Deep Learning for QSM Reconstruction without Labels

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ABSTRACT

Current deep learning (DL) techniques for quantitative susceptibility mapping (QSM) reconstruction demonstrated improved performance of QSM reconstruction compared with conventional non-DL methods. However, these end-to-end supervised DL techniques usually require a large amount of labeled training pairs and can be limited to the inherent difficulties of measuring ‘ground-truth’ in QSM. In light of these, we presented an unsupervised DL method for QSM inversion denoted as uQSM. Without accessing to QSM labels, uQSM was trained to perform QSM reconstruction using the physical model. When evaluating multi-orientation QSM datasets, uQSM results have achieved higher levels of quantitative accuracy compared to TKD, TV-FANSI, and MEDI approaches. Additionally, uQSM can better preserve susceptibility anisotropy and microstructures in comparison with QSMnet and COSMOS. In addition, uQSM was evaluated on a large number of single-orientation QSM datasets. Visual assessment showed that uQSM outperformed conventional non-DL QSM reconstruction methods.

Keywords: QSM, Unsupervised Learning.

1. INTRODUCTION

Quantitative susceptibility mapping (QSM) is a MRI technique that can be utilized to estimate tissue magnetic susceptibility values. Tissue magnetism can provide useful image contrast and construct magnetism biomarkers of materials including iron, calcium, and gadolinium. QSM estimates tissue magnetic susceptibility values from the MRI Larmor frequency sensitive phase images, and assumes that the phase shift is primarily caused by tissue-susceptibility-induced magnetic field perturbation. The local field perturbation can be modeled as the convolution of susceptibility distributions with the dipole kernel in k-space.\(^2,3\)

\[
\Delta B(\vec{k}) = \chi(\vec{k}) \cdot d(\vec{k})
\]

\[
d(\vec{k}) = \frac{1}{3} - \frac{k_z^2}{k_x^2 + k_y^2 + k_z^2}
\]

where \(\Delta B(\vec{k})\) is the the field variation related to the source magnetization in k-space along the main magnetic field, \(\chi(\vec{k})\) is the Fourier transform of susceptibility distribution, \(d(\vec{k})\) is the dipole kernel in the k-space.

While the source-to-field forward model can be efficiently computed using Fast-Fourier-Transforms (FFT), the field-to-source inversion faces technical challenges due to division of zeros when \(d(\vec{k}) \approx 0\). Noise amplification upon inversion often causes streaking artifacts and susceptibility quantification errors. Acquiring multiple head orientations data can sufficiently improve the conditioning of the inverse problem.\(^4\) Though infeasible in clinical practice, calculation of susceptibility through multiple orientation sampling (COSMOS) remains the empirical gold-standard for in vivo QSM assessment. Single-orientation susceptibility maps are computed by either thresholding of the convolution operator\(^5-7\) or sophisticated regularization methods.\(^8-11\) However, these conventional methods have difficulties in providing accurate and reliable susceptibility estimation.

Deep learning (DL) have recently been explored to solve varieties of inverse problems, which usually relies on large amounts of training data for end-to-end learning. Some researchers utilized DL techniques to address QSM reconstruction challenges, such as QSMnet,\(^12\) DeepQSM,\(^13\) QSMGAN,\(^14\) which have shown promising with comparison to conventional non-DL methods. QSMnet and QSMGAN used COSMOS results as QSM labels, while DeepQSM were trained using purely synthetic data simulated using the physical model.
Though these end-to-end supervised learning techniques have shown promising in addressing QSM reconstruction challenges, they have several associated constraints. First, the data-driven DL methods require large amounts of labeled data for training. However, acquiring large number of COSMOS data is not only expensive but also time consuming. In addition, it is impractical to acquire multi-head-orientation QSM data from patients with severe diseases. Therefore, the DL methods which are trained using COSMOS data from healthy subjects may not be able to capture the clinical and pathological characteristics of patients and may encounter performance degradation when applying to pathological data. In addition, though COSMOS is widely used the ‘gold standard’, it neglects of the susceptibility anisotropy and can contain errors from registration procedure. Though synthetic data can provide a reliable and cost-effective way for training, the generalizability is questionable when the test data deviate from the training data.

Due to the difficulties of collecting large amounts of training data or measuring the ‘ground truth’ in standard supervised DL, unsupervised DL and self-supervised learning (SSL) are emerging research direction for solving inverse problems. Deep image prior (DIP) used neural network structure as regularization without prior training to solve inverse problems such as noise reduction, super-resolution, and inpainting. Early stopping was often used in DIP to avoid overfitting to the noise in the input data. Senouf et al. proposed SSL as solver of accelerated MRI reconstruction using forward model for training. Yaman et al. presented a novel SSL approach for MRI Reconstruction without fully-sampled data by dividing the acquired sub-sampled points for each scan into training and validation subsets, which can perform similarly to the supervised approach that is trained with fully-sampled references. In addition, there are some papers applying unsupervised DL for MR imaging on R2* map calculation, metal artifact correction.

In this work, we extended unsupervised DL techniques for QSM dipole inversion. The unsupervised DL approach, denoted as uQSM, required no QSM labels during training. By taking local field and brain mask as the inputs, uQSM was trained using 3D convolutional neural networks (CNNs) with encoder-decoder architecture. The physical model used in the loss function enforced the neural network to update the network weights and learn how to do dipole inversion.

For quantitative evaluation, uQSM was applied on 9 datasets acquired with multiple head orientations. When compared with TKD, MEDI, TV-FANSI with COSMOS as a reference, the proposed uQSM achieved better quantitative metrics score. In addition, uQSM can better preserve susceptibility anisotropy and microstructures compared with QSMnet and COSMOS. Moreover, four hundred single-orientation datasets were used to qualitative evaluation of the reconstructed maps of TKD, MEDI, TV-FANSI, QSMInvNet and uQSM.

2. METHODS

A 3D convolutional neural network with encoder-decoder structure was trained for a 3D dipole deconvolution. This network takes local field patches and a brain mask as inputs to infer resulting susceptibility maps. The neural network architecture is shown in Figure.2.
During uQSM training, the target susceptibility maps were not provided. To enable the neural network to learn to update the weights and QSM outputs, the loss function incorporated the data consistency term.

\[ L_\chi = \| W (e^{jdx} - e^{jdy}) \|_1 \]  

(3)

where \( W \) was data weighting term which can be the magnitude image or noise weight matrix. Since noise is spatially variant in the field measurements, the nonlinear dipole inversion as above is widely used in conventional QSM reconstruction methods to get more robust QSM estimations.\(^\text{24,25}\) Therefore, we applied the nonlinear dipole convolution data consistency loss in the loss function.

\[ L_{TV} = \| G_x (\chi) \|_1 + \| G_y (\chi) \|_1 + \| G_z (\chi) \|_1 \]  

(4)

where \( G_x, G_y, \) and \( G_z \) are image gradient operator. The total variation loss of the reconstructed susceptibility map was included to serve as a regularization term to preserve important details such as edges whilst removing unwanted noise in the reconstructed susceptibility map.

\[ L_{Total} = L_\chi + \omega L_{TV} \]  

(5)

The loss function combined of data consistency loss and the total variation loss. \( \omega \) was a penalty term which was a hyperparameter of the neural network.

2.1 Data

2.1.1 Multi-orientation Data

9 QSM datasets were acquired using five head orientations and a 3D single-echo gradient recalled echo (GRE) scan with voxel size 1x1x1mm\(^3\). QSM data processing was implemented as below, whereby offline GRAPPA reconstruction was used to reconstruct magnitude and phase images from saved k-space data,\(^\text{26}\) coil combination using sensitivities estimated with ESPIRiT,\(^\text{27}\) BET was used (FSL, FMRI, Oxford, UK) for brain mask extraction,\(^\text{28}\) the Laplacian method for phase unwrapping,\(^\text{29}\) and RESHARP for background field removal\(^\text{30}\) with spherical mean radius 4mm. COSMOS results were calculated using the 5 head orientation data registered using FLIRT (FSL, FMRI, Oxford, UK).

In the training phase, local field patches from a total of 45 scans from 9 datasets were cropped with patch size 96x96x96 voxels with an overlapping scheme of 16.6 percent overlap between adjacent patches. A total of 2950 patches were generated for training and validation with split ratio 9/1. In the loss function, \( \lambda \) was set 0.03. The ADAM optimizer was used for the deep learning model training. An initial learning rate was set as 0.0001, with exponentially decay at every 200 steps. \( W \) was set the magnitude image. Two NVIDIA Tesla k40 GPUs were used for training with batch size 4. The model was trained and evaluated using Keras with Tensorflow as a backend. After training, the full local field at normal head orientation was inputted in the trained DL model to get QSM estimates.

The reconstructed QSM maps using uQSM, TKD, TV-FANSI, and MEDI were compared with respect to the gold-standard COSMOS QSM maps in 9 datasets. Peak signal-to-noise ratio (pSNR), normalized root mean squared error (NRMSE), high-frequency error norm (HFEN), and structure similarity index (SSIM) were used as quantitative metrics to measure the QSM reconstruction quality. When comparing uQSM and QSMnet, 5 out of 9 datasets were used since they were used as the testing datasets in the QSMnet publication.\(^\text{12}\)
2.1.2 Single-orientation Data

400 QSM datasets were collected on a 3T MRI scanner (GE Healthcare MR750) from a commercially available susceptibility-weighted software application (SWAN, GE Healthcare). The data acquisition parameters were as follows: in-plane data matrix 320x256, field of view 24 cm, voxel size 0.5x0.5x2.0 mm³, 4 echo times [10.4, 17.4, 24.4, 31.4] ms, repetition time 58.6 ms, autocalibrated parallel imaging factors 3x1, total acquisition time 4 minutes.

Complex multi-echo images were reconstructed from raw k-space data using GE Orchestra. The brain masks were obtained using the SPM tool. After background field removal using the RESHARP method with spherical mean radius 4mm, susceptibility inversion was performed using TKD, TV-FANSI, MEDI, and QSMInvNet.

For uQSM training, 8000 patches with patch size 128x128x64 of local field maps, and brain masks from 200 QSM datasets were used. In the loss function, \( \lambda \) was set 0.01 for training. \( W \) was set the noise standard deviation on the field map. After training, the trained DL model took the full local field to get QSM estimates.

3. RESULTS

Table 1 summarized quantitative metrics of four reconstruction methods on nine QSM datasets with COSMOS as reference. Compared to TKD, TV-FANSI, and MEDI, uQSM results achieved the best metric scores in RMSE, SSIM, and HFEN, suggesting the best performances for all criteria.

| Method | pSNR(dB) | NRMSE(%) | HFEN(%) | SSIM  |
|--------|----------|----------|---------|-------|
| TKD    | 43.4 ± 0.5 | 101.4 ± 7.2 | 77.8 ± 6.9 | 0.83 ± 0.01 |
| TV-FANSI | 41.5 ± 0.7 | 84.7 ± 6.2  | 76.7 ± 6.7 | 0.88 ± 0.02 |
| MEDI   | 41.5 ± 0.7 | 125.3 ± 8.5 | 106.2 ± 9.7 | 0.90 ± 0.01 |
| uQSM   | 44.6 ± 0.4 | 87.8 ± 6.6  | 74.7 ± 6.6 | 0.88 ± 0.01 |

Table 2. Means and standard deviations of the quantitative performance metric, pSNR, NRMSE, HFEN, and SSIM of QSMnet and uQSM results on 5 test datasets.

| Method   | pSNR(dB) | NRMSE(%) | HFEN(%) | SSIM  |
|----------|----------|----------|---------|-------|
| QSMnet   | 45.8 ± 0.3 | 76.1 ± 4.7 | 64.1 ± 4.7 | 0.90 ± 0.02 |
| uQSM     | 44.8 ± 0.3 | 85.4 ± 6.5 | 71.4 ± 5.0 | 0.88 ± 0.01 |

In Table 2, quantitative metrics of 5 testing data from QSMnet and uQSM displayed. uQSM achieved comparable metrics scores compared with QSMnet.
Figure 2. QSM maps reconstructed by the six methods from a multi-orientation data. TKD (a), TV-FANSI (b) and MEDI (c) maps showed oversmoothing and/or streaking artifacts. The uQSM (e) map shows preserved details and invisible artifacts.

Fig. 2 displayed QSM maps from a representative dataset in three planes. TKD showed well-preserved details, yet streaking artifacts. TV-FANSI and MEDI maps showed increased blurring due to their heavy use of spatial regularization. uQSM results demonstrated the superior sharpness as the same time minimal observed streaking artifacts. QSMnet can generate COSMOS-like maps, showing contrast loss in regions of globus pallidus and putamen.
Figure 3. uQSM and QSMnet images in 5 head orientations from a multi-orientation data. QSMnet (i) images showed consistent across five head orientations, while uQSM (ii) displayed large variability in QSM results for the multiple head orientations.

Fig. 3 displayed the QSM image of five head orientations reconstructed by QSMnet and uQSM from a multi-orientation data. QSMnet images showed consistent in five head orientations, while uQSM had large variability in QSM results for the multiple head orientations.

4. COMPARISON WITH DIP

We compared uQSM with DIP. DIP was trained with the same neural network architecture as Fig. 2. DIP performed QSM inversion for each individual dataset without prior network training. By taking full local field map and brain mask as the inputs, DIP used the loss 5 to update the QSM output. To avoid overfitting which can result in severe streaking artifacts in the reconstructed QSM images, DIP stopped after a certain number of steps.
Figure 4. Comparison of QSM results from two multi-orientation datasets reconstructed by DIP and uQSM. DIP and uQSM can produce visually comparable QSM images.

Fig. 4 displayed QSM images from two multi-orientation datasets reconstructed by DIP and uQSM. We can note that DIP and uQSM results showed comparable image quality.
Figure 5. Comparison of QSM results from two single-orientation datasets reconstructed by DIP and uQSM. DIP results had visible streaking and shading artifacts (black arrows). uQSM can produce better QSM images with non-visible image artifacts.

Fig.5 displayed QSM images from two single-orientation datasets reconstructed by DIP and uQSM. DIP results showed inferior susceptibility maps with streaking artifacts while uQSM generated better susceptibility maps.

5. IMPACT OF DATA CONSISTENCY LOSS

In the loss function of uQSM, the nonlinear dipole inversion data consistency loss was adopted. Here, we investigated the impact of three different data consistency losses.

The first was linear dipole inversion (LDI),

$$L_{LDI} = \| d^*\chi - y \|_1$$ (6)

The second was weighted linear dipole inversion (WLDI),

$$L_{WLDI} = \| W(e^{ldx} - e^{ly}) \|_1$$ (7)

The third was weighted nonlinear dipole inversion (NDI),

$$L_{NDI} = \| W(d^*\chi - y) \|_1$$ (8)
Figure 6. Comparison of QSM results from a multi-orientation data reconstructed using three data consistency loss in uQSM training. LDI, WDI, and NDI generated comparable QSM images.

Fig. 6 displayed the QSM results of a multi-orientation data reconstructed using three data consistency loss in neural network training. It was observed that LDI, WDI, and NDI images have comparable image quality.
Figure 7. Comparison of QSM results from a single-orientation data reconstructed using different data consistency loss in uQSM training. LDI, WDI results showed black shading artifacts close to vessels (black arrows), while NDI can generate better QSM images.

Fig. 7 displayed the QSM results of a single-orientation data reconstructed using three data consistency loss in network training. It was observed that LDI, WDI images displayed black shading artifacts close to brain vessels with high susceptibility values, while NDI can suppress the artifacts in QSM images.

5.1 Impact of TV loss
In the uQSM loss, the TV loss was incorporated in order to suppress the noise in the reconstructed QSM images.
Figure 8. Comparison of QSM results from two multi-orientation datasets reconstructed with/without loss in network training. uQSM trained without TV loss has high noise in the QSM images, while uQSM trained with TV loss can suppress the noise and achieve higher SNR.

Fig.8 displayed QSM results from two multi-orientation datasets reconstructed with/without loss in neural network training. uQSM trained without TV loss had high noise in the QSM images, while uQSM trained with TV loss can suppress the noise and achieved higher SNR.

6. DISCUSSION

In this work, an unsupervised DL method for QSM dipole deconvolution was proposed. uQSM was trained using 3D encoder-decoder CNNs. Without accessing to QSM labels during training, uQSM learned to perform dipole inversion through physical model.

From quantitative evaluation using multi-orientation QSM datasets, uQSM outperformed TKD, TV-FANSI, and MEDI with COSMOS as a reference. While compared with QSMnet which was trained using COSMOS results as QSM labels, uQSM can achieve comparable quantitative metric scores. From visual assessment, uQSM can better preserve microstructures and have less image artifacts.

When using single-orientation datasets for qualitative assessment, uQSM results show better image quality than conventional non-DL methods. TKD, MEDI, and TV-FANSI results have streaking artifacts while uQSM
results show non-visible streaking artifacts. At the same time, uQSM can better preserve microstructures while other methods suffer from oversmoothing.

Four variant encoder-decoder architectures produce comparable QSM images, which may indicates there are many different network architecture can be used for QSM reconstruction. The four variant encoder-decoder 3D CNNs require different calculations and memory consumption. Since the network architecture may not have much influence on QSM results, it is preferable to choose the network architecture with less memory consumption and less calculation.

When comparing three different data consistency loss, it is found that linear dipole inversion loss and weighted linear dipole inversion are prone to introduce streaking artifacts in the reconstructed QSM images. The nonlinear dipole inversion can better suppress the artifacts and produce better QSM images.

When investigating the effect of TV loss, it is found that uQSM trained with TV loss can greatly suppress the noises in the multi-orientation datasets. This is maybe that the multi-orientation datasets have low SNR since they were acquired using a single echo pulse sequence with each orientation scan time about 1 minute. Therefore, it is important to incorporate the TV loss in the loss function when the data have high noise.

We also compared uQSM with DIP. DIP has the advantage that it requires no prior training. However, DIP needs early-stopping to avoid overfitting. In the experiment, it is found that DIP are prone to generate QSM image with streaking artifacts when overfitting, while uQSM does not have this problem. In addition, DIP requires hundreds of steps to get the results, which can take long times for each individual dataset. However, uQSM can predict QSM in a couple of seconds once trained.

The proposed unsupervised DL technique for QSM reconstruction approach has several advantages of the proposed uQSM. First, uQSM is unsupervised-based which requiring no training pairs. It can greatly solve the difficulties of preparing large amount of labeled data for end-to-end training. Second, uQSM trained using physical model can better reflect susceptibility anisotropy. Though COSMOS results were treated as gold standard of QSM, it neglects susceptibility anisotropy and can suffer from registration error.

There are still some limitations of uQSM. First, uQSM was relying on the physics-based training formalism. More work can be done by using more sophisticated model. Moreover, these DL-based QSM dipole inversion methods can still be affected by the performance of background field removal algorithms. More work is needed to evaluate the effects of the background field removal performance on QSM quantification.

7. CONCLUSION

In summary, this work has introduced an unsupervised DL-based QSM inversion approach relying on a physics-based training formalism. This approach can substantially improve addressing the difficulties of obtaining COSMOS data. This new capability opens a wide array of potential QSM investigations using deep learning to derive QSM maps.

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