QR and LQ Decomposition Matrix Backpropagation Algorithms for Square, Wide, and Deep Matrices and Their Software Implementation

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Abstract

This article presents matrix backpropagation algorithms for the QR decomposition of matrices $A_{m,n}$, that are either square ($m = n$), wide ($m < n$), or deep ($m > n$), with rank $k = \min(m,n)$. Furthermore, we derive a novel matrix backpropagation result for the LQ decomposition for deep input matrices. Differentiable QR decomposition offers a numerically stable, computationally efficient method to solve least squares problems frequently encountered in machine learning and computer vision. Software implementation across popular deep learning frameworks (PyTorch [10], TensorFlow [1], MXNet [3]) incorporate the methods for general use within the deep learning community. Furthermore, this article aids the practitioner in understanding the matrix backpropagation methodology as part of larger computational graphs, and hopefully, leads to new lines of research.

1 Background

The QR decomposition is the thread that connects most of the algorithms of numerical linear algebra, including methods for least squares, eigenvalue, and singular value problems, as well as iterative methods for all of these and also for systems of equations [13]. Despite the critical nature of the decomposition, the QR factorization and its gradient have lagged behind in deep learning research. We surmise one reason is the absence of complete autodiff software implementations in the most common deep learning frameworks. The QR decomposition and the gradient of this decomposition have many uses in machine learning including for canonicalization of tensor networks in quantum computing [7], fitting least squares and Bayesian statistics [12], and for optimum experimental design [14]. Other differentiable matrix decompositions were used in structured layers as part of end-to-end learning of computer vision models [6]. Both QR (in the Householder implementation) and SVD solutions are backward stable and the one with the least computational cost can be chosen for full-rank least squares problems. The QR decomposition is a faster alternative [15], as well as a faster alternative to solving the least squares solution for approximately square matrices [13]. Recent work [4] compares SVD alternatives for solving least squares problems and provides an end to end solution to ellipse points fitting and human pose estimation applications. QR is a valid alternative for solving the least squares and could be considered in experiments.

In this document we refer to the process of calculating the gradient of the input matrix $A$ interchangeably as QR matrix backprop or auto-diff QR. In [12] an argument for the LQ auto-diff was presented for wide and square matrices. In [7] a different formula for the QR auto-diff was given. In [14] the authors derive an analytical gradient for the square and deep case only. We fully derive new analyt-

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ical formulae for all input matrix orders, clearly state the necessary assumptions, provide proofs, a supporting appendix, software implementations and numerical checks via central differences.

The contributions of this article are:

- A review of the QR and LQ decompositions with a view toward auto-diff. We include a full derivation of the QR decomposition matrix backprop for square, wide, and deep matrices $A$, including their software implementations in popular deep learning frameworks.
- Using the partitioning trick, we derive a novel result for the LQ decomposition backprop for deep matrices. A Github repository contains TensorFlow code for LQ backprop and corresponding numerical checks.
- A systematic process for deriving matrix backprop for the decomposition of deep, square, and wide inputs.

The exposition shows how the partitioning trick is applicable more broadly to cases where matrices are not of full rank. Once the input matrix is partitioned, the sub-matrices have full rank, thereby facilitating our derivations. The remainder of the article is structured as follows: in Section 2 we give an introduction to the QR and LQ decompositions. We also introduce the matrix backprop process and state basic results in matrix algebra that we use throughout the article. Then in Section 3 we derive expressions for the gradient through matrix backpropagation for QR (Deep and Square) case in Section 3.1, QR Wide case in Section 3.2, and LQ Deep case in Section 3.3. We then conclude with a few final notes. An extensive Appendix is available which includes derivations of results omitted for brevity.

2 Preliminaries

2.1 The QR and The LQ Decomposition

The algebra of a QR decomposition is included in standard matrix algebra texts [11]. Implementations of the QR decomposition are usually products of Householder rotations and are numerically stable. The implementation of the QR decomposition used in packages such as Numpy [9] and MXNet [3] typically wrap calls to the LAPACK [2] library, as a sequence of two routines $\text{geqrf}$, and $\text{orgqr}$. The first LAPACK routine used in the sequence, $\text{geqrf}$, determines the Householder reflections whose matrix product determines $Q$ and then returns the matrix $R$ directly. The second LAPACK routine, $\text{orgqr}$, returns the $Q$ matrix. For GPU implementations, CuSolver (in the NVIDIA CUDA library [8]), is employed in the MXNet [3] implementation. Note that TensorFlow uses the Eigen library for linear algebra implementations. The decomposition typically returns, for an input matrix $A$ of order $(m, n)$, matrices $Q_{m,k}$ and $R_{k,n}$ with $k = \min(m, n)$, with $k$ typically the rank of the input matrix. This is the reduced mode decomposition. The first $k$ columns of $Q$ form an orthonormal basis in the vector space spanned by the leading $k$ columns of the matrix $A$. Notice that for wide input matrices (more columns than rows), $Q$ is $m \times m$ with $k = m$, so $Q$ is a square, orthogonal, full-rank matrix and all $m$ columns of $Q$ are returned. In the case of deep matrices (more rows than columns, $m > n$), for the default (reduced) call to the decomposition, only the first $n$ columns of $Q$ are included. In this case $R$ is a square matrix while $Q$ is not. This article assumes that the reduced mode QR (or LQ) is performed on the forward pass. The full (or complete) mode decomposition is also available and return matrices are of order $Q_{m,m}$ and $R_{m,n}$ but the reduced mode is typically the default because of computational efficiency considerations when solving least square problems [13]. A further assumption we make throughout this article is that the rank of the input matrix is $k = \min(m, n)$.

There is a relationship between the QR and the LQ decomposition. If $A = QR$ is the QR decomposition of $A$ then $A^T = R^T Q^T$ is the LQ decomposition of $A^T$. The relationship implies that an algebraic result for the deep case of the LQ corresponds to the wide case of the QR and vice-versa. For ease of exposition and because of the aforementioned correspondence with the LQ decomposition, we focus our exposition primarily on the QR decomposition.

2.2 Auto-differentiating Linear Algebra

A collection of useful auto-diff results for linear algebra operators are given in [12] and [5] and are used throughout this article. In [6] a two step process for matrix backprop in the context of deep
learning layers is described. We can view the calculation of the QR decomposition as successive computational layers. Each layer represents a matrix operation, with the matrix $A$ preceding $Q$ and $R$ in the computational graph as depicted in Figure 1.

![Figure 1: Forward pass calculations indicated with solid arrows and back-prop calculations depicted with dashed arrows. The matrices inside the nodes are the forward pass matrix decomposition values while the matrices with bars are the auto-diff matrices.](image)

The goal of auto-diff through matrix backprop is to obtain an analytical formula for the gradient of matrix $A$, given the gradient of matrices closer to the end of the topological order of the computational graph. In this article we refer to reverse mode auto-diff calculation of the gradient of $A$, the QR matrix backprop process, as simply matrix backprop. From [5], if $C$ is an intermediate variable computed at a node in the computational graph and $C$ is given as $C = f(A, B)$ a function of matrices $A$ and $B$ computed at a layer further ahead in the computational graph, then, from differential calculus,

$$dC = \frac{\partial f}{\partial A} dA + \frac{\partial f}{\partial B} dB.$$ (1)

In reverse mode auto-diff the infinitesimal perturbations are taken to be due to changes in the output $L$. Note that $L$ could be either a scalar valued loss function or an upstream layer in the computational graph. The sensitivities are computed starting at $L$ and working backwards. By definition, an infinitesimal change in $L$ and using the expression for $dC$ in 1,

$$dL = Tr(\bar{C}^T dC)$$

$$= Tr(\bar{C}^T \frac{\partial f}{\partial A} dA) + Tr(\bar{C}^T \frac{\partial f}{\partial B} dB).$$

We identify $\bar{A} = \frac{\partial f}{\partial A} C$ and $\bar{B} = \frac{\partial f}{\partial B} C$, which are the gradients sought.

Now assume that the gradient $\bar{C}$ propagated from upstream in the topological ordering is the identity matrix $I$. Then $\bar{A} = \frac{\partial f}{\partial A}$ and $\bar{B} = \frac{\partial f}{\partial B}$. Since for the QR decomposition $A = QR$, with gradients of $Q$ and $R$ being backpropagated from upstream (denoted $L$ in Figure 1), the tables are turned on the $C = f(A, B)$ with $Q, R = f(A)$. The trace identity remains similar

$$Tr(\bar{A}^T dA) = Tr(\bar{Q}^T dQ) + Tr(\bar{R}^T dR),$$ (2)

which is an identity we use repeatedly throughout the rest of the article.

The two-step backprop approach we repeatedly use in subsequent sections can be summarized as:

1. Derive formulas for the variations of $Q$ and $R$ (or $L, Q$), denoted $dQ$ and $dR$, respectively, as a function of $dA$.
2. Using the variations derived in step one, and the trace identity in Equation 2 identify the gradient matrix, denoted $\bar{A}$.

### 2.3 A Collection of Useful Matrix Results

Before proceeding to the QR and LQ matrix backprop derivations, it is useful to review a few matrix definitions and properties with proofs in any standard matrix algebra text such as [11].

**Definition 2.1.** If $A$ is a square matrix, let $\text{sym}(A) = \frac{A + A^T}{2}$ denote a symmetric matrix.
Definition 2.2. If a matrix $X$ satisfies $X = -X^T$, then $X$ is called a skew-symmetric matrix.

Some useful properties of the trace operator:

1. $\text{Tr}(ABC) = \text{Tr}(CAB) = \text{Tr}(BCA)$, Invariance to Cyclic Permutations (ICP).
2. $\text{Tr}(A) = \text{Tr}(A^T)$ Invariance to Transpose (IT).
3. From [12], for a square matrix $M$, $\text{Tr}(MT \text{sym}(E \circ C)) = \text{Tr}(\text{sym}(M \circ E)C)$, commutativity of products and symmetry (CPS).

Useful properties of matrices:

1. From [12], if $A$ is a lower (upper) triangular matrix (all the elements above the main diagonal are zero), write $A = \text{sym}(A) \circ E$, ($A = \text{sym}(A) \circ E^T$) where the masking matrix $E$ is defined as

   $e_{ij} = \begin{cases} 0, & i < j \\ 1, & i = j \\ 2, & i > j \end{cases}$

2. From [12], write $\text{copyltu}(A) = \text{sym}(M \circ E)$ (copy lower to upper) for a square matrix $A$.

We will use these properties repeatedly in derivations in the sequel.

3 QR and LQ Backpropagation Algorithms

In this section we derive formulae for the gradient of $A$ from the gradients of $Q$ and $R$ (or $L$ and $Q$ in the LQ decomposition) through matrix backprop. The matrix backprop algorithm takes as input the output of the forward pass of the decomposition ($Q$, $R$ or $L$, $Q$), in some cases the initial input matrix $A$ (used in the partitioning trick), and the upstream gradients of $\bar{Q}$, $\bar{R}$ (or $\bar{L}$, $\bar{Q}$ in the LQ decomposition). We treat separately the QR decomposition backprop for deep (and square) matrices, the QR backprop for wide matrices, LQ backprop for wide (and square) matrices and finally LQ backprop for deep matrices. The derivation differs depending on the input matrix order (shape). As stated earlier, we assume rank $k$ of the input matrix.

The proceeding sections stand alone and can be independently consulted if the reader is interested in only one of the matrix orders or techniques presented.

3.1 QR Backpropagation: Square and Deep Matrices

In the forward pass, the QR decomposition of the input matrix $A$ is obtained as described in Section 2. On the backward pass the gradient is obtained using the two matrix backprop steps. A key assumption in the derivation for square and deep input matrix $A$ is that the matrix $R$ is full rank. That $R$ has full rank is a consequence of the assumption $\text{rank}(A) = \min(m, n)$, an assumption implicit as well in the derivations in [12] for the wide input LQ decomposition gradient derivation.

Proposition 1. Let $A = QR$ be the QR decomposition of a square or a deep matrix $A$, $A \in \mathbb{R}^{m,n}$, with $m \geq n$, such that $Q \in \mathbb{R}^{m,n}$ and $R \in \mathbb{R}^{n,n}$, with $R$ an upper triangular matrix and $Q$ orthogonal with $Q^TQ = I_m$.

Then in the reverse mode auto-diff,

$$\bar{A} = \left[\bar{Q} + Q \text{copyltu}(M)\right] R^{-T},$$

where $M = RR^T - \bar{Q}^T \bar{Q}$.

Proof. We apply the two step process described in Section 2.2. The proof is similar to the LQ decomposition auto-diff technique in [12] for wide matrices. The LQ decomposition of a wide matrix parallels the QR decomposition of its transpose (a deep matrix).

BP Step 1: Variations Calculate the variations $dQ$ and $dR$ for a given variation $dA$. 

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Lemma 1. For a deep matrix $A$ with QR decomposition $A = QR$, the variations of $Q$ and $R$ for a given variation $dA$ of $A$, $dQ$ and $dR$ respectively, are
\[
\begin{align*}
    dQ &= (dA - QdR)R^{-1} \\
    dR &= (\text{sym}(C) \circ E^T)R
\end{align*}
\]
with $C = Q^T dAR^{-1}$.

The proof of Lemma 1 is left to the Appendix.

BP Step 2: Partial Derivatives In the second step of the process for matrix backprop laid out in Section 2.2 one obtains partial derivatives using the variations from step one and the trace identity
\[
\text{Tr}(\bar{A}^T dA) = \text{Tr}(\bar{Q}^T dQ) + \text{Tr}(\bar{R}^T dR) \tag{4}
\]
The goal is to express $dQ$ and $dR$ variations on the r.h.s. of the trace identity as a function of $dA$ and then identify the coefficients of $dA$. First, replace the $dQ$ expression in Lemma 1 on the r.h.s. to get
\[
\text{Tr}(\bar{Q}^T dQ) + \text{Tr}(\bar{R}^T dR) = \text{Tr}(\bar{Q}^T (dA - QdR)R^{-1}) + \text{Tr}(\bar{R}^T dR). \tag{5}
\]
Next replace $dR$ from Lemma 1, use the ICP property of trace, and arrange the terms to isolate $dA$. Considering the non $dA$ terms only,
\[
\text{Tr}((\bar{R}^T - R^{-1} \bar{Q}^T Q)(\text{sym}(C) \circ E^T)R) = \text{Tr}(M(\text{sym}(C) \circ E^T)), \tag{6}
\]
where we define $M = R\bar{R}^T - \bar{Q}^T Q$. Next use the definition of $C$ from Lemma 1, as well as the ICP property from Section 2.2 to simplify the trace to
\[
\text{Tr}(\text{sym}(C) \circ E^T)) = \text{Tr}((\text{sym}(M^T) \circ E^T)C) = \text{Tr}((\text{sym}(M^T) \circ E^T)Q^T dAR^{-1}) = \text{Tr}(R^{-1}(\text{sym}(M^T) \circ E^T)Q^T dA).
\]
Returning to the r.h.s. expression in Equation 4 containing both terms, we use ICP and IT to get
\[
\text{Tr}(R^{-1} \bar{Q}^T dA) + \text{Tr}(R^{-1} (\text{sym}(M^T) \circ E^T)Q^T dA) = \text{Tr}((\bar{Q} + Q(\text{sym}(M) \circ E)R^{-T})^T dA). \tag{7}
\]
The matrix that left multiplies $dA$ in Equation 4 is $\bar{A}^T$, and Equation 8 identifies
\[
\bar{A} = [\bar{Q} + Q_{\text{copytu}}(M)] R^{-T}. \tag{7}
\]
Note that the expression derived in Proposition 1 is equivalent to the result in [14]. In [14], the QR gradient for deep or square input matrices $A$ is given in their Equation 42,
\[
\bar{A} = Q(\bar{R} + P_L \circ (R\bar{R}^T - \bar{R}R^T + Q^T \bar{Q} - \bar{Q}^T Q)R^{-T}) + (\bar{Q} - QQ^T \bar{Q})R^{-T}. \tag{8}
\]
Equation 8 (their Equation 42) simplifies to our Equation 4. The matrix $P_L = (i > j)$ in 8 is a strictly lower tridiagonal matrix with all ones below the diagonal and zeroes along and above the main diagonal. The equivalence of Equation 3 and Equation 8 is proved in Appendix 5.2.

3.2 QR Backpropagation: Wide Matrices

As in the previous section, we assume that the reduced mode QR decomposition is performed on the forward pass as described in Section 2.1. On the backward pass, the gradient derivations for the wide case are complicated by the fact that $R$ is no longer square and full rank. We employ a partitioning trick. Let $A = QR$ be the QR decomposition of a wide matrix $A$, with $A \in \mathbb{R}^{m,n}$, and $Q \in \mathbb{R}^{m,m}$ a square orthogonal matrix, $R \in \mathbb{R}^{m,n}$ an upper triangular matrix, and $m < n$. Throughout this article matrix $A$ is assumed to be full rank $k = \text{min}(m,n)$. In the wide input case, a further assumption is that the first $k$ columns of $A$ form a square full rank matrix. This is a strong assumption, generally met for random matrices. A pivoted QR decomposition, where $AP = QR$, can assure that the assumption is met. However the pivoted forward implementation is not available in the popular deep learning framework at the time of this writing.

Proposition 2.
Figure 2: A graphical depiction of the QR auto-diff computation. Forward pass results are indicated with solid arrows and back-prop calculations depicted with dashed arrows. Note that the partitioning is only employed as a device on the backward pass. The matrices inside the nodes are the forward pass matrix decomposition values while the matrices with overbars are the gradient matrices. In the backward pass we employ the split and concatenate operations: \( A = [X|Y] \), \( R = [U|V] \), \( \bar{R} = [\bar{U}|\bar{V}] \) to finally obtain \( \bar{A} = [\bar{X}|\bar{Y}] \).

On the backward pass let us assume that the input matrices \( A, R \) and \( \bar{R} \) are partitioned as \( A = [X|Y] \), \( R = [U|V] \) and \( \bar{R} = [\bar{U}|\bar{V}] \) respectively with \( X, \bar{R}, \bar{R} \in \mathbb{R}^{m,m} \), and \( Y, V, \bar{V} \in \mathbb{R}^{m,n-m} \). Then \( \bar{A} = [\bar{X}|\bar{Y}] \), where

\[
\bar{X} = [\bar{Q}_{\text{prime}} + Q_{\text{copylu}}(M)]U^{-T}, \quad \text{and} \quad (9)
\]

\[
\bar{Y} = QV, \quad \text{and} \quad (10)
\]

with \( \bar{Q}_{\text{prime}} = \bar{Q} + Y\bar{V}^T \), and \( M = U\bar{U}^T - \bar{Q}_{\text{prime}}^TQ \).

Proof.

We follow the general process backprop outlined in Section 2.2 and employ the partitioning trick. For wide \( A, Q \) is square, orthogonal, and full rank and the columns of \( Q \) form an orthogonal basis for the first \( m \) columns of \( A \). We can formulate the QR decomposition as a multi-step sequential calculation which facilitates the gradient computation. The chain of operations is:

1. Partition \( A = [X|Y] \), with \( X \) a square matrix of full rank \( m \).
2. Calculate the QR decomposition of \( X \), \( X = QU \). The \( Q \) from the QR decomposition of \( X \) is the same \( Q \) in the QR decomposition of \( A \) produced on the forward pass. The matrix \( U \) is square and full-rank.
3. Transform the remaining \( n - m \) columns of \( A \), the \( Y \) partition, to get \( V = Q^TY \).
4. The reverse mode auto-diff employs this sequence in reverse order to get the partitioned \( [X|Y] \) gradient. Then the full \( A \) gradient is obtained by a simple concatenation node in the computational graph.

The reader may find Figure 2 instructive to study for the backprop computations with a partitioning trick. Next we apply the chain rule and the two-step backprop algorithm to obtain \( \bar{A} \).
BP Step 1: Variations First calculate the variations of $Q$, $R$, $dQ$, and $dR$, for a given variation $dA$ of $A$.

Lemma 2. The variations of $A$ and $R$ are partitioned $dA = [dX \mid dY]$ and $dR = [dU \mid dV]$. Then

$$
dQ = (dX - QdU)U^{-1}
$$

$$
dV = Q^T(dY - dQV)
$$

$$
dU = \text{sym}(C) \circ E^T U,
$$

with $C = Q^T dX U^{-1}$ and $Q^T dQ$ is skew-symmetric.

Proof. The proof of Lemma 2 is left to the appendix.

BP Step 2: Partial Derivatives On the second step of the matrix backprop process we derive $[\hat{X} \mid \hat{Y}]$ and consequently $\hat{A}$. We begin by using the partitioned form to rewrite Equation 14

$$
Tr(X^T dX) + Tr(Y^T dY) = Tr(Q^T dQ) + Tr(U^T dU) + Tr(V^T dV).
$$

(14)

Replace the variations $dQ$, $dU$ and $dV$ in the r.h.s. of Equation 14 with their expressions as functions of the $dX$, and $dY$ from Lemma 2. Now both the l.h.s. and r.h.s. are functions of only $dX$ and $dY$ and are orthogonal to each other due to the nature of the partitioning. Matching the pre-multiplying matrices from the l.h.s. and r.h.s. of Equation 14 we identify the gradients $\hat{X}$ and $\hat{Y}$.

Focusing on the r.h.s. of Equation 14 first replace $dV$ from Lemma 2 to get

$$
Tr(\hat{Q}^T dQ) + Tr(\hat{U}^T dU) - Tr(\hat{V}^T Q^T dQV) + Tr(\hat{V}^T Q^T dY).
$$

We identify the transpose of the $dY$ coefficient in Equation 14 as $\hat{Y} = Q \hat{V}$. Now that we have identified the gradient $\hat{Y}$, we omit the corresponding terms from both the l.h.s. and r.h.s. of Equation 14 and focus on identifying $dX$. We have

$$
Tr(\hat{X}^T dX) = Tr(\hat{Q}^T dQ) + Tr(\hat{U}^T dU) - Tr(\hat{V}^T Q^T dQV).
$$

The last trace can be simplified by replacing $Q^T dQ$, using skew-symmetry and $V = Q^T Y$ from the partitioning argument, and the orthogonality of $Q$ to get

$$
Tr(\hat{V}^T Q^T dQV) = -Tr(\hat{V}^T (dQ^T Q)V)
$$

$$
= -Tr(\hat{V}^T ((dQ^T Q)(Q^T Y))
$$

$$
= -Tr(\hat{V}^T Q^T Y).
$$

Further use the ICP and the IT property from Section 2.3 to write

$$
Tr(\hat{V}^T dQ^T Y) = Tr(Y \hat{V}^T dQ^T) = Tr(\hat{V}^T Y dQ).
$$

With this result simplify the r.h.s. of Equation 14

$$
Tr(\hat{Q}^T dQ) + Tr(\hat{U}^T dU) + Tr(\hat{V}^T Y dQ) = Tr(\hat{Q}^T + \hat{V}^T Y \hat{Q}^T) dQ) + Tr(\hat{U}^T dU)
$$

(15)

$$
= Tr(\hat{Q}^T dQ) + Tr(\hat{U}^T dU),
$$

(16)

where we use the notation $Q_{\text{prime}} = \hat{Q} + Y \hat{V}^T$. The rest of the argument for the $dX$ term is similar to the argument in Section 3.1 since $X$ and $U$ are square. Next, we follow the same process as in the proof of Proposition 1, with $X$ in place of $A$, $U$ in place of $R$ and $Q_{\text{prime}}$ in place of $Q$. We use $Q_{\text{prime}}$ instead of simply $Q$ since $Q$ is used in multiple node computations in the computational graph showed in Figure 2. Consequently, using the result in Section 3.1, we get

$$
X = (Q_{\text{prime}} + Q_{\text{create}}(M))U^{-T},
$$

with $M = UU^T - Q_{\text{prime}}Q$. Now that we have identified both $X$ and $Y$, we concatenate them to obtain

$$
\hat{A} = [(Q_{\text{prime}} + Q_{\text{create}}(M))U^{-T} | QV],
$$

7
as proposed. Notice that the calculation of $\bar{X}$ in the wide case employs the techniques in Section 3.1 hence either Equation 3 or the equivalent Equation 8 can be employed. In Appendix 5.2 we prove that Equation 3 and Equation 8 are equivalent. Where possible we prefer to use Equation 3 for computational efficiency considerations.

The connection to the square case simplifies software implementations considerably. Although memory is re-used as much as possible for efficiency, additional memory must still be allocated for intermediary results. In the MXNet software implementation (C++) Equation 3 is implemented as a helper and then used directly to either obtain $\bar{A}$ directly when $A$ is square or deep, or to obtain $\bar{X}$ when $A$ is deep. TensorFlow had already implemented a QR backward method decomposition for square and deep input matrices (Python) and the Equation 8 was used. We implemented Equation 8 as a helper and calculated $\bar{X}$ directly using the helper function. However, Equation 3 has a more computationally efficient implementation and should be preferred when possible. After obtaining $\bar{X}$ and $\bar{Y}$ we re-assemble the gradient $A$ via matrix concatenation. Numerical tests to test the correctness of the gradient via central differences were implemented as part of the typical test driven development approach. These tests can be referred to in the backend of the aforementioned deep learning frameworks on Github.

3.3 LQ Backpropagation: Square, Wide and Deep

In [12], the reverse mode auto-diff for the LQ decomposition is derived for square and wide matrices, $A \in \mathbb{R}^{m,n}, m \leq n$, as:

$$\bar{A} = L^{-T} \left[ \tilde{Q} + copyltu(M)Q \right],$$

where $M = L^T \tilde{L} - \tilde{Q}Q^T$. A key assumption in the proof is that $L$ is full rank. For the deep case, the reverse mode AD derivation is stymied by the shapes of $L$ and $Q$ and by the fact that $L$ is not full rank. We again employ the partitioning trick to get the LQ decomposition gradient for deep input matrices. To the best of our knowledge this result is novel.

**Proposition 3**

Let $A = LQ$ be the LQ decomposition of a deep matrix $A$, with $A \in \mathbb{R}^{m,n}, Q \in \mathbb{R}^{n,n}$ a square orthogonal matrix, $L \in \mathbb{R}^{m,n}$ a lower triangular matrix, and $m > n$, with the top $n$ rows of $A$ forming a square full-rank matrix. In the reverse mode auto-diff $A$, $L$ and $\tilde{L}$ are partitioned into

$$A = \begin{bmatrix} X \\ Y \end{bmatrix}, \quad L = \begin{bmatrix} U \\ V \end{bmatrix}, \quad \text{and} \quad \tilde{L} = \begin{bmatrix} \tilde{U} \\ \tilde{V} \end{bmatrix},$$

respectively with $X, U, \tilde{U} \in \mathbb{R}^{n,n}$, $Y, V, \tilde{V} \in \mathbb{R}^{m-n,n}$. Then we calculate $\bar{A}$ as the concatenation of $\bar{X}$ and $\bar{Y}$ along the row axis with $\bar{X} = U^{-T}(Q_{\text{prime}} + copyltu(M)Q)$ and $\bar{Y} = VQ$, with $M = U^TU - Q_{\text{prime}}Q^T$, and $Q_{\text{prime}} = \tilde{Q} + \tilde{V}^TY$.

The proof of Proposition 3 parallels the proof of Proposition 2 and is left to the Appendix. The LQ decomposition and its gradient can be obtained using the TensorFlow based code in this Github repository.

4 Final Notes

In this article we presented the reverse mode automatic differentiation algorithms for QR and LQ decompositions that can be used in matrix backprop derivations for any full-rank matrix orders. As a result of this work the QR decomposition (forward and backward, for all input shapes) was implemented in MXNet [3]. In TensorFlow Core [1] and PyTorch [10] the gradient for wide inputs was implemented. All frameworks support CPU and GPU implementations. In these frameworks the QR decomposition can be applied in batches and performed on the last two dimensions of larger tensors. The software implementation of the methods across the popular deep learning frameworks allows researchers and engineers to use the differentiable QR across common frameworks. We hope this article allows the practitioner to understand the derivations of the implemented routines.

**References**

[1] Martín Abadi, Paul Barham, Jianmin Chen, Zhifeng Chen, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Geoffrey Irving, Michael Isard, et al. Tensorflow: A system for large-scale machine learning. In 12th {USENIX} Symposium on Operating Systems Design and Implementation ({OSDI} 16), pages 265–283, 2016.
[2] Edward Anderson, Zhaojun Bai, Christian Bischof, Susan Blackford, Jack Dongarra, Jeremy Du Croz, Anne Greenbaum, Sven Hammarling, Alan McKenney, and Danny Sorensen. LA-PACK Users’ guide, volume 9. Siam, 1999.

[3] Tianqi Chen, Mu Li, Yutian Li, Min Lin, Naiyan Wang, Minjie Wang, Tianjun Xiao, Bing Xu, Chiyuan Zhang, and Zheng Zhang. MXNet: A flexible and efficient machine learning library for heterogeneous distributed systems. arXiv preprint arXiv:1512.01274, 2015.

[4] Z. Dang, K. M. Yi, Y. Hu, F. Wang, P. Fua, and M. Salzmann. Eigendecomposition-free training of deep networks for linear least-square problems. IEEE Transactions on Pattern Analysis and Machine Intelligence, pages 1–1, 2020.

[5] Mike B Giles. Collected matrix derivative results for forward and reverse mode algorithmic differentiation. In Advances in Automatic Differentiation, pages 35–44. Springer, 2008.

[6] Catalin Ionescu, Orestis Vantzos, and Cristian Sminchisescu. Training deep networks with structured layers by matrix backpropagation. arXiv preprint arXiv:1509.07838, 2015.

[7] Hai-Jun Liao, Jin-Guo Liu, Lei Wang, and Tao Xiang. Differentiable programming tensor networks. Physical Review X, 9(3):031041, 2019.

[8] CUDA Nvidia. Nvidia cuda c programming guide. Nvidia Corporation, 120(18):8, 2011.

[9] Travis E Oliphant. A guide to NumPy, volume 1. Trelgol Publishing USA, 2006.

[10] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, et al. Pytorch: An imperative style, high-performance deep learning library. In Advances in neural information processing systems, pages 8026–8037, 2019.

[11] Shayle R Searle and Andre I Khuri. Matrix algebra useful for statistics. John Wiley & Sons, 2017.

[12] Matthias Seeger, Asmus Hetzel, Zhenwen Dai, Eric Meissner, and Neil D Lawrence. Auto-differentiating linear algebra. arXiv preprint arXiv:1710.08717, 2017.

[13] Lloyd N Trefethen and David Bau III. Numerical linear algebra, volume 50. Siam, 1997.

[14] Sebastian F Walter and Lutz Lehmann. Algorithmic differentiation of linear algebra functions with application in optimum experimental design (extended version). arXiv preprint arXiv:1001.1654, 2010.
5 Appendix

5.1 Lemma 1.

For a deep matrix with QR decomposition $A = QR$, the variations of $Q$ and $R$ for a given variation $dA$ of $A$, denoted $dQ$ and $dR$ respectively, are

$$dQ = (dA - QdR)R^{-1}$$
$$dR = (\text{sym}(C) \circ E^T)R,$$

with $C = Q^T dAR^{-1}$.

Proof First calculate the variations of $Q$ and $R$, where the following hold:

- $R$ and $dR$ are square, upper triangular and full rank.
- $Q$ is orthogonal with $Q^T Q = I$ and hence (after taking the first variation)

$$dQ^T Q + Q^T dQ = 0$$

so $Q^T dQ$ is skew-symmetric with $Q^T dQ = -dQ^T Q$.

Take the first variation of the QR decomposition $A = QR$

$$dA = dQR + QdR.$$  

Right multiply by $R^{-1}$ to get

$$dQ = (dA - QdR)R^{-1}.$$  

(20)

Next, find an expression for $dR$. First left-multiply Equation (20) by $Q^T$ to get

$$Q^T dQ = Q^T (dA - QdR)R^{-1}.$$  

Now $Q^T dQ$ is skew-symmetric, so the r.h.s. is also skew-symmetric, and

$$Q^T (dA - QdR)R^{-1} = -R^{-T} (dA - QdR)^T Q$$

which simplifies to

$$Q^T dAR^{-1} + (Q^T dAR^{-1})^T = dRR^{-1} + (dRR^{-1})^T.$$  

Consequently, with some left to right algebraic manipulations,

$$\text{sym}(C) = \text{sym}(dRR^{-1}),$$

with $C = Q^T dAR^{-1}$. In Equation (21) $dRR^{-1}$ is upper triangular so we express $dR$, using the notation of Lemma 1, as $dR = (\text{sym}(C) \circ E^T)R$.

5.2 Equivalence of Equation 3 in Proposition 1 and Equation 8 in Section 3.1

In Section 3.1 we derived the gradient for the QR decomposition of square and deep input matrices and noted that the resulting formula is equivalent to the one given in 8, albeit more compact and computationally efficient. We prove the equivalence next.

Proof We need to prove that Equation 8

$$\hat{A} = Q(R + P_L \circ (RR^T - RR^T + Q^T Q - Q^T Q)R^{-T}) + (Q - QQ^T Q)R^{-T},$$

with $P_L = (i > j)$, a strictly lower tridiagonal matrix with all ones below the diagonal and zeroes along and above the main diagonal, simplifies to Equation 3

$$\hat{A} = [\hat{Q} + Q_{copyltu}(M)] R^{-T},$$

where $M = RR^T - Q^T Q$. 

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First, in Equation 8 we rearrange and simplify the innermost parenthesis as
\[ M = \bar{M} + (\bar{R} - M^T)R^{-T} + Q^TQ - Q^TQ. \]

Now we can re-write Equation 8 as
\[ \bar{A} = Q(\bar{R}R^T + P_L \circ (M - M^T)R^{-T}) + (\bar{Q} - QQ^T)R^{-T}. \]

Next we factor out \( R^{-T} \)
\[ \bar{A} = [Q(\bar{R}R^T + P_L \circ (M - M^T)) + \bar{Q} - QQ^T]R^{-T}. \]

Then we re-arrange terms and factor out \( Q \)
\[ \bar{A} = [\bar{Q} + Q(P_L \circ (M - M^T) + \bar{R}R^T - Q^T\bar{Q})]R^{-T}. \]

We now identify matrix \( M^T \) and rewrite
\[ \bar{A} = [\bar{Q} + Q(P_L \circ (M - M^T) + M^T)] R^{-T}. \]

Note that \( E = 2P_L - I \) by definition, so one can write \( P_L = 0.5(E + I) \) and
\[ \bar{A} = [\bar{Q} + Q(0.5(E + I) \circ M - 0.5(E + I) \circ M^T + M^T)] R^{-T} \]
\[ = [\bar{Q} + Q(0.5E \circ M + 0.5E \circ M^T)] R^{-T} \]
\[ = [\bar{Q} + Q(E \circ \text{sym}(M))] R^{-T} \]
\[ = [\bar{Q} + Q\text{cyl}(\text{sym}(M))] R^{-T}, \]

which proves the equivalence of Equation 5 and 8.

5.3 Lemma 2.

When \( A \) is wide, full rank, and with the first \( k \) columns forming a square full rank matrix, the variations of \( A \) and \( R \) can be partitioned similarly to \( A \) and \( R \) as \( d\bar{A} = [dX \mid dY] \) and \( d\bar{R} = [dU \mid dV] \) with corresponding orders such that
\[ d\bar{Q} = (dX - QdU)U^{-1}, \]
\[ dV = Q^T(dY - dQV), \]
\[ dU = (\text{sym}(C) \circ E^T)U, \]
with \( C = Q^TdXU^{-1}. \)

**Proof.** We want to calculate the variations \( d\bar{Q} \) and \( [dU \mid dV] \) for given \( [dX \mid dY] \), where
- \( d\bar{R} \) and \( dU \) are upper triangular matrices.
- \( Q \) is orthogonal with
  \[ dQ^TQ + Q^TdQ = 0. \]  
  \[ (22) \]

The exposition is continued using partitioned matrices. Taking the first variation of the QR decomposition of \( X \), we have
\[ d\bar{X} = dQU + QdU. \]
Then right multiply by \( U^{-1} \) to get
\[ d\bar{Q} = (dX - QdU)U^{-1}. \]
\[ (23) \]

Similarly take the first variation of \( Y = QV \) in Equation 9 to get \( d\bar{Y} = QdV + dQV \) and then \( dV = Q^T(dY - dQV) \). Next, we use Equation 23 to find an expression for \( dU \). First left-multiply by \( Q^T \) to get
\[ Q^Td\bar{Q} = Q^T(dX - QdU)U^{-1}. \]
Now the l.h.s. is skew-symmetric, so the r.h.s. is also skew-symmetric, with
\[ Q^T (dX - QdU)U^{-1} = -U^{-T}(dX - QdU)^T Q, \]
which simplifies to
\[ Q^T dXU^{-1} + (Q^T dXU^{-1})^T = dUU^{-1} + (dUU^{-1})^T. \]
Then write
\[ sym(dUU^{-1}) = sym(C), \]
with \( C = Q^T dXU^{-1} \). Matrix \( dUU^{-1} \) is upper triangular so we express \( dU \), using the notation in Lemma 2,
\[ dU = (sym(C) \circ E^T)U. \]

6 Proposition 3. LQ BP For Deep Input Matrices

Proof. The proof follows closely the proof of Proposition 2.

If \( A \) is deep, of rank \( k \), with the top \( k \) rows forming a square full-rank matrix, and partitioned as illustrated in Section 3.3, Proposition 3, then
\[ X = UQ \]
is the LQ decomposition of \( X \), with \( Q \) and \( U \) square, full-rank invertible matrices. Then \( Y = VQ \).
Hence we can apply the chain rule and the two step matrix backprop to obtain \( \bar{A} \).

BP Step 1: Variations
First calculate the variations of \( L \) and \( Q \), \( dQ \) and \( dL \) for a given variation \( dA \) of \( A \). The variations of \( A \) and \( L \) can also be partitioned as \( dA = [dX | dY] \) and \( dL = [dU | dV] \) with corresponding orders such that
\[
\begin{align*}
    dQ &= U^{-1}(dX - dUQ) \\
    dV &= (dY - VdQ)Q^T. \\
    dU &= U(sym(C) \circ E).
\end{align*}
\]
with \( C = U^{-1}dXQ^T \).

Proof. We want to calculate the variations \( dQ \) and \( [dU, dV] \) for given \( [dX, dY] \), where
- \( dL \) and \( dU \) are lower triangular matrices.
- \( Q \) is orthogonal with
\[ dQQ^T + QdQ^T = 0 \]
Taking the first variation of the LQ decomposition of \( X \), we have
\[ dX = dUQ + UdQ, \]
Then left multiply by \( U^{-1} \) to get
\[ dQ = U^{-1}(dX - dUQ) \]
Similarly take the first variation of \( Y = VQ \) to get \( dY = dVQ + VdQ \) and then \( dV = (dY - VdQ)Q^T. \) Next, find an expression for \( dU \). First right-multiply by \( Q^T \) in Equation 26 to get
\[ dQQ^T = U^{-1}(dX - QdU)Q^T. \]
The l.h.s. is skew-symmetric, so the r.h.s. is also skew-symmetric, and we can write
\[ U^{-1}dXQ^T + (U^{-1}dXQ^T)^T = U^{-1}dU + (U^{-1}dU)^T. \]
Then
\[ sym(U^{-1}dU) = sym(C), \]
with \( C = U^{-1}dXQ^T \). Matrix \( U^{-1}dU \) is lower triangular so we can express \( dU \)
\[ dU = U(sym(C) \circ E). \]
**BP Step 2: Partial Derivatives** We proceed to the second step of the process for matrix backprop process to get $A$. We use the trace identity $Tr(A^T dA) = Tr(L^T dL) + Tr(Q^T dQ)$. Replace the partitioned matrices and the calculated variations $dQ$, $dU$ and $dV$ and get the l.h.s. and r.h.s. coefficients of $dX$ and $dY$ to find $X$ and $Y$.

First replace $dV$ to get

$$Tr(Q^T dQ) + Tr(U^T dU) - Tr(V^T Y Q^T) + Tr(V^T Y Q^T).$$

Identify the $dY$ coefficient and get $Y = V Q$. Next identify $dX$. We have

$$Tr(X^T dX) = Tr(Q^T dQ) + Tr(U^T dU) - Tr(V^T Y Q^T).$$

The last trace can be simplified by replacing $dQQ^T$, using skew-symmetry and $V = Y Q^T$ from the partitioning argument, the orthogonality of $Q$, and ICP and IT properties to get

$$Tr(V^T V dQQ^T) = -Tr(V^T Y Q^T Qd(Q^T)) = -Tr(Y^T Y dQ).$$

With this result simplify the r.h.s. of the trace equality

$$Tr(Q^T dQ) + Tr(U^T dU) - Tr(Y^T Y dQ) = Tr(Q_{prime}^T dQ) + Tr(U^T dU).$$

Since $X$, $U$ are square, the rest of the argument for the $dX$ term is the argument for LQ decomposition gradient with square input and we get $X = U^{-T} [Q_{prime} + copyltu(M)Q]$, with $M = U^T U - Q_{prime} Q^T$, and $Q_{prime} = Y + Y^T Y$ as proposed.