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Mean square optimal NUFFT approximation for efficient non-Cartesian MRI reconstruction

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Abstract

The fast evaluation of the discrete Fourier transform of an image at non-uniform sampling locations is key to efficient iterative non-Cartesian MRI reconstruction algorithms. Current non-uniform fast Fourier transform (NUFFT) approximations rely on the interpolation of oversampled uniform Fourier samples. The main challenge is high memory demand due to oversampling, especially when multi-dimensional datasets are involved. The main focus of this work is to design an NUFFT algorithm with minimal memory demands. Specifically, we introduce an analytical expression for the expected mean square error in the NUFFT approximation based on our earlier work. We then introduce an iterative algorithm to design the interpolator and scale factors. Experimental comparisons show that the proposed optimized NUFFT scheme provides considerably lower approximation errors than our previous scheme that rely on worst case error metrics. The improved approximations are also seen to considerably reduce the errors and artifacts in non-Cartesian MRI reconstruction.

Keywords

interpolators; non-uniform fast Fourier transform; histogram; non-Cartesian MRI

1. Introduction

Non-Cartesian MRI schemes (e.g., spiral and radial trajectories) offer several advantages over Cartesian sampling, including higher speed, robustness to undersampling, and low motion sensitivity. While gridding is the most popular reconstruction method [1], iterative algorithms are being increasingly used due to their improved accuracy, ability to handle image priors, and account for non-idealities during acquisition [2, 3, 4, 5]. Since the exact evaluation of the discrete time Fourier transform of the Fourier sum is computationally prohibitive, these algorithms approximate the non-Cartesian Fourier transform. While approximation schemes for specific trajectories are available [6, 7], the common approach is to compute the non-uniform samples as the interpolation of the uniform Fourier transform. The uniform Fourier samples are computed efficiently using the fast Fourier transform, while support limited functions (e.g., Kaiser–Bessel, Gaussian) are used for interpolation [8, 2, 9, 1, 10, 11]. This approximation is often termed as the non-uniform fast Fourier

transform (NUFFT). NUFFT schemes often weight the signal with suitable scale factors before evaluating the uniform FFT to minimize the approximation error [12, 13, 14, 15].

Classical choices of interpolator and scale factors (e.g., Gaussian interpolator and cosine scale factors) require the Fourier transform to be evaluated on a fine uniform grid to keep the approximation error reasonably low [12, 13, 15]. The common choice is to compute the Fourier transform on a $K \times K$; $K = 2N$ uniform grid for an $N \times N$ image. Unfortunately, the oversampling of the Fourier grid significantly increases the memory demands of the algorithm. For example, the reconstruction of a three dimensional dataset with $K = 2N$ requires eight times more memory than the original dataset. This often makes it difficult to accelerate such algorithms using graphical processing units (GPUs) that have limited on-board memory, especially when large datasets are involved [16]. Several researchers have developed design strategies to improve the approximation properties of the NUFFT scheme [14, 17, 18, 19, 20, 13]. These schemes rely on analytical expressions for point-wise errors in the Fourier domain. The main challenge with these expressions is the difficulty in decoupling the effects of the interpolator and the scale factors. Hence, the above schemes derive the optimal interpolator, assuming the scale factors to be fixed [17] or have simple parametric expressions [14]. Since the constraints on the scale factors were too restrictive, the performance of the optimized NUFFT schemes were only comparable to the one using Kaiser-Bessel (KB) functions [14]. The NUFFT scheme was reinterpreted as a shift invariant approximation of the discrete Fourier transform (DTFT) in [21]. A worst case error metric, which was independent of the scale factors and the signal, was introduced in [21]. The optimization of this metric yielded an NUFFT scheme that provided considerably lower worst case errors than the conventional NUFFT scheme [21].

We studied the utility of the optimized interpolators [14, 21] in MR image reconstruction problems. Unfortunately, we observed that in the $K \approx N$ regime, the approximation properties of the optimized NUFFT schemes were not considerably better than that of classical methods for many images, even though the optimized NUFFT schemes yielded far lower error bounds. The main reason for this discrepancy is the use of the worst case error metrics [14, 21]. Specifically, these upper bounds for the approximation error are unrealistically high and are not achieved for practical signals. For example, the image which provides the worst case error in [21, 22] has most of its energy concentrated along the image edges/borders. Since MR brain images are often support limited to a disc region within the rectangular support, the worst case error is never achieved for such MR signals. In this context, it is desirable to derive the mean square optimal NUFFT schemes from error metrics that are more representative of real-world signals.

The main objective of this paper is to improve the framework in [21, 22] in the context of MR imaging applications and to demonstrate its utility in non-Cartesian MRI reconstruction. Specifically, we depart from the worst case setting considered in [21] and focus on a mean-square error metric. This error metric is dependent on the expected spatial energy distribution of the signal. Hence, it can be customized to real world applications (e.g., when the image is support limited to specific regions). The error metric decouples the effect of the scale factors and the interpolators into two positive terms. This enables us to derive the mean square optimal scale factors; the use of these scale factors corresponds to the

projection of the DTFT of the signal to the space spanned by the integer shifts of the interpolator [21]. We adapt the iterative reweighted algorithm introduced in [21] to derive the mean square optimal interpolator and scale factors. When the spatial energy distribution of the class of signals is known *a priori* (e.g., learned from exemplar images), it will be used to derive the interpolator. Empirically, we observe that the NUFFT scheme that is derived with the assumption of uniform energy distribution is comparable to the one using known energy distribution for many practical signals; the assumption of uniform energy distribution is a better alternative than using the worst case scenario when the energy distribution is unknown.

We validate the proposed mean square optimal NUFFT scheme using simulations and experimental MRI data. Our experiments show that the proposed scheme is capable of providing good approximations of the non-uniform DTFT for modest oversampling factors ($K < 1.1 \times N$) and short interpolators ($J \leq 6$). The image reconstruction experiments show that the proposed scheme provides more accurate reconstructions than classical NUFFT schemes, when low oversampling factors are considered. The low oversampling factor will in turn translate to memory efficient algorithms which will enable its implementation on faster devices such as GPUs that have limited onboard memory. While the reduction in memory demand may come in with a slight increase in computational complexity compared to $K = 2N$, the speedups offered by faster parallel computing devices are expected to more than make up for the performance.

2. Methods

2.1. NUFFT approximation: Background

The NUFFT scheme approximates the discrete Fourier transform (DTFT) of the uniform support limited signal $x[n]$; $n = -N/2, \dots, N/2 - 1$:

$$\hat{x}(\nu) = \sum_{n=-N/2}^{N/2-1} x[n] e^{-\frac{j2\pi n\nu}{N}} \quad (1)$$

at non-uniform k-space locations ν_m ; $m = 0, \dots, M - 1$. The exact evaluation of the discrete time Fourier transform of this sum is computationally expensive. In their seminal work [12], Dutt and Rokhlin have shown that an exponential with arbitrary frequency ν can be efficiently approximated as:

$$e^{-\frac{j2\pi n\nu}{N}} \approx \underbrace{\exp(b|n|^2)}_{h[n]} \sum_{k=\nu/T-J/2}^{k=\nu/T+J/2} \varphi\left(\frac{\nu}{T} - k\right) e^{-\frac{j2\pi kT}{N}}. \quad (2)$$

Here, φ is the Gaussian interpolation function and $T = N/K < 1$, where K is an appropriately chosen integer. In [23], the authors extended the above approximation using alternate interpolation functions and associated weighting functions. The NUFFT scheme is obtained by substituting the approximation specified by (2) into (1). Thus, the NUFFT approximation involves two key steps. The K -point FFT ($K > N$) of the sequence $h[n]x[n]$ is first computed as

$$c[k] = \sum_{n=-N/2}^{N/2-1} h[n] x[n] e^{-\frac{j2\pi kn}{K}}, \quad (3)$$

where $h[n]$; $n = -N/2, \dots, N/2 - 1$ are scale factors¹. Once the coefficients $c[k]$ are available, the NUFFT approximation of the DTFT is obtained as:

$$\hat{x}_{\text{app}}(\nu) = \sum_{k=-K/2}^{K/2-1} c[k] \varphi_p\left(\frac{\nu}{T} - kT\right), \quad (4)$$

where $T = N/K$ is the sampling step and $\varphi_p(x) = \sum_{k \in \mathbb{Z}} \varphi(x - kN)$ is the K -periodized version of φ .

2.2. Current NUFFT design strategies

The error in the NUFFT approximation of a signal $x[n]$ at a specific frequency point ν is specified by

$$\underbrace{\hat{x}(\nu) - \hat{x}_{\text{app}}(\nu)}_{\epsilon(\nu)} = \left\langle x[n], \underbrace{e^{-\frac{j2\pi n\nu}{N}} - h[n] \sum_{k=-K/2}^{K/2-1} \varphi\left(\frac{\nu}{T} - k\right) e^{-\frac{j2\pi nk}{K}}}_{q_\nu[n]} \right\rangle \quad (5)$$

Several researchers have derived the upper-bound of the approximation error based on this expression [15, 20, 14]:

$$\|\epsilon(\nu)\| \leq \|x\|_{\ell_2} \cdot \|q_\nu\|_{\ell_2} \quad (6)$$

and used it to derive the optimal interpolator. For example, the Nguyen *et al.*, and Nieslony *et al.*, proposed to determine the interpolator φ by minimizing $\|q_\nu\|_2$, assuming pre-selected scale factors (e.g., Gaussian, Kaiser-Bessel, Cosine) [15, 20]. Since this is a quadratic optimization problem, the optimal interpolator is solved analytically. However, the assumption of fixed scale factors makes it difficult for the scheme to exploit the full flexibility to lower the approximation error. This approach is similar to [14], where they additionally used a min-max scheme to also search for the scale factors. However, since their search was restricted to small parametric families, this approach could not exploit the full potential of the NUFFT approximation.

All of the above NUFFT design schemes evaluated the point-wise error in the Fourier domain $\epsilon(\nu)$. Duijndam *et al.*, focussed on numerically optimizing the INUFFT approximation scheme in [24]. They assume the signal in the Fourier domain to be modeled as a linear combination of Diracs at the non-uniform sampling locations:

¹In the Gaussian case, the scale factors are specified by $\exp(b|n|^2)$.

$$\hat{x}(\nu) = \sum_i d_i \delta(\nu - \nu_i),$$

and derive the expression for the error in the spatial domain as

$$\|x[n] - x_{\text{INUFFT}}[n]\|^2 = \|x[n]\|^2 D\left(\frac{2\pi n}{K}\right). \quad (7)$$

Here,

$$D(\nu) = \sum_{l \neq 0} \frac{|\hat{\varphi}(\nu + lK)|^2}{|\hat{\varphi}(\nu)|^2}. \quad (8)$$

Here, they assumed the scale factors to be chosen as $h[n] = 1/\hat{\varphi}(2\pi n/K)$. They proposed a numerical algorithm to determine the mean square optimal INUFFT interpolator that minimizes the mean square error $\sum_n \|x[n] - x_{\text{INUFFT}}[n]\|^2$. Although this INUFFT design scheme has conceptual similarities with the proposed schemes, it cannot be directly applied to our NUFFT setting. Besides, their error expression is very different from the proposed scheme since they assume a specific signal model and scale factors.

2.3. Mean square error metric in NUFFT approximation

We have shown that the NUFFT scheme is the shift invariant approximation of $\hat{x}(\nu)$ in the periodic shift invariant space V_{φ} , spanned by the function φ [21]. Specifically, the coefficients can be seen as the inner-products between the exact DTFT of $x[n]$ and shifted versions of the analysis function:

$$c[k] = \left\langle \hat{x}(\nu), \tilde{\varphi}_p^*\left(\frac{\nu}{T} - k\right) \right\rangle_{L_2[-\pi, \pi]}.$$

The analysis function is the DTFT of the scale factors $\tilde{\varphi}_p(\nu) = \sum_{n=-N/2}^{N/2-1} h[n] e^{-j\frac{2\pi\nu}{K}}$. The re-interpretation of the NUFFT scheme as a shift invariant representation enables us to use the theoretical tools developed for periodic shift invariant representations to analyze and optimize the NUFFT scheme.

We have derived an expression for the error in the NUFFT approximation as [25, 21]:

$$\eta(x, \varphi, \tilde{\varphi}, K) = \sum_{n=-N/2}^{N/2-1} |x[n]|^2 E_{\varphi, \tilde{\varphi}}\left(\frac{2\pi n}{K}\right), \quad (9)$$

where the error kernel $E_{\varphi, \tilde{\varphi}}(\omega)$ is given by

$$E_{\varphi, \tilde{\varphi}}(-\omega) = \underbrace{1 - \frac{|\hat{\varphi}(\omega)|^2}{\hat{a}_{\varphi}(\omega)}}_{E_{\min, \varphi}} + \underbrace{\hat{a}_{\varphi}(\omega) \left| \hat{\varphi}(\omega) - \hat{\varphi}_d(\omega) \right|^2}_{E_{\text{res}, \varphi, \tilde{\varphi}}}. \quad (10)$$

Here, $\hat{\varphi}(\omega) = \int_{-\infty}^{\infty} \varphi(\nu) e^{-j\nu\omega} d\nu$ is the Fourier transform of the interpolator $\varphi(\nu)$ and $\hat{a}_{\varphi}(\omega) = \sum_{k \in \mathbb{Z}} |\hat{\varphi}(\omega + 2k\pi)|^2$ is the discrete Fourier transform of the autocorrelation sequence of the interpolator $a_{\varphi}(k) = \langle \varphi(\nu), \varphi(\nu - k) \rangle$. The dual function of the interpolator, denoted by φ_d in (10) is specified by

$$\hat{\varphi}_d(\omega) = \hat{\varphi}(\omega) / \hat{a}_{\varphi}(\omega). \quad (11)$$

2.4. Selection of scale factors

Note that $E_{\min, \varphi}(\omega)$ and $E_{\text{res}, \varphi, \tilde{\varphi}}$ are positive functions of ω . The first term

$$E_{\min, \varphi}(\omega) = \frac{\sum_{k \neq 0} |\hat{\varphi}(\omega + 2K\pi)|^2}{\sum_{k \in \mathbb{Z}} |\hat{\varphi}(\omega + 2k\pi)|^2} \quad (12)$$

is independent of the analysis function $\tilde{\varphi}$. This term quantifies the error in orthogonally projecting the DTFT of the signal to the subspace spanned by the shifts of the interpolator

$\left\{ \varphi\left(\frac{\nu}{T} - k\right), k = -K/2, \dots, K/2 \right\}$. Note that when $|\varphi(\omega + 2k\pi)| \ll \|\varphi(\omega)\|, \forall k \neq 0$, we have $E_{\min, \varphi}(\omega) \rightarrow 0$. This may partially explain the relatively good performance of support limited functions, whose energy is concentrated in a certain frequency range (e.g., Kaiser-Bessel, prolate spheroidal functions) [18, 13, 23].

The second term $E_{\text{res}, \varphi, \tilde{\varphi}}$ will vanish if $\tilde{\varphi}_d(\omega) = \varphi_d(\omega)$. This choice corresponds to the mean square optimal scale factors

$$h_d[n] = \frac{\hat{\varphi}(2\pi n/K)}{\sum_{k \in \mathbb{Z}} |\hat{\varphi}(2\pi n/K + 2k\pi)|^2}. \quad (13)$$

2.5. Optimization of the interpolator

A careful optimization of the interpolator and scale factors is essential to minimize the approximation error, while keeping resources such as memory and computational complexity to a minimum. If the scale factors are chosen as in (13), the NUFFT approximation is the orthogonal projection of the exact DTFT (1) of the signal to the shift

invariant subspace spanned by $\left\{ \varphi\left(\frac{\nu}{T} - k\right), k \in \mathbb{Z} \right\}$. This minimum achievable error is specified by

$$\eta_{\min}(x, \varphi, K) = \sum_{n=-N/2}^{N/2-1} |x[n]|^2 E_{\min, \varphi} \left(\frac{2\pi n}{K} \right). \quad (14)$$

Note that this expression is only dependent on the interpolator φ , the signal $x[n]$, and the sampling step $T = N/K$. Evaluating the expectation on both sides of the above expression, we obtain

$$e(\varphi, K) = \mathbb{E}(\eta_{\min}) = \sum_{n=-N/2}^{N/2-1} s[n] E_{\min, \varphi} \left(\frac{2\pi n}{K} \right), \quad (15)$$

where $s[n] = \mathbb{E}(|x[n]|^2)$ is the energy distribution of the class of the signals. Note that if

$$s[n] = 1, \forall n, \text{ then } e(\varphi, K) = \sum_{n=-N/2}^{N/2-1} E_{\min, \varphi} \left(\frac{2\pi n}{K} \right).$$

2.6. Mean square NUFFT optimal interpolator

We derive the mean square optimal NUFFT interpolator as the one that minimizes the expected error specified by (15) subject to the energy constraint $\|\varphi\|_{L_2} = 1$:

$$\varphi_{\text{opt}} = \underset{\varphi}{\operatorname{argmin}} e(\varphi, K) \text{ such that } \sum_{n \in \mathbb{Z}} \left| \hat{\varphi} \left(\frac{2\pi n}{K} \right) \right|^2 = 1. \quad (16)$$

Substituting for the expression of $E_{\min, \varphi}$ from (10) and using the relation

$$\hat{a}_{\varphi}(\omega) = \sum_{k \in \mathbb{Z}} |\hat{\varphi}(\omega + 2k\pi)|^2, \text{ we obtain:}$$

$$e(\varphi, K) = S - \sum_{n=-N/2}^{N/2-1} s[n] \left(\frac{|\hat{\varphi}(-2\pi n/K)|^2}{\sum_{k \in \mathbb{Z}} |\hat{\varphi}(-2\pi n/K + 2k\pi)|^2} \right), \quad (17)$$

where the constant $S = \sum_{n=-N/2}^{N/2-1} s[n]$ is the total energy of the signal. Omitting S , the optimization simplifies to the minimization of the second part of (17). Note that the above criterion is a non-quadratic expression of the Fourier coefficients of the interpolator. Since the direct minimization of this expression is difficult, we propose to adapt the iterative reweighted minimization algorithm introduced in [21] to determine the mean square optimal interpolator. Using (17), we rewrite (16) as

$$\begin{aligned} \varphi_{\text{opt}} &= \underset{\varphi}{\operatorname{argmax}} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}-1} w[n] \left| \hat{\varphi} \left(-\frac{2\pi n}{K} \right) \right|^2 \\ &\text{such that } \sum_{n \in \mathbb{Z}} \left| \hat{\varphi} \left(\frac{2\pi n}{K} \right) \right|^2 = 1. \end{aligned} \quad (18)$$

Here, the weights $w[n]$ are specified by

$$w[n] = \frac{s[n]}{\sum_{k \in \mathbb{Z}} |\hat{\varphi}(-2\pi n/K + 2k\pi)|^2}. \quad (19)$$

We use an iterative scheme that alternates between (18) and (19). At each iteration, the algorithm assumes the weights $w[n]$ to be constants and solves (18) to determine the interpolator. Once interpolator is obtained by solving (18), the weights $w[n]$ are re-estimated. The steps (18) and (19) are repeated in an alternating fashion until the cost function does not change considerably². We initialize the algorithm by setting the weights as $w[n] = s[n]$.

2.7. Discretization of the interpolator

The NUFFT approximation of the signal (4) at a specified non-uniform location $\nu \in \mathbb{R}$ requires the evaluation of the samples of the interpolator $\varphi(\nu - m); m \in \mathbb{Z}$. The exact evaluation of the discrete time Fourier transform of the samples at several non-Cartesian locations is computationally prohibitive in MR image reconstruction algorithms, even when the interpolator has analytical expressions (e.g., Gaussian or Kaiser-Bessel interpolators). Hence, it is a general practice to pre-compute the interpolator on a fine uniform grid and store it as a lookup table; the samples of the interpolators are then obtained as a linear interpolation of these uniformly sampled values. Note that the performance loss in discretizing the interpolator could be ignored if the grid is densely sampled. The evaluation for each interpolator sample requires two multiplications and one addition; the computational complexity is independent of the grid density. Assuming an even interpolator oversampling factor O , we assume the interpolator φ to be represented as:

$$\varphi(\nu) = \sum_{k=-JO/2+1}^{JO/2-1} q[k] \beta(O\nu - k). \quad (20)$$

Here, $q[k] = \varphi\left(\frac{k}{O}\right)$, $k = -JO/2+1, \dots, JO/2-1$ are the uniform samples of the interpolator and β denotes the linear B-spline function. The Fourier transform of the interpolator is given

by $\hat{\varphi}(\omega) = \hat{q}\left(e^{j\frac{\omega}{O}}\right) \hat{\beta}\left(\frac{\omega}{O}\right)$. Substituting the expression of $\hat{\varphi}(\omega)$ back in (18), we obtain

$$\begin{aligned} \mathbf{q}_{\text{opt}} &= \underset{\mathbf{q}}{\text{argmax}} \sum_{n=-\frac{N}{2+1}}^{\frac{N}{2}} u[n] \left| \hat{q}\left(-\frac{2\pi n}{K}\right) \right|^2 \\ &\text{such that } \sum_{n=-RN}^{RN} b[n] \left| \hat{q}\left(e^{-\frac{2\pi n}{K}}\right) \right|^2 = 1. \end{aligned} \quad (21)$$

Here, the weights are specified by

²We currently do not have guarantees for the convergence of this algorithm to the global minimum of the cost function. Nevertheless, the interpolator and prefilter obtained by the proposed algorithm are observed to considerably reduce the approximation error over classical schemes.

$$u[n] = w[-n] \left| \hat{\beta} \left(\frac{2\pi n}{KO} \right) \right|^2, \quad \text{and} \quad (22)$$

$$b[n] = \left| \hat{\beta} \left(\frac{2\pi n}{KO} \right) \right|^2. \quad (23)$$

Note that the second summation is now restricted to a finite range $[-RN, RN]$, where R is a sufficiently large number (we chose it as 20 in this study³). –

Since the interpolator is support limited, the DTFT of the sequence $q[k]$; $n = -JO/2+1, \dots, JO/2-1$ simplifies to a finite summation. Hence, $\hat{\mathbf{q}} = \mathbf{F}\mathbf{q}$, where $\hat{\mathbf{q}}$ is the vector of Fourier samples, $\mathbf{q}$ is the vector of coefficients, and $\mathbf{F}$ is the $(2RN) \times (JO-1)$ discrete Fourier transform matrix. Thus, the optimization problem specified by (18) can be reformulated in the matrix form as

$$\mathbf{q}_{\text{opt}} = \arg \max_{\mathbf{q}} \mathbf{q}^T (\mathbf{F}^T \mathbf{U} \mathbf{F}) \mathbf{q} \quad \text{subject to} \quad \mathbf{q}^T \mathbf{B} \mathbf{q} = 1 \quad (24)$$

Here, $\mathbf{U} = \text{diag}(u[n])$ and $\mathbf{B} = \text{diag}(b[n])$. Note that (24) is the generalized eigenvalue problem [26]; the solution is obtained as the eigenvector corresponding to the maximum eigenvalue of the pair of matrices $(\mathbf{F}^T \mathbf{U} \mathbf{F}, \mathbf{B})$. The iterative reweighted algorithm proceeds by alternating between the generalized eigenvalue problem (24) and re-evaluation of the weights $w[n]$, and hence the diagonal matrix $\mathbf{U}$, until convergence. The pseudo-code of the algorithm is shown below. The implementation of the NUFFT algorithm as well as sample codes for MRI reconstruction from non-Cartesian samples are available for download at <https://research.engineering.uiowa.edu/cbig/content/software>.

2.8. Experiments

We assess the utility of the proposed NUFFT approximation algorithms in recovering images from their non-Cartesian Fourier samples. We consider numerical simulations in Fig. 3 and Fig. 4, where the non-Cartesian Fourier samples were generated using the exact discrete Fourier transform on radial trajectories. The image $f(\mathbf{r})$ is recovered from the non-Cartesian samples specified by the vector $\mathbf{b}$ using the total variation (TV) regularized reconstruction scheme:

$$f_{\text{recon}} = \arg \min_f \|\mathcal{A}(f) - \mathbf{b}\|^2 + \lambda \|\nabla f\|_{\ell_1}. \quad (25)$$

Here, $\mathcal{A}$ is discrete Fourier transform of the image f computed at the non-Cartesian sampling locations. We solve the optimization problem (25) using the iterative reweighted approach described in detail in [27, 28].

We study the impact of different NUFFT approximations of $\mathcal{A}$ operator on the quality of the reconstructions. Specifically, we compare the proposed mean square optimal least square

³We studied the dependence of the approximation on R and determined that $R = 20$ results in minimal truncation error.

(MOLS) interpolator, MOLS interpolator which assumes uniform energy distribution (MOLS-U), worst case mean square optimal least square (WOLS) interpolator [21], and the least square interpolator proposed in [20] based on Kaiser-Bessel scale factors (LS-KB). We rely on the discretization of the interpolators, specified by (20), to compute the mean square optimal scale factors. Note that these scale factors provide improved approximations over scale factors used in classical NUFFT schemes.

The *in vivo* brain dataset in Fig. 4 was acquired on a Siemens TIM Trio 3T MR scanner using a 12 channel head coil. This data was acquired from a healthy adult volunteer in accordance with the institutional review board at the University of Iowa. We used a variable density multi-shot spiral sequence with the following specifications: # interleaves=24, FOV=20 cm, 192×192 matrix, resulting in an in-plane spatial resolution of 1.04×1.04 mm². Each of the channels were independently recovered using (25), before combining them using the sum of squares approach.

3. Results

The proposed optimization scheme is designed to minimize the error in approximating the exact DTFT of support limited images. We first determine the utility of the interpolators in obtaining a good approximation of the discrete Fourier transform. Second, the impact of the NUFFT approximation quality on recovering MR images from its non-Cartesian k-space samples is then determined using both numerical simulations and experimental data. The proposed mean square optimal (MOLS) interpolators are compared against the interpolators optimized using the worst case interpolation error metric (termed as WOLS interpolators) as well as the least square interpolators using Kaiser-Bessel scale factors (LS-KB).

3.1. Analysis of NUFFT approximation error

We study the impact of the scale factors on the NUFFT approximation in Fig. 1. Specifically, we compare the NUFFT schemes in [20, 15, 14] with KB, Gaussian, and cosine scale factors, against the proposed MOLS-U approach. We observe that the conventional schemes result in considerably higher error kernels than the MOLS-U method. We observe that the errors provided by the classical schemes can be considerably reduced if their scale factors are recomputed according to (13); the errors are more comparable to the MOLS scheme than the original LS NUFFT schemes [20, 15, 14]. These results demonstrate the benefit in using the proposed mean square optimal scale factors.

We illustrate the ability of the NUFFT interpolators to reduce approximation errors for signals with a known energy distribution in Fig. 2. Specifically, we assume the spatial energy distribution $s[n]$ to be a truncated Gaussian function, shown in Fig.2(j). We set $K = 68$ and $N = 64$ ($K/N = 1.0625$), while the interpolators were discretized on a grid assuming $O = 101$. The optimal interpolators and scale factors corresponding to worst case error metric (WOLS) [21], the proposed mean square error metric (MOLS), the MOLS scheme assuming a uniform error distribution (MOLS-U), and the least square interpolator with KB scale factors (LS-KB) computed according to [20, 15, 14] are shown in Fig.2.(a)-(f). The error

kernels $E_{\min, \varphi} \left(\frac{2\pi n}{K} \right)$ corresponding to WOLS, LS-KB, MOLS and MOLS-U are shown in

Fig.2.(g)-(i), respectively. We observe that the worst case interpolator results in flatter error kernels, which lead to roughly the same level of errors in all image regions. This is expected since it is minimizing the worst case error. In contrast, the MOLS interpolators provide lower value of error kernels in the central regions corresponding to the peak of $s[n]$ at the expense of slightly higher errors close to the image boundaries. Since $s[n]$ has smaller values at the boundaries, the MOLS interpolators will result in lower expected error. While the LS-KB interpolator generally have lower errors in the central regions, we observe that the errors with this method is considerably higher than the proposed schemes. The poor performance of LS-KB scheme can be mainly attributed to the sub-optimal scale factors. The plot of the mean square errors, computed according to (15), and worst case errors computed as described in [21] as a function of the size of the interpolator are shown in (k) and (l), respectively. We observe from (l) that the WOLS interpolators provide considerably lower worst case errors at higher values of J . However, the mean-square performance of these interpolators are worse than the MOLS interpolators as seen from (k). We also observe that the performance of MOLS-U interpolator is not considerably worse than the MOLS scheme; this approximation can be used when the exact energy distribution is unknown.

3.2. Improved MRI reconstruction using MOLS NUFFT: Numerical simulations

We first perform simulation studies to determine the utility of the proposed scheme in MR image reconstruction. We consider the recovery of the 64×64 Shepp-Logan phantom from its Fourier samples acquired on 30 radial lines using total variation regularized recovery. We choose $J = 4$ and $K = 66$ to obtain a computationally efficient algorithm with low memory

demand. Note that the oversampling factor is $\frac{K}{N} \approx 1.03$; This choice is far lower than the routine value, $\frac{K}{N}=2$, in current image reconstruction schemes. Hence, the proposed algorithm requires about four times less memory and is computationally more efficient than the current algorithms. We reconstruct the images from their non-Cartesian k-space samples using WOLS, LS-KB, MOLS and MOLS-U interpolators. We compare the reconstructions against the one obtained using the iterative algorithm with exact non-uniform DTFT instead of the NUFFT approximation. Note that the run time of this algorithm with the exact DTFT is considerably higher than the one with the NUFFT approximation. We assumed the same regularization parameters in all the experiments. We observe that the LS-KB scheme results in higher errors close to the image edges. The worst case interpolator is capable of minimizing the error at the edges quite significantly, however at the expense of an increase in the center of the image (see regions pointed by the arrow). We observe that the MOLS interpolators are able to lower the errors at most locations, resulting in a recovered image with low overall errors.

We consider the reconstruction of the 128×128 MRI knee image from its samples on 84 radial lines in Figure 4. It is challenging to approximate the DTFT of this image using classical NUFFT schemes since the image has high energy close to the top and bottom edges. We set $K = 130$; $J = 6$ and recover the images using different NUFFT

approximations. Note that the oversampling factor is $\frac{K}{N}=1.016$. We compare the TV reconstructions using NUFFT approximations against reconstructions using the exact DTFT.

We observe that the use of LS-KB NUFFT scheme results in considerable line-like artifacts at the top of the image (see (b) and (g)). Similar to the Shepp-Logan example, the worst case interpolator is able to significantly lower the streak-like artifacts at the expense of increased error towards the center of the image. By contrast, the mean-square interpolators are capable of reducing the overall error without significantly increasing artifacts. We compute the energy distribution of the signal by averaging the energy distribution of the rows and columns of the original image. Since the energy distribution of the signal to be recovered is often not known *a priori*, this interpolator is only included as a best case example. It is interesting to observe that the MOLS-U NUFFT scheme that assumes uniform energy distribution is a good surrogate for MOLS NUFFT scheme, when the exact energy distribution of the signal is unknown.

3.3. Effect of NUFFT approximation in MRI reconstruction: Experimental comparisons

We determine the use of the proposed NUFFT approximation in the recovery of experimental MR image data in Fig. 5. Since the exact energy distributions of the signals are unknown, we only consider the MOLS-U interpolator. Here, we set $K = 194$ and $J = 4$ while

the size of image N is 192; $\frac{K}{N} = 1.01$. The comparison of the TV reconstructed images with NUFFT approximations against the ones with the exact DTFT are shown in Fig. 4. We observe that this is a challenging experiment since the ground truth is not known and the measurements are corrupted by measurement noise. It is observed that the MOLS-U interpolator is capable to provide reconstructions that closely match the exact DTFT. The WOLS scheme is observed to introduce oscillatory textures in the reconstruction, indicated by red arrows. These artifacts can also be appreciated from the error image and can be explained by the oscillatory nature of the WOLS error kernel close to the image boundaries (see Fig. 2. g-i). The LS-KB scheme introduces considerably larger errors as seen from the error image. These consist of systematic reduction in intensity, indicated by the black arrow and oscillatory artifacts denoted by red arrows. We observe that the error distribution is not as oscillatory as the WOLS scheme. This behavior can also be easily seen from the LS-KB error kernels in Fig. 2. g-i, which is much higher in amplitude but smoother; the resulting errors may be thought of as the image content being modulated by the error kernel. These results demonstrate the value of the error kernels in predicting the distribution of the errors due to the NUFFT approximations in the reconstructions. These experiments confirm that the use of the proposed interpolators can provide substantially lower error than classical interpolators. Thus, the proposed algorithms can achieve relatively high accuracy with considerably lower memory demands than classical schemes.

4. Discussion and Conclusion

We introduce a design strategy to determine the mean square optimal interpolator and scale factors in the NUFFT approximation. Our main goal is to improve the quality of the approximation when low oversampling factors ($K/N \approx 1$) are involved. We determine the mean square optimal NUFFT scheme by minimizing a novel analytical expression for the expected mean square error in a NUFFT approximation. We observe that the proposed error expression is more representative of real-world signals compared to the worst case one in

[21]. Our experiments demonstrate that we could obtain good non-Cartesian MRI images by using the mean square optimal interpolators and scale factors, even when $\frac{K}{N} < 1.1$ and $J = 6$. Thus, the proposed scheme enables us to considerably reduce the memory demand for non-Cartesian reconstructions, which makes it possible to accelerate these algorithms using graphical processing units.

Our experiments show that the LS-KB scheme provides higher errors comparing with WOLS method. However, we also observe that the spatial distribution of the errors with the LS-KB are smoother than that of the OLS schemes. Note that this can be completely explained in terms of the smoothness of LS-KB error kernels compared to the WOLS kernels (see Fig. 2). Hence, the LS-KB reconstructions may be visually pleasing, even-though the square errors are higher. While this behavior may be acceptable in anatomical imaging, the spatial modulation of variance may be un-acceptable in applications such as functional imaging. Note that our optimization criterion only depends on the magnitude of the error kernel and did not account for its smoothness; it may be possible to also account for smoothness of the kernel in the NUFFT optimization to yield lower square errors that are unstructured.

Our theoretical findings show that the errors due to classical schemes (LS-KB) may be relatively lower in specific image regions (e.g., center of the image), as seen from Fig. 3 and 5. While higher errors at the image boundaries may be acceptable for brain imaging, it may not be acceptable for other applications (e.g. knee images considered in Fig. 4). We observe that the performance of the OLS schemes, which have the same computational complexity as the KB methods, are considerably better in most image regions.

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Algorithm : MOLS NUFFT($s[n]$, K , N , J , Ofactor)

$\varphi \leftarrow$ Kaiser Bessel function

$\text{err} = 1 \times 10^{10}$

do $\left\{ \begin{array}{l} \text{err} \leftarrow e(\varphi, K), \text{ specified by (15)} \\ \text{Update } w[n] \text{ using (19)} \\ \mathbf{U} \leftarrow \text{diag}(u[n]), \text{ where } u[n] \text{ is specified by (22)} \\ \mathbf{B} \leftarrow \text{diag}(b[n]), \text{ where } b[n] \text{ is specified by (23)} \\ \text{Compute } \mathbf{q}_{\text{opt}} \text{ using (24)} \end{array} \right.$

Compute $\mathbf{h}_{\text{opt}}$ using (13)

return ($\mathbf{q}$, $\mathbf{h}_{\text{opt}}$)

Figure 1.

Effect of scale factors on NUFFT approximation: the solid lines correspond to least square methods introduced in [20, 15, 14] with KB, Gaussian, and cosine scale factors. Note that all of these methods results in considerably higher error kernels than the proposed MOLS-U interpolator, shown in black dotted lines. To demonstrate the improvement offered by mean-square optimal scale factors specified by (13), we re-compute the scale factors of the LS schemes [20, 15, 14]; the corresponding methods are termed as LS-KB*, LS-Cosine*, and LS-Gaussian*, which are denoted by dotted lines. We observe that the error kernels of these methods are considerably lower and more comparable to the proposed scheme than the original LS methods. These results demonstrate the role played by the scale factor in NUFFT approximation.

Figure 2.

Comparison of different NUFFT approximation schemes: the optimized interpolators, scale factors, and the corresponding error kernels specified by (10) are shown in the top three rows. Here, we assume the energy distribution to be a Gaussian shown in (j).

The columns correspond to the interpolators with different lengths ($J = 4, 6, 8$), computed assuming $K = 68$, $N = 64$ and $O = 101$. We observe that the error kernels associated with the LS-KB scheme is much higher than the proposed one, mainly due to the sub-optimality of the scale factors as shown in Fig. 1. The decay of the NUFFT approximation error for a random k-space sampling pattern are shown in (k) and (l). We observe from (k) that the MOLS schemes provide the lowest mean-square errors. However, their worst case performance is much worse than the WOLS scheme as seen from (l), since they result in higher errors at the image boundaries.

Figure 3.

Recovery of the 64×64 Shepp-Logan phantom from under sampled radial acquisition (30 lines) using total variation reconstruction scheme, specified by (25). We set $K=66$ and $J=4$ to obtain a memory and computationally efficient iterative reconstruction algorithm. The comparison of the reconstructions using different NUFFT approximations with the ones obtained using the exact DTFT are shown in bottom row. These error images are scaled by a factor of 6.67 compared to the original images for better visualization. Note that the MOLS and MOLS-U interpolators provide low errors at most image regions. In contrast, the WOLS scheme results in higher errors at the image center, while the errors associated with the LS-KB scheme are considerably higher.

Figure 4.

Reconstructed images and error images using different interpolators, when $K=130$ and $J=6$. It is observed from the top row that

LS-KB kernel results in large errors close to the image boundaries, indicated by the red arrows. It also results in subtle differences in the texture in the central regions. As in the case of the Shepp-Logan example, the WOLS scheme is able to reduce these structured artifacts at the expense of increased in the image center. By contrast, the MOLS and MOLS-U schemes result in lower and un-structured artifacts. The behavior can be better appreciated from the error images shown in the bottom row, obtained by comparing the reconstructions against ones obtained using the exact DTFT. For better visualization, the error images are scaled by a factor of 10 compared to the original images.

Figure 5.

Reconstructed images and error images using different interpolators, when $K=194$ and $J=4$. The MOLS-U scheme provides considerably less reconstruction errors compared to WOLS and LS-KB reconstructions. All the error images are scaled by the factor of 12. We observe that the LS-KB scheme results in higher errors. Specifically, we observe the systematic reduction in intensity indicated by the black arrows, as well as oscillatory artifacts indicated by red arrows. We also observe that the errors in the LS-KB case are more unstructured and hence not as visually disturbing as the WOLS scheme. This can be explained in terms of the smoothness of LS-KB error kernel (see Fig. 2). Specifically, the variance of the errors is spatially modulated by the error kernel and the intensity of the image. While this behavior may be acceptable in anatomical imaging, it may be undesirable in functional imaging.