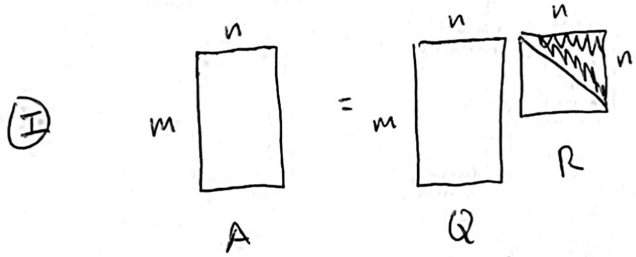
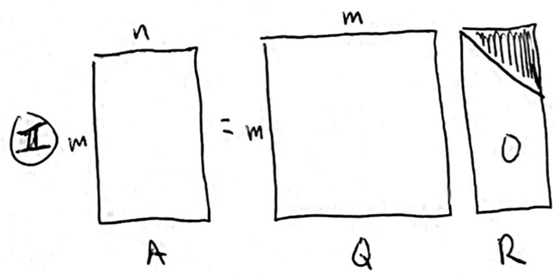
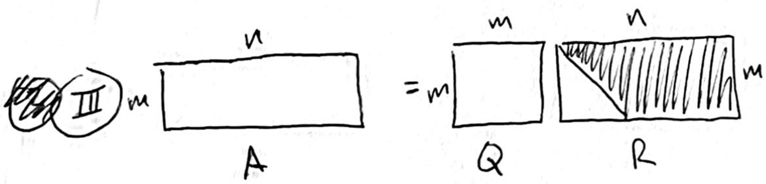
The QR-factorization ← the foundation of NLA, in some sense. (Mention least squares solution.)

Three scenarios





"Full QR"



Assuming rank $A = \min(m,n)$, reduced-rank next

There are two basic approaches for computing QR:

1. Gram-Schmidt triangular ↓ orthogonalization
2. Householder reflection triangularization ↑ orthogonal

Consider type I first.

$$A = QR \quad \Leftarrow\Rightarrow \quad \underbrace{A R^{-1}} = \underset{\text{orthogonal}}{Q}$$

This says to compute entris of R^{-1} such that they <u>orthogonalize</u> the columns of A $\Rightarrow$ Gram-Schmidt

I.e. if $A = (\vec{a}_1\ \vec{a}_2 \cdots \vec{a}_n)$

$Q = (\vec{q}_1\ \vec{q}_2 \cdots \vec{q}_n)$

then

$$\left.\begin{aligned} \vec{a}_1 &= r_{11}\vec{q}_1 \\ a_2 &= r_{12}\vec{q}_1 + r_{22}\vec{q}_2 \\ &\vdots \\ \vec{a}_n &= r_{1n}\vec{q}_1 + \dots + r_{nn}\vec{q}_n \end{aligned}\right\} \quad (*)$$

<u>G-S</u>: Turn $\vec{a}_1, \dots, \vec{a}_n$ into $\vec{q}_1 \cdots \vec{q}_n$

On step j, set $\vec{v}_j = \vec{a}_j - (\vec{q}_1, \vec{a}_j)\vec{q}_1 - \dots - (\vec{q}_{j-1}, \vec{a}_j)\, q_{j-1}$

and then $\vec{q}_j = \dfrac{\vec{v}_j}{\|\vec{v}_j\|}$

~~Comparing with (*) we see that~~

~~$a_j = \vec{v}_j$~~ Comparing with $(*)$ this implis that $r_{ij} = (\vec{q}_i, \vec{a}_j)$

and $|r_{jj}| = \|\vec{a}_j - \sum_{i=1}^{j-1} r_{ij}\vec{q}_i\|$

since $\quad r_{jj}\vec{q}_j = \vec{a}_j - r_{1j}\vec{q}_1 - \dots r_{j-1,j}\vec{q}_{j-1}$

(and take norms)

CODE

do ~~for~~ $j=1,n$ $\quad \left(\hat{q}_1 = \dfrac{\vec{a}_1}{\|\vec{a}_1\|}\right)$

$\vec{v}_j = \vec{a}_j$

do $i=1,j-1$

$r_{ij} = (\hat{q}_i, \vec{a}_j)$

$\vec{v}_j = \vec{v}_j - r_{ij}\hat{q}_i$

end

$r_{jj} = \|\vec{v}_j\|$

$\hat{q}_j = \vec{v}_j / r_{jj}$

end

This G-S algorithm is unstable!

round-off error can accumulate

An alternative way to think about this algorithm:

Define $\hat{Q}_{j-1}$ as $\hat{Q}_{j-1} = (\hat{q}_1\ \hat{q}_2 \cdots \hat{q}_{j-1})$

and P_j as the projector onto the subspace orthogonal to $\mathrm{col}(\hat{Q}_{j-1})$: $P_j = I - \hat{Q}_{j-1}\hat{Q}_{j-1}^*$

The "classical" G-S algorithm is then

$$\hat{q}_1 = \frac{\vec{a}_1}{\|\vec{a}_1\|} = \frac{P_1 \vec{a}_1}{\|P_1 \vec{a}_1\|}$$

$$\vdots$$

$$\hat{q}_j = \frac{P_j \vec{a}_j}{\|P_j \vec{a}_j\|}$$

"Modified" G-S is stable, and writes this projection in a different form:

$$P_j = I - \hat{Q}_{j-1} Q_{j-1}^*$$

$$= \underbrace{\left(I - \hat{q}_{j-1}\hat{q}_{j-1}^*\right)}_{P_{\perp \hat{q}_{j-1}}} \underbrace{\left(I - \hat{q}_{j-2}\hat{q}_{j-2}^*\right)}_{P_{\perp \hat{q}_{j-2}}} \cdots \left(I - \hat{q}_1 \hat{q}_1^*\right)$$

These are mathematically equivalent, but numerically different.

CODE

```
DO j=1,n
   v_j = a_j
END
```

$\}$ initialize the $\vec{v}_j$'s $\}$ cost: $\theta(mn)$, no-ops

...

DO $i = 1, n$

$r_{ii} = \|\vec{v}_i\|$ .... $\mathcal{O}(m)$

$\hat{q}_i = \vec{v}_i / r_{ii}$ .... $\mathcal{O}(m)$

DO $j = 1+i, n$

$\left.\begin{array}{l} r_{ij} = (\hat{q}_i, \vec{v}_j) \\ \vec{v}_j = \vec{v}_j - r_{ij}\hat{q}_i \end{array}\right\} P_{\perp \hat{q}_i}$ .... $\mathcal{O}(m)$, $\mathcal{O}(m)$

END

END

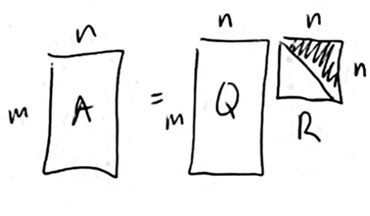
~~A.~~ This is the G-S algorithm used in practice.

How expensive is it? (See flop counts above)

$$\sum_{i=1}^{n}\left(3m + \sum_{j=1+i}^{n}(2m+2m)\right) \sim \sum_{i=1}^{n}\sum_{j=1+i}^{n} 4m \sim \boxed{\mathcal{O}(2mn^2)}.$$

- This is a cubic algorithm (like Gaussian elim, basically).

- Suited to Type I factorizations:



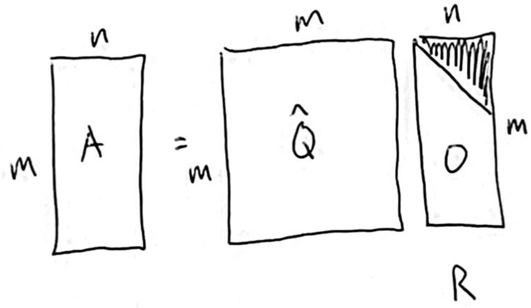
Aside: "big-oh" notation

$f(n) \sim \mathcal{O}(g(n))$ if

$f(n) \le C\,g(n)$ for

all $n > n_0 > 0$.

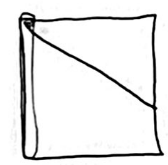
Next, consider Type II:



G-S will <u>not</u> produce an orthonormal basis for $\mathbb{R}^m$ when $m > n$ — we need an alternative.

Consider the following: If $A = \hat{Q}R$ (as above) then $\hat{Q}^* A = R$. Can we construct a $\hat{Q}^*$ that transforms A into an upper triangular matrix? Yes! Using "Householder Reflections".

<u>Step 1</u> Consider the first column of R:



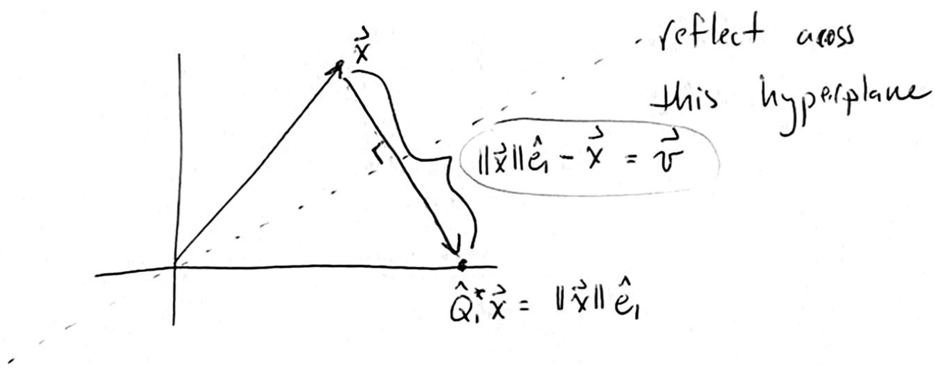
→ Every element is zero except for the first one.

Q: Can we find $\hat{Q}_1^*$ such that $\hat{Q}_1^* \vec{a}_1 = \begin{bmatrix} \bullet \\ 0 \end{bmatrix}$?

It must be that $\|\vec{r}_1\| = \|\vec{a}_1\|$ since $\hat{Q}_1^*$ is orthogonal. This can be achieved using a Householder reflection.

(numerically as, or more, stable than Gram-Schmidt).

Geometrically:



$$\hat{Q}_1^* \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix} = \begin{pmatrix} \|\vec{x}\| \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \|\vec{x}\| \hat{e}_1$$

Easy to show that this $\hat{Q}_1^*$ is given by $\hat{Q}_1^* = I - 2\dfrac{\vec{v}\vec{v}^*}{\vec{v}^*\vec{v}}$

(One could also reflect the "other" way to $-\|\vec{x}\|\hat{e}_1$, should choose the direction <u>farthest</u> from $\vec{x}$ for stability reasons.)

What about $\hat{Q}_k^*$?

Need $\cancel{\hat{Q}_k^* \hat{A}_k = \hat{Q}_k^* \begin{pmatrix} a_{1k} \\ a_{2k} \\ \vdots \\ a_{mk} \end{pmatrix}}$

$$\hat{Q}_k^* \vec{x} = \hat{Q}_k^* \begin{pmatrix} x_1 \\ \vdots \\ x_k \\ x_{k+1} \\ \vdots \\ x_m \end{pmatrix} = \begin{pmatrix} x_1 \\ \vdots \\ x_{k-1} \\ \|x_k \cdots x_m\| \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} I_{k-1} & 0 \\ 0 & F_{m-k+1} \end{pmatrix}$$

Reflector of size $(m-k+1) \times (m-k+1)$.