

# Numerical Linear Algebra for Computational Science and Information Engineering

## Lecture 07 Orthogonalization and Least-Squares Problems

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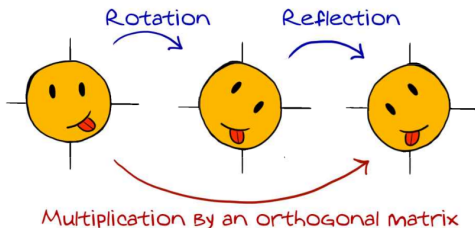
# QR factorization

Section 4 in Darve & Wootters (2021)

## QR factorization

- ▶ A QR factorization decomposes a matrix as the **product of an orthogonal matrix  $Q$  with an upper-triangular matrix  $R$ .**
- ▶ Recall that a matrix  $Q$  is orthogonal if  $Q^T Q = I$ .
- ▶ If a matrix is orthogonal, then  $\|Qx\|_2 = \|x\|_2$  for all  $x$ , i.e.,  $Q$  doesn't change the length of vectors.

The operations that do not change the length of vectors are **rotations** and **reflections**, so an orthogonal matrix can be thought of as a map that combines a rotation with a reflection.



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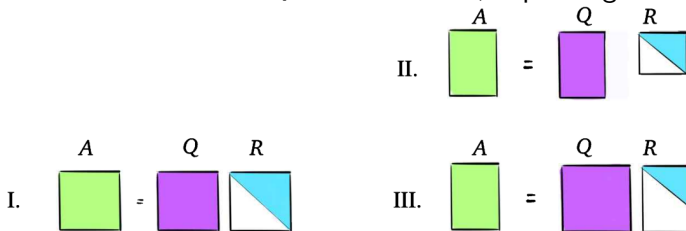
# QR factorization, cont'd

## QR factorization

- Let  $A$  be a real  $m \times n$  matrix with  $m \geq n$ . Then, there is an orthogonal matrix  $Q$  and an upper-triangular matrix  $R$  such that  $A = QR$ . This is called the **QR factorization**.
- When  $A$  is complex, there is still a factorization  $A = QR$ , but  $Q$  is unitary, i.e.,  $Q^H Q = I$ .

For the rest of this lecture, we assume  $A$  is real, but QR factorizations do exist for complex matrices.

► There are different forms of QR factorizations, depending on the shape of  $A$ :



# Applications of the QR factorization

The QR factorization has several applications in numerical linear algebra:

- 1 It can be used to solve least-squares problems, i.e., problems of the form  $\arg \min_x \|Ax - b\|_2$  where  $A$  is tall and skinny.
- 2 It is used as part of eigen- and singular value algorithms for small dense matrices.
- 3 It is also used in iterative methods to solve linear systems and compute eigenvalues, such as in Krylov methods.

## QR factorization and least-squares problems

To see why the QR factorization can be useful, let's look briefly at the least-squares problem:

- Let  $A \in \mathbb{R}^{m \times n}$  with  $m > n$ . We want to find  $x$  such that  $Ax$  is closest to  $b$  in Euclidean distance. That is

$$x^* = \arg \min_x \|Ax - b\|_2.$$

To do this, we use the QR factorization, with a square  $Q$ , i.e., case III from slide #2:

$$\|Ax - b\|_2 = \|Q^T(Ax - b)\|_2 = \|Q^T(QRx - b)\|_2 = \|Rx - Q^Tb\|_2$$

where we used the fact that for any vector  $y$ ,  $\|Q^Ty\|_2 = \|y\|_2$  because

$$\|Q^Ty\|_2^2 = (Q^Ty)^T(Q^Ty) = y^TQQ^Ty = y^T(Q^TQ)^Ty = y^TI^Ty = y^Ty = \|y\|_2^2.$$

As it turns out, it is easier to find  $x$  that minimizes  $\|Rx - Q^Tb\|_2$  than it is to minimize  $\|Ax - b\|_2$ .



# Householder reflections

Section 4.1 in Darve & Wootters (2021)

# Householder reflections

- ▶ Householder reflections are one of the most reliable methods to compute a QR factorization with a square  $Q$ , i.e., cases I and III.
- ▶ That is, we ask the question, does there exist a matrix  $Q$  s.t.  $Q^T A = R$ .
- ▶ Our goal is thus to create zero entries below the diagonal. Starting by the first column, we have:

$$Q_1^T \quad A \quad = \quad \begin{array}{|c|} \hline \text{blue} \\ \hline \text{green} \\ \hline \end{array}$$

Let's focus on this column

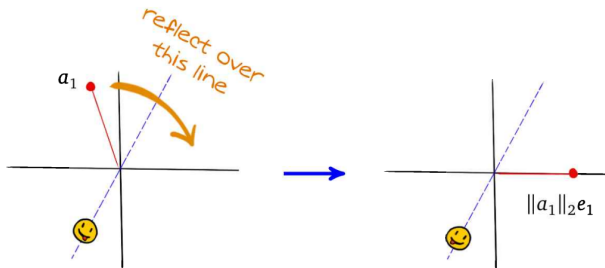
- ▶ We need to apply an orthogonal transformation  $Q_1^T$  to transform the first column of  $A$  into a vector in the direction of  $e_1$ .

Let's write  $A = [a_1 | \dots | a_n]$ . Then, since  $Q_1^T$  does not change the norm of  $a_1$ , we should have:

$$Q_1^T \quad a_1 \quad = \quad \begin{array}{|c|} \hline \text{blue} \\ \hline \text{white} \\ \hline \end{array} \quad \pm \|a_1\|_2 e_1$$

## Householder reflections, cont'd<sub>1</sub>

- ▶ A logical choice for  $Q_1^T$  would be a rotation that maps  $a_1$  parallel to  $e_1$ . However, rotations in high dimensions are not so easy to set up. Thus, we'll instead choose  $Q_1^T$  to be a **reflection** that maps  $a_1$  parallel to  $e_1$ :

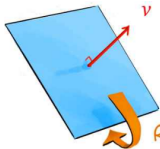


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Now that we have an idea of what the reflection should be doing, we need to figure out its mathematical formula.

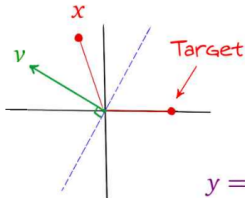
## Householder reflections, cont'd<sub>2</sub>

- Let us consider reflections in general. A reflection is defined by a vector:

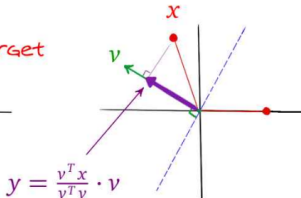


Reflect over the hyperplane orthogonal to  $v$

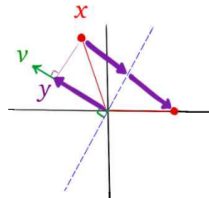
Given  $v$ , we can reason geometrically about what a reflection is:



Say we want to reflect  $x$  with respect to the hyperplane orthogonal to  $v$



Consider the projection  $y$  of  $x$  onto  $v$



Then the target is  $x - 2y = \left(I - \frac{2vv^T}{v^T v}\right)x$

# Householder reflections, cont'd<sub>3</sub>

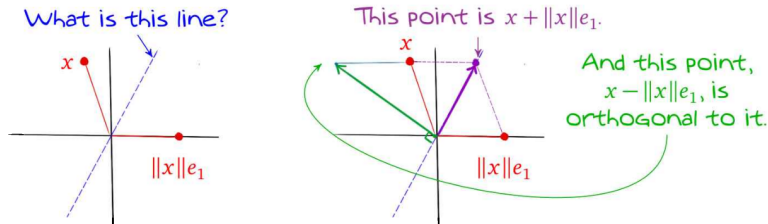
## Reflection

Let  $P$  be the matrix which represents a reflection over the hyperplane orthogonal to some vector  $v$ . Then  $P$  is given by

$$P = I - \beta vv^T \text{ where } \beta = \frac{2}{v^T v}.$$

- Now we need to pick  $v$  to arrive at a Householder reflection, i.e., to get a transformation from  $x$  to  $\|x\|_2 e_1$ .

The following geometric argument shows that  $v = x - \|x\|_2 e_1$  will work



## Householder reflections, cont'd<sub>3</sub>

Let  $v = x - \|x\|_2 e_1$ , then we see that

$$\begin{aligned} Px &= \left( I - 2 \frac{vv^T}{v^T v} \right) x \\ &= \left( I - 2 \frac{(x - \|x\|_2 e_1)(x - \|x\|_2 e_1)^T}{(x - \|x\|_2 e_1)^T (x - \|x\|_2 e_1)} \right) x \\ &= \left( I - 2 \frac{(x - \|x\|_2 e_1)(x - \|x\|_2 e_1)^T}{2(\|x\|_2^2 - 2\|x\|_2 x_1)} \right) x \\ &= x - \frac{(x - \|x\|_2 e_1)(\|x\|_2^2 - \|x\|_2 x_1)}{(\|x\|_2^2 - 2\|x\|_2 x_1)} \\ &= x - (x - \|x\|_2 e_1) \\ &= \|x\|_2 e_1 \end{aligned}$$

so that, indeed, a reflection over the hyperplane orthogonal to  $v = x - \|x\|_2 e_1$ , is a Householder reflection of  $x$ .

## Iterating Householder reflections

- Now that we know how to operate a first Householder reflection from  $a_1$  to  $\|a_1\|_2 e_1$ , we can apply a series of Householder transformations to progressively reduce  $A$  to an upper-triangular form.

We proceed by first zeroing entries in the first column, then in the second column, and so on.

In the end, for  $A \in \mathbb{R}^{m \times n}$  with  $m \geq n$ , we have

$$Q_{n-1}^T \dots Q_1^T A = R,$$

which is equivalent to

$$A = Q_1 \dots Q_{n-1} R = QR$$

where  $Q = Q_1 \dots Q_{n-1} \in \mathbb{R}^{m \times m}$ , and  $R$  has zeros in the  $m - n$  rows if  $m > n$ .

- In practice, when reducing  $A$  to  $R$ , the matrix  $P$  is never formed explicitly, instead we compute  $PA = A - \beta v(v^T A)$  which carries a cost  $\mathcal{O}(2mn)$ , instead of  $\mathcal{O}(m^2n)$  when  $P$  is assembled and applied, i.e., as  $P$  is dense.

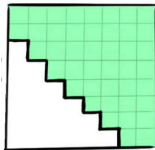
# Givens rotations

Section 4.2 in Darve & Wootters (2021)



## Givens rotations

- ▶ When the matrix  $A$  is upper Hessenberg, i.e., where  $a_{ij} = 0$  for all  $i > j + 1$ , most of the subdiagonal components are already zero, and using Householder transformations in this situation is a bit of an overkill:

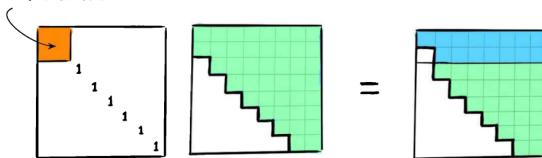


$A$

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- ▶ On every column of  $A$ , only one entry needs to be zeroed, so that 2D rotations, which are easy to set up, can be deployed for the job:

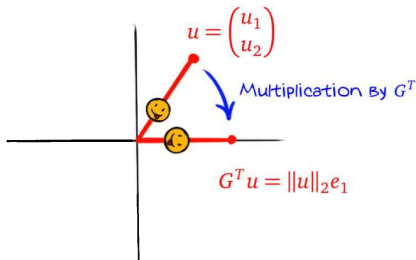
2D rotation



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## Givens rotations, cont'd<sub>1</sub>

- Zeroing a single subdiagonal entry can be reduced to considering a 2D vector  $u = (u_1, u_2)$  and finding a rotation  $G^T$  such that the vector  $u$  becomes aligned with  $e_1$ :



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With some algebra, we find:

### Givens rotation

A **Givens rotation** which rotates  $u = (u_1, u_2)^T$  to  $\|u\|_2 e_1$  is the  $2 \times 2$  matrix defined by

$$G^T = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}, \quad c = \frac{u_1}{\|u\|_2}, \quad s = -\frac{u_2}{\|u\|_2}.$$

## Givens rotations, cont'd<sub>2</sub>

- ▶ For an upper Hessenberg matrix  $A$  of size  $m \times n$ , we can compute its QR factorization using a sequence of Givens rotations.
- ▶ The algorithm is as follows:
  1. For each column  $j = 1, \dots, n - 1$  :
  2. Construct a Givens rotation matrix  $G^T$  that zeros  $a_{j+1,j}$
  3. Apply  $G^T$  to rows  $j$  and  $j + 1$  of  $A$

# CholeskyQR

# CholeskyQR factorization

- ▶ The **CholeskyQR** algorithm builds an economic factorization (i.e., case III) of  $A \in \mathbb{R}^{m \times n}$ , typically for  $n \ll m$ .
- ▶ It proceeds by first obtaining the  $R$  factor through a Cholesky factorization of the Gram matrix  $A^T A$ , then retrieving the  $Q$  factor by forward substitution:

The algorithm is as follows:

1.  $X := A^T A$  // BLAS 3
2. Find the upper triangular  $R$  s.t.  $R^T R = X$  // Cholesky factorization
3.  $Q := AR^{-1}$  // triangular solves

- ▶ CholeskyQR reaches higher arithmetic intensity and requires less synchronizations than Householder QR:

$\implies$  favored for distributed implementations.

- ▶ But, unlike Householder QR, CholeskyQR suffers from instability, with

$$\text{LOO}(Q) \in \mathcal{O}(u \cdot \kappa(A)).$$

## Reorthogonalized variants

- ▶ The lack of stability of an orthogonalization procedure can be partly remedied by repetition. The repetition of CholeskyQR is referred to as **CholeskyQR2**:

1.  $(Q_1, R_1) \leftarrow \text{CholeskyQR}(A)$
2.  $(Q, R_2) \leftarrow \text{CholeskyQR}(Q_1)$
3.  $R := R_2 R_1$

Repeating CholeskyQR significantly improves orthogonality, yielding  $\text{LOO}(Q) \in \mathcal{O}(u)$  under the condition that  $\kappa(A) \in \mathcal{O}(u^{-1/2})$ .

- ▶ Another way to improve the stability of CholeskyQR is to shift the Gram matrix, decreasing its condition number, thus improving the stability of the Cholesky factorization. The resulting **Shifted CholeskyQR** is given by:

1.  $X := A^T A$
2.  $s := 11(mn + n(n + 1))u\|A\|_2^2$  // calculate shift
3.  $X := X + sI_n$  // shift Gram matrix
4. Find the upper triangular  $R$  s.t.  $R^T R = X$  // Cholesky factorization
5.  $Q := AR^{-1}$  // triangular solves

which ensures  $\kappa(Q) \in \mathcal{O}(u^{-1/2})$  as long as  $\kappa(A) \in \mathcal{O}(u^{-1})$ .

## Reorthogonalized variants, cont'd

► Therefore, Shifted CholeskyQR can be used as a preconditioner to CholeskyQR2. This procedure is referred to as **Shifted CholeskyQR3**:

1.  $(Q_1, R_1) \leftarrow \text{Shifted CholeskyQR}(A)$
2.  $(Q, R_2) \leftarrow \text{CholeskyQR2}(Q_1)$
3.  $R := R_2 R_1$

which yields  $\text{LOO}(Q) \in \mathcal{O}(u)$  as long as  $\kappa(A) \in \mathcal{O}(u^{-1})$ .

Yamamoto, Y., Nakatsukasa, Y., Yanagisawa, Y., & Fukaya, T. (2015). Roundoff error analysis of the CholeskyQR2 algorithm. *Electron. Trans. Numer. Anal*, 44(01), 306-326.

Fukaya, T., Kannan, R., Nakatsukasa, Y., Yamamoto, Y., & Yanagisawa, Y. (2020). Shifted Cholesky QR for computing the QR factorization of ill-conditioned matrices. *SIAM Journal on Scientific Computing*, 42(1), A477-A503.

# Tall-and-skinny QR



## Tall-and-skinny QR (TSQR)

- ▶ Householder QR is unconditionally stable but memory-bound, and CholeskyQR variants, although they achieve high arithmetic intensity, offer limited stability.
- ▶ Tall-and-skinny (TSQR) algorithms offer both unconditional stability and high arithmetic intensity.

TSQR is particularly relevant when only the upper triangular factor  $R$  is needed.

- ▶ The key idea of TSQR is to **partition the matrix  $A$  into blocks** and compute QR factorizations hierarchically.

## Tall-and-skinny QR (TSQR), cont'd<sub>1</sub>

- ▶ For a matrix  $A \in \mathbb{R}^{m \times n}$  with  $m \gg n$ , we partition  $A$  into  $p$  blocks:

$$A = \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_p \end{bmatrix}$$

where each  $A_i \in \mathbb{R}^{(m/p) \times n}$ .

- ▶ We then compute the QR factorization of each block independently:

$$A_i = Q_i R_i, \quad i = 1, \dots, p.$$

- ▶ This gives us:

$$A = \begin{bmatrix} Q_1 R_1 \\ Q_2 R_2 \\ \vdots \\ Q_p R_p \end{bmatrix} = \begin{bmatrix} Q_1 & & & \\ & Q_2 & & \\ & & \ddots & \\ & & & Q_p \end{bmatrix} \begin{bmatrix} R_1 \\ R_2 \\ \vdots \\ R_p \end{bmatrix}.$$

## Tall-and-skinny QR (TSQR), cont'd<sub>2</sub>

- ▶ Next, we need to compute the QR factorization of the stacked  $R$  matrices:

$$\begin{bmatrix} R_1 \\ R_2 \\ \vdots \\ R_p \end{bmatrix} = \tilde{Q} \tilde{R}$$

where  $\tilde{Q} \in \mathbb{R}^{(pn) \times n}$  and  $\tilde{R} \in \mathbb{R}^{n \times n}$ .

- ▶ The final QR factorization is then:

$$A = \begin{bmatrix} Q_1 & & & \\ & Q_2 & & \\ & & \ddots & \\ & & & Q_p \end{bmatrix} \tilde{Q} \tilde{R} = Q \tilde{R}$$

where  $Q = \text{diag}(Q_1, Q_2, \dots, Q_p) \tilde{Q}$ .

- ▶ **Key advantage:** Each block can be processed independently, making TSQR highly parallelizable.

## Tall-and-skinny QR (TSQR), cont'd<sub>3</sub>

► The TSQR algorithm is as follows:

1. Partition  $A$  into  $p$  blocks:  $A = [A_1^T, A_2^T, \dots, A_p^T]^T$
2. Parallelizable step: Compute  $(Q_i, R_i) = \text{QR}(A_i)$  for  $i = 1, \dots, p$
3. Stack the  $R$  factors:  $\tilde{A} = [R_1^T, R_2^T, \dots, R_p^T]^T$
4. Compute  $(\tilde{Q}, \tilde{R}) = \text{QR}(\tilde{A})$
5. If only  $R$  is needed, return  $\tilde{R}$ . Otherwise,  $Q = \text{diag}(Q_1, \dots, Q_p)\tilde{Q}$

► The loss of orthogonality of TSQR is such that  $\text{LOO}(Q) \in \mathcal{O}(u)$  irrespective of  $A$ , i.e., TSQR is unconditionally stable.

► TSQR combines the best of both worlds: numerical stability of Householder QR with high arithmetic intensity and parallelizability.  
 $\implies$  TSQR favored for high-performance implementations.

# Gram-Schmidt procedures

Section 4.3 in Darve & Wootters (2021)

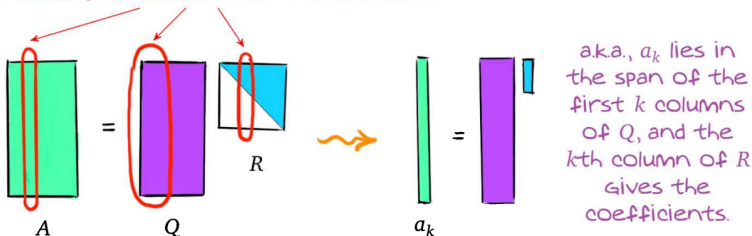
# Gram-Schmidt procedures

- ▶ Householder reflections and Givens rotations produce a square matrix  $Q \in \mathbb{R}^{m \times m}$ , even when  $A \in \mathbb{R}^{m \times n}$  with  $m > n$ , i.e., case III.  
On the other hand, **Gram-Schmidt** procedures will **produce a rectangular, tall-and-skinny matrix**  $Q \in \mathbb{R}^{m \times n}$ , i.e., like in case II.
- ▶ Another peculiarity of **Gram-Schmidt** procedures is that they **work column-by-column**, i.e., to compute  $q_i$  in  $Q = [q_1, \dots, q_n]$ , you only need access to  $a_i$  from  $A = [a_1, \dots, a_n]$  and  $q_1, \dots, q_{i-1}$ .  
This feature of the Gram-Schmidt procedures is particularly **useful in Krylov methods** where  $A$  is not available all at once, and the new column  $a_i$  to orthogonalize is only available after an performing a full iteration of computations.
- ▶ The first  $k$  columns  $q_1, \dots, q_k$  formed by Gram-Schmidt procedure in  $Q$  are an **orthonormal basis** of the subspace spanned by  $a_1, \dots, a_k$ .

## Gram-Schmidt procedures, cont'd<sub>1</sub>

- ▶ Visualizing the column  $a_k = QR_{:,k}$ , and the fact that  $R_{:,k}$  has  $k$  non-zero entries followed by  $m - k$  zeros on the subdiagonal, we can write  $a_k = Q_{:,1:k}R_{1:k,k}$ :

Consider just this part of the equation



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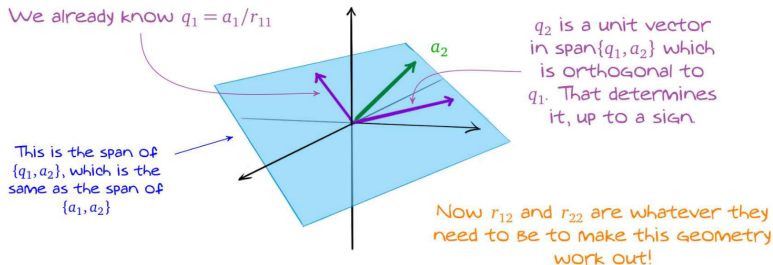
That is,  $a_k$  is formed by linear combination of  $q_1, \dots, q_k$ :

$$a_k = r_{1k}q_1 + \dots + r_{kk}q_k.$$

- ▶ Thus, instead of searching for the matrix  $Q$  that makes  $Q^T A$  upper triangular, we are rather going to search for the upper triangular matrix  $R$  such that every  $a_k$  is given by linear combination of  $q_1, \dots, q_k$ .

## Gram-Schmidt procedures, cont'd<sub>2</sub>

- ▶ First, since we have  $a_1 = r_{11}q_1$ , and  $q_1$  has unit norm, we set  $r_{11} = \|a_1\|_2$  and  $q_1 = a_1/r_{11}$ .
- ▶ Then, we continue iteratively, i.e.,  $a_2 = r_{12}q_1 + r_{22}q_2$  so that  $q_2$  is a unit vector in  $\text{span}\{q_1, a_2\} = \text{span}\{a_1, a_2\}$ , orthogonal to  $q_1$ :



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Then  $r_{12}$  and  $r_{22}$  are found to close the system.



# Classical Gram-Schmidt (CGS) procedure

- More formally, for each  $1 \leq k \leq n$ , we write

$$a_k = \sum_{i=1}^k r_{ik} q_i = r_{kk} q_k + \sum_{i=1}^{k-1} r_{ik} q_i$$

Assuming we already know  $q_j$  and  $r_{ij}$  for all  $j < k$  and  $i \leq j$ , we can then use this formula to find expressions for the  $r_{ik}$ 's and  $q_k$ .

First, multiplying by  $q_i^T$  and invoking the orthonormality of the basis given by  $q_1, \dots, q_k$ , we get

$$q_i^T a_k = \sum_{j=1}^k r_{jk} q_i^T q_j = r_{ik} \implies r_{ik} = q_i^T a_k \text{ for } i < k.$$

Next, to find  $r_{kk}$ , we have  $q_k r_{kk} = a_k - \sum_{i=1}^{k-1} r_{ik} q_i$  where  $q_k$  has unit norm so that

$$r_{kk} = \left\| a_k - \sum_{i=1}^{k-1} r_{ik} q_i \right\|_2.$$

## Classical Gram-Schmidt (CGS) procedure, cont'd<sub>1</sub>

Note that  $r_{kk}$  could also be chosen to be negative. However, it is standard to let  $R$  have positive components on the diagonal.

Finally, we have

$$q_k = \frac{1}{r_{kk}} \left( a_k - \sum_{i=1}^{k-1} r_{ik} q_i \right).$$

This procedure is referred to as the **classical Gram-Schmidt** algorithm.

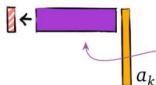
We see indeed that, in order to compute  $q_k$ , you need access to  $a_k$  and  $q_1, \dots, q_{k-1}$ .

# Classical Gram-Schmidt (CGS) procedure, cont'd<sub>2</sub>

When we get the  $k$ th column of  $A$ :

The first  $k-1$  columns,  $q_1, \dots, q_{k-1}$ , have already been orthogonalized.

STEP 1: Set the  $k$ th column of  $R$



This matrix has rows that are  $q_1, \dots, q_{k-1}$ .

STEP 2: Update  $a_k$



This matrix projects  $a_k$  onto the space orthogonal to  $q_1, \dots, q_{k-1}$ .

$$= a_k - \begin{bmatrix} q_1 & \dots & q_{k-1} \end{bmatrix} \begin{bmatrix} r_{k1} \\ \vdots \\ r_{k,k-1} \end{bmatrix} = \left( \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} - \begin{bmatrix} q_1 & \dots & q_{k-1} \end{bmatrix} \begin{bmatrix} r_{k1} \\ \vdots \\ r_{k,k-1} \end{bmatrix} \right) a_k$$

STEP 3: Renormalize  $a_k$  and set  $r_{kk}$  appropriately.

Now we've turned  $a_k$  into  $q_k \perp q_1, \dots, q_{k-1}$ ! Move on to the next column.

## Classical Gram-Schmidt (CGS) procedure, cont'd<sub>3</sub>

► So the CGS algorithm is implemented as follows:

1.  $r_{11} := \|a_1\|_2; q_1 := a_1/r_{11}$
2. For each  $k = 2, \dots, n$  :
3.  $R_{1:k-1,k} := Q_{:,1:k-1}^T a_k$  // BLAS 2
4.  $q_k := a_k - Q_{:,1:k-1} R_{1:k-1,k}$  // BLAS 2
5.  $r_{kk} := \|q_k\|_2; q_k := q_k/r_{kk}$

so that CGS relies on two BLAS 2 calls per iteration.

Similarly, we can write

1.  $r_{11} := \|a_1\|_2; q_1 := a_1/r_{11}$
2. For each  $k = 2, \dots, n$  :
3.  $q_k := \Pi_{k-1} a_k$
4.  $r_{kk} := \|q_k\|_2; q_k := q_k/r_{kk}$

where  $\Pi_{k-1} := I_m - Q_{:,1:k-1} Q_{:,1:k-1}^T$  is an **orthogonal projector** onto the subspace  $\text{range}(Q_{:,1:k-1})^\perp$  so, indeed,  $q_k$  is made orthogonal to the previously formed vectors  $q_1, \dots, q_{k-1}$ .

# Instability of CGS

- ▶ CGS is known to **not** being very **stable**.

- ▶ For example, consider the matrix  $A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix}$ .

If we assume  $\varepsilon^2$  is smaller than the unit roundoff  $u$ , then the  $Q$  matrix

generated by CGS is  $Q = \begin{bmatrix} 1 & 0 & 0 \\ \varepsilon & -1/\sqrt{2} & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix}$ .

Then we see that  $q_2$  and  $q_3$  are far from being orthogonal as we have  $q_2^T q_3 = 1/2$ .

- ▶ Numerical stability is measured with respect to the loss of orthogonality, LOO, defined by  $\text{LOO}(Q) := \|I_m - Q^T Q\|_2$ .
- ▶ With CGS, the LOO depends on  $A$ , i.e.,  $\text{LOO} \in \mathcal{O}(u \cdot \kappa^{n-1}(A))$ , irrespective of  $\kappa(A)$ , although this bound is not sharp.

## Re-orthogonalization, CGS2

- An alternative is to orthogonalize twice by CGS, leading to CGS2:

- |   |   |
|---|---|
| 1. $r_{11} := \ a_1\ _2; q_1 := a_1/r_{11}$ | 1. $r_{11} := \ a_1\ _2; q_1 := a_1/r_{11}$ |
| 2. For each $k = 2, \dots, n$ :             | 2. For each $k = 2, \dots, n$ :             |
| 3. $q_k := \Pi_{k-1} a_k$                   | 3. $R_{1:k-1,k} := Q_{:,1:k-1}^T a_k$       |
| 4. $q_k := \Pi_{k-1} q_k$                   | 4. $q_k := a_k - Q_{:,1:k-1} R_{1:k-1,k}$   |
| 5. $r_{kk} := \ q_k\ _2; q_k := q_k/r_{kk}$ | 5. $S_{1:k-1} := Q_{:,1:k-1}^T q_k$         |
|   | 6. $q_k := q_k - Q_{:,1:k-1} S_{1:k-1}$     |
|   | 7. $r_{kk} := \ q_k\ _2; q_k := q_k/r_{kk}$ |
- where  $\Pi_{k-1} := I_m - Q_{:,1:k-1} Q_{:,1:k-1}^T$ .

- The loss of orthogonality becomes  $\text{LOO}(Q) \in \mathcal{O}(u)$  under the assumption that  $\kappa(A) \in \mathcal{O}(u^{-1})$ .
- However, CGS2 requires  $4mn^2$  FLOPs instead of  $2mn^2$  for CGS.

# Modified Gram-Schmidt, MGS

- Another alternative to CGS, referred to as modified Gram-Schmidt (MGS), is obtained by letting  $\Pi_{k-1} := (I_m - q_{:,k-1}q_{:,k-1}^T) \cdots (I_m - q_{:,1}q_{:,1}^T)$  in

1.  $r_{11} := \|a_1\|_2$ ;  $q_1 := a_1/r_{11}$
2. For each  $k = 2, \dots, n$  :
3.  $q_k := \Pi_{k-1}a_k$
5.  $r_{kk} := \|q_k\|_2$ ;  $q_k := q_k/r_{kk}$

Assuming perfect arithmetic, this is equivalent to CGS, but it relies on BLAS 1 instead BLAS 2 operations:

1.  $r_{11} := \|a_1\|_2$ ;  $q_1 := a_1/r_{11}$
2. For each  $k = 2, \dots, n$  :
3.  $q_k := a_k$
4. For each  $\ell = 1, \dots, k-1$  :
3.  $r_{\ell k} := q_\ell^T q_k$  // BLAS 1
4.  $q_k := q_k - r_{\ell k}q_\ell$  // BLAS 1
5.  $r_{kk} := \|q_k\|_2$ ;  $q_k := q_k/r_{kk}$

## Modified Gram-Schmidt, MGS, cont'd

- ▶ The loss of orthogonality of MGS is  $\text{LOO}(Q) \in \mathcal{O}(u \cdot \kappa(A))$ , irrespective of  $\kappa(A)$ , so that it is more stable than CGS.

- ▶ Considering once again the matrix  $A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix}$  where  $\varepsilon^2 < u$ ,

MGS yields a  $Q$  matrix  $A = \begin{bmatrix} 1 & 0 & 0 \\ \varepsilon & -1/\sqrt{2} & -1/\sqrt{6} \\ 0 & 1/\sqrt{2} & -1/\sqrt{6} \\ 0 & 0 & \sqrt{2}/\sqrt{3} \end{bmatrix}$ .

Contrarily to CGS, we see that  $q_2$  and  $q_3$  are exactly orthogonal, i.e.,  $q_2^T q_3 = 0$ , and  $q_1$  is nearly orthogonal to  $q_2$  and  $q_3$ , with  $|q_1^T q_2| = \varepsilon/\sqrt{2}$  and  $|q_1^T q_3| = \varepsilon/\sqrt{6}$ .

- ▶ In practice, MGS and CGS2 are used instead of CGS.
- ▶ MGS is often preferred by default, but CGS2 is more stable and reaches higher arithmetic intensity.

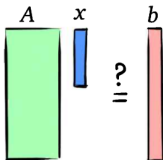


# Least-squares problems

Section 4.4 in Darve & Wootters (2021)

# Geometry of least-squares

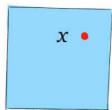
- One of the applications of the QR decomposition is the solving of least-squares problems  $\arg \min_x \|Ax - b\|_2$ :



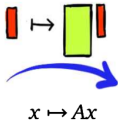
Since  $A$  is tall and skinny, there are more equations than unknowns! So there may not be some  $x$  so that  $Ax = b$ . The least-squares problem is to find the  $x$  so that  $Ax$  is closest to  $b$ , in 2-norm.

with a tall-and-skinny matrix  $A \in \mathbb{R}^{m \times n}$  and a vector  $b \in \mathbb{R}^n$ .

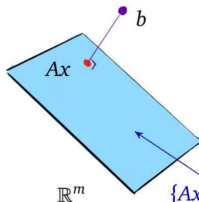
- To minimize the 2-norm from a point  $b$  to a subspace  $\{Ax, x \in \mathbb{R}^n\}$ , we can just do an orthogonal projection:



$\mathbb{R}^n$



$x \mapsto Ax$



The point  $Ax$  which is closest to  $b$  in 2-norm is the orthogonal projection of  $b$  onto the subspace  $\{Ax : x \in \mathbb{R}^n\}$ .

## Method of normal equations

- As per property of orthogonal projections, the  $x$  that minimizes  $\|Ax - b\|_2$  has an error  $e := Ax - b$  which is orthogonal to the range of  $A$ . This can be written as

$$A^T(Ax - b) = 0. \quad (1)$$

Assuming  $A$  is full-rank, this equation can be used to solve for  $x$  by a method called **normal equations**.

Eq. (1) may also be derived from calculus, namely, the optimal  $x$  which minimizes the cost function

$$f(x) = \|Ax - b\|_2^2 = (Ax - b)^T(Ax - b) = x^T A^T A x - 2x^T A^T b + b^T b$$

is obtained for  $\nabla f(x) = 0$  where

$$\nabla f(x) = 2A^T A x - 2A^T b,$$

which equivalently yields Eq. (1).

## Method of normal equations, cont'd

- ▶ Assuming  $A$  is full-rank,  $A^T A$  is SPD so that we may compute its Cholesky factorization and solve for  $x$  in  $A^T A x = A^T b$ .

### Normal equations

Finding the solution  $x$  to the least-squares problem  $\arg \min \|Ax - b\|_2$  by solving the system  $A^T A x = A^T b$  is called the method of **normal equations**.

- ▶ Since the condition number of  $A^T A$  is the square of that of  $A$ , the method of normal equations can run into issues when  $A$  is poorly conditioned.
- ▶ For cases where  $A$  is poorly conditioned, the QR factorization can be used to yield a more accurate computation of the solution  $x$  to the least-squares problem.

## QR factorization for least-squares problems

- The origin of the method of normal equations stems from saying that the error  $Ax - b$  is orthogonal to the range of  $A$ .

But if we know a QR factorization  $A = QR$  where  $Q \in \mathbb{R}^{m \times n}$ , then the range of  $A$  is the same as the range of  $Q$ .

The orthogonality condition can then be re-stated as

$$Q^T(Ax - b) = 0. \quad (2)$$

Since  $Q$  is orthogonal, it is necessarily well-conditioned, and the conditioning problem of the method of normal equations can be avoided.

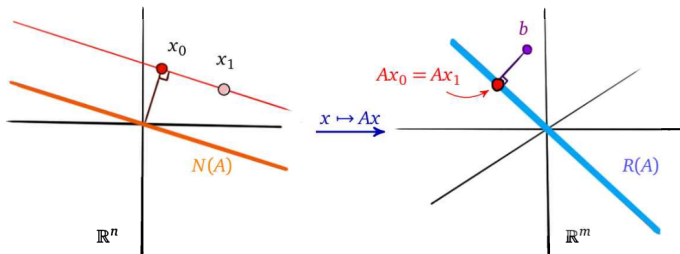
Since  $A = QR$ , due to the orthogonality of  $Q$ , we have  $Q^T A = R$  so that Eq. (2) becomes

$$Rx = Q^T b$$

where  $R$  is non-singular as long as  $A$  is non-singular, so that there exists a unique solution  $x$ .

## Case of rank-deficient $A$

- ▶ If  $A$  is rank-deficient, the null space of  $A$  is non-trivial. Then, for some  $x$  that minimizes  $\|Ax - b\|_2$ , there are infinitely many  $\delta x \in \text{null}(A)$  such that  $A(x + \delta x) = Ax$ . Hence, the solution to the least-squares problem is not unique.
- ▶ In case of non-uniqueness of solution, one can search for the unique  $x_0$  which minimizes both  $\|Ax - b\|_2$  and  $\|x\|_2$ :



Darve, E., & Wootters, M. (2021). Numerical linear algebra with Julia. Society for Industrial and Applied Mathematics.

We can see the  $x_0$  we are after is orthogonal to the null space of  $A$ , while any other solution  $x_1$  is of the form  $x_0 + \delta x$ .

## SVD method for solving least-squares with rank-deficient $A$

- Let  $A \in \mathbb{R}^{m \times n}$  be of rank  $r < n < m$  have an SVD given by  $A = U\Sigma V^T$  with  $U \in \mathbb{R}^{m \times m}$ ,  $V \in \mathbb{R}^{n \times n}$  and  $\Sigma \in \mathbb{R}^{m \times n}$  where  $\Sigma$  has zeros from row  $r + 1$  to  $m$ .

Then we can ignore the columns of  $U$  and  $V$  that correspond to zeros in  $\Sigma$  to create the thin SVD  $A = \tilde{U}\tilde{\Sigma}\tilde{V}^T$ :

$$A = U \Sigma V^T = \tilde{U} \tilde{\Sigma} \tilde{V}^T$$

Darve, E., & Wootters, M. (2021). Numerical linear algebra with Julia. Society for Industrial and Applied Mathematics.

- Now,  $Ax = 0$  if and only if  $\tilde{V}^T x = 0$ , which means that the null space of  $A$  is the same as that of  $\tilde{V}^T$ , i.e.,  $\text{null}(A) = \text{null}(\tilde{V}^T)$ .

## SVD method for solving least-squares with rank-deficient $A$

- We know that any solution  $x$  to the least-squares problem satisfies

$$\begin{aligned}A^T A x &= A^T b \\(\tilde{U} \tilde{\Sigma} \tilde{V}^T)^T \tilde{U} \tilde{\Sigma} \tilde{V}^T x &= (\tilde{U} \tilde{\Sigma} \tilde{V}^T)^T b \\ \tilde{V} \tilde{\Sigma}^T \tilde{\Sigma} \tilde{V}^T x &= \tilde{V} \tilde{\Sigma}^T \tilde{U}^T b \\ \tilde{\Sigma} \tilde{V}^T x &= \tilde{U}^T b\end{aligned}$$

where  $r < n$  so that  $\tilde{\Sigma} \tilde{V}^T$  is not full-column-rank and this equation admits infinitely many solutions.

- However, we can find one solution as follows.

First, let's solve the system  $\tilde{\Sigma} \omega = \tilde{U}^T b$  for  $\omega \in \mathbb{R}^r$ . This gives

$$\omega_i = \frac{\tilde{u}_i^T b}{\tilde{\sigma}_{ii}}$$

where  $\tilde{U} = [\tilde{u}_1, \dots, \tilde{u}_r]$  and  $\tilde{\Sigma} = \text{diag}(\tilde{\sigma}_{11}, \dots, \tilde{\sigma}_{rr})$ .



## SVD method for solving least-squares with rank-deficient $A$

Then, since  $\omega = \tilde{\Sigma}^{-1}\tilde{U}^T b$ , we have

$$\tilde{\Sigma}\tilde{V}^T(\tilde{V}\omega) = \tilde{\Sigma}\tilde{V}^T\tilde{V}\tilde{\Sigma}^{-1}\tilde{U}^T b = \tilde{U}^T b$$

so that  $x_0 := \tilde{V}\omega$  is solution of  $\tilde{\Sigma}\tilde{V}^T x_0 = \tilde{U}^T b$  and thus, as explained before, it is also solution of the least-squares problem.

Note that  $x_0 := \tilde{V}\omega$  is the solution with smallest norm.

To see this, we need to show  $x_0 \perp \text{null}(A)$ . First, let

$$\text{null}(\tilde{V}^T) = \{y \in \mathbb{R}^n, \tilde{V}^T y = 0\}$$

and consider that for each  $y \in \text{null}(\tilde{V}^T)$ , we have

$$x_0^T y = (\tilde{V}\omega)^T y = \omega^T \tilde{V}^T y = 0$$

so that  $x_0 \perp \text{null}(\tilde{V}^T)$ .

But since  $\text{null}(\tilde{V}^T) = \text{null}(A)$ , we have that  $x_0 \perp \text{null}(A)$ .

# LSQR

## Iterative solve of normal equations

- ▶ We saw that the least-squares solution  $x_*$  of  $\min_{x \in \mathbb{R}^n} \|Ax - b\|_2$  for  $A \in \mathbb{R}^{m \times n}$  and  $b \in \mathbb{R}^m$  with  $m > n$  is such that  $A^T A x_* = A^T b$ , i.e.,  $x_*$  is solution of the normal equation.
- ▶ For very large matrices, the cost of computing a QR factorization by Householder QR, or even by CholeskyQR, can be prohibitive. When the matrix is sparse, computing a QR factorization is generally an overkill.
- ▶ In future lectures, we will look into iterative methods to solve linear systems of the form  $Bx = b$  with a square matrix  $B \in \mathbb{R}^{n \times n}$ .

In particular, if  $A$  is full-rank, one can use the conjugate gradient algorithm to solve  $A^T A x_* = b$ .

However, in practice, for cases where  $A$  is ill-conditioned, this approach can suffer from significantly delayed convergence.

- ▶ **LSQR** is an algorithm proposed by Paige and Sanders (1982) which, in case of exact arithmetic, reproduces the iterates of the conjugate gradient algorithm applied to the normal equation but, in practice, is **more reliable**.

Paige, C. C., & Saunders, M. A. (1982). LSQR: An algorithm for sparse linear equations and sparse least squares. ACM Transactions on Mathematical Software (TOMS), 8(1), 43-71.

# Bidiagonalization

- Bidiagonalization is a procedure proposed by Golub and Kahan (1965) which reduces any general matrix  $A \in \mathbb{R}^{m \times n}$  into lower bidiagonal form. Let  $x_0 \in \mathbb{R}^n$  be an initial approximation of  $x_*$  with residual  $r_0 := b - Ax_0$ . Starting the bidiagonalization procedure with  $r_0$  goes as follows:

$$\left. \begin{aligned} \beta_1 u_1 &= r_0, \quad \alpha_1 v_1 = A^T u_1 \\ \beta_{i+1} u_{i+1} &= A v_i - \alpha_i u_i \\ \alpha_{i+1} v_{i+1} &= A^T u_{i+1} - \beta_{i+1} v_i \end{aligned} \right\} \text{ for } i = 1, 2, \dots$$

where the scalars  $\alpha_i \geq 0$  and  $\beta_i \geq 0$  are chosen so that  $\|u_i\|_2 = \|v_i\|_2 = 1$ . Let  $U_k := [u_1, \dots, u_k]$ ,  $V_k := [v_1, \dots, v_k]$ ,

$$B_k := \begin{bmatrix} \alpha_1 & & & & \\ \beta_2 & \alpha_2 & & & \\ & \ddots & \ddots & & \\ & & \beta_k & \alpha_k & \end{bmatrix} \quad \text{and} \quad \underline{B}_k := \begin{bmatrix} \alpha_1 & & & & \\ \beta_2 & \alpha_2 & & & \\ & \ddots & \ddots & & \\ & & \beta_k & \alpha_k & \\ & & & \beta_{k+1} & \end{bmatrix}.$$

Golub, G., & Kahan, W. (1965). Calculating the singular values and pseudo-inverse of a matrix. *Journal of the Society for Industrial and Applied Mathematics, Series B: Numerical Analysis*, 2(2), 205-224.

Paige, C. C. (1974). Bidiagonalization of matrices and solution of linear equations. *SIAM Journal on Numerical Analysis*, 11(1), 197-209.

## Bidiagonalization, cont'd

Then, we have

$$U_{k+1}(\beta_1 e_1) = r_0 \quad (e_1 := I_{k+1}[:, 1])$$

$$AV_k = U_{k+1}\underline{B}_k = U_k B_k + \beta_{k+1} u_{k+1} e_k^T \quad (e_k := I_k[:, k])$$

$$A^T U_{k+1} = V_k \underline{B}_k^T + \alpha_{k+1} v_{k+1} e_{k+1}^T. \quad (e_{k+1} := I_{k+1}[:, k+1])$$

In exact arithmetic, we have  $U_k^T U_k = I_k$  and  $V_k^T V_k = I_k$ .

Clearly,  $U_{k+1}^T AV_k = \underline{B}_k$ ,  $U_k^T AV_k = B_k$ ,  $\alpha_k = u_k^T Av_k$  and  $\beta_k = u_k^T Av_{k-1}$ .

Moreover, the columns of  $U_k$  and  $V_k$  are orthonormal bases of Krylov subspaces of  $AA^T$  and  $A^T A$ , respectively, i.e.,

$$\text{range}(U_k) = \mathcal{K}_k(AA^T, u_1) = \text{span} \left\{ u_1, AA^T u_1, \dots, (AA^T)^{k-1} u_1 \right\},$$

$$\text{range}(V_k) = \mathcal{K}_k(A^T A, v_1) = \text{span} \left\{ v_1, A^T A v_1, \dots, (A^T A)^{k-1} v_1 \right\}.$$

Bidiagonalization is an orthogonal equivalence transformation which plays a key role in the iterative solve of singular value decompositions.

Golub, G., & Kahan, W. (1965). Calculating the singular values and pseudo-inverse of a matrix. *Journal of the Society for Industrial and Applied Mathematics, Series B: Numerical Analysis*, 2(2), 205-224.

Paige, C. C. (1974). Bidiagonalization of matrices and solution of linear equations. *SIAM Journal on Numerical Analysis*, 11(1), 197-209.

# LSQR

- LSQR defines a sequence of iterates  $x_1, x_2, \dots, x_k$  which approximate the solution  $x_*$  of  $\min_{x \in \mathbb{R}^n} \|b - Ax\|_2$  by

$$x_k \in x_0 + \mathcal{K}_k(A^T A, v_1).$$

That is, we search for  $x_k = x_0 + V_k y_k$  such that

$$\begin{aligned} x_k = \arg \min_{x \in x_0 + \text{range}(V_k)} \|b - Ax\|_2 &\implies y_k = \arg \min_{y \in \mathbb{R}^k} \|b - A(x_0 + V_k y)\|_2 \\ &= \arg \min_{y \in \mathbb{R}^k} \|r_0 - U_{k+1} \underline{B}_k y\|_2 \\ &= \arg \min_{y \in \mathbb{R}^k} \|U_{k+1}(\beta_1 e_1) - U_{k+1} \underline{B}_k y\|_2 \\ &= \arg \min_{y \in \mathbb{R}^k} \|\beta_1 e_1 - \underline{B}_k y\|_2. \end{aligned}$$

In exact arithmetic, the LSQR iterates exhibit monotonic decrease of residual norm, i.e.,  $\|r_{k+1}\|_2 \leq \|r_k\|_2$ .

## LSQR, cont'd

► A basic implementation of the LSQR algorithm goes as follows:

1.  $r_0 := b - Ax_0$
2.  $u_1 := r_0$ ,  $\beta_1 := \|u_1\|_2$ ,  $u_1 := u_1/\beta_1$
3.  $v_1 := A^T u_1$ ,  $\alpha_1 := \|v_1\|_2$ ,  $v_1 := v_1/\alpha_1$
4. for  $i = 1, 2, \dots$
5.  $u_{i+1} := Av_i - \alpha_i u_i$ ,  $\beta_{i+1} := \|u_{i+1}\|_2$ ,  $u_{i+1} := u_{i+1}/\beta_{i+1}$
6.  $v_{i+1} := A^T u_{i+1} - \beta_{i+1} v_i$ ,  $\alpha_{i+1} := \|v_{i+1}\|_2$ ,  $v_{i+1} := v_{i+1}/\alpha_{i+1}$
7.  $y_i := \arg \min_{y \in \mathbb{R}^i} \|\beta_1 e_1 - \underline{B}_i y\|_2$

When convergence is achieved, the iterate  $x_i := x_0 + V_i y_i$  is formed.

Convergence monitoring is reliant on the evaluation of  $\|r_i\|_2$  and  $\|A^T r_i\|_2$ .

Note that we have

$$\begin{aligned}\|r_i\|_2 &= \|b - A(x_0 + V_i y_i)\|_2 = \|\underline{t}_i\|_2 \quad \text{where } \underline{t}_i := \beta_1 e_1 - \underline{B}_i y_i \\ \|A^T r_i\|_2 &= \|A^T U_{i+1} \underline{t}_i\|_2 = \|(V_i \underline{B}_i^T + \alpha_{i+1} v_{i+1} e_{i+1}^T) \underline{t}_i\|_2 = \|\underline{B}_{i+1}^T \underline{t}_i\|_2\end{aligned}$$

so that convergence can be monitored without forming neither  $x_i$  nor  $r_i$ .

# Homework problems



## Homework problem

Turn in **your own** solution to the following problem:

**Pb. 17** Let  $A = \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix}$  and  $b = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$ .

- (a) Find a QR decomposition of  $A$  applying a Gram-Schmidt procedure with a pen and paper.
- (b) Find the least-squares problem solution  $x_* = \arg \min_x \|Ax - b\|_2$  making use of the QR factorization.

# Practice session

## Practice session

- 1 Implement and test and time your implementation of Householder QR.
- 2 Implement CholeskyQR, CholeskyQR2 and Shifted CholeskyQR3.
- 3 Compare the runtime, loss of orthogonality and residual obtained with each CholeskyQR implementation for multiple tall-and-skinny matrices with different conditioning numbers.
- 4 Implement CGS, CGS2 and MGS procedures.
- 5 Compare the runtime, loss of orthogonality and residual obtained with each Gram-Schmidt implementation for multiple tall-and-skinny matrices with different conditioning numbers.
- 6 Implement the Golub-Kahan bidiagonalization procedure. Then, compare  $U_{k+1}^T A V_k$  to  $\underline{B}_k$ , and check the loss of orthogonality of  $U_{k+1}$  and  $V_k$ . What do you observe?
- 7 Implement LSQR using the following stopping criterion:

$$\frac{\|A^T r_i\|_2}{\|A\|_F \|r_i\|_2} < \varepsilon_{tol}.$$

Apply your algorithm to large sparse least-squares problems.