Efficient Inverse-Free Incremental and Decremental Algorithms for Multiple Hidden Nodes in Extreme Learning Machine

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Abstract—The inverse-free extreme learning machine (ELM) algorithm proposed in [4] was based on an inverse-free algorithm to compute the regularized pseudo-inverse, which was deduced from an inverse-regularized recursive algorithm to update the inverse of a Hermitian matrix. Before that recursive algorithm was applied in [4], its improved version had been utilized in previous literatures [9], [10]. Accordingly from the improved recursive algorithm [9], [10], several efficient inverse-free algorithms for ELM were proposed in [13] to reduce the computational complexity. In this paper, we propose two inverse-free algorithms for ELM with Tikhonov regularization, which can remove multiple hidden nodes in an iteration. On the other hand, we also propose two efficient decremental learning algorithms for ELM with Tikhonov regularization, which can remove multiple redundant nodes in an iteration.

Index Terms—Extreme learning machine (ELM), inverse-free, fast recursive algorithms, inverse LDLT factorization, neural networks.

I. INTRODUCTION

The extreme learning machine (ELM) [1] is an effective solution for Single-hidden-layer feedforward networks (SLFNs) due to its unique characteristics, i.e., extremely fast learning speed, good generalization performance, and universal approximation capability [2]. Thus ELM has been widely applied in classification and regression [3].

The incremental ELM proposed in [2] achieves the universal approximation capability by adding hidden nodes one by one. However, it only updates the output weight for the newly added hidden node, and freezes the output weights of the existing hidden nodes. Accordingly those output weights are no longer the optimal least-squares solution of the standard ELM algorithm. Then the inverse-free algorithm was proposed in [4] to update the output weights of the added node and the existing nodes simultaneously, and the updated weights are identical to the optimal solution of the standard ELM algorithm. The ELM algorithm in [4] was based on an inverse-free algorithm to compute the regularized pseudo-inverse, which was deduced from an inverse-free recursive algorithm to update the inverse of a Hermitian matrix.

Before the recursive algorithm to update the inverse was utilized in [4], it had been mentioned in previous literatures [5]–[9], while its improved version had been utilized in [9], [10]. Accordingly from the improved recursive algorithm [9], [10], several efficient inverse-free algorithms for ELM were proposed in [13] to reduce the computational complexity. In [13], two proposed inverse-free ELM algorithms compute the output weights directly from the inverse and the LDLT factors of the inverse, respectively, to avoid computing the regularized pseudo-inverse that is usually bigger than the inverse.

In each iteration, the inverse-free algorithms in [4, 13] for ELM with Tikhonov regularization can only increase one hidden node. In this paper, we develop two inverse-free algorithms for ELM with Tikhonov regularization, which can increase multiple hidden nodes in an iteration. On the other hand, it is also required to prune redundant nodes [19]–[24] by decremental learning algorithms in machine learning. Thus in this paper, we will propose efficient decremental learning algorithms to remove multiple redundant nodes in an iteration.

II. ARCHITECTURE OF THE ELM

In the ELM model, the n-th input node, the i-th hidden node, and the m-th output node can be denoted as xn, hi, and zm, respectively, while all the N input nodes, l hidden nodes, and M output nodes can be denoted as x=[x1 x2 ⋯ xN]T ∈ RN, h=[h1 h2 ⋯ hl]T ∈ Rl, and z=[z1 z2 ⋯ zM]T ∈ RM, respectively. Accordingly the ELM model can be represented in a compact form as

\[ h = f(Ax + d) \]

and

\[ z = Wh \]

where A=[ai,j] ∈ RN×N, d=[d1 d2 ⋯ dl]T ∈ RN, W=[wmi] ∈ RM×l, and the activation function f(•) is entry-wise, i.e., f(A)=[f(ai,m)] ∈ RN×N for a matrix input A=[ai,m] ∈ RN×N. In (1), the activation function f(•) can be chosen as linear, sigmoid, Gaussian models, etc.

Assume there are totally K distinct training samples, and let xk ∈ RN and zk ∈ RM denote the k-th training input and the corresponding k-th training output, respectively, where k=1, 2, ⋯, K. Then the input sequence and the output sequence in the training set can be represented as

\[ X = [ x_1 \ x_2 \ ⋯ \ x_K ] ∈ RN×K, \]

and

\[ Z = [ z_1 \ z_2 \ ⋯ \ z_K ] ∈ RM×K, \]

respectively. We can substitute (3) into (1) to obtain

\[ H = f(AX + 1T ⊗ d), \]
where \( H = [ \mathbf{h}_1 \mathbf{h}_2 \cdots \mathbf{h}_K ] \in \mathbb{R}^{l \times K} \) is the value sequence of all \( l \) hidden nodes, and \( \otimes \) is the Kronecker product \([4]\). Then we can substitute (5) and (4) into (2) to obtain the actual training output sequence

\[
Z = WH. \tag{6}
\]

In an ELM, only the output weight \( W \) is adjustable, while \( A \) (i.e., the input weights) and \( d \) (i.e., the biases of the hidden nodes) are randomly fixed. Denote the desired output as \( Y \). Then an ELM simply minimizes the estimation error

\[
\mathbf{E} = \mathbf{Y} - Z = \mathbf{Y} - WH \tag{7}
\]

by finding a least-squares solution \( W \) for the problem

\[
\min_{W} \| \mathbf{E} \|^2_F = \min_{W} \| \mathbf{Y} - WH \|^2_F, \tag{8}
\]

where \( \| \cdot \|_F \) denotes the Frobenius norm.

For the problem (8), the unique minimum norm least-squares solution is \([1]\)

\[
W = YH^T(\mathbf{HH}^T)^{-1}. \tag{9}
\]

To avoid over-fitting, the popular Tikhonov regularization \([14, 15]\) can be utilized to modify (9) into

\[
W = YH^T(\mathbf{HH}^T + k_0^2 I)^{-1}, \tag{10}
\]

where \( k_0^2 > 0 \) denotes the regularization factor. Obviously \([3]\) is just the special case of (10) with \( k_0^2 = 0 \). Thus in what follows, we only consider (10) for the ELM with Tikhonov regularization.

III. The Existing Inverse-Free ELM Algorithms in \([13]\)

In machine learning, it is a common strategy to increase the hidden node number gradually until the desired accuracy is achieved. However, when this strategy is applied in ELM directly, the matrix inverse operation in (10) for the conventional ELM will be required when a few or only one extra hidden node is introduced, and accordingly the algorithm will be computational prohibitive. Accordingly an inverse-free strategy was proposed in \([4]\), to update the output weights incrementally with the increase of the hidden nodes. In each step, the output weights obtained by the inverse-free algorithm are identical to the solution of the standard ELM algorithm using the inverse operation.

Assume that in the ELM with \( l \) hidden nodes, we add one extra hidden node, i.e., the hidden node \( l + 1 \), which has the input weight row vector \( \mathbf{a}_{l+1}^T = [a_{l+1,1} a_{l+1,2} \cdots a_{l+1,N}] \in (\mathbb{R}^N)^T \) and the bias \( d_{l+1} \). Then from (5) it can be seen that the extra row \( \tilde{\mathbf{H}}_{l+1} = f(\tilde{\mathbf{a}}_{l+1}^T \mathbf{X} + d_{l+1} I^2) \) needs to be added to \( \mathbf{H} \), i.e.,

\[
\mathbf{H}^{l+1} = \begin{bmatrix} \mathbf{H}^l & \tilde{\mathbf{H}}_{l+1} \end{bmatrix}, \tag{11}
\]

where \( \mathbf{H}^i \) (\( i = l, l+1 \)) denotes \( \mathbf{H} \) for the ELM with \( i \) hidden nodes. In \( \tilde{\mathbf{a}}_{l+1}, \tilde{\mathbf{h}}_{l+1}, \tilde{d}_{l+1} \) and what follows, we add the underline to emphasize the extra vector or scalar, which is added to the matrix or vector for the ELM with \( l \) hidden nodes.

After \( \mathbf{H} \) is updated by (11), the conventional ELM updates the output weights by (10) that involves an inverse operation. To avoid that inverse operation, the algorithm in \([4]\) utilizes an inverse-free algorithm to update

\[
\mathbf{B} = \mathbf{H}^T(\mathbf{H}H^T + k_0^2 I)^{-1} \tag{12}
\]

that is the regularized pseudo-inverse of \( \mathbf{H} \), and then substitutes (12) into (10) to compute the output weights by

\[
\mathbf{W} = \mathbf{YB}. \tag{13}
\]

In \([4]\), \( \mathbf{B}^{l+1} \) (i.e., \( \mathbf{B} \) for the ELM with \( l + 1 \) hidden nodes) is computed from \( \mathbf{B}^l \) iteratively.

Let

\[
\mathbf{R} = \mathbf{HH}^T + k_0^2 \mathbf{I} \tag{14}
\]

and

\[
\mathbf{Q} = \mathbf{R}^{-1} = (\mathbf{HH}^T + k_0^2 \mathbf{I})^{-1}. \tag{15}
\]

Then we can write (12) as

\[
\mathbf{B} = \mathbf{H}T \mathbf{Q}. \tag{16}
\]

From (14) we have

\[
\mathbf{R}^{l+1} = \mathbf{H}^{l+1} (\mathbf{H}^{l+1}T + k_0^2 \mathbf{I})^{-1}, \tag{17}
\]

into which we substitute (11) to obtain

\[
\mathbf{R}^{l+1} = \begin{bmatrix} \mathbf{R}^l & \mathbf{p}_l^T \\ \mathbf{p}_l & \tilde{\mathbf{H}}_{l+1}^T \tilde{\mathbf{h}}_{l+1} + k_0^2 \end{bmatrix}, \tag{18}
\]

where \( \mathbf{p}_l \), a column vector with \( l \) entries, satisfies

\[
\mathbf{p}_l = \mathbf{H}^T \tilde{\mathbf{h}}_{l+1}. \tag{19}
\]

The inverse-free recursive algorithm in \([13]\) computes

\[
\mathbf{Q}^{l+1} = \begin{bmatrix} \tilde{\mathbf{Q}}^l & \mathbf{t}_l \\ \mathbf{t}_l^T & \tau_l \end{bmatrix}, \tag{20}
\]

where

\[
\begin{cases} 
\tau_l = 1 / \left( (\tilde{\mathbf{h}}_{l+1}^T \tilde{\mathbf{h}}_{l+1} + k_0^2) - \mathbf{p}_l^T \mathbf{Q}^l \mathbf{p}_l \right) \\
\mathbf{t}_l = -\tau_l \mathbf{Q}^l \mathbf{p}_l \\
\tilde{\mathbf{Q}}^l = \mathbf{Q}^l + (1/\tau_l) \mathbf{t}_l \mathbf{t}_l^T 
\end{cases} \tag{21}
\]

and update the output weight \( \mathbf{W} \) by

\[
\mathbf{W}^{l+1} = \begin{bmatrix} \tilde{\mathbf{W}}^l & \tilde{\mathbf{w}}_{l+1} \end{bmatrix}, \tag{22}
\]

where

\[
\begin{cases} 
\tilde{\mathbf{W}}^l = \mathbf{W}^l + (\tilde{\mathbf{w}}_{l+1}/\tau_l) \mathbf{t}_l \\
\tilde{\mathbf{w}}_{l+1} = \tau_l (\mathbf{Y} \tilde{\mathbf{h}}_{l+1} - \mathbf{W}^l \mathbf{p}_l) \end{cases} \tag{23}
\]

are computed from \( \mathbf{t}_l \) and \( \tau_l \) in \( \mathbf{Q}^{l+1} \).

Since the processor units are limited in precision, the recursive algorithm utilized to update \( \mathbf{Q} \) may introduce numerical instabilities, which occurs only after a very large number of iterations \([12]\). Thus instead of the inverse of \( \mathbf{R} \) (i.e., \( \mathbf{Q} \)), we can also update the inverse \( \mathbf{LDL}^T \) factors \([11]\) of \( \mathbf{R} \), since usually the \( \mathbf{LDL}^T \) factorization is numerically stable \([16]\). The inverse \( \mathbf{LDL}^T \) factors include the upper-triangular \( \mathbf{L} \) and the diagonal \( \mathbf{D} \), which satisfy

\[
\mathbf{LDL}^T = \mathbf{Q} = \mathbf{R}^{-1}. \tag{24}
\]
From (23) we can deduce
\[ L^{-T}D^{-1}L^{-1} = R, \]  
(24)
where the lower-triangular \( L^{-T} \) is the conventional LDL\( ^T \) factor \( [16] \) of \( R \).

The inverse LDL\( ^T \) factors can be computed from \( R \) directly by the inverse LDL\( ^T \) factorization in (11), i.e.,
\[
\begin{align*}
L^{i+1} &= \begin{bmatrix} L^i & \tilde{t}_l \\ 0^T & 1 \end{bmatrix} \\
D^{i+1} &= \begin{bmatrix} D^i & 0 \\ 0^T & \tau \end{bmatrix},
\end{align*}
\]
(25a, 25b)
where
\[
\begin{align*}
\tilde{t}_l &= -L^iD^i(L^i)^T p_l \\
\tau_l &= 1/((\tilde{H}_{l+1}^T H_{l+1} + k^2_d) - p_l^T L^iD^i(L^i)^T p_l). 
\end{align*}
\]
(26a, 26b)
We can show that \( \tilde{t}_l \) in (26a) and \( t_l \) in (20b) satisfy
\[ \tilde{t}_l = t_l / \tau_l, \]
(27)
and \( \tau_l \) in (26b) is equal to \( \tau_l \) in (20a), by substituting (23) into (26a) and (26b), respectively. After updating \( L \) and \( D \), we compute the output weight \( W \) by (22b),
\[
\tilde{W}^l = W^l + \tilde{w}_{l+1} T_l^T,
\]
(28)
and (21), where (28) is deduced by substituting (27) into (22a).

IV. THE PROPOSED INVERSE-FREE ELM ALGORITHMS TO REMOVE MULTIPLE HIDDEN NODES BY ONE ITERATION

In (10), \( \tau_l \) was extended to be the \( 2 \times 2 \) Alamouti [17] sub-block, while \( t_l \) was extended to be the block vector consisting of \( 2 \times 2 \) Alamouti sub-blocks. In this paper, we extend (11), (17) and (19) to be
\[
\begin{align*}
H^{i+\delta} &= \begin{bmatrix} H^i \\ \bar{H} \end{bmatrix}, \\
R^{i+\delta} &= \begin{bmatrix} R^i & P \\ PT & F \end{bmatrix}, \\
Q^{i+\delta} &= \begin{bmatrix} \bar{Q}^i \\ T^T G \end{bmatrix}, \end{align*}
\]
(29, 30, 31)
respectively, where \( \bar{H}^i \in \mathbb{R}^{n \times K}, P \in \mathbb{R}^{n \times d}, T \in \mathbb{R}^{d \times d}, F \in \mathbb{R}^{d \times d}, \) and \( G \in \mathbb{R}^{d \times d} \). Moreover, \( T, G \) and \( \bar{Q} \) in (31) can be computed by
\[
\begin{align*}
G &= (F - PT Q^i P)^{-1} \\
T &= -Q^i \bar{P} \bar{G}, \\
\bar{Q} &= Q^i - Q^i \bar{P} \bar{T},
\end{align*}
\]
(32a, 32b, 32c)
which will be deduced in Appendix A.

Accordingly we update the output weight \( W \) by
\[
W^{i+\delta} = \left[ \begin{bmatrix} W^l + (Y(H^i)^T - W^l P) T_l^T \\ (Y(H^i)^T - W^l P) G \end{bmatrix}^T \right]^T, \]
(33)
which will be deduced in Appendix B.

We can also utilize the LDL\( ^T \) factors, which can be written as
\[
\begin{align*}
L^{i+\delta} &= \begin{bmatrix} L^i & U \\ 0^T & V \end{bmatrix}, \\
D^{i+\delta} &= \begin{bmatrix} D^i & 0 \\ 0^T & S \end{bmatrix},
\end{align*}
\]
(34a, 34b)
where \( U \in \mathbb{R}^{n \times \delta}, V \in \mathbb{R}^{\delta \times \delta} \) and \( S \in \mathbb{R}^{\delta \times \delta} \) can be computed by
\[
\begin{align*}
U &= -L^i D^i (L^i)^T PV \\
V S V^T &= (F - PT Q^i P)^{-1}.
\end{align*}
\]
(35a, 35b)
Accordingly we can update the output weight \( W \) by
\[
W^{i+\delta} = \begin{bmatrix} (W^l + (Y(H^i)^T - W^l P) V S V^T)^T \\ (Y(H^i)^T - W^l P) V S V^T \end{bmatrix}^T.
\]
(36)

We will deduce (35) and (36) in Appendix C. Notice that in (35b), the upper-triangular \( V \) and the diagonal \( S \) are the inverse LDL\( ^T \) factors of \( F - PT Q^i P \) and can be computed by the inverse LDL\( ^T \) factorization in (11), or by invert and transpose the traditional LDL\( ^T \) factors of \( F - PT Q^i P \).

V. THE PROPOSED INVERSE-FREE ELM ALGORITHMS TO REMOVE MULTIPLE HIDDEN NODES

Assume the \( \tau \) nodes corresponding to the rows \( i_1, i_2, \ldots, i_\tau \) (\( i_1 < i_2 < \cdots < i_\tau \)) in \( H^l \) needs to be removed. Then let us permute the rows \( i_1, i_2, \ldots, i_\tau \) in \( H^l \) to be the last \( 1^{st}, 2^{nd}, \ldots, \tau^{th} \) rows, respectively, and the permuted \( H^l \) can be written as
\[
H^l = \begin{bmatrix} H^{l-\tau} \\ H^\tau \end{bmatrix},
\]
(37)
where \( H^\tau \) includes the \( \tau \) rows to be removed. Since (37) and (29) have the same form, we can write (31) as
\[
Q^i = \begin{bmatrix} \bar{Q}^{i-\tau} \\ T^T \tau \end{bmatrix} G, \tau, \]
(38)
respectively, where \( T^\tau, \tau \in \mathbb{R}^{(l-\tau) \times \tau} \) and \( G, \tau \in \mathbb{R}^{\tau \times \tau} \). From (32b) we can deduce \( Q^i P = -TG^{-1} \), which is substituted into (32a) to obtain \( Q^i = \bar{Q} = T^T TG^{-1} \), i.e.,
\[
Q^{i-\tau} = \bar{Q}^{i-\tau} - T, G, \tau \]
(39)
Correspondingly \( Q^{i-\tau} \) for the remaining \( l - \tau \) nodes can be computed by (39).

Substitute (39) into (38), and then substitute (38) and (37) into (33) to obtain
\[
W^l = Y \left[ H^{l-\tau} \begin{bmatrix} H^{l-\tau} \\ H^\tau \end{bmatrix}^T \begin{bmatrix} \bar{Q}^{l-\tau} + T, G, \tau T^T \tau \\ P \end{bmatrix} \right], \tau, \]
(40)
where
From (40) we can deduce

\[
\begin{align*}
W_{l:1:l-\tau}^l &= W_{l:1:l-\tau}^l + \left( Y(H^{l-l})^T T^\tau \right) G_{\tau}^{-1} T^\tau, \\
W_{l:l-\tau+1:l}^l &= Y(H^{l-l})^T T^\tau + Y(H^{l})^T G_{\tau},
\end{align*}
\]

(41a)

(41b)

where \( W_{l:1:l-\tau}^l \) and \( W_{l:l-\tau+1:l}^l \) denote the first \( l - \tau \) columns and the last \( \tau \) columns in \( W_l \), respectively. Then we can substitute (41b) into (41a) to deduce \( W_{l:1:l-\tau}^l = W_{l:1:l-\tau}^l + W_{l:l-\tau+1:l}^l G_{\tau}^{-1} T^\tau \), i.e.,

\[
W_{l:1:l-\tau}^l = W_{l:1:l-\tau}^l - W_{l:l-\tau+1:l}^l G_{\tau}^{-1} T^\tau.
\]

(42)

Permute the rows \( i_1, i_2, \ldots, i_\tau \) in \( L_l \) to be the last 1st, 2nd, \ldots, \( \tau \)th rows, respectively. Since the permuted \( L_l \) is no longer triangular, we can utilize the wide-sense Givens rotation described in Appendix D to upper-triangularize \( L_l \), and update \( D_l \) accordingly. Then \( L_{l:1:l-\tau}^l \) and \( D_{l:1:l-\tau}^l \) for the remaining \( l - \tau \) nodes are the sub-matrix \( L_{l:1:l-\tau}^l \) in \( L_l \) and the sub-matrix \( D_{l:1:l-\tau}^l \) in \( D_l \), respectively.

\[
\begin{align*}
\bar{L}_l &= \begin{bmatrix} L_{l:1:l-\tau}^l & U_{\tau} \\ 0^T & V_{\tau} \end{bmatrix} \\
\bar{D}_l &= \begin{bmatrix} D_{l:1:l-\tau}^l & 0 \\ 0^T & S_{\tau} \end{bmatrix},
\end{align*}
\]

(43a)

(43b)

Substitute (43a) and (38) into (23) to obtain

\[
\begin{align*}
\times \begin{bmatrix} U_{\tau} S_{\tau} V_{\tau}^T \\ V_{\tau} S_{\tau} V_{\tau}^T \end{bmatrix} &= \begin{bmatrix} \bar{Q}_{l:1:l-\tau}^l & T_{\tau} \\ T_{\tau}^T & G_{\tau} \end{bmatrix},
\end{align*}
\]

(44)

where \( \times \) denotes the irrelevant entries. From (44) we can deduce

\[
\begin{align*}
T_{\tau} &= U_{\tau} S_{\tau} V_{\tau}^T \\
G_{\tau} &= V_{\tau} S_{\tau} V_{\tau}^T,
\end{align*}
\]

(45a)

(45b)

which are then substituted into (32) to obtain \( W_{l:1:l-\tau}^l = W_{l:1:l-\tau}^l - W_{l:l-\tau+1:l}^l (V_{\tau} S_{\tau} V_{\tau}^T)^{-1} (U_{\tau} S_{\tau} V_{\tau}^T) \), i.e.,

\[
W_{l:1:l-\tau}^l = W_{l:1:l-\tau}^l - W_{l:l-\tau+1:l}^l V_{\tau}^{-1} U_{\tau}^T.
\]

(46)

The wide-sense Givens rotation \( \Psi_{k+j}^{i+1} \) is equal to \( I_k \) except the 2 \times 2 sub-block in the \( j \)th and \( (j+1) \)th rows and columns, which is

\[
\begin{bmatrix} \psi_{k+j, k+j}^{i+1} & \psi_{k+j, k+j+1}^{i+1} \\ \psi_{j+1+j}^{i+1} & \psi_{j+1+j+1}^{i+1} \end{bmatrix} = \frac{1}{\rho} \begin{bmatrix} l_{k+j, d_{j+1}}^{i+1} & l_{k+j, d_{j+1}}^{i+1} \\ -l_{j+1,d_{j+1}}^{i+1} & l_{j+1, d_{j+1}}^{i+1} \end{bmatrix},
\]

(47)

where \( l_{k+j, d_{j+1}}^{i+1} \) is the \( i \)th entry in the last \( k+j \)th row of \( L_k \), and

\[
\rho = (l_{k+j, d_{j+1}}^{i+1})^2 + (l_{j+1, d_{j+1}}^{i+1})^2.
\]

(48)

The wide-sense Givens rotation \( \Psi_{k+j}^{i+1} \) is equal to \( I_k \) except the 2 \times 2 sub-block in the \( j \)th and \( (j+1) \)th rows and columns, which is

\[
\begin{bmatrix} \psi_{k+j, k+j}^{i+1} & \psi_{k+j, k+j+1}^{i+1} \\ \psi_{j+1+j}^{i+1} & \psi_{j+1+j+1}^{i+1} \end{bmatrix} = \frac{1}{\rho} \begin{bmatrix} l_{k+j, d_{j+1}}^{i+1} & l_{k+j, d_{j+1}}^{i+1} \\ -l_{j+1,d_{j+1}}^{i+1} & l_{j+1, d_{j+1}}^{i+1} \end{bmatrix},
\]

(49)

where \( l_{k+j, d_{j+1}}^{i+1} \) is the \( i \)th entry in the last \( k+j \)th row of \( L_k \), and

\[
\rho = (l_{k+j, d_{j+1}}^{i+1})^2 + (l_{j+1, d_{j+1}}^{i+1})^2.
\]

(50)

VI. Conclusion

In this paper, we develop two inverse-free algorithms for ELM with Tikhonov regularization, which can increase multiple hidden nodes in an iteration. On the other hand, we also develop two efficient decremental learning algorithms for ELM with Tikhonov regularization, which can remove multiple redundant nodes in an iteration.

APPENDIX A

DERIVATION OF (32)

From (15) we can deduce \( R^T P = I \), into which we can substitute (30) and (31) to obtain

\[
\begin{bmatrix} R^T & P \end{bmatrix} \begin{bmatrix} \bar{Q}^T \\ T^T \end{bmatrix} = I.
\]

(51)

Then from (31) we can obtain

\[
\begin{align*}
R^T + P G &= 0 \\
P^T T + F G &= I \\
R^T \bar{Q}^T + P T^T &= I.
\end{align*}
\]

(52a)

(52b)

(52c)

From (52a) we can deduce \( T = -(R^T)^{-1} P G \), i.e., (32a), which can be substituted into (52b) to obtain \( -P^T \bar{Q}^T P G + F G = I \), i.e., (32b). Moreover, from (52c) we can deduce \( \bar{Q}^T + (R^T)^{-1} P T^T = (R^T)^{-1} \), i.e., (32c).

APPENDIX B

DERIVATION OF (33)

Substitute (15) into (10) to obtain

\[
W^{l+i} = Y(H^{l+i})^T Q^{l+i},
\]

(53)

into which substitute (29) and (31) to obtain \( W^{l+i} = Y(H^T)^T \begin{bmatrix} \bar{Q}^T \\ T^T \end{bmatrix} G \), i.e.,

\[
W^{l+i} = \begin{bmatrix} Y(H^T)^T \bar{Q}^T + Y(H^T)^T T^T \end{bmatrix} \begin{bmatrix} Y(H^T)^T T^T \end{bmatrix} G \end{bmatrix}.
\]

(54)

Substitute (32b) into the first entry in the right side of (54) to write it as

\[
Y(H^T)^T \bar{Q}^T - Y(H^T)^T Q^T P T^T + Y(H^T)^T T^T,
\]

(55)

and substitute (32b) into the second entry in the right side of (54) to write it as

\[
Y(H^T)^T G - Y(H^T)^T Q^T P G.
\]

(56)

Substitute (33) into (55) and (56) to write them as

\[
W^l + \begin{bmatrix} Y(H^T)^T - W^l P \end{bmatrix} T^T
\]

(57)

and

\[
\begin{bmatrix} Y(H^T)^T - W^l P \end{bmatrix} G,
\]

(58)

respectively. Then the first and second entries in the right side of (54) can be replaced with (57) and (58), respectively, to obtain (33).
APPENDIX C
DERIVATION OF (55) AND (36)
Substitute (34a), (34b) and (31) into (23) to obtain
\[
\begin{bmatrix}
L_f^T U & D_f^T & 0 & L_f^T U \\
0^T & 0^T & S & 0^T \\
\end{bmatrix} \begin{bmatrix}
D_f^T & 0 \\
0^T & V \\
\end{bmatrix} = \begin{bmatrix}
Q_f^T & T \\
T^T & G \\
\end{bmatrix}, \text{ i.e.,}
\]
\[
\begin{bmatrix}
(L_f^T (L_f^T)^T + USV^T)USV^T \\
(USV^T)^T \\
VSV^T \\
\end{bmatrix} = \begin{bmatrix}
Q_f^T & T \\
T^T & G \\
\end{bmatrix}. \tag{59}
\]
From (59) we can obtain
\[
\begin{cases}
VSV^T = G \\
USV^T = T.
\end{cases} \tag{60a} \tag{60b}
\]
We can substitute (32a) into (60a) to deduce (35b). On the other hand, we can substitute (32b) into (60b) to obtain \(USV^T = -Q^TPG\), into which we substitute (60a) to obtain \(USV^T = -Q^PVSV^T\), i.e., \(U = -Q^PV\), into which we can substitute (23) to obtain (35a).
Moreover, to deduce (36), we only need to substitute (60a) and (60b) into (33).

APPENDIX D
THE DERIVATION OF THE WIDE-SENSE GIVENS ROTATION
In this section we derive the wide-sense Givens rotation \(\Psi_k^{j,j+1}\) that is computed by (28) and (47). Let \(D_k^2\) denote a diagonal matrix of real valued weights \(\sqrt{d_j} = d_k^2\). Then we can represent (23) as
\[
\tilde{Q}_k = L_k D_k^2 \tilde{d}_k^2 \tilde{L}_k. \tag{61}
\]
Denote the \(i^{th}\) column of \(L_k\) as \(l_i\), and define
\[
\tilde{L}_k = L_k D_k^2 = \begin{bmatrix}
1 \sqrt{d_1} & 1 \sqrt{d_2} & \cdots & 1 \sqrt{d_k} \\
\end{bmatrix}. \tag{62}
\]
Then substitute (62) into (61) to obtain \(\tilde{Q}_k = \tilde{L}_k \tilde{L}_k^H\), from which we can deduce
\[
\tilde{Q}_k = \tilde{L}_k \tilde{L}_k^H = \tilde{L}_k \Omega \left(\tilde{L}_k \Omega\right)^H, \tag{63}
\]
where \(\Omega\) can be any unitary transformation, e.g., a Givens rotation.
Let \(\tilde{l}_k^j\) denotes the \(i^{th}\) entry in the last \(k^{th}\) row of \(\tilde{L}_k\). Then let \(\Omega_k^{j,j+1}\) denote a Givens rotation that rotates \(\begin{bmatrix}
\tilde{l}_k^j \\
\tilde{l}_k^{j+1} \\
\end{bmatrix}\) (in the last row of \(\tilde{L}_k\)) into \(\begin{bmatrix}
0 \\
\tilde{l}_k^j \\
\end{bmatrix}\). We can employ the efficient Givens rotation (13). Then \(\Omega_k^{j,j+1}\) is equal to \(L_k\) except the 2 \times 2 sub-block in the \(j^{th}\) and \((j+1)^{th}\) rows and columns, which is (13)
\[
\frac{1}{\sqrt{d_j}} \begin{bmatrix}
1 & \tilde{l}_k^{j+1} \\
\tilde{l}_k^j & \sqrt{d_j} \end{bmatrix} \left[ \begin{bmatrix}
\tilde{l}_k^{j+1} \\
\tilde{l}_k^j \\
\end{bmatrix} \right]. \tag{64}
\]
We can obtain \(\tilde{l}_k^j = l_k^j \sqrt{d_k}\) from (62), which is substituted into (64) to get
\[
\frac{1}{\sqrt{d_j}} \begin{bmatrix}
\tilde{l}_k^{j+1} & \sqrt{d_j} \tilde{l}_k^{j+1} \\
-\sqrt{d_j} \tilde{l}_k^{j+1} & \tilde{l}_k^j \\
\end{bmatrix} \begin{bmatrix}
\tilde{l}_k^{j+1} \\
\tilde{l}_k^j \\
\end{bmatrix}. \tag{65}
\]
where
\[
\tilde{\rho} = \left|\frac{l_k^{j+1}}{d_k^j}\right| \left|\sqrt{d_j+1} + \frac{l_k^{j+1}}{d_k^j} \right| d_j+1 + \frac{l_k^j}{d_k^j} d_j. \tag{66}
\]
Now we have got \(\Omega_k^{j,j+1}\). From (62), we can obtain
\[
\tilde{L}_k \Omega_k^{j,j+1} = L_k D_k^2 \Omega_k^{j,j+1}. \tag{67}
\]
It can be seen from (65) that \(D_k^2 \Omega_k^{j,j+1}\) in (67) is equal to \(D_k^2\) except the 2 \times 2 sub-block in the \(j^{th}\) and \((j+1)^{th}\) rows and columns, which is
\[
\frac{1}{\tilde{\rho}} \begin{bmatrix}
\tilde{l}_k^{j+1} & \sqrt{d_j+1} & \sqrt{d_j} \tilde{l}_k^{j+1} & d_j+1 \\
-\sqrt{d_j} \tilde{l}_k^{j+1} & \tilde{l}_k^j & \tilde{l}_k^{j+1} & d_j+1 \\
\end{bmatrix}, \tag{68}
\]
Decompose (68) into
\[
\frac{1}{\tilde{\rho}} \begin{bmatrix}
\tilde{l}_k^{j+1} & \sqrt{d_j+1} & \sqrt{d_j} \tilde{l}_k^{j+1} & d_j+1 \\
-\sqrt{d_j} \tilde{l}_k^{j+1} & \tilde{l}_k^j & \tilde{l}_k^{j+1} & d_j+1 \\
\end{bmatrix} \times \begin{bmatrix}
\tilde{d}_k^j & 0 \\
0 & \tilde{d}_j+1 \\
\end{bmatrix}, \tag{69}
\]
i.e.,
\[
\frac{1}{\tilde{\rho}} \begin{bmatrix}
\tilde{l}_k^{j+1} & \sqrt{d_j+1} & \sqrt{d_j} \tilde{l}_k^{j+1} & d_j+1 \\
-\sqrt{d_j} \tilde{l}_k^{j+1} & \tilde{l}_k^j & \tilde{l}_k^{j+1} & d_j+1 \\
\end{bmatrix} \times \begin{bmatrix}
\tilde{d}_k^j & 0 \\
0 & \tilde{d}_j+1 \\
\end{bmatrix}, \tag{70}
\]
where
\[
\rho = \tilde{\rho} \tilde{d}_k^j. \tag{71}
\]
We can write (70) as
\[
\frac{1}{\rho} \begin{bmatrix}
\tilde{l}_k^{j+1} & \sqrt{d_j+1} & \sqrt{d_j} \tilde{l}_k^{j+1} & d_j+1 \\
-\sqrt{d_j} \tilde{l}_k^{j+1} & \tilde{l}_k^j & \tilde{l}_k^{j+1} & d_j+1 \\
\end{bmatrix} \begin{bmatrix}
\tilde{d}_k^j & 0 \\
0 & \tilde{d}_j+1 \\
\end{bmatrix}, \tag{72}
\]
from which we can deduce (47). Moreover, we can substitute (66) into (71) to obtain \(\rho = \frac{\tilde{l}_k^j}{d_k^j} \sqrt{d_j+1} + \frac{l_k^{j+1}}{d_j} d_j\), i.e., (48).

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