ENSURE: ENSEMBLE STEIN’S UNBIASED RISK ESTIMATOR FOR UNSUPERVISED LEARNING

Hemant Kumar Aggarwal, Mathews Jacob

University of Iowa, Iowa, USA

ABSTRACT

Deep learning accelerates the MR image reconstruction process after offline learning of a deep neural network from a large volume of clean and fully sampled data. Unfortunately, fully sampled images may not be available or are difficult to acquire in several application areas such as high-resolution imaging. Previous studies have utilized Stein’s Unbiased Risk Estimator (SURE) as a mean square error (MSE) estimate for the image denoising problem. Unrolled reconstruction algorithms, where the denoiser at each iteration is trained using SURE, has also been introduced. Unfortunately, the end-to-end training of a network using SURE remains challenging since the projected SURE loss is a poor approximation to the MSE, especially in the heavily undersampled setting. We propose an ENsemble SURE (ENSURE) approach to train a deep network only from undersampled measurements. In particular, we show that training a network using an ensemble of images, each acquired with a different sampling pattern, can closely approximate the MSE. Our preliminary experimental results show that the proposed ENSURE approach gives comparable reconstruction quality to supervised learning and a recent unsupervised learning method.

Index Terms—Unsupervised learning, SURE, fine-tuning, parallel MRI.

1. INTRODUCTION

MRI is a non-invasive imaging modality that gives better soft-tissue contrast than PET/CT. Accelerating the MR scanning process is an active research area since it can reduce the scanning cost and lead to patient comfort. One way to accelerate MRI is by acquiring fewer samples in k-space and use a compressed sensing (CS) based algorithm during reconstruction. The CS based algorithms can help in reducing the acquisition time, but at the cost of computational complexity. Deep learning based techniques help to speed-up the reconstruction time after training on large datasets. Unfortunately, fully sampled and noise-free training data is not available or hard to be acquired in several MR applications, such as high-resolution MRI. The main focus of this work is on unsupervised deep learning, where no ground-truth is needed for training.

There are a large number of successful supervised deep learning methods for MR image reconstruction problem. We broadly classify these methods into two categories, namely direct-inversion and model-based methods. The model-based methods, such as [12], explicitly ensure the data-consistency as oppose to direct-inversion methods, such as [3][4]. This work focuses on unsupervised training that is applies to both of these training approaches.

The unsupervised learning for image reconstruction is a comparatively scarcely studied and challenging problem since it requires training a neural network only from undersampled measurements. The deep image prior (DIP) [5] suggests that a CNN can act as an implicit regularizer; therefore, mean-square-error minimization only on the measured and reconstructed k-space can reconstruct a fully sampled image. However, DIP requires to stop the algorithm manually and results in a sub-optimal reconstruction quality compared to supervised learning methods. [6] proposes a CycleGAN based method for dynamic contrast enhancement in MR angiography based on optimal transport theory. SSDU [7] suggests partitioning the measured k-space into two disjoint sets. The first set is used in the data consistency step, and another set is used for measuring the MSE loss.

Stein’s unbiased risk estimator (SURE) [8] is an estimator for mean-square-error (MSE) and has been widely used to find regularization parameters in denoising problems [9] and recently to train deep denoisers [10]. The generalized SURE (GSURE) approach extended SURE to inverse problems, where an estimate of the projection of the MSE to the range of the measurement operator was considered [10]; this approach also used to determine regularization parameters of inverse problems. A challenge in directly using GSURE to train deep image reconstruction algorithm is the poor approximation of the MSE by the projected MSE, especially in compressed sensing applications.

LDAMP-SURE also proposes to learn the reconstruction network on patches of color images as layer-by-layer training where each layer trains a denoiser independently using
SURE. Approach in [12] shows the application of LDAMP-SURE to parallel MRI but requires fully sampled data to pre-train a single denoiser.

In this proposed ensemble SURE (ENSURE) approach, we first show that projected MSE is equivalent to a weighted MSE when estimated over an ensemble of sampling operators. We also derive an unbiased estimate for this weighted MSE, following [10]. We further consider two special cases of single-channel and multichannel MRI. The preliminary experiments demonstrate that proposed ENSURE approach can give comparable results to supervised training in both direct-inversion and model-based settings.

2. BACKGROUND

2.1. Inverse problems

We consider the case where an image \( \rho \) is only known through its measurements \( y_s \) from the acquisition operator \( A_s \) parameterized by the random vector \( s \). The vector \( s \) can be viewed as the k-space sampling mask. The forward model representing the measurement process is given by

\[
y_s = A_s \rho + n. \tag{1}
\]

We assume the noise \( n \) to be Gaussian distributed with zero mean and covariance matrix \( C \) such that \( n \sim \mathcal{N}(0, C) \). The probability density of \( y_s \) is given by \( p(y_s|s) = \mathcal{N}(A_s \rho, C) \).

2.2. Deep learning based image recovery

Deep learning methods have been introduced to reconstruct fully sampled image \( \hat{\rho} \) from noisy and undersampled measurements \( y_s \). The recovery using a deep neural network \( f_\Phi \) with trainable parameters \( \Phi \) can be represented as

\[
\hat{\rho} = f_\Phi(y_s). \tag{2}
\]

Here \( f_\Phi \) can be a direct-inversion or a model-based deep neural network. Most of the current deep learning solutions rely on supervised training, where fully sampled images are used as ground truth. However, it is challenging to acquire fully sampled data in many cases.

2.3. Unsupervised learning for inverse problems

The unsupervised learning of denoising methods (i.e., when \( A = I \)) have been extensively studied, resulting in popular schemes such as Noise2Noise [13] and Noise2Void [14]. Recently, several researchers have adapted the Stein’s unbiased risk estimate (SURE) [8] for the unsupervised training of deep image denoisers [11][12]. When \( C = \sigma^2 I \), SURE methods use an unbiased estimate of the mean-square error (MSE) as

\[
\mathbb{E}[\|\hat{\rho} - \rho\|^2] = \mathbb{E}[\|\hat{\rho} - y_s\|^2] + 2\sigma^2 \mathbb{E}[\nabla_y \cdot h(y_s)] - N\sigma^2. \tag{3}
\]

This scheme has been demonstrated in [11][12] in the training of deep learned denoisers.

SURE methods have been extended to inverse problems in [10] with rank deficient \( A_s \) operators, where the original MSE is approximated by the projected MSE as

\[
\text{MSE}_s = \mathbb{E}_{\hat{\rho}} \| P_s (\hat{\rho} - \rho) \|^2, \tag{4}
\]

where \( P_s = A_s^H (A_s A_s^H)^{-1} A_s \) is the projection operator to the range space of \( A_s^H \). This extension was considered for the training of deep learned inverse problems in [11]. However, in applications involving heavily undersampled measurements, \( \text{MSE}_s \) is a poor approximation of \( \text{MSE} \); current methods report poor results using SURE. LDAMP-SURE algorithm in [11] instead rely on layer-by-layer training of deep learning denoisers, assuming the noise at each iteration to be Gaussian distributed. The independent training of the denoisers is expected to be sub-optimal compared to end-to-end training. This approach suffers from two deficiencies. First, this approach relies on approximate message passing algorithm and is not directly applicable to any unrolled iterative algorithm. Second, LDAMP-SURE performed limited result evaluation on small patches of natural images with Gaussian measurement matrices. Our proposed ENSURE approach is applicable to any direct-inversion as well as model-based unrolled networks. In this work, we evaluate our proposed approach on more general measurement matrices with complex-valued parallel MR images.

3. PROPOSED ENSEMBLE SURE (ENSURE)

To overcome the poor approximation of the MSE by \( \text{MSE}_s \), we propose to consider an ensemble of sampling operators. Specifically, we assume the sampling mask \( s \) to be a random vector drawn from the distribution \( S \). Note that this acquisition scheme is realistic and can be implemented in many applications. For instance, it may be difficult to acquire a specific image in a fully sampled fashion due to time constraints. However, one could use a different undersampling mask for each image \( \rho \in I \).

Instead of the projected MSE in (4), we first consider the expectation of the projected MSE, computed over different sampling patterns and images, which simplifies to a weighted MSE. Let \( u_s = \frac{1}{\sigma^2} A_s^H y_s \) be the sufficient statistic for the model in (1) then

\[
Q = \mathbb{E}_{\rho \sim S} \left[ \mathbb{E}_{u_s} \left[ \| P_s (f_\Phi(u) - \rho) \|^2 \right] \right]. \tag{5}
\]

Using properties of Expectation and projection matrices, (5) simplifies to weighted MSE term

\[
Q = \mathbb{E}_{u_s} \left[ \| W (f_\Phi(u) - \rho) \|^2 \right]. \tag{6}
\]

If the sampling patterns are chosen appropriately, we can guarantee that \( W \) is a full-rank matrix with high probability.
Although, this framework is extendible to rank-deficient case as well, in this work we consider full-rank $W$. Depending on $S$, some subspace components may be weighted more than others. To compensate for this weighting, we now consider the weighted version of the projected MSE using the matrix $W^{-1}$. We hence consider a weighted version of (6), denoted by

$$\mathcal{L} = \mathbb{E}_{u_s}\left[\mathbb{E}_{s}\left[\|W_s(f_\phi(u_s) - \rho)\|^2\right]\right]$$

Specifically, we choose the operator $W_s = W^{-1}P_s$ depending on the sampling pattern. The expression in (7) opens the door to estimating the true MSE from only the undersampled measurements. It is impossible to compute (7) since it depends on $\rho \in \mathbb{I}$. We thus approximate it by its unbiased ENSURE estimate.

**Lemma 1** Let $A_s; s \in S$ denote a family of sampling operators measuring images $\rho \in \mathbb{I}$, and let $f_\phi$ be a weakly differentiable reconstruction network. Then the weighted projected loss $\mathcal{L}$ in (8) is equal to

$$\mathcal{L} = \mathbb{E}_{u_s}\left[\mathbb{E}_{s}\left[\|W_s f_\phi(u_s) - \rho_{ML,s}\|_2^2\right]\right] + \frac{2\mathbb{E}_{u_s}[\nabla_{u_s} \cdot f_\phi(u_s) + K\text{ constant}]}{\mathbb{E}_{u_s}[\|\nabla_{u_s} f_\phi(u_s)\|_2^2]}$$

where

$$\rho_{ML,s} = -\left(A_s^H C^{-1} A_s\right)^\dagger A_s^H C^{-1} y_s$$

is the maximum likelihood solution of (1). $\nabla_{u_s}$ represents the divergence of the network $f_\phi$ with respect to its input $u_s$.

We now consider two special cases of single-channel and multi-channel MRI.

### 3.1. Single-channel MRI

In the single-channel setting $A_s(\rho) = SF(\rho)$, where $F$ is the Fourier transform and $S$ is the sampling matrix. Here, $\rho_{ML,s} = F^H S^H y_s$. We assume the probability of a specific k-space sample to be acquired as a Bernoulli distribution with a probability $w_{ij}$, which may be varying spatially; a variable density distribution with higher density in the center of k-space is a common choice in compressed sensing application. The expectation of the projection operators $P_s$ in this case yields $W = F^H \text{diag}(w) F$. In this case, (8) simplifies to

$$\mathcal{L} = \mathbb{E}_{s}\mathbb{E}_{u_s}\left[\|W^{-1}(A_s f_\phi(u_s) - y_s)\|^2\right] + \mathbb{E}_{u_s}\left[\|\nabla_{u_s} f_\phi(u_s)\|_2^2\right]$$

We evaluate the divergence term using Monte-Carlo SURE approach [15].

![Fig. 1](image-url) Visual representation of the proposed ENSURE estimate in (9). Here, $\oplus$ and $\otimes$ represent the addition and inner-product, respectively.

### 3.2. Multichannel MRI

In the context of parallel MRI, the sampling operator is given by $A(\rho) = SFC y$, where $C$ denotes the coil sensitivity weighting, $F$ denotes the Fourier transform and $S$ denotes the multichannel sampling matrix. Here, we rely on $\rho_{ML,s}$ computed using the conjugate gradient SENSE algorithm, which solves

$$\rho_{ML,s} = \arg\min_{\rho} \|A_s \rho - y_s\|^2 + \lambda \|\rho\|^2$$

with $\lambda \to 0$. The projection $P_s \rho$ of $\rho$ onto the range space of $A^H_s$ is obtained by solving (11). In this work, we will choose $W = F^H \text{diag}(w) F$ for simplicity, which will undo the low-pass weighting of the MSE introduced by the averaging in (4). The outline of the data term and the divergence term are shown in Fig. 1.

Note that for each sampling pattern, we compare the difference between the reconstructed image and the corresponding SENSE solution. However, we only compare the projections of the errors onto the range space of the measurement operator, evaluated using CG-SENSE. An additional weighting is used to compensate for the non-uniform density of the sampling patterns in k-space. The divergence term may be viewed as a network regularization, which serves to minimize noise amplification. The divergence term is computed using Monte-Carlo approximation [15]. Note that the use of the data term alone will result in overfitting, similar to observations in deep image prior methods as the number of epochs increase. As shown by the theory, the averaging of the sum of the error measures and divergence terms over a variety of sampling patterns closely approximate the MSE, without requiring ground truth images.
4. EXPERIMENTS AND RESULTS

We consider a parallel MRI brain data using a 3-D T2 CUBE sequence with Cartesian readouts using a 12-channel head coil at the University of Iowa on a 3T GE MR750w scanner. The matrix dimensions were $256 \times 232 \times 208$ with a 1 mm isotropic resolution. Fully sampled multi-channel brain images of nine volunteers were collected, out of which data from five subjects were used for training, while the data from two subjects were used for testing and the remaining two for validation.

We compare the proposed ENSURE approach with a supervised learning approach named MoDL and a recent unsupervised learning approach named SSDU. We also compared the performance in direct-inversion and model-based frameworks. The direct inversion approach had a standard 18-layer ResNet architecture with 3x3 filters and 64 feature maps at each layer. Both SSDU and MoDL had the same architecture with 5-repetitions of ResNet and data consistency steps with shared weights. For SSDU, we used 60% of measured k-space for data consistency step and 40% for MSE estimation, as suggested in the [7]. The real and imaginary components of complex data were used as channels in all the experiments.

Table 1 shows results of proposed ENSURE approach on the test dataset at six-fold acceleration and noise of standard deviation $\sigma = 0.01$. Table 1 shows comparison of self-supervised learning via data undersampling (SSDU)[7] and the proposed ENSURE approach. The proposed approach results in higher peak signal to noise ratio (PSNR) and structural similarity index (SSIM) as compare to a recent existing unsupervised algorithm (SSDU).

Figure 2 compares the visual quality obtained from the proposed unsupervised learning using the ENSURE approach with a supervised learning and an existing unsupervised learning (SSDU) approach at six-fold acceleration and noise std=0.03. It is clear from the zoomed region that the proposed ENSURE approach provides cleaner reconstruction than the existing SSDU approach.

| Framework            | Direct-Inversion | Model-Based |
|----------------------|------------------|-------------|
| Algorithm            | PSNR  | SSIM  | PSNR  | SSIM  |
| SSDU [7]             | 31.85 | 0.79  | 37.89 | 0.94  |
| ENSURE               | 32.67 | 0.88  | 38.44 | 0.96  |
| Supervised           | 34.85 | 0.95  | 39.31 | 0.98  |

Table 1. Quantitative comparison of PSNR and SSIM values in the direct-inversion and model-based framework at six-fold acceleration in the presence of Gaussian noise of standard deviation=0.01.
5. CONCLUSIONS

We proposed an unsupervised learning approach for linear inverse problems for the non-trivial measurement operator. We showed that projected MSE is equivalent to weighted MSE when expected over an ensemble of sampling operators. We further derive an unbiased estimate, termed ENSURE, for the inverse weighted MSE. Here, we omitted the proof of Lemma 1 due to space constraints. The current experiments are limited to a relatively small dataset as proof of concept.

6. REFERENCES

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