Projector matrices and the QR decomposition

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Recall: Last time, we "fixed" the stability issues in the Gaussian Elimination and LU decomposition algorithms by introducing the idea of "pivoting": permuting rows (or rows and columns) before each round of elimination to pick the diagonal entry (pivot) that was biggest in absolute value (out of the lower right block). This led us to two new algorithms: Gaussian Elimination with Partial Pivoting and with Complete Pivoting.

Part of any pivoting algorithm is to store and return the row permutation vector p (row and column permutation vectors p,q for complete), so we can use it later (this is especially important for LU decomposition). If we use partial pivoting, then A[p, :] = L U , and so the LU solver must solve L U x = b(p).

Today, we will discuss the **Gram-Schmidt algorithm** and its connection to the **QR decomposition**. We will take a brief detour into projections and projector matrices, and then we will introduce a **stable algorithm (Householder QR)** to compute QR (Gram-Schmidt is incredibly un-stable!).

ORTHOGONALITY – VERY USEFUL TOOL IN INNER PRODUCT (HILBERT) SPACES.

- Continuous LS – Polynomial, Fourier, ...
- Discrete LS
- Gaussian quadrature
- Orthogonal bases

Gram-Schmidt: $\{v_1, v_2, \dots, v_n\}$ basis (LI)

→ Produce orthonormal basis $\{q_1, q_2, \dots, q_n\}$ that spans the same thing.

$$\langle q_i, q_j \rangle = \delta_{ij} = \begin{cases} 0 ; & i \neq j \\ 1 ; & i = j \end{cases}$$

$$Q = \begin{bmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_n \\ | & | & & | \end{bmatrix} \longrightarrow Q^* Q = I$$

Gram-Schmidt

(1) $\tilde{q}_1 = v_1 ; \quad q_1 = \tilde{q}_1 / \|\tilde{q}_1\|.$

$v_1 = \|\tilde{q}_1\| \, q_1 .$

(2) $\tilde{q}_2 = v_2 - \dfrac{\langle v_2, q_1 \rangle}{\cancel{\langle q_1, q_1 \rangle}} \cdot q_1$

$q_2 = \tilde{q}_2 / \|\tilde{q}_2\|$

$v_2 = (\langle v_2, q_1 \rangle) q_1 + (\|\tilde{q}_2\|) \, q_2$

$\vdots$

(K) $\tilde{q}_k = v_k - \sum_{j=1}^{k-1} \langle v_k, q_j \rangle q_j$

$q_k = \tilde{q}_k / \|\tilde{q}_k\| .$

$v_k = \sum_{j=1}^{k} \langle v_k, q_j \rangle q_j + \|\tilde{q}_k\| q_k$

$q_k = \tilde{q}_k / \|\tilde{q}_k\|$. $\qquad j=1$

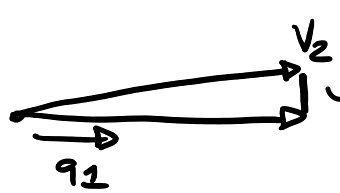
$$\begin{bmatrix} | & | & & | \\ v_1 & v_2 & \cdots & v_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} \|\tilde{q}_1\| & \langle v_2, q_1\rangle & & \langle v_k, q_1\rangle \\ 0 & \|\tilde{q}_2\| & & \langle v_k, q_2\rangle \\ \vdots & 0 & \cdots & \vdots \\ \vdots & \vdots & & \|\tilde{q}_k\| \\ 0 & 0 & & 0 \\ & & & \vdots \end{bmatrix}$$

$$\mathbb{A} = \mathbb{Q} \qquad \mathbb{R}$$

Useful:

- $\mathbb{A}x = b$ ($\mathbb{A}$ inv) $\to \mathbb{Q}\mathbb{R}x = b$
  $\mathbb{R}x = \mathbb{Q}^* b$
  + back solve. $\quad O(n^2)$
- $\min \|\mathbb{A}x - b\|^2 \to$ solve $\mathbb{R}x = \mathbb{Q}^* b$
- $\mathbb{Q}\mathbb{R}$ iteration (find eigendecomposition).

Gram-Schmidt is very unstable.



$v_2 - \langle v_2, q_1\rangle q_1 = \tilde{q}_2$

$q_2 = \tilde{q}_2 / \|\tilde{q}_2\|$.

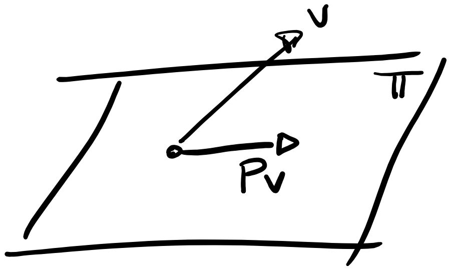
Two ways to fix

- Modified / Double GS.
- Different Approach "$\mathbb{R} = \mathbb{Q}^* \mathbb{A}$"
  - Householder
  - Givens

Projector matrix

Givens

Projector matrix



$$\boxed{\mathbb{P}^2 = \mathbb{P}.}$$

$\mathbb{P}$ projects onto $\underline{\underline{\mathcal{R}(\mathbb{P})}}$

$$\mathcal{N}(\mathbb{P}) = \{ y = x - \mathbb{P}x \}$$

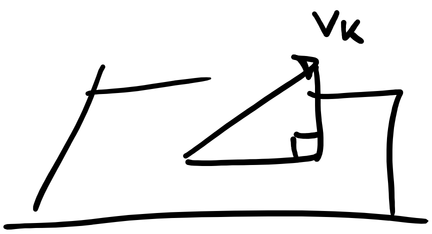
$$\mathbb{P}(\mathbb{I} - \mathbb{P}) = \mathbb{P} - \mathbb{P}^2 = \mathbb{O}.$$

$\mathbb{P}$ & $\mathbb{I} - \mathbb{P}$ are both proj w $\mathcal{R}(\mathbb{P}) = \mathcal{N}(\mathbb{I} - \mathbb{P})$

$\mathcal{R}(\mathbb{I} - \mathbb{P}) = \mathcal{N}(\mathbb{P})$

- Orthogonal Projectors

$$\left.\underline{\mathbb{P}^2 = \mathbb{P}, \quad \mathbb{P}^* = \mathbb{P}.}\right\} \quad \begin{array}{l} \mathcal{R}(\mathbb{P}) \perp \mathcal{N}(\mathbb{P}) \\ \mathcal{R}(\mathbb{P}) \oplus \mathcal{N}(\mathbb{P}) = \mathbb{R}^n. \end{array}$$



$$\{ q_1, q_2, \dots, q_n \}$$

$$\sum_{i=1}^{k} q_i q_i^* \to \mathbb{P}$$

$$\parallel$$

$$\mathbb{Q}\mathbb{Q}^*$$

$$\mathbb{I} - \sum q_i q_i^* = \underline{\underline{\mathbb{I} - \mathbb{Q}\mathbb{Q}^*}}$$

$$\mathbb{R} = \mathbb{Q}^* \mathbb{A}$$

$$\begin{bmatrix} r_{11} & | & \cdot \\ 0 & | & \end{bmatrix} \qquad \mathbb{Q}^* \begin{bmatrix} | & \\ \vec{a}_1 & \end{bmatrix}$$

$$\begin{bmatrix} r_{11} & & \\ 0 & & \\ 0 & & \\ \vdots & & \\ 0 & & \end{bmatrix} = Q^* \begin{bmatrix} \vec{a}_1 & & \end{bmatrix}$$

"Householder reflectors"

Given $w \in \mathbb{R}^n$ ($\mathbb{C}^n$) of unit length. Then,

$$H_w = I - 2ww^*$$

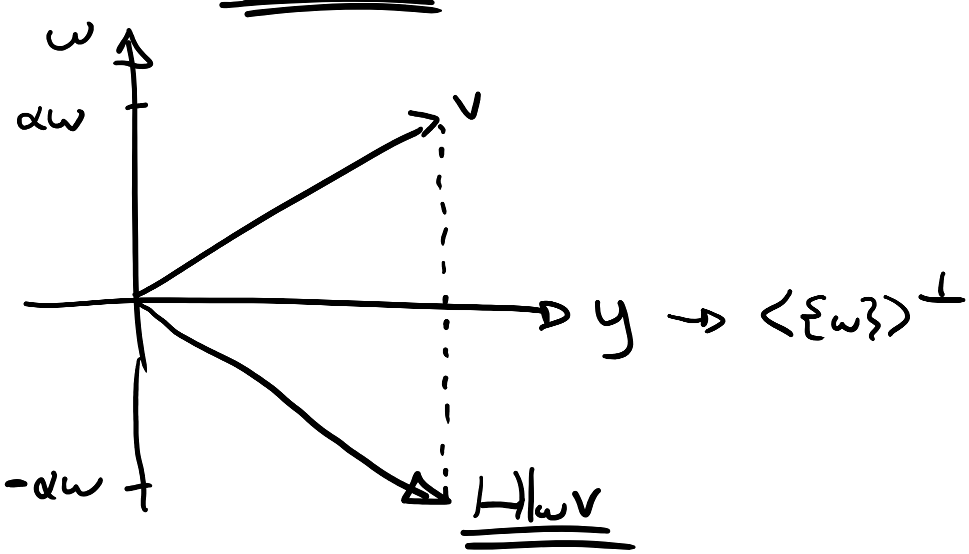
$H_w^2 = H_w$, $H_w^* = H_w$. (HW)

$\vec{v} \in \mathbb{R}^n \longrightarrow v = \alpha w + y$ where $\langle y, w \rangle = 0$.

$$H_w \cdot w = (I - 2ww^*)w = w - 2w(\overset{1}{\cancel{w^* w}}) = -w$$

$$H_w \cdot y = (I - 2ww^*)y = y - 2w(w^* y) = y.$$

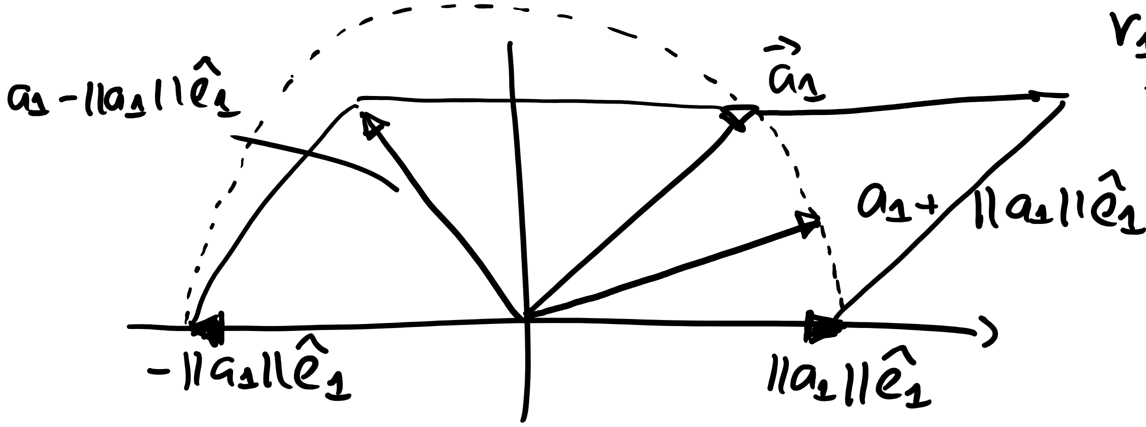
$$H_w v = \underline{\underline{y - \alpha w}}$$



Find w_1 s.t. $H_{w_1} \cdot \vec{a}_1 = r_{11} \cdot \hat{e}_1$, $|r_{11}| = \|a_1\|$

Find w_1 s.t. $H_{w_1} \cdot a_1 = r_{11} \cdot e_1$, $|r_{11}| = \|a_1\|$

$r_{11} = \pm \|a_1\|$



Best pick: $\boxed{\tilde{w}_1 = a_1 + \mathrm{sgn}(a_{11})\|a_1\|\hat{e}_1}$

$w_1 = \tilde{w}_1 / \|\tilde{w}_1\|$.

$$H_{w_1} \cdot A = \left[\begin{array}{c|ccc} r_{11} & a_{12}^{(2)} & & \\ \hline 0 & a_{22}^{(2)} & & \\ 0 & a_{23}^{(2)} & \ddots & \\ \vdots & \vdots & & \ddots \\ 0 & & & \end{array}\right]$$

$\hookrightarrow \underline{\underline{a_2^{(2)}}}$

$w_2 = a_2^{(2)} - \mathrm{sgn}(a_{2\,1}^{(2)})\|a_2^{(2)}\|\hat{e}_1$

$$H_2 = \begin{bmatrix} 1 & \boxed{0} \\ \boxed{0} & H_{w_2} \end{bmatrix}$$

$$H_2 H_1 A = \left[\begin{array}{cc|c} r_{11} & r_{12} & \\ 0 & r_{22} & \\ \vdots & 0 & \\ \vdots & \vdots & a_3^{(3)} \quad \boxed{} \\ 0 & 0 & \end{array}\right]$$

$\vdots$

$$\vdots$$

$$\mathbb{H}_k = \begin{bmatrix} I_{k-1} & 0 \\ 0 & H_{w_k} \end{bmatrix}$$

$$\underbrace{(\;\cdot\;\mathbb{H}_{n-1} \cdots \mathbb{H}_1)}\, A = \mathbb{R}$$

$$A = \underbrace{(\mathbb{H}_1 \mathbb{H}_2 \cdots \mathbb{H}_{n-1})}_{\mathbb{Q}}\, \mathbb{R}$$

- Compute $\mathbb{R}$ (and maybe apply $\mathbb{Q}^*$)
- Compute $\underline{\mathbb{R} \text{ and } \mathbb{Q}}$.

$$\mathbb{H}_k = \left[\begin{array}{c|c} I_{k-1} & 0 \\ \hline 0 & \underbrace{I - 2ww^*}_{n-(k-1)} \end{array}\right] \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right]$$

$$\mathbb{H}_{k-1} A = \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline H_w \underbrace{A_{21}}_{\text{often } 0} & H_w A_{22} \end{array}\right] \qquad \underbrace{A_{22} - 2(A_{22}w)w^*}_{O((n-(k-1))^2)}$$

Algo 1: ($\mathbb{R}$ and apply $\mathbb{Q}^*$) $\to \sim \frac{4}{3}n^3$ (2GE, 1LU)

Algo 2: (Compute $\mathbb{Q}, \mathbb{R}$) $\to \sim \frac{8}{3}n^3$ (4GE, 2LU)

EIGENVALUES / EIGENVECTORS

$\to A = U D U^*$, U unitary
D diagonal.

DEF: (Eigenpair) Given $A \in \mathbb{C}^{n \times n}$, then $\lambda \in \mathbb{C}$ is an eigenvalue of A iff there is $\vec{x} \neq 0$ s.t.

$$A\vec{x} = \lambda\vec{x} \leftrightarrow \underline{(A - \lambda I)\vec{x} = \vec{0}}$$

$x \to$ eigenvector (for λ)
$(\lambda, x) \to$ eigenpair of A
set of λ's $\to$ spectrum

$N(A - \lambda I)$ $\to \{0\}$ — λ is not an eigen.
$N(A - \lambda I)$ $\to \neq \{\vec{0}\}$ — λ is an eigenvalue.

$\updownarrow$

$A - \lambda I$ is singular — $\underbrace{\det(A - \lambda I)} = 0$

$P_A(\lambda) = \det(A - \lambda I)$ char. poly of A (deg $=$: n)

$\to$ eigenvalues = roots of P_A.

Notation: $\mathcal{E}_\lambda = N(A - \lambda I)$ "eigenspace"

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Multiplicity of λ:
- $p_A(\lambda) = (\lambda - \lambda_0)^k q(\lambda)$, $q(\lambda_0) \neq 0$.
- $\underline{\dim(\mathcal{E}_\lambda)}$.

SIMILARITY: $\mathbb{A}$, $\mathbb{B}$ $n \times n$, I say they are similar if $\exists\ \mathbb{P}$ invertible s.t.

$$\mathbb{B} = \mathbb{P}^{-1} \mathbb{A} \mathbb{P}$$

$\to$ $\mathbb{A}$, $\mathbb{B}$ are the same linear op but $\mathbb{P}$ is a change of basis.

I want $\mathbb{P}$ to be unitary

$$\mathbb{B} = \mathbb{P}^* \mathbb{A} \mathbb{P}$$

cols of $\mathbb{P}$ are orthonormal.

Invariants under similarity:

- $p_{\mathbb{A}}(\lambda) = p_{\mathbb{B}}(\lambda)$
- Eigenvalues are the same.

$(\lambda, \vec{x}_A)$ eigenpair for $\mathbb{A}$ $\leftrightarrow$ $(\lambda, \mathbb{P}^{-1} x_A)$ eigenpair for $\mathbb{B}$.

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random $\mathbb{A} \neq \mathbb{U} \mathbb{D} \mathbb{U}^*$ this is not always possible.

(Schur decomposition): for $A \in \mathbb{C}^{n \times n}$, there exists a unitary U s.t.

$$T = U^* A U$$

where T is upper triangular (Schur form) and eigen of $A \to$ diagonal (T).

- Algo (iterative) that produces $\approx (T, U)$

Spectral theorems (2):

Real case: ($\lambda \in \mathbb{R}$) - A be symmetric (hermitian) ($A = A^*$) $\leftrightarrow$ there is an orthonormal basis of eigenvectors w/ $\lambda \in \mathbb{R}$, $\underline{A = U D U^*}$

Complex case ($\lambda \in \mathbb{C}$) - A be normal $\to AA^* = A^*A$. $\leftrightarrow$ there is orth. basis of complex eigenvec/values $\leftrightarrow A = UDU^*$.

Sketch proof (Schur)

(i) $A = A^* \leftrightarrow T = T^* \to T = D$

(ii) $AA^* = A^*A \leftrightarrow TT^* = T^*T$

$\leftrightarrow \underline{T = D}$

Statement: There are no direct methods

$\boxed{\text{\underline{Statement}: There are \underline{no} direct methods to find eigendecomposition / all eigenvalues of } \mathbb{A} \text{ (for } n \geq 5)}$

If there was, you would have a formula for roots of $P_{\mathbb{A}}$.

$\mathbb{Q}\mathbb{R}$ iteration:

Start $\mathbb{A}_0 = \mathbb{A}$

while (algo has not converged)

$$[\mathbb{Q}_k, \mathbb{R}_k] = qr(\mathbb{A}_k)$$

$$\mathbb{A}_{k+1} = \underbrace{\mathbb{R}_k}\mathbb{Q}_k = \underline{\mathbb{Q}_k^* \mathbb{A}_k \mathbb{Q}_k}$$

$$\ldots \lim_{k \to \infty} \mathbb{A}_k = \underline{\underline{\mathbb{T}}}, \quad \lim_{k \to \infty} (\mathbb{Q}_1 \ldots \mathbb{Q}_k) = \underline{\underline{\mathbb{U}}}$$