Direct Inversion Formula of the Multi-coil MR Operator under Arbitrary Trajectories

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Abstract. This study introduces a novel inversion formula for the multi-coil MRI forward operator applicable to arbitrary sampling trajectories. Traditional MRI reconstruction leverages fast Fourier transforms (FFTs) for Cartesian sampling and nonuniform FFTs for non-Cartesian patterns. However, subsampled k-space reconstruction typically relies on iterative least-squares (LS) solutions, which are computationally intensive due to the complex structure introduced by multiple coil sensitivities. We hypothesize that the MRI multi-coil forward operator exhibits the low displacement rank (LDR) property, enabling an efficient inversion using triangular Toeplitz operators with a computational complexity of $\mathcal{O}(\alpha N \log^2 N)$, with α being a small integer. The hypothesis is supported through numerical simulations. For demonstration of the feasibility of such inversion formula, we propose a learning-based approach to determine the necessary LDR parameters, demonstrating successful forward and inverse operator representations across various sampling patterns, including Cartesian and radial trajectories. The proposed inversion formula offers a significant acceleration in MR reconstruction, reducing computational complexity by a factor of approximately 26 compared to conventional conjugate gradient methods. The proposed inversion formula will greatly enhance reconstruction speed and simplify reconstruction pipelines, including iterative reconstructions and deep learning solutions incorporating data-consistency layers. Future work will focus on deriving the LDR parameters analytically to further streamline the inversion process. The code is available at https://github.com/mikecjz/structured-nets.

Keywords: Inverse Problem · Displacement Rank · Toeplitz Inversion · Compressed Sensing

1 Introduction

The reconstruction of MRI image from fully sampled k-space is straightforward with fast Fourier transforms (FFTs) for Cartesian sampling patterns and regridding with density-compensated nonuniform fast Fourier transforms (NUFFTs) for non-Cartesian sampling patterns. The reconstruction of subsampled k-space, however, requires more advanced algorithm design. Most of the image reconstruction techniques have a common element: data consistency constraints posed as SENSE-style [20] regularized least-squares (LS) subproblems entailing computationally expensive matrix inversions of the forward operator. Under single-coil settings, the forward operator is circulant given Cartesian sampling trajectories [13] and is Toeplitz [2,6,29] given non-Cartesian sampling trajectories. Simple formulas exist for inversion of the forward operator under single-coil settings for Cartesian and non-Cartesian trajectories [7,9]. However, there are generally no practical avenues for direct inversion of multi-coil forward operators because multiple coil sensitivities introduce channelwise shift variance, complicating the originally well-structured single-coil forward operator. Therefore, solving these LS problems often rely on gradient-based iterative algorithms [3,8,24] and is often the most time-consuming step in MR reconstruction. In deep learning applications, the LS solution is often approximated by conjugate gradient (CG) steps [1,32], potentially complicating network gradient back propagation.

To accelerate the reconstruction, many studies consider preconditioning [5,13,14,19,22,25,27,30,31], a technique to improve the condition number on the forward operator, and thus convergence can be achieved in fewer steps. We note that with preconditioning, the number of evaluations of the forward operator is reduced, but to a number larger than one. Additionally, most preconditioning techniques increase computation at each iteration step and at the end of the iteration, the inverse of the preconditioner needs to be evaluated. Direct solution to the LS problem has been explored with hierarchically semi-separable solvers [4] demonstrated in $\mathcal{O}(N)$ time complexity. However, the implementation of such algorithm remains non-trivial.

In this study we aim to validate an inversion formula for the multi-coil MR forward operator given a hypothesis that the multi-coil forward operator is not strictly Toeplitz, but "Toeplitz-like". Specifically, we hypothesize the operator in question has a modified Toeplitz structure, possessing low displacement rank (LDR) properties [11], which enables an easy formula for inversion involving only triangular Toeplitz operators with an overall complexity of $\mathcal{O}(\alpha N \log^2 N)$, with α being a small integer. In this study we will provide rationale and introduce empirical evidence to support this hypothesis. We will also demonstrate that the inversion formula for the multi-coil operator achieves good inversion results and that evaluation of the inversion formula can be done in roughly the same floating point operations (FLOPS) as one evaluation of the forward operator. Such inversion formula will dramatically accelerate solving the LS problem in MR reconstruction compared to iterative methods and will also serve as an alternative to the more complicated CG-based data consistency layer embedded in any end-to-end MR reconstruction network for arbitrary trajectories.

2 Theory

2.1 MR multi-coil forward operator

Consider the SENSE [20,21]-style LS reconstruction problem and its equivalent normal equation:

$$\hat{x} = \arg\min_{x} \|Ax - b\|_2^2 \Rightarrow \hat{x} = \left(A^H A\right)^{-1} A^H b \tag{1}$$

where $x \in \mathbb{C}^N$ is the image to be reconstructed, and b being the multi-channel k-space signal. $A = \Lambda \mathcal{F} S$ with the diagonal matrix Λ being the subsampling mask, $\mathcal{F}$ being the Fourier operator (either uniform or non-uniform), and S being the sensitivity maps. Note that $A^H A = S^H \mathcal{F}^H \Lambda^H \Lambda \mathcal{F} S$ and that $\mathcal{F}^H \Lambda^H \Lambda \mathcal{F}$ is Toeplitz under arbitrary sampling trajectories (Circulant if trajectory is Cartesian) [2,6,13,29]. The invertibility of $A^H A$ can be improved with regularization. For example, consider the ℓ_1- norm regularized compressed sensing [15,16,18,33] objective incorporating SENSE-style parallel imaging:

$$\arg\min_{x} \frac{1}{2}\|Ax - b\|_2^2 + \lambda \|\Psi x\|_1 \tag{2}$$

where Ψ is a sparsifying transform (e.g. wavelet or total variation(TV)). Many optimization techniques can be used to solve expression 2 including alternating directional method of multipliers (ADMM) [3] or split Bregman (SB) [8] iterations. Using ADMM as an example, the iterative steps are the following:

$$x^{k+1} := (A^H A + \rho \Psi^H \Psi)^{-1} (A^H b + \rho \Psi^H (z^k - u^k)) \tag{3}$$

$$z^{k+1} := S_{\lambda/\rho}(\Psi x^{k+1} + u^k) \tag{4}$$

$$u^{k+1} := u^k + \Psi x^{k+1} - z^{k+1} \tag{5}$$

where $S_{\lambda/\rho}$ is the soft-thresholding operator with threshold λ/ρ. The most time-consuming operation is evaluating $(A^H A + \rho \Psi^H \Psi)^{-1}$, and is often solved with CG. Note that $\Psi^H \Psi$ is simply the identity if Ψ is wavelet transform or tridiagonal Toeplitz if Ψ is TV.

In this paper, we define $A^H A$, or its regularized variant (e.g. $A^H A + \rho \Psi^H \Psi$), as the MR multi-coil forward operator.

2.2 Displacement rank

Let Z be the lower shift matrix:

$$Z = \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & 0 & 0 \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \tag{6}$$

with ones only along the subdiagonal. Define the displacement operator with respect to Z :

$$\nabla_Z X = X - ZXZ^H = R \tag{7}$$

it can be shown that any Hermitian Toeplitz matrix T will have a rank-2 residual after the displacement operator.

$$\nabla_Z T = \begin{bmatrix} t_1 & t_2 & t_3 & \cdots & t_N \\ t_1^H & t_1 & t_2 & \cdots & t_{N-1} \\ t_2^H & t_1^H & t_1 & \cdots & t_{N-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_N^H & t_{N-1}^H & t_{N-2}^H & \cdots & t_1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & t_1 & t_2 & \cdots & t_{N-1} \\ 0 & t_1^H & t_1 & \cdots & t_{N-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & t_{N-1}^H & t_{N-2}^H & \cdots & t_1 \end{bmatrix} = \begin{bmatrix} t_1 & t_2 & t_3 & \cdots & t_N \\ t_1^H & 0 & 0 & \cdots & 0 \\ t_2^H & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_N^H & 0 & 0 & \cdots & 0 \end{bmatrix} \tag{8}$$

Then, Toeplitz matrices are said to have displacement rank of 2. Following this property, a matrix $\tilde{T}$ is defined to be Toeplitz-like if it has low displacement rank (LDR) $\alpha \ll N$.

2.3 Inversion of LDR matrices

Kailath et al. [10,11] showed that if a matrix $\tilde{T}$ has a displacement rank α, its inverse $\tilde{T}^{-1}$ also has the same displacement rank α. Furthermore, both $\tilde{T}$ and $\tilde{T}^{-1}$ can be calculated by sum of products of Toeplitz matrices. Using $\tilde{T}^{-1}$ as an example:

$$\widetilde{T}^{-1} = \sum_{i=1}^{\alpha} L\left(g_i\right) L^H\left(h_i\right) \tag{9}$$

where $L(v)$ denotes a lower triangular Toeplitz matrix whose first column is v and that

$$\nabla_Z \widetilde{T}^{-1} = GH^H \tag{10}$$

given $G \in \mathbb{C}^{N\times\alpha}$ and $H \in \mathbb{C}^{N\times\alpha}$ are a set of vectors $G = [g_1, g_2, \ldots, g_\alpha]$, $H = [h_1, h_2, \ldots, h_\alpha]$. The complexity to evaluate $\widetilde{T}^{-1}$ is therefore $\mathcal{O}\left(\alpha N \log^2 N\right)$.

2.4 LDR hypothesis of the MR multi-coil forward operator

Hypothesis 1 *The multi-coil MR operator in the form of*

$$A^H A = \sum_{i=i}^{N_{coil}} S_i^H T S_i$$

with T being a Toeplitz matrix, is Toeplitz-like and has low displacement rank $\alpha \ll N$ with respect to Z and therefore has an inversion formula with complexity $\mathcal{O}\left(\alpha N \log^2 N\right)$. It then easily follows that $\sum_{i=i}^{N_{coil}} S_i^H T S_i + \rho \Psi^H \Psi$ also has low displacement rank $\widehat{\alpha} \approx \alpha$.

In the following sections, we will use numerical simulations and experiments to demonstrate that Hypothesis 1 might be true.

3 Methods

First, following from section 2.3, it is sufficient to demonstrate the forward operator $A^H A$ has low-displacement rank as we know its analytical expression. For this task, we use numerical simulation to show this is true. The simulation is based on the fully sampled 2D multi-coil kspace data from the fastMRI dataset [12]. The k-space data is trimmed to the center 128×128 for ease of calculation. A set of coil sensitivity maps are estimated using the center 24×24 k-space with ESPIRiT [28] without any eigenvalue thresholding to ensure $\sum_{i=1}^{N_{coil}} S_i^H S = I$. Without loss of generality, a 1D line from the center of coil sensitivity maps is used to simulate $4\times$ Cartesian undersampling in 1D. We then analyze $\nabla_Z A^H A$ with singular value decomposition (SVD).

Second, assume $A^H A$ and $\left(A^H A\right)^{-1}$ has low displacement rank with respect to Z, then the residual result of the displacement operation ∇_Z, in the form of outer products GH^H is unknown. Knowing $G,\ H$ is necessary to evaluate $A^H A$ or $\left(A^H A\right)^{-1}$. Therefore, we propose to treat $G,\ H$ as parameters that can be learned from simulated data. For this task, we first reconstruct a fully sampled 2D image $x \in \mathbb{C}^{128\times 128}$ from the 128×128 k-space via inverse FFTs and coil combination. Then we simulate three types of sampling pattern; 1) a $2\times$ Cartesian undersampling pattern, 2) a $4\times$ Cartesian undersampling pattern, 3) a non-Cartesian 280-spoke radial sampling data with golden-angle ordering. The output of the forward operator is then simply denoted as $A^H Ax$. Then we initiate $G,\ H$, with a fixed rank α randomly and build the $\sum_{i=1}^{\alpha} L\left(g_i\right) L^H\left(h_i\right)$ operation using padded FFTs as a single network layer in PyTorch and learn $G,\ H$ via standard gradient back propagation. Switching between x and $A^H Ax$ as inputs and outputs, we can train $\sum_{i=1}^{\alpha} L\left(g_i\right) L^H\left(h_i\right)$ to represent both the forward and the inverse process per section 2.3. The PyTorch implementation is built upon the infrastructure provided by Thomas et al. [26].

Training was done on a Linux server with 96 core intel Xeon CPUs, Nvidia GeForce 3090 (24GB) and 256GB RAM. Learning rate is 3×10^{-5}, optimizer is AMSGrad [23] with momentum 0.9. Only one image slice is sufficient for this learning process.

4 Results

Figure 1 demonstrates the absolute value of the singular value spectrum of $\nabla_Z A^H A$ simulated with $4\times$ 1D Cartesian undersampling with coil sensitivities. The displacement rank of the multi-coil forward operator can be clearly seen as $\alpha = 6$, which we will use for all trainings going forward. Figure 2 demonstrate the learned inverse operator output. Figure 3 demonstrate the comparison between the learned inverse LDR format operators and 20 CG iterations without preconditioning and starting with 0, and their difference compared to the

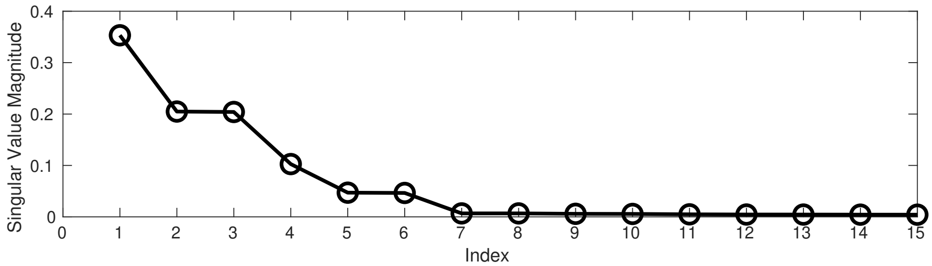

Fig. 1. The singular values spectrum (first 15) of the displacement operator output of the multi-coil operator, i.e. $\nabla_Z A^H A$ simulated with $4\times$ 1D Cartesian undersampling with coil sensitivities.

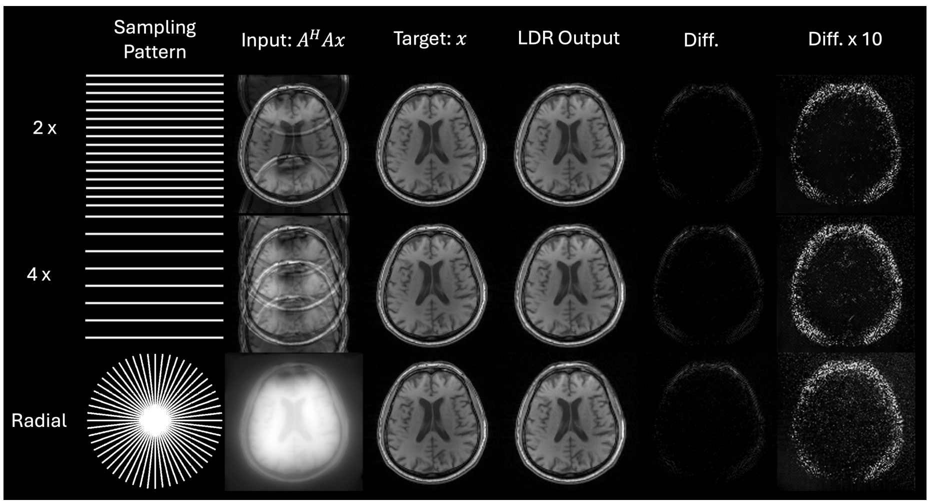

Fig. 2. Learned LDR forward operator output under different sampling patterns and the difference to the target.

ground truth. For all trajectories, each epoch is found to take 6 - 7 ms. It took 4k epochs for the Cartesian undersampling cases to converge and 24k epochs for the non-Cartesian case to converge.

5 Discussion

In this work, demonstrate a new formula to invert the multi-coil MR forward operator. We utilize the established theory that operators with underlying Toeplitz structure, in the form of low displacement rank with respect to the lower shift matrix Z (defined in expression 6), has an inversion formula involving only sum of products of triangular Toeplitz matrices, which can be implemented with FFTs with $\mathcal{O}\left(\alpha N \log^2 N\right)$ complexity. We provide some empirical evidence that

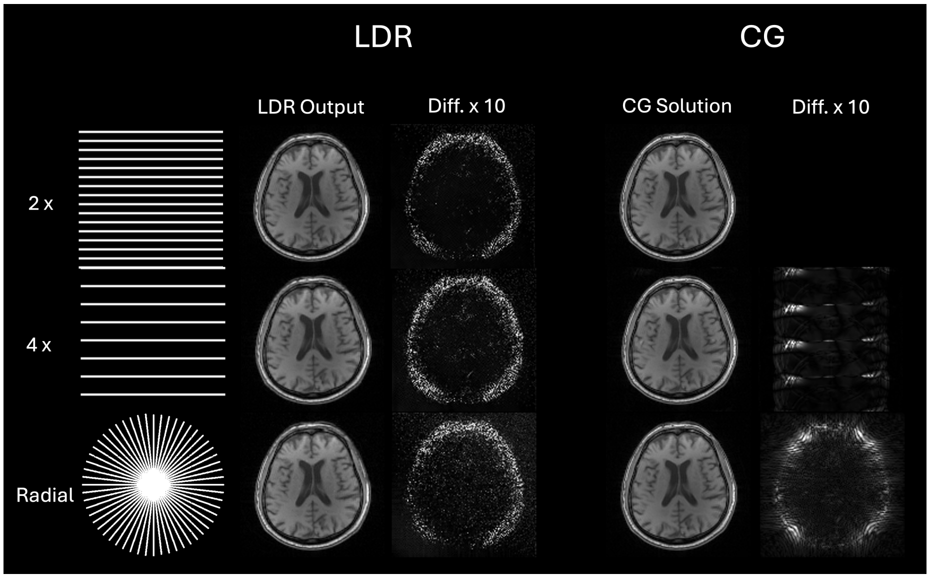

Fig. 3. Comparison between the learned inverse LDR format operators output under different trajectories and 20 CG iterations without preconditioning and starting with 0, and their difference compared to the ground truth.

the MR multi-coil operator does at least approximately possess the low displacement rank property. Then we proceed to showcase the feasibility of this inversion formula. The inversion formula requires the low-rank parameters be known prior to evaluation. In the case of the multi-coil forward operator, these parameters for its inverse are not currently found to be immediately derivable. To get around of this limitation, we propose to learn these parameters from numerical simulations and with the gradient back propagation provided by PyTorch. The learning process appears to be successful; it can be seen in the results that the LDR operators are successfully learned to perform the inverse operations. The error seems to accumulate around the boundary between brain and air. We hypothesize that this is because the sharp transition in the boundary region is making the learning process more difficult.

The convergence of the learned operators for Cartesian sampling trajectories appears to be quicker than the non-Cartesian radial sampling pattern. We again hypothesize that it is because both the forward and inverse operator of the radial sampling pattern has a higher condition number, leading to slow convergence, a phenomenon well documented in classic iterative algorithms. We note that the learning process is only intended for the demonstration of the inversion formula's feasibility. For practical use, the LDR parameters need to be derived efficiently either analytically or through a greatly accelerated learning process, which we consider to be outside the scope of this study.

This inversion formula will have several potential impacts to the field of MR reconstruction. First there is a direct acceleration benefit to the reconstruction speed. For example, an inversion of the forward operator under non-Cartesian trajectory using, for example, 20 CG steps and $N_{coil} = 16$ coils, will have the computation complexity $\mathcal{O}\left(20 \times 16 \times N\log^2 N\right)$, whereas the proposed inversion formula will have complexity $\mathcal{O}\left(2 \times \alpha \times N\log^2 N\right)$. With $\alpha = 6$ in our demonstrated case, there is an acceleration factor of 26.

Second, the easy inversion formula will help reduce implementation difficulty of end-to-end MR reconstruction network involving ℓ_2- norm data consistency layers for both the Cartesian and non-Cartesian trajectories. Previously, the solution to the data consistency layers involves hand-building CG iterations [1] and using backward gradient-enabled NUFFT packages [17] for non-Cartesian trajectories. Our proposed formula on the other hand, is a direct, lightweight linear operation that will only require FFTs, which is a standard built-in function in both TensorFlow and PyTorch.

6 Conclusion

We have showcased an easy formula for the MR multi-coil forward operator and its inversion under arbitrary sampling trajectories. Building on the theories of low displacement rank and whose parameter can be learned from simulated data, such formula will significantly speed up MR iterative reconstruction and potentially provide a lightweight and direct solution for deep learning MR reconstruction learned end-to-end with data consistency layers. The learning process of the LDR operator is only for demonstration of feasibility. The practical solution to quickly derive the necessary parameters will be investigated in future studies.

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