Iterative RAKI with Complex-Valued Convolution for Improved Image Reconstruction with Limited Scan-Specific Training Samples

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Abstract

**Purpose:** To investigate the influence of the training data (auto-calibration signals, ACS) on the reconstruction quality of Robust Artificial-neural-networks for K-space Interpolation (RAKI) for standard 2D imaging, and to evaluate an iterative learning approach (iterative RAKI) for enhanced performance, when only a limited amount of original ACSs are available for RAKI training.

**Methods:** RAKI was implemented using complex-valued convolutional neural networks for simultaneous multi-coil k-space interpolation. In the iterative learning approach, RAKI is initially trained using augmented ACS obtained from an initial GRAPPA reconstruction, which allows to increase the convolution filter size assigned to the first layer. Subsequently, RAKI is further trained iteratively using augmented ACS extracted from the RAKI reconstruction of the previous iteration step. Evaluation was carried out on retrospective undersampled in-vivo datasets.

**Results:** For limited training data (8% of full matrix size), iterative RAKI outperforms standard RAKI by reducing residual artefacts occurring at accelerations factors R=4 and R=5 and yields strong noise suppression when compared to standard parallel imaging, underlined by quantitative reconstruction quality metrics. Combination with a phase-constraint yields further improvement. Additionally, iterative RAKI shows better performance than GRAPPA and RAKI in case of pre-scan calibration and strongly varying contrast between training- and undersampled data.

**Conclusion:** The iterative learning approach with RAKI enables to benefit from standard RAKI’s well known noise suppression but requires less original training data for the reconstruction of standard 2D images.

K E Y W O R D S Parallel imaging, GRAPPA, RAKI, deep learning, complex-valued machine learning.
1. **Introduction**

Since its invention, magnetic resonance imaging (MRI) has raised to one of the most widespread clinical diagnostic techniques nowadays. It offers numerous benefits such as absence of ionizing radiation, non-invasiveness and the capability of showing soft tissue structures. However, MRI acquisitions can be time consuming and the total scanning time remains a crucial factor. Almost all MRI applications such as dynamic MR angiographies, perfusion MRI, or imaging of the cardiac function require accelerated imaging to cover their typical time scales. Strategies to shorten the scan times based on hardware modifications have reached engineering as well as physiological limits, for example due to peripheral nerve stimulations. In order to further decrease scan time, data acquisition techniques based on gradient sub-encoding were considered. By introducing phased arrays [1] in 1990, Parallel Imaging (PI) is nowadays the most common strategy in clinical routine. In PI, the MR signal is acquired simultaneously with multiple, independent receiver coils, while the inverse image space (also known as k-space) is sub-sampled. Dedicated PI reconstruction methods make use of the inherent spatial encoding capabilities of the phased arrays to recover the full image content, and can be classified to operate either in image- or k-space domain. Image domain methods are essentially based on the sensitivity encoding (SENSE) [2] method that recovers an artifact-free image by utilizing explicit spatial coil-sensitivity information. On the other hand, GeneRalized Autocalibrating Partial Parallel Acquisition (GRAPPA) [3] is a widely used reconstruction method operating in k-space, and relies on a linear regression using least squares method to derive convolution filters, and thus, can be considered a data-driven machine learning approach. GRAPPA estimates missing k-space signals by a convolution of adjacent multichannel k-space signals. The convolution filters (also known as GRAPPA kernel) is calibrated by linear least-squares fit using several fully sampled auto-calibration signals (ACS) that serve as scan-specific training data. However, severe noise enhancement at high accelerations is a major limitation in all PI methods. To overcome this limitation, Nonlinear GRAPPA [4] has been presented, where additional virtual channels are generated by the non-linear combination of physical channels. Both physical and virtual channels are then used to interpolate missing k-space signals in standard GRAPPA. Nonlinear GRAPPA
outperforms its standard counterpart at high accelerations. However, it requires an increased amount of ACS as the convolution model has more degrees of freedom. More recently, GRAPPA has been generalized within the machine learning framework by the deep learning method Robust Artificial-Neural-Networks for k-space interpolation (RAKI) [5]. In contrast to GRAPPA, where only one convolution filter layer is applied on the acquired k-space signals for interpolation, RAKI makes use of multi-layer feature extraction. In RAKI, non-linearity is introduced by applying a non-linear activation function element-wise to the convolution-layers. The combination of multiple convolution layers with non-linear activation functions are essential features of a convolutional neural network (CNN). Similar to GRAPPA, the neural network parameters in RAKI (i.e. the convolution filter weights within the CNN) are calibrated using scan-specific ACS as training data. In previous studies, RAKI has demonstrated better performance in comparison to GRAPPA [5,6,7]. However, similar to Nonlinear GRAPPA, RAKI requires more training data due to its increased parameter space, which may limit its application in standard 2D imaging. In this work, we investigate the influence of training data on the RAKI reconstruction in standard 2D imaging. The particular focus is on the training data amount and contrast information contained in the ACS. We extend RAKI by an iterative learning approach (iterative RAKI, iRAKI) for improved reconstruction quality when only a limited number of ACS lines is available for training. RAKI network modifications were made by implementing complex-valued convolutions, instead of splitting the complex-valued k-space data into real-valued, separate CNN-channels. Additional network modifications were made by using only one single CNN for simultaneous multi-coil interpolation. We show that iRAKI provides improved reconstruction quality in comparison to GRAPPA and standard RAKI in standard 2D imaging. Furthermore, we show that iRAKI training yields significantly improved signal-to-noise ratio in combination with the Virtual Conjugate Coils (VCC) concept that incorporates additional image- and coil-phase information into the reconstruction process. Part of this work has been presented at the annual meeting of the ISMRM 2021 congress [9] and the ESMRMB 2021 congress [10].
2. Methods

We first describe the architecture of the convolutional neural network used in this work and point out the differences to the original RAKI architecture [5]. Afterwards, we investigate the influence of the training data amount, the convolution filter size as well as the contrast information contained by the training data on the reconstruction quality for both standard RAKI and GRAPPA. Finally, we introduce the general principle in the iterative learning approach.

2.1. Network Architecture

The network architecture developed in this work differs from the original RAKI model in two ways: We implemented one single CNN for simultaneous multi-coil k-space interpolation, instead of assigning each coil one CNN. Furthermore, instead of performing real-valued convolution, we implemented its complex-valued equivalent [11,12]. Complex-valued convolution, which can be exactly mimicked by connecting real-valued neural network components [11,12], prevents the mathematical correlation between the real- and imaginary part of k-space data from being dismissed within the CNN. It has been shown to be beneficial to use complex-valued convolutions rather than real-valued convolutions within CNNs for magnitude- [13,14,15] and phase-sensitive image reconstructions [12] in image domain. Note that the influence of complex-valued convolution in k-space based deep-learning approaches, like RAKI, has not been studied profoundly yet, and is beyond the scope of this work. However, we noted a reduction of residual artefacts at the cost of minor noise enhancement, when replacing real-valued convolution by its complex-valued equivalent (see Supporting Information Fig. S1).

Throughout the entire k-space reconstruction process, the complex-valued structure of k-space data is preserved. Within the complex CNN, k-space data is stored as complex numbers in one single channel, in contrast to original RAKI, in which real- and imaginary signal components are assigned two separate channels. In the forward propagation, linear complex-valued convolutions are applied using complex-valued convolution filters. A complex convolution of a signal vector \( z = a + ib \) with a filter \( W = H + iK \) can be decomposed into four real-valued convolutions according to [11,12]:

\[
z \odot W = (a + i b) \odot (H + i K) = (a * H - b * K) + i(a * K + b * H), \tag{1}
\]
where \( \oplus \) denotes a complex-valued convolution, \( * \) denotes a real-valued convolution, \( i \) is the imaginary unit, \( z \) denotes a complex number with \( a \) and \( b \) its real- and imaginary part, respectively, \( W \) denotes a complex-valued convolution filter with \( H \) and \( K \) being two real-valued convolution filters. As nonlinear activation function, we use the complex rectifier linear unit (CReLU) \([12,16]\), defined as:

\[
\text{CReLU}(z) = \text{ReLU}(\text{Re}(z)) + i \text{ReLU}(\text{Im}(z)),
\]

with \( \text{Re}(z) \) and \( \text{Im}(z) \) denoting the real and imaginary part of \( z \), respectively, and \( \text{ReLU} \) is the standard real-valued rectifier linear unit \([17]\).

The network architecture used in this work is depicted in Fig. 1. The input layer \( s_1 \) takes in the complex-valued, zero-filled multi-coil k-space data, resulting into \( N_c \) total input channels, with \( N_c \) being the number of receiver coils. The hidden layers \( s_2 \) and \( s_3 \) are then calculated through linear, complex-valued convolution, and an element-wise activation using a complex Rectifier Linear Unit CReLU: \( s_2 = \text{CReLU}(s_1 \oplus W^1_C) \) and \( s_3 = \text{CReLU}(s_2 \oplus W^2_C) \), with the complex convolution matrix \( W^1_C \) of size \( k_y \times k_x = 2 \times 5 \) and \( W^2_C \) of size \( k_y \times k_x = 1 \times 1 \) in Phase- and Read-out encoding direction, respectively. The first hidden layer \( s_2 \) is assigned 256 channels and the second hidden layer \( s_3 \) is assigned 128 channels. Note that the total number of hidden layers, the assigned channel-numbers as well as the kernel sizes for each layer are hyperparameters, which were determined heuristically, as currently there are no existing methods for optimally tuning the network-architecture in deep learning applications \([18,5]\). The output layer \( s_4 \) predicts all missing points across all coils simultaneously, thus having \( (R - 1) \times N_c \) channels, where \( R \) denotes the undersampling rate. It is activated with the identity function \( \gamma(x) = x \), thus reading \( s_4 = \gamma(s_3 \oplus W^3_C) \), with \( W^3_C \) of size \( k_y \times k_x = 1 \times 5 \). The mean-squared-error (MSE) \( L(y, \hat{y}) \) of signal prediction \( y \) to its groundtruth \( \hat{y} \) was used as cost-function for training, reading

\[
L(y, \hat{y}) = \frac{1}{N} \left( \sum_{i=0}^{N} |y_i - \hat{y}_i|^2 \right),
\]

with \( N \) denoting the total number of training samples. The Adaptive Moment Estimation (Adam) optimizer \([19]\) was used as optimization algorithm to minimize the mean-squared-error of estimated k-space data to its ground-truth. Bias terms were excluded in the CNN, as they may cause issues with k-space scaling \([5]\). The CNN was implemented within the
PyTorch package 1.8.0 [20]. To obtain the final reconstructed image, the interpolated k-spaces are Fourier-transformed and combined by root sum-of-squares. All reconstructions were performed on a high-performance-computing-cluster with Intel® Xeon® Gold 6134 (CPU). Note that the GRAPPA k-space reconstruction via convolution can be formulated as $s_{\text{int}} = \gamma(s_1 \odot W_C^e)$, where $s_{\text{int}}$ denotes the interpolated k-space signals, $s_1$ denotes the undersampled, multi-coil k-space data, $W_C^e$ is the GRAPPA kernel, and $\gamma$ is the identity function assigned to the only convolution layer. Thus, the model in GRAPPA can be obtained from the RAKI model by omitting the hidden layers, which are used for abstract multi-layer feature extraction of k-space signals.

![Architecture of the Convolutional Neural Network (CNN) used for RAKI implementation in this work.](image)

**Figure 1:** Architecture of the Convolutional Neural Network (CNN) used for RAKI implementation in this work. Throughout the entire CNN, the complex-valued k-space data structure is preserved. Convolution is performed with complex-valued filter matrices. The input-layer takes in the zero filled, complex-valued k-space data, thus having $N_c$ channels, with $N_c$ denoting the number of receiver coils. The first and second hidden layer are assigned 256 and 128 channels, respectively. The output layer predicts all missing k-space data across all coils, thus having $(R - 1) \cdot N_c$ channels, with $R$ denoting the undersampling rate.
2.2. Training Data Considerations

As k-space interpolation is based on correlations between adjacent points and redundancies induced by coil-sensitivity profiles, the convolution filter size determines the extension in which the k-space footprint of spatially varying coil sensitivity profiles is captured [21]. Thus, model complexity of the CNN in RAKI is significantly determined by its convolution filter sizes. However, analogous to GRAPPA, the choice of the filter sizes affects the total number of available training data, given a fixed number of ACS lines [22]. As both complexity and total number of training data are crucial factors for the performance of the CNN, a more detailed evaluation for this trade-off is obligatory. For this purpose, we vary the number of ACS lines between \( N_{\text{ACS}} = 20, \ldots, 100 \) with step size 5, and assign two different convolution filter sizes to the first convolution filter in the CNN (denoted as \( W_C^1 \) in the previous section): \( k_y \times k_x = 2 \times 5 \) and \( 6 \times 7 \), respectively. Image reconstruction quality is assessed qualitatively via error images and quantitatively via the normalized mean squared error (NMSE) of the magnitude image w.r.t. the fully sampled reference image. Since the CNN weights are initialized randomly in the training procedure, there is an inherent stochasticity incorporated in RAKI. To take this point into account, each reconstruction is repeated one hundred times to minimize effects of outliers on the evaluation. For comparison, the NMSE of the corresponding GRAPPA reconstruction is evaluated. In all cases, ACS were not re-inserted into the reconstructed k-space for a more valid comparison.

In this work, we also study the effect of the contrast information contained by the training data. To this purpose, ACS with different contrast information were used for RAKI training and subsequent k-space interpolation. We acquired 2D data with T1- and T2-weighted contrast, and used T1-weighted ACS for RAKI training to reconstruct both T1- and T2-weighted data. ACS were not re-inserted and the results were compared to corresponding GRAPPA reconstructions.

2.3. Iterative Training

The workflow of iRAKI is motivated by observations from training data considerations as described in the previous section. As illustrated in Fig. 2, the iterative procedure includes different amounts of original and augmented ACS [9], as well as different convolution filter
Figure 2: Workflow of iRAKI. In the first iteration step, RAKI is trained with augmented ACS obtained from an initial GRAPPA reconstruction. The latter is performed using 8% of the total number of PE-lines at k-space center as original ACS, and a kernel size $2 \times 5$. The first hidden layer in RAKI is assigned a convolution filter size $6 \times 7$. From the initial GRAPPA reconstruction, $N$ central k-space lines are used as training samples for RAKI training (in this work, we set $N = 100$). In subsequent iteration steps, the CNN weights are further optimized using $N' = 100$ central lines from the RAKI reconstruction of the previous iteration step as ACS. Original ACS are inserted after each reconstruction step. The learning rate is decreased by a constant factor after each iteration step, which determines the total iteration number, given an initial learning rate.

The goal is to enhance RAKI image quality when only a reduced amount of original acquired ACS is available. Given 8% fully sampled central k-space region as original, low-resolution ACS, an initial GRAPPA reconstruction is performed in order to obtain augmented ACS of increased amount for an initial RAKI training with an increased convolution filter size. Note that the approach to use an initial GRAPPA reconstruction to increase the training data amount for RAKI has been discussed in the original RAKI paper [5]. In this work, GRAPPA is assigned a kernel size $2 \times 5$, while the first hidden layer in RAKI is assigned a filter size $6 \times 7$ in PE- and RO-direction, respectively. Augmented ACS is extracted from $N = 100$ central lines of the initial GRAPPA k-space reconstruction. It should be noted that the original ACS are reinserted before the initial RAKI reconstruction. In order to further improve performance, subsequent iteration steps follow. In each iteration, the CNN weights are transferred, and further optimized using $N' = 100$ central lines (including reinserted original ACS) from the RAKI reconstruction of the previous iteration. The initial learning rate
\( \eta_0 \) passed to the Adam optimizer is decreased by a constant factor \( \Delta \eta \) after each subsequent iteration step. Thus, the learning rate at iteration step number \( i \) reads \( \eta_i = \eta_0 - i \cdot \Delta \eta \). In this work, we set \( \eta_0 = 0.05 \) and \( \Delta \eta = 0.003 \) for \( R = 4 \), and \( \Delta \eta = 0.004 \) for \( R = 5 \). We chose \( \Delta \eta \) such that the cost-function (MSE) does not diverge at late iteration steps, ensuring robustness in the iterative training procedure. Accordingly, the total number of iterations \( N_{\text{iter}} \) amounts to \( N_{\text{iter}} = \eta_0 / \Delta \eta \). The final optimized CNN interpolates the multi-coil sub-sampled k-spaces simultaneously, which are then Fourier-transformed to image domain, and combined via root-sum-of-squares coil-combination to obtain the final reconstructed image, in analogy to GRAPPA. All image reconstructions were evaluated qualitatively via error images, as well as quantitatively using the NMSE, the peak-signal-to-noise ratio (PSNR) and the structural similarity index (SSIM) [24]. Specifying the original ACS to be 8% fully sampled center region was motivated by the requirements given in the fastMRI challenge for 4-fold accelerated data [25].

In order to investigate the performance of iRAKI regarding noise resilience, we estimated SNR maps via the pseudo-replica method [26]: The image reconstruction procedure is conducted repeatedly (100 times in this work) using k-space data, which are superimposed with randomly generated noise at each repetition step. The synthetic noise-data is correlated and scaled appropriately using a noise covariance-matrix, obtained from a noise-only scan. The SNR map is then estimated by dividing the mean across the image-stack by its standard deviation at each voxel. It should be noted that for GRAPPA, there exists an analytical expression to derive the SNR-and g-factor maps [27]. However, for both standard RAKI and iRAKI, this analytical expression cannot be applied or transferred simply, as the non-linearity induced by the activation functions, need to be considered appropriately, which is beyond the scope of this work.

It is worth mentioning that within the general machine learning context, the common strategy to handle the issue of limited training data amount is to use data augmentation techniques to synthetically enlarge the effective amount of training data [28,29]. Sandino et al. trained unrolled neural networks on augmented 2D cardiac cine MRI data in image space [30], e.g. by random flipping along readout- and phase encoding direction, or random circular translations along phase-encoding direction. However, these augmentation techniques do not work in standard 2D imaging, since the multi-channel k-space correlations must be
preserved for k-space interpolation. Nencka et al. performed RAKI on multi-band imaging, and augmented training data by creating synthetically aliased k-space data via linear combination of the k-space acquisitions for subsets of slices in the excited package [23]. For standard 2D imaging, however, this approach is not applicable due to the lack of multiple slice excitations.

2.4. Phase-Constrained Reconstruction

The Virtual Conjugate Coils (VCC) concept [8] has been introduced to improve parallel MRI performance by utilizing conjugate symmetry properties of the k-space, and can be seen as a phase-constrained reconstruction technique. From actual coils, additional virtual coils are generated which contain conjugate symmetric k-space signals. Thereby, additional image- and coil-phase information is utilized to improve reconstruction conditions. The VCC concept has been presented as a practical approach especially in combination with GRAPPA, since no explicit spatial phase information is required. In this work, we study the influence of VCCs on the reconstruction quality of RAKI and iRAKI in comparison to GRAPPA. The additional k-space signals from a virtual coil can be generated from an actual coil $i$ according to

$$s_{i+N_c}(\mathbf{k}) = s_i^*(-\mathbf{k}), i = 1 \ldots N_c,$$

where $N_c$ denotes the number of actual, physical coils in the phased array, $\mathbf{k}$ denotes a k-space vector and $s_i^*$ is the complex-conjugate signal assigned to coil $i$. The stack of virtually received k-spaces thus contains two times as many coils as actual coils. The reconstruction process is carried out by first generating the virtual coils for both ACS and undersampled data according to Eq. 4, and subsequently perform a k-space reconstruction using a standard GRAPPA-, RAKI- or iRAKI reconstruction. The resulting images of the physical coils are then combined using a root sum-of-squares combination.

2.5. Experiments

Three in-plane brain imaging datasets were acquired on healthy volunteers at 3 T (Siemens Magnetom Skyra, Siemens Healthineers, Erlangen, Germany) using a 20-channel head-coil array (with only 16 coils activated). The study was approved by our institutional review
board. Written informed consent was obtained before each in vivo study. Additionally, a FLAIR multi-slice dataset from the fastMRI neuro database [25] was considered.

**Variable Density Acquisition Scheme**

In this work, four full-sampled datasets of 2D anatomical brain imaging were used for evaluation (acquisition parameters summarized in Tab. 1). The datasets were retrospectively undersampled uniformly to mimic the variable density acquisition scheme [31,32]. We extracted 8% of the total number of Phase-encoding lines at the central k-space region to obtain the scan-specific ACS for GRAPPA and RAKI training. Specifically, the training data considerations were carried out on a dataset referred to as neuro(1), which was acquired using a TSE sequence with T1-weighting. Another dataset with T2-weighting was acquired subsequently to study the influence of contrast information in the training process on reconstruction quality for both RAKI and GRAPPA. The performance of iRAKI was evaluated using the dataset neuro(1) in order to consider the case of limited training data amount (18 ACS lines, i.e. 8% of 224 Phase-encoding lines in total). Two further datasets were used for evaluation: One dataset was acquired using a FLASH sequence with T1-weighting, referred to as neuro(2), and the TSE-multi-slice fastMRI FLAIR dataset, referred to as neuro(3).

Tab. 1: The sequence and imaging parameters for the 2D neuro imaging experiments used for evaluation in this work.

|                  | neuro(1) T1 | neuro(1) T2 | neuro(2) T1 | neuro(3) FLAIR | neuro(4) T1 |
|------------------|-------------|-------------|-------------|----------------|-------------|
| Sequence/Turbofactor | TSE / 2     | TSE / 2     | FLASH       | TSE / 2        | FLASH       |
| Rep.-/Echo-Time [ms] | 500/10      | 4500/102    | 250/2.9     | 9000/181       | 250/3.1     |
| Inversion-Time [ms] |             |             |             | 2500           |             |
| Flip Angle [°]    | 90/180      | 90/180      | 70          | 90/150         | 70          |
| FOV [mm²]         | 193 x 220   | 193 x 220   | 230 x 230   | 220 x 220      | 195 x 250   |
| Matrix Size       | 224 x 256   | 230 x 256   | 320 x 320   | 320 x 320      | 250 x 320   |
| Slice Thickness [mm] | 4.0         | 4.0         | 3.0         | 5.0            | 4.0         |

**Pre-Scan Calibration**

In the variable density acquisition scheme, the scan-specific training data used to calibrate the GRAPPA kernel and the model-weights in iRAKI can be re-inserted into the reconstructed
k-spaces, since the ACS are an integral part of the image scan. Alternatively, the training data can be obtained by acquiring a fully-sampled, low-resolution pre-scan before the actual undersampled image scan series. As no contrast information is needed in the pre-scan, its sequence parameters like repetition- and echo-time can be adjusted to maximize SNR, or to minimize the total acquisition time. However, in this case the training data cannot be re-inserted into the reconstructed k-space of the actual image scan. Thus, the performance of iRAKI needs to be investigated separately for pre-scan ACS with different contrast. For this purpose, we acquired a proton-density weighted pre-scan of size $64 \times 64$ in PE-and RO-direction, which was used to calibrate GRAPPA, RAKI and iRAKI. The calibrated models were then used to reconstruct a subsequently acquired, 4-fold undersampled 2D neuro image scan with T1-weighting (referred to as neuro(4)). We also compared the image reconstructions to those obtained with scan-specific ACS as training data. To this purpose, we additionally performed a 4-fold undersampled T1-weighted image scan on the same subject using the variable density acquisition scheme. The ACS was limited to 20 central k-space lines (i.e. 8% of 250 PE-lines in total), and re-inserted into the interpolated k-spaces in GRAPPA, RAKI and iRAKI.

### 3. Results

#### 3.1. Amount of Training Data

The distribution of the normalized mean squared error (NMSE) versus the number of ACS lines for the 4-fold undersampled neuro(1) T1-dataset is depicted in boxplot-form in Fig. 3 (A). The NMSE is depicted for two convolution filter sizes assigned to the first hidden layer. For comparison, the NMSE of the corresponding GRAPPA reconstruction is depicted. Based on the presented results, we can analyze the trade-off between training data amount and convolution filter size, i.e. between number of training samples and model complexity. It turns out that for large training data amounts, an increased convolution filter size is beneficial. We note that for a reduced training data amount (< 45 ACS lines), the NMSE of RAKI tends to increase more intensely the less ACS lines are given. This underlines the difficulty to train RAKI even with small convolution filter size, when there is only a limited training data amount available. This observation is emphasized by the representative images.
depicted in Fig. 3 (B), where blurring and contrast-loss artefacts are observed for RAKI with small filter size, which was trained on 25 ACS lines (i.e. 11% of total PE-lines). The more ACS data is available for training, the more beneficial becomes the convolution filter with increased size (6 × 7) over the smaller convolution filter (2 x 5), for both RAKI and GRAPPA (see also Fig. 3 (C) for corresponding representative images).

Figure 3: A) Boxplots of normalized mean squared error (NMSE) distributions for standard RAKI image reconstructions of 4-fold retrospective undersampled neuro(1) T1-dataset w.r.t. the fully sampled reference image. RAKI reconstruction was repeated one hundred times to take the inherent stochasticity of its initialization and training process into account. The amount of training data (ACS) was varied by using central k-space lines in range 20 – 100 with stepsize 5. Additionally, we assigned two convolution filter sizes (2 × 5 and 6 × 7 in Phase-Encoding and Read-Out-direction, respectively) to the first hidden layer. Corresponding results of GRAPPA reconstructions are depicted for comparison, too. B) Representative RAKI and GRAPPA image reconstructions using 25 and C) using 100 central k-space lines as ACS for both convolution filter sizes (2 × 5 left, and 6 × 7 right in PE- and RO direction)
3.2. Different Contrasts in Training and Interpolation

We used 30 central k-space lines of the neuro(1) T1-dataset for standard RAKI and GRAPPA training, and used the calibrated models to reconstruct 4-fold retrospectively undersampled datasets of the neuro(1) dataset with both T1- and T2-weighting (see Fig. 4). Standard RAKI outperforms GRAPPA in the T1-weighted dataset as it provides an enhanced noise resilience, however, it shows poor performance when the contrast information between training data (T1-weighted) and data to be reconstructed differs strongly, as indicated by the T2-weighted image reconstruction. On the other hand, GRAPPA shows only few additional artefacts for the reconstruction of the T2-weighted image.

Figure 4: Both T1- and T2-weighted acquisitions were 4-fold retrospectively undersampled, and reconstructed with GRAPPA (bottom row) and standard RAKI (top row), both of which were calibrated on 30 central lines of the T1-weighted dataset only. ACS data were not re-inserted (error images scaled for display).
3.3. Iterative Training

Variable Density Acquisition Scheme

In Fig. 5 (A), image reconstructions by GRAPPA, standard RAKI and iRAKI are depicted for 4-fold retrospective undersampling of the neuro(3) FLAIR-dataset. GRAPPA exhibits pronounced noise enhancement, which is successfully suppressed in standard RAKI. However, RAKI exhibits residual artefacts, which are successfully suppressed in iRAKI. Its improved reconstruction quality is also underlined by quantitative metric measures, as indicated by the PSNR, the NMSE as well as the SSIM (see Fig. 5 B). Note that 25 original ACS lines were used in training for this datasets (i.e. 8% of 320 Phase-encoding lines).

Figure 4: Both T1- and T2-weighted acquisitions were 4-fold retrospectively undersampled, and reconstructed with GRAPPA (bottom row) and standard RAKI (top row), both of which were calibrated on 30 central lines of the T1-weighted dataset only. ACS data were not re-inserted (error images scaled for display).
For reconstruction of the neuro(1) T1-dataset, 18 original ACS lines were used in training (i.e. 8% of 224 Phase-encoding lines) for 4-fold retrospective undersampling (see Fig. 6 A).

Figure 6: A) GRAPPA, standard RAKI and iRAKI in comparison at 4-fold retrospective undersampling of the T1 neuro(1) dataset, and B) of the T1 neuro(2) dataset. Note that 18 and 25 ACS lines were used for training, respectively (8%). In addition, corresponding phase-constrained image reconstruction via VCCs are shown for standard and iRAKI, too. Error images are shown below, and scaled for display. The artefacts in the posterior region in A) can be attributed to pulsatile flow.

While standard RAKI suffers from severe residual artefacts and contrast-loss, which deteriorate its visual appearance, iRAKI provides an improved visual appearance, as it strongly reduces the artefacts as well as the pronounced noise enhancement apparent in GRAPPA. It also outperforms both standard RAKI and GRAPPA regarding SSIM, PSNR and NMSE (see Supporting Information Tab. S1 for numeric results). Moreover, iRAKI preserves
noise resilience of standard RAKI. This observation is indicated by SNR maps of GRAPPA, standard RAKI and iRAKI depicted in Fig. 7 (B, top), which were obtained from the neuro(2) T1-dataset at 4-fold retrospective undersampling using 25 ACS lines (i.e. 8% of 320 Phase-encoding lines). The SNR is decreased in GRAPPA, especially at image-center due to g-factor noise amplification. However, standard RAKI shows strongly improved SNR regarding GRAPPA (see also Fig. 6 B for depiction of image reconstructions). In comparison to standard RAKI, iRAKI shows further improved noise suppression.

![Figure 7: A) SNR map of the fully-sampled reference image of the T1 neuro(2) dataset. B) SNR maps of GRAPPA, standard RAKI and iRAKI at 4-fold retrospective undersampling (top), and including VCC (bottom). Corresponding image reconstructions are depicted in Fig. 6 (B). C) Mean SNR within the ROI marked in A), which is scaled with the square-root of the effective acceleration factor $R_{eff}$. For this example (4-fold undersampling), $R_{eff} = 3.2$, as 25 original ACS lines were used for training (8% of 320 Phase-encoding lines).](image)

An additional improvement in reconstruction performance is achieved by the phase-constrained reconstruction using VCCs: We observe that standard RAKI provides a strongly improved SNR (see Fig. 7 (B, bottom) for SNR maps of the neuro(2) dataset), however, this benefit comes along with residual artefacts (see Fig. 6 A and B). On the other hand, iRAKI prevents the emerge of residual artefacts in standard RAKI, but also preserves its greatly
improved noise resilience, as it yields similarly improved SNR, thus, providing a strongly enhanced visual appearance for both datasets.

Iterative RAKI in combination with VCCs also yields the best SSIM, PSNR and NMSE for both datasets and for both \( R = 4 \) and \( R = 5 \) (see Supporting Information Tab. S1 for numerical results). Similar results were observed for the neuro(1) T2-dataset (see Supporting Information Fig. S3 for image depiction).

Note that in Figure 7 C, the mean of the SNR within a ROI (\( \overline{SNR}_{ROI} \)) is scaled by \( \sqrt{R_{\text{eff}}} \) to compensate for the impact of k-space undersampling (with \( R_{\text{eff}} \): effective acceleration rate) and to indicate the noise-enhancement or -suppression caused by the reconstruction algorithm analogous to the g-factor [2, 27]. For both standard and iRAKI this value is increased compared to the reference image, and hence shows the denoising capabilities of RAKI, especially when VCCs are employed. In analogy to GRAPPA this would represent a g-factor \( g < 1 \).

At 5-fold retrospective undersampling, noise enhancement appears more severely in GRAPPA, and residual artefacts are more apparent in standard RAKI for all evaluated datasets (see Fig. 8 (A), for the neuro(1) T1-dataset, Fig. 8 (B) for the neuro(2) T1-dataset, and Supporting Information Fig. S2 (A) for the neuro(3) FLAIR-dataset. However, iRAKI still shows strong suppression of both residual artefacts (compared to standard RAKI) and noise enhancement (compared to GRAPPA), and yields outperforming SSIM, PSNR and NMSE (see Supporting Information Tab. S1, and Fig. S2 B). Additional exemplary image reconstructions at 4-and 5-fold undersampling are provided in the supplementary material (see Supporting Information Fig. S3 and Fig. S4). For these additional datasets, similar results are observed as described above.
Figure 8: A) GRAPPA, standard RAKI and iRAKI in comparison at 5-fold retrospective undersampling of the T1 neuro(1) dataset, and B) of the T1 neuro(2) dataset. Note that 18 and 25 ACS lines were used for training, respectively (8%). In addition, corresponding phase-constrained image reconstruction via VCCs are shown for standard and iRAKI, too. Error images are shown below, and scaled for display. The artefacts in the posterior region in A) can be attributed to pulsatile flow.

Pre-Scan Calibration

Fig. 9 (B) depicts results of GRAPPA, standard RAKI and iRAKI using the pre-scan (Fig. 9 A) as training data to reconstruct the 4-fold accelerated neuro(4)-dataset. Note that the contrast information in the pre-scan (proton-density) varies from that of the undersampled image scan (T1). We observe that the standard RAKI reconstruction is deteriorated due to contrast-loss artefacts, which are not present in iRAKI. Moreover, iRAKI still preserves its improved
noise resilience, without the cost of emerging blurring artefacts. Using the variable density acquisition scheme, iRAKI yields a further improved reconstruction quality with enhanced visual appearance (Fig. 9 bottom), given only 20 ACS lines as training data (i.e. 8% of total Phase-encoding lines). Standard RAKI, on the other hand, suffers from pronounced aliasing artefacts (emphasized by arrows), and GRAPPA shows severe noise amplification at the image center, which leads to severe deterioration of the reconstruction quality.

4. Discussion

This study investigated the influence of scan-specific training data on the reconstruction quality of the deep-learning method RAKI, with particular focus on the amount and the contrast information. Moreover, it evaluated an iterative k-space interpolation approach to
improve the reconstruction quality in case of limited scan-specific training data for standard 2D imaging at medium acceleration factors \((R = 4\) and \(R = 5\)). It was demonstrated that the iterative learning approach yields superior reconstruction quality by avoiding the emerge of residual artefacts encountered in standard RAKI. Additionally, it preserves standard RAKI's suppression of noise enhancement compared to GRAPPA using the variable density acquisition scheme as training data for various T1, T2 and FLAIR datasets. Thus, iRAKI incorporates benefits from both GRAPPA and RAKI by suppressing residual artefacts and g-factor noise enhancement, respectively, for a limited amount of ACS as training data enabling higher net acceleration-rates. To overcome the issue of limited training data in standard RAKI, the application of an initial GRAPPA reconstruction has been proposed, but not demonstrated in the original RAKI article [5]. Subsequently to the initial calibration of the CNN-weights in RAKI, the iterative learning approach proposed here incorporates both original ACS lines and reconstructed k-space lines as augmented training data for further refinement of the CNN-weights. This approach is similar to iterative GRAPPA in which the GRAPPA kernel is re-estimated iteratively including reconstructed lines into the GRAPPA-kernel estimation [4]. For iterative GRAPPA, a convergence criterion is incorporated to determine the total number of iteration steps. In iRAKI, on the other hand, the total number of iteration steps is determined from the initial learning rate \((0.05)\), which is decreased constantly after each iteration step by \(0.003\) \((R = 4)\) and \(0.004\) \((R = 5)\). These parameters were chosen heuristically such that the cost-function does not diverge in later iteration steps, and ensure robust performance. The final iteration step is reached, when the learning rate has decayed to zero, and thus, no CNN-weights update happens in the training process. This approach has the advantage of keeping the total reconstruction time limited and predictable, which is particularly beneficial in deep-learning methods as the training procedure is particularly time-consuming. The total training time in iRAKI amounts to \(\approx 180\) s and \(\approx 170\) s for \(R = 4\) and \(R = 5\), respectively, exceeding standard RAKI \((\approx 12s\) and \(\approx 20s)\) and GRAPPA \((< 1.5\) s both \(R = 4\) and \(R = 5\)). Future work should focus on optimizing the training speed to apply Iterative RAKI in clinical applications.

As has been demonstrated, the size of the convolution kernel assigned to the first hidden layer should be increased for better reconstruction performance. However, this requires a sufficient number of ACS lines for training. In this study, the larger kernel provided
significantly improved image reconstructions on the neuro(1) dataset for 50 ACS lines. As for any other deep-learning method with supervised learning procedure, it was shown in this work that the number of training samples is crucial for RAKI's generalization performance. However, in the special case of k-space interpolation, one has to take into account that the number of training samples is determined by the size of the ACS region, as well as by the convolution filter size. The latter determines the extent at which the coil-sensitivity profiles are captured in k-space. Previously, Bauer et al. [22] have shown the benefit of a larger kernel size in terms of the trade-off to the effective number of training samples for standard GRAPPA-based reconstructions. In this work, it was demonstrated that the larger kernel size should be preferred for RAKI, given an increased amount of training data. It was also shown that the reconstruction quality in iRAKI can be further enhanced by incorporating additional image- and coil-phase information into the reconstruction procedure via the virtual conjugate coil (VCC) concept. iRAKI with VCCs reconstructed all test datasets with high SNR and only minor artefacts, while standard RAKI with VCCs yielded severe residual artefacts. However, the VCC concept may be limited in its applicability, as it requires consistent k-space information to avoid residual artefacts. This condition is not necessarily ensured in all imaging experiments. Through the pre-scan calibration experiments, it was shown that iRAKI enables to profit from RAKI's noise-suppression for strongly varying contrast information between calibration- and undersampled data, as it prevents the emerge of contrast-loss artefacts in standard RAKI. The results from Fig. 9 (and also Fig. 4) indicate that RAKI, as modeled in this work with simultaneous multi-coil interpolation, does process contrast information besides the coil-sensitivity information in the k-space data, probably due to its increased number of unknowns. In contrast, iRAKI lacks of the contrast-loss present in standard RAKI, as its training data originate from an initial GRAPPA reconstruction with matching contrast.

Future studies will focus on further optimizing hyperparameters, and including more datasets, e.g. dynamic cardiac imaging. Furthermore, higher acceleration factors may be enabled by combining iRAKI with CAIPRINHA [34].
5. Conclusion

The number and contrast of training samples are essential for standard RAKI reconstruction quality. Given a limited training data amount, the proposed iRAKI combines beneficial features of GRAPPA and standard RAKI and yields reconstructions with strong suppression of both noise and residual artefacts for standard 2D imaging.

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Supporting Information

Supporting Information Table S1

*Tab. S1: Quantitative reconstruction quality measures (Structural Similarity Index Measure, SSIM; Peak Signal-to-noise Ratio, PSNR and Normalized Mean Squared Error, NMSE) for images depicted in Fig. 6 (R=4) and Fig. 8 (R=5).*

|         | SSIM (10^-2) | PSNR | NMSE | SSIM (10^-2) | PSNR | NMSE |
|---------|--------------|------|------|--------------|------|------|
| R=4     |              |      |      |              |      |      |
| GRAPPA  | 87.00        | 36.40| 9.52 | 70.29        | 29.72| 44.33|
| RAKI    | 91.73        | 38.40| 6.16 | 87.38        | 35.67| 11.26|
| VCC-RAKI| 94.44        | 40.68| 3.70 | 92.40        | 38.78| 5.50 |
| iRAKI   | 92.78        | 39.11| 5.10 | 89.24        | 37.17| 8.00 |
| VCC-iRAKI| 94.96      | 41.10| 3.24 | 92.71        | 39.54| 4.61 |
| R=5     |              |      |      |              |      |      |
| GRAPPA  | 86.10        | 36.29| 7.40 | 73.34        | 30.99| 25.05|
| RAKI    | 89.04        | 37.58| 5.50 | 85.19        | 35.64| 8.58 |
| VCC-RAKI| 91.93        | 39.05| 3.91 | 88.70        | 37.32| 5.83 |
| iRAKI   | 91.10        | 38.49| 4.46 | 87.37        | 36.67| 6.74 |
| VCC-iRAKI| 92.65      | 39.57| 3.48 | 89.36        | 37.76| 5.27 |
Supporting Information Figure S1

**Figure S1:** Standard RAKI image reconstructions of two slices from the FLAIR fastMRI dataset (referred to as neuro(3) in the main text) using real- and complex-valued convolution at retrospective undersampling (R=4) and 25 ACS lines for training (8%).
Figure S2:  A) GRAPPA, standard RAKI and iRAKI in comparison for 5-fold retrospective undersampling of the FLAIR fastMRI dataset using 25 original ACS lines as training data (8%). Error images are shown below, and scaled for display. B) Corresponding quantitative reconstruction quality metrics.
Supporting Information Figure S3

**Figure S3**: GRAPPA, standard RAKI and iRAKI image reconstructions of the TSE T2-dataset (referred to as neuro(1) in the main text) at retrospective undersampling **A) R=4** and **B) R=5** using 18 ACS lines for training (8%). Error images are shown below, and scaled for display.
Supporting Information Figure S4

**Figure S4:** GRAPPA, standard RAKI and iRAKI image reconstructions of the FLAIR fastMRI dataset at **A)** 4-fold- and **C)** 5-fold retrospective undersampling using 25 ACS lines as training data (8%). Error images are shown below and are scaled for display. Corresponding quantitative reconstruction quality measures are shown below **B)** for 4-fold and **D)** for 5-fold undersampling.