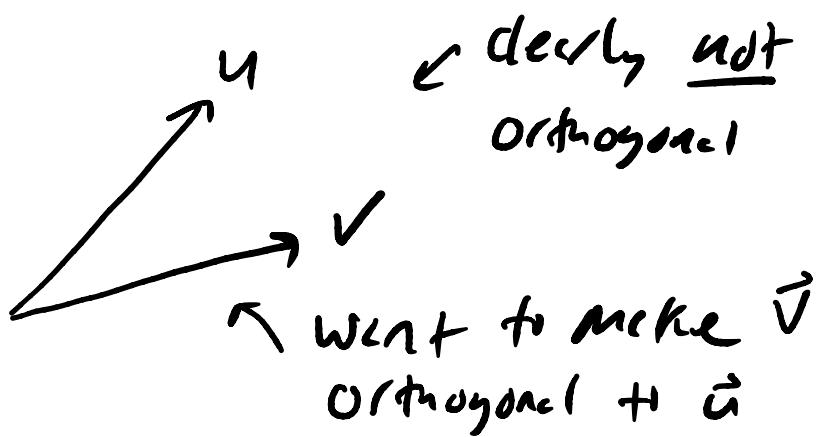


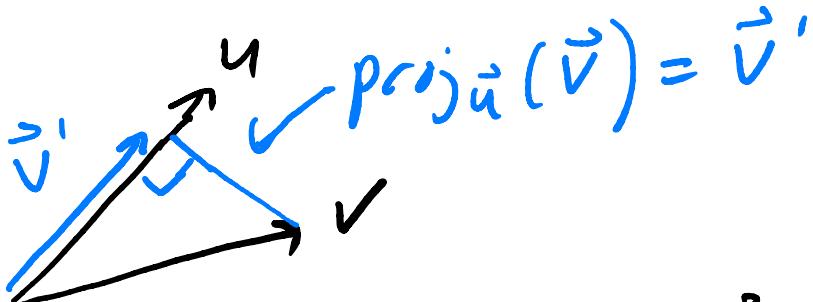
Gram - Schmidt algorithm (intuition) :

Idea: make column vectors orthogonal from one another by subtracting out "overlapping" components via projection:

2D example:

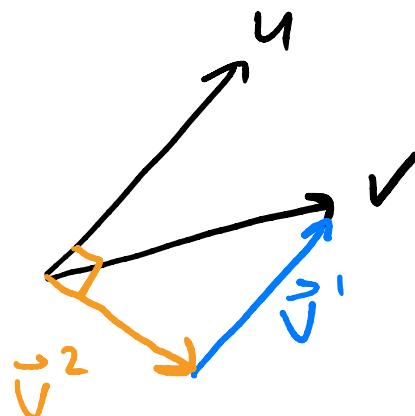


$\Rightarrow \text{proj}_{\vec{u}}(\vec{v}) = \text{project } \vec{v} \text{ onto } \vec{u}$



Then to make \vec{u}, \vec{v}' orthogonal:

$$\vec{v}^2 = \vec{v} - \underbrace{\text{proj}_{\vec{u}}(\vec{v})}_{\vec{v}'}$$



General Case: To make column vectors

$$[\vec{v}_1, \vec{v}_2, \vec{v}_3, \dots, \vec{v}_n]$$

$$\text{Orthogonal} - [\vec{u}_1, \vec{u}_2, \vec{u}_3, \dots, \vec{u}_n]$$

progressively subtract out projections
onto previous column vectors:

Orthogonal original vectors



$$u_1 = v_1$$

$$u_2 = v_2 - \text{proj}_{\vec{u}_1}(\vec{v}_2)$$

$$u_3 = v_3 - \text{proj}_{\vec{u}_1}(\vec{v}_3) - \text{proj}_{\vec{u}_2}(\vec{v}_3)$$

⋮

Gram-Schmidt algorithm (details) :

- 1) Initialize Q to an $(N, M+1)$ matrix.
 - 2) Visit columns in A from left-to-right.
Call the index of current column i .

$$\begin{bmatrix} \vdots \\ \downarrow \\ \vdots & \vdots & \vdots & \cdots \end{bmatrix}$$

- 3) with a separate "pointer" j , revisit all columns to the left of i in Q. $j < i$

$$(Q: \begin{bmatrix} \vdots & \vdots & \vdots & \ddots \end{bmatrix})$$

$j=1 \quad j=2$
 $\downarrow \rightarrow \downarrow$

$$A := \begin{bmatrix} & & & \\ & \vdots & \vdots & \vdots \\ & \vdots & \vdots & \vdots \\ & & & \dots \end{bmatrix}$$

purpose of j : visit vectors already
Mutually orthogonal.

4) For all valid j , add to a copy of column i of A
the following:

- $\underbrace{\langle \vec{\text{col}}(i), \vec{\text{col}}(j) \rangle}_{\text{dot product}} \cdot \vec{\text{col}}(j)$

$\xrightarrow{\text{element-wise multiplication}}$

Vector

Dot product \rightarrow Scalar

result = $(N, 1)$ "subtract off Scaled version of vector j "

i.e. $\underbrace{\vec{\text{col}}(i)}_{\text{temp variable}} = \vec{\text{col}}(i) - \sum_{j=1}^{i-1} \langle \vec{\text{col}}(i), \vec{\text{col}}(j) \rangle \cdot \vec{\text{col}}(j)$

— Don't modify A

5) After subtracting off all columns j from the current i column, normalize $\vec{\text{col}}(i)$ by its length / norm :

$$\vec{\text{col}}(i) = \frac{\vec{\text{col}}(i)}{\|\vec{\text{col}}(i)\|_2} = \frac{\vec{\text{col}}(i)}{\sqrt{x_{i,1}^2 + x_{i,2}^2 + \dots}}$$

Components
of column
 i .

6) $\vec{c}_{\text{ol}(i)}$, derived from A , becomes $\vec{c}_{\text{ol}(i)}$ of Q .

7) Repeat for all columns $i \rightarrow$ Done!

8) Compute $R = Q^T A$

• Solve least squares problem with QR decomposition

$$A \vec{c} = \vec{Y}$$

$$Q R \vec{c} = \vec{Y}$$

$$R \vec{c} = \underbrace{Q^T \vec{Y}}_{\text{Shape} = (M+1, 1)}$$

Solve for \vec{c} efficiently, without inversion by
back substitution b/c R upper triangular matrix.

Form:

$$\begin{array}{c|c} R & Q^T \vec{Y} \\ \left[\begin{array}{cccc|c} 0 & * & * & * & 1 \\ * & 0 & * & * & 2 \\ * & * & 0 & * & 3 \\ * & * & * & 0 & 2 \end{array} \right] & \left[\begin{array}{c} 1 \\ 2 \\ 3 \\ 2 \end{array} \right] \end{array}$$

i.e.

$$\begin{array}{ccccccc} & & & & = & \vdots \\ & & & & = & \vdots \\ & & & & = & \vdots \\ & & & & & & \end{array}$$

$$c_{n-1} + 2c_n = 3$$

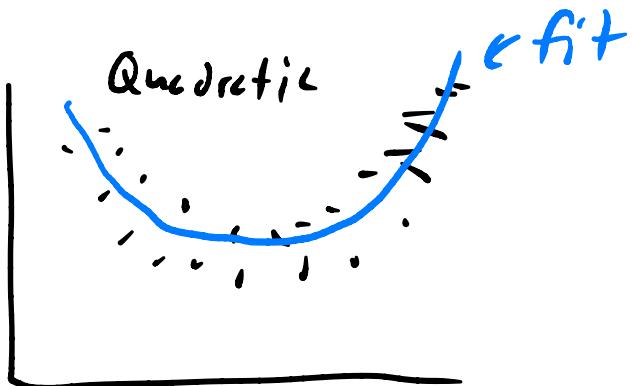
$$c_n = 2$$

- In project, can use Scipy function to do back substitution for you
 - `Scipy.linalg.solve_triangular`

$$\begin{matrix} R C & \longrightarrow & (n+1, 1) \\ \sqcup \quad \sqcup & & \sqcup \\ (n+1, n+1) & (n+1, 1) & n+1 \text{ equations} \\ & & n+1 \text{ unknowns} \end{matrix}$$

Polynomial regression

- In project, you will explore fitting a polynomial regression model to one independent/dependent variable pair:



This will allow you to better fit nonlinear data — data that does not exhibit a linear relationship between independent and dependent variable.

Example: $\vec{x}_1 = \begin{bmatrix} 2 \\ 4 \\ 1 \\ 3 \\ 5 \end{bmatrix}$ $\vec{Y} = \begin{bmatrix} 15 \\ 5 \\ 2 \\ 11 \\ 4 \end{bmatrix}$

fit the data to the cubic polynomial model:

$$Y = C_0 + C_1 X_1 + C_2 X_1^2 + C_3 X_1^3$$

$$\vec{Y} = \vec{A} \vec{C}$$

$$\begin{bmatrix} 15 \\ 5 \\ 2 \\ 11 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 4 & 8 \\ 1 & 4 & 16 & 64 \\ 1 & 1 & 1 & 1 \\ 1 & 3 & 9 & 81 \\ 1 & 5 & 25 & 125 \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \end{bmatrix}$$

Let's use polynomial regression on actual data!

[Boston housing data]

problem with polynomial regression: overfitting to data

[show slides]