A RANK REVEALING FACTORIZATION USING ARBITRARY NORMS

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Abstract.
The classic rank-revealing QR factorization factorizes a matrix $A$ as $AP = QR$ where $P$ permutes the columns of $A$, $Q$ is an orthogonal matrix, and $R$ is upper triangular with non-increasing diagonal entries. This is called rank-revealing because careful choice of $P$ allows the user to truncate the factorization for a low-rank approximation of $A$ with an error term computed in the $l^2$ norm. In this paper I generalize the QR factorization to use any arbitrary norm and prove analogous properties for $Q$ and $R$ in this setting. I then show an application of this algorithm to compute low-rank approximations to $A$ with error term in the $l^1$ norm instead of the $l^2$ norm. I provide Python code for the $l^1$ case as demonstration of the idea.

Key words. QR factorization, rank-revealing QR factorization, low-rank approximation

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1. Introduction. Low-rank approximation allows the user to compress an input matrix in a very informative way. The low-rank factors can provide useful information about the data which comprises the input matrix, which forms the basis of Principal Component Analysis (PCA). The gold-standard of low-rank approximations is the SVD factorization, which gives optimal low-rank approximations with respect to the Euclidean norm $\| \cdot \|_2$. The problem with SVD is that algorithms for it typically must be iterative in nature, or even probabalistic. A non-iterative and deterministic algorithm which reveals rank information can therefore be useful.

The rank-revealing QR factorization [2] is a deterministic and non-iterative algorithm which provides rank information on the input matrix by way of the diagonal entries of its upper triangular factor. It turns out this factorization can in fact be used directly for low-rank approximation also, bypassing the SVD entirely, and this has been exploited heavily in areas such as hierarchical compression of matrices [3],[4]. Like with the SVD the quality of this low-rank approximation is often best in the Euclidean norm $\| \cdot \|_2$ because the $QR$ factorization is explicitly based on the Euclidean dot product. This optimality in the Euclidean norm has some undesirable properties in other fields however.

For some applications of data analysis the optimality of a low-rank approximation in the Euclidean norm results in unfavorable low-rank factors, because outliers in data can quickly overwhelm the Euclidean norm of that data, resulting in poor approximations. This has led to the field of “L1 PCA” which tries to find optimal low rank approximations in the $l^1$ norm instead of the $l^2$ norm [8],[6],[7]. Unfortunately, since the $QR$ factorization is highly specialized to the Euclidean norm this suggests that rank-revealing $QR$ strategies can not help in domain. Thus this new area of low-rank approximation has moved in the direction of iterative or probabalistic SVD-like algorithms [7].

In this paper I show that the $QR$ factorization can be generalized to norms other than the Euclidean norm. I derive the algorithm, state and prove analogous properties of the resulting $Q$ and $R$ factors, and then show numerical results. This yields a deterministic and non-iterative algorithm with rank-revealing properties with the potential to give optimality in norms besides the Euclidean norm.

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The paper is organized as follows. The main theory and algorithm is presented in section 2, an implementation of this algorithm in python for the special case of the $l^1$ norm is in section section 3, experimental results are in section 4, and the conclusions follow in section 5.

2. Main results. I start by presenting the algorithm that this paper is based on. This algorithm accepts a matrix $A \in \mathbb{R}^{m \times m}$ and any norm $\|\cdot\|$ on $\mathbb{R}^m$ and returns a permutation $P$, an upper triangular matrix $R$ with nonincreasing diagonal, and $Q$ such that $AP = QR$. I then prove key facts about this algorithm (theorem 2.1) and state a conjecture (conjecture 1). I also prove that when the input norm is equal to the Euclidean norm, then the factorization reduces to a classical $QR$ - in the sense that $Q$ becomes orthogonal. This is theorem 2.2. I start first with the algorithm 2 below.
Algorithm 2.1 Arbitary-norm rank-revealing QR Factorization

Start with an input $A \in \mathbb{R}^{m \times m}$ and any norm $\| \cdot \|$ on $\mathbb{R}^m$.

I use the notation $e_k$ to mean the $k$th column of the identity matrix, and I use

\begin{align*}
(2.1) & \quad A = (A_1, A_2, A_3, \ldots, A_m) \\
(2.2) & \quad Q = (Q_1, Q_2, Q_3, \ldots, Q_m) \\
(2.3) & \quad P = (P_1, P_2, P_3, \ldots, P_m)
\end{align*}

to represent $A, P$ and $Q$ by their respective columns. Furthermore I define $Q^i \in \mathbb{R}^{m \times i}$ as the first $i$ columns of $Q$:

$$Q^i = (Q_1, Q_2, \ldots, Q_i).$$

I now define the $P, Q$ and $R$ factors inductively as follows:

\begin{align*}
(2.4) & \quad k = \arg \max_i \|A_i\| \\
(2.5) & \quad P_1 = e_k \\
(2.6) & \quad Q_1 = A_k/\|A_k\| \\
(2.7) & \quad R(1, 1) = \frac{1}{\|A_k\|}
\end{align*}

and for any $1 \leq j \leq m - 1$ I define

\begin{align*}
(2.8) & \quad k_j = \arg \max_i \min_{c_j \in \mathbb{R}} \|A_i - Q^j c_j\| \\
(2.9) & \quad c_j = \arg \min_{c_j \in \mathbb{R}} \|A_{k_j} - Q^j c_j\| \\
(2.10) & \quad \gamma_j = \|A_{k_j} - Q^j c_j\| \\
(2.11) & \quad P_{j+1} = e_{k_j} \\
(2.12) & \quad Q^{j+1} = (Q^j, \gamma_j^{-1}(A_{k_j} - Q^j c_j)) \\
(2.13) & \quad R(j, 1 : j - 1) = c_j \\
(2.14) & \quad R(j, j) = \gamma_j
\end{align*}

The key theoretical result of this paper is summarized in theorem 2.1. Following this theorem is a conjecture which seems true based on numerical evidence supporting it (see section section 4) but a full proof remains elusive. Finally I prove in theorem 2.2 that if $\| \cdot \| = \| \cdot \|_2$ then algorithm 2 outputs $Q$ as orthogonal.

**Theorem 2.1 (Arbitrary-norm Rank-Revealing QR Factorization ).**

Suppose that $A \in \mathbb{R}^{m \times m}, \| \cdot \|$ is a norm, and that $P, Q, R$ are output by algorithm 2.

Then the following properties hold:

\begin{align*}
(2.15) & \quad AP = QR
\end{align*}
(2.16) \( R \) is upper triangular with nonincreasing diagonal entries

There exists a constant \( C_1 > 0 \) independent of \( A \) such that

\[
\max_{\|x\|=1} \|Qx\| \leq C_1
\]

**Conjecture 1 (Inverse Bound).** Suppose that \( A \in \mathbb{R}^{m \times m}, \|\cdot\| \) is a norm, and that \( P, Q, R \) are output by algorithm 2.

Then there exists a constant \( C_2 > 0 \) that depends only on the norm \( \|\cdot\| \) such that

\[
\min_{\|x\|=1} \|Qx\| \geq C_2
\]

Properties 2.15 and 2.16 are standard and precisely match the classical QR factorization with column pivoting. Properties 2.17 and 2.18 perhaps require more explanation. In the classical QR factorization the matrix \( Q \) is orthogonal \((Q^TQ = I)\). Strictly speaking we could insist that \( Q \) also be orthogonal in the above theorem, but the utility of orthogonality is lost when using norms different from the \( l^2 \) norm. This utility stems from the fact that the \( l^2 \) norm is derived from an inner product, so orthogonality has strong implications on the conditioning of \( Q \) in this norm.

Thus to find an analogue to orthogonality I require that the matrix \( Q \) be well conditioned. The bounds 2.17 and 2.18 prove that \( Q \) is invertible (full-rank), but also that the conditioning of \( Q \) does not depend on the conditioning of \( A \), which the theorem allows to be highly numerically singular. By way of example, if we were to state this theorem for \( \|\cdot\| = \|\cdot\|_2 \) then we would actually have \( C_1 = C_2 = 1 \).

I now prove theorem 2.1, minus the conjecture:

**Proof.** To prove equation 2.15 note that \( AP^1 = Q^1R(1,1) \) follows directly from the base case definitions of these quantities. Now assume \( AP^j = Q^jR(1:j,1:j) \) for some \( j \). Then

\[
Q^{j+1}R(1:j+1,1:j+1) = (Q^j,Q_{j+1})\begin{bmatrix} R(1:j,1:j) & c_j \\ 0 & \gamma_j \end{bmatrix} = (Q^jR(1:j,1:j),Q_jc + \gamma_jQ_{j+1}) = (AP^j,A_{k_j}) = AP^{j+1}
\]

For 2.16 it’s clear that \( R \) is upper triangular, but to show that its diagonal entries are nonincreasing observe that from the optimality property of \( c_j \) we have

\[
R(1,1) = \arg \max_i \|A_i\| \\
\geq \|A_{k_1}\| \\
\geq \|A_{k_1} - Q^1c\| \\
= R(2,2)
\]

and for any \( j > 1 \):
\[ R(j, j) = \max_i \min_{c_j \in \mathbb{R}} \| A_i - Q^j c_j \| \]
\[ \geq \max_i \min_{c_{j+1} \in \mathbb{R}} \| A_i - Q^{j+1} c_{j+1} \| \]
\[ = R(j+1, j+1) \]

and finally for the conditioning properties 2.17 and 2.18 observe that if \( \| x \| = 1 \) then

\[ \| Qx \| = \| \sum_{i=1}^{m} Q_i x_i \| \]
\[ \leq \sum_{i=1}^{m} \| Q_i x_i \| \]
\[ \leq \sum_{i=1}^{m} \| Q_i \| \| x_i \| \]
\[ \leq \| x \|_1 \]

where the final inequality is a consequence of Holder’s inequality. Finally we may apply norm equivalence between all norms in finite dimensional spaces to choose \( C_1 > 0 \) such that \( \| x \|_1 \leq C_1 \| x \| \) holds for all \( x \) to complete the proof of 2.17. The bound 2.18 remains conjecture, but is supported by numerical evidence in section section 4.

**Theorem 2.2 (Classic QR as Special Case).** Suppose that \( A \in \mathbb{R}^{m \times m}, \| \cdot \|_2 \) is the \( l^2 \) norm, and that \( P, Q, R \) are output by algorithm 2. Then \( Q \) is orthogonal, i.e. \( Q^T Q = I \).

**Proof.** By the inductive definition of \( Q \) in 2.8 we have

\[ Q^{j+1} = (Q^j, \gamma_j^{-1}(A_k - Q^j c_j)) \]

Recall that \( c_j \) solves the minimization problem

\[ c_j = \arg \min_{c_j \in \mathbb{R}} \| A_k - Q^j c_j \| \]

which means it is forming the \( l^2 \) projection of \( A_k \) onto the space \( V = \text{span}(Q_1, \ldots, Q_j) \). Since \( Q_{j+1} \) is the residual of this projection, it is orthogonal to the whole space \( V \).

**3. Implementation for \( l^1 \) norm using linear programming.** The key ingredient of algorithm 2 is the ability to compute solutions to minimum-norm linear problems such as \( \arg \min \| b - Ax \|_1 \).

For the \( l^2 \) case there are already established and robust algorithms for this problem, but it's less obvious for other norms. For the \( l^1 \) norm we can cast it as a linear program. In other words:

\[ \arg \min_{x} \| b - Ax \|_1 \]

is equivalent to the linear program
\[
\arg\min \sum_{i=1}^{m} t_i \\
\text{Subject to} \quad b - Ax \leq t \\
Ax - b \leq t \\
t \geq 0
\]

This is implemented in python below using SciPy [5] and [9].

```python
import numpy as np
import scipy.optimize as opt

def lst1norm(A, b):
    (m, n) = A.shape
    nvars = m+n
    ncons = 2*m
    cons = np.zeros((ncons, nvars))
    cons[0:m, 0:m] = -np.identity(m)
    cons[0:m, m:m+n] = A
    cons[m:2*m, 0:m] = -np.identity(m)
    cons[m:2*m, m:m+n] = -A
    c = np.zeros(nvars)
    c[0:m] = 1.0
    ub = np.zeros(ncons)
    ub[0:m] = b
    ub[m:2*m] = -b
    bounds = []
    for i in range(0, m):
        bounds.append((0, None))
    for i in range(m, m+n):
        bounds.append((None, None))
    out = opt.linprog(c, cons, ub, None, None, bounds,
                      options={'maxiter': 10000, 'tol': 1e-6},
                      method='interior-point')
    return out
```

Furthermore I have also implemented the relations 2.4 and 2.8 as a function in python.

```python
import numpy as np
import scipy.optimize as opt

def l1rrqr(A):
    (m, n) = A.shape
    Q = np.zeros((m, n))
    R = np.zeros((n, n))
    k = np.argmax([np.linalg.norm(A[:, i], ord=1) for i in range(0, n)])
    perm = [k]
    sout = set(perm)
    sin = set([i for i in range(0, n)]).difference(sout)
```
i=0
Q[ :, i]=A[ :, k]/np.linalg.norm(A[ :, k], ord=1)
R[i, i]=np.linalg.norm(A[:, k], ord=1)
while sin:
   i=i+1
   V=Q[ :, 0 : i]
   vals=[lst1norm(V[ :, i]).fun for i in sin]
   ids=[i for i in sin]
   k=ids[np.argmax(vals)]
   sout.add(k)
   sin=sin.difference(sout)
   perm.append(k)
   soln=lst1norm(V,A[:, k])
   c=soln.x[m:m+n]
   y=A[:, k]−V@c
   Q[ :, i]=y/np.linalg.norm(y, ord=1)
   R[0 : i, i]=c
   R[i, i]=np.linalg.norm(y, ord=1)
return (Q,R,perm)

I now proceed to show numerical results of this algorithm.

4. Experimental results. The results below are designed to validate some of the theoretical properties proven and asserted earlier. These include properties like the well-conditioning of $Q$ and the non-increasing property for the diagonal of $R$. I also include results on low-rank approximation from this factorization as that was the primary motivation of deriving this algorithm.

4.1. Diagonal Entries of $R$. These experiments test the theorem result 2.16. Here I take $A \in \mathbb{R}^{m \times m}$ constructed explicitly as an SVD factorization $A=U\Sigma V^T$ with diagonal entries of $\Sigma$ varying in relative size, which I indicate with $\sigma_m \arg\min_{\Sigma_{ii}} \sigma_{i,i}$ and $\sigma_1 = \arg\max_{\Sigma_{ii}} \Sigma_{i,i}$.

If $R$ truly has rank-revealing properties then it should exhibit rapid decay of diagonal entries when $A$ becomes progressively more singular.
Fig. 1. Scaling of diagonal entries for $m = 10$
These results suggest that $R$ is capturing low rank information.

4.2. Conditioning of $Q$. An important part of successful rank-revealing factorization $AP = QR$ is the conditioning of $Q$ should be independent of the conditioning of $A$. The key theoretical result which would prove this would be 2.18, but unfortunately I was unable to prove this. Here I give numerical evidence that it does appear to be true.

I take $A \in \mathbb{R}^{m \times m}$ constructed explicitly as an SVD factorization $A = U \Sigma V^T$ with diagonal entries of $\Sigma$ varying in relative size. I compute the condition numbers $\|A\|_1 \|A^{-1}\|_1, \|Q\|_1 \|Q^{-1}\|_1$ and plot them against each other in figure 3.
4.3. Factorization error. Next I illustrate that the factorization error \( \|AP - QR\| \) also does not depend on the conditioning of \( A \).

I take \( A \in \mathbb{R}^{m \times m} \) constructed explicitly as an SVD factorization \( A = U\Sigma V^T \) with diagonal entries of \( \Sigma \) varying in relative size. I compute the condition numbers \( \|A\|_1 \|A^{-1}\|_1 \), and factorization errors \( \|AP - QR\|_1 \) and plot them against each other in figure 4.
4.4. Low-rank approximation. With the rank-revealing properties validated I now show an example of low-rank approximation.

For this test I again generate A by forming it as an explicit SVD factorization $A = U \Sigma V^T$ with $\max_i \Sigma_{i,i} = 1$ and $\min_i \Sigma_i, i = 10^{-6}$. I then compute two factorizations of $A$:

\begin{align}
(4.1) \quad & A P_1 = Q_1 R_1 \text{ 11 RRQR factorization} \\
(4.2) \quad & A P_2 = Q_2 R_2 \text{ Classic RRQR factorization}
\end{align}

Next I truncate the factorizations to be a rank-$k$ approximation to $A$ as follows:

\begin{align}
(4.3) \quad & A \approx Q_1(:,1:k) R_1(1:k,:) P_1^T \\
(4.4) \quad & A \approx Q_2(:,1:k) R_2(1:k,:) P_2^T
\end{align}

For the first study I compare the induced $l^1$ matrix norm error of these approximations for $k = 1, \ldots, 60$ this is in figure 5.
This result suggests that there is little difference in results between $l^1$ and $l^2$ rank revealing factorizations. The next section 4.5 shows the subtle difference between $l^1$ and $l^2$ norms for low-rank approximations, and why the $l^1$ norm may be preferred in some situations.

4.5. Resistance of $l^1$ norm to outliers. One of the original motivations for deriving algorithm 2 was to be able to do $l^1$ low-rank approximations, which can be very robust with respect to outliers in data [1].

I show here that to some extent this appears to be reflected in the $l^1$ version of the rank revealing factorization. To illustrate this I first show a "clean" example without outliers, and then do rank $k$ approximations for $k = 1, 2, 3$ for both classical RRQR and $l^1$ RRQR. Then I introduce outliers to this same data and show the classical RRQR algorithm quickly is drawn to over-resolve outlier data because of how it dominates the Euclidean norm.

The first case are the low-rank approximations without outliers in the input data.
Fig. 6. Low rank approximations of clean data using both classical and $l^1$ RRQR factorizations

The next case I introduce two outliers of much larger magnitude than surrounding data. The classical RRQR quickly gravitates to the columns containing these outliers because the outlier data gets squared in the Euclidean norm and then dominates it. In the $l^1$ norm however this effect is much less pronounced. See figure 7 below.
5. Conclusions. I derived a rank-revealing factorization that shares some similarities to classic rank-revealing QR with column pivoting. Instead of the $Q$ factor being orthogonal it has conditioning that is independent of the conditioning of $A$. Furthermore the rank-revealing factorization presented here does not depend strictly on using dot products and the $l^2$ norm. I validated that claim by implementing the algorithm for the $l^1$ norm case, where least-norm-solution is equivalent to a linear program.

While I was able to numerically validate the conditioning properties of $Q$ I was unable to mathematically prove them. The key fact to be proven remains conjecture (1). Without orthogonality properties available in the $l^2$ case most avenues for proof
are lost. I believe however that careful use of the optimality properties for the least-
norm solution $c_j$ (see eqns 2.8) may be able to overcome the loss of orthogonality.

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