

Noise Estimation in Zero-Shot Plug-and-Play Reconstruction for 3D MPI Data [†]

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Abstract

In Magnetic Particle Imaging (MPI), the scans of delta concentrations can be collected in a system matrix and a target distribution of particles injected in a specimen can be retrieved by regularized inversion of the associated linear system, using the scan of the specimen as data. Recent publications show that ill-posed inverse problems can be solved with Plug-and-Play (PnP) algorithms, which split at each iteration the general regularized inversion into a simpler Tikhonov-type problem and a Gaussian denoising problem. By substituting the Gaussian denoising step with machine learning-based denoisers, it is possible to leverage the performance of Neural Networks in the denoising task. In particular, it has been shown that it is possible to employ publicly available and general-purpose denoisers into the MPI reconstruction task in a Zero-Shot fashion (no ad hoc training necessary). In the specific algorithm considered, each denoising step takes as input the noise level of the Tikhonov subproblem and works in particular with a very coarse estimation of the noise level as variance of the iterate. In this work we explore the benefit of using a better estimation of the noise level using convolution with the Laplacian.

Keywords: Magnetic Particle Imaging; system matrix; Plug-and-Play; noise estimation

1. Introduction

Magnetic Particle Imaging (MPI) is an emerging tracer-based imaging modality that employs superparamagnetic nanoparticles as tracer and dynamic magnetic fields for the scanning procedure. Indeed, the nanoparticles injected in a specimen have a non-linear magnetization response to the time-changing magnetic fields that cause a voltage to be induced in receive coils. Such voltage is digitalized into a signal from which the spatial distribution of the nanoparticles is to be reconstructed. After its introduction in 2005 by Gleich and Weizenecker [1], MPI has gained popularity among researchers and a plethora of medical applications have been proposed, among which we would like to mention cancer detection [2] and imaging [3], stem cell tracing [4] and blood flow imaging [5]. Further applications can be found in [6]. The scanning procedure can be described as follows: the practitioners inject a tracer containing the nanoparticles in a specimen to be scanned; the magnetic fields are applied to the specimen in the scanner and the magnetization response of the particles induces a voltage in receiving coils; and the voltage thus collected



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during a scan constitutes the signal from which the distribution of the nanoparticles is to be reconstructed. There are two main reconstruction approaches. Model-based approaches consider models coming from physics to simulate the MPI operator and measurement-based approaches consider a system matrix collected by scanning known delta concentrations. An example of popular model-based approaches are the so called X-Space approaches [7–9], which employ the Langevin theory of paramagnetism [10], from which it is also possible to distill a two-stage algorithm for MPI reconstruction [11,12] that has various points of flexibility for reconstruction quality enhancement [13] and potential applications in multi-patch [14] and reconstruction from partial data [15]. In the measurement-based approach, a calibration procedure is performed by scanning a delta-probe and collecting the responses into a system matrix; given the scan of a specimen, the particle distribution can be reconstructed via regularized inversion of the linear system associated to the system matrix [16]. Classical reconstruction approaches involve Tikhonov regularization [17,18], usually with the Kaczmarz method but also with ℓ^1 priors for noise compression [19]. Recently, machine learning-based approaches have been introduced, among which are the Deep Image Prior (DIP) [20,21] and Deep Equilibrium Models [22]. One particular approach that leverages machine learning is Plug-and-Play (PnP), which has been used in MPI [23]. In [23], the Gaussian denoiser is trained for the MPI reconstruction task on MPI-friendly data. In contrast, in [24], we suggested the ZeroShot- ℓ^1 -PnP approach that employs an openly available general-purpose denoiser [25] that can take noise level maps as inputs and requires no additional training (ZeroShot) specifically for MPI. Because the noise level functions as a parameter in the ZeroShot- ℓ^1 -PnP approach, it is possible to couple it with the Tikhonov reconstruction parameter and produce an automatic parameter update after the first iteration of the ZeroShot- ℓ^1 -PnP algorithm. In particular, the noise level map in [24] has been estimated with the variance of the iterate; in this work we consider a more sophisticated noise level estimation that involves convolution with the Laplacian, similarly to [26] but in 3D. We evaluate the benefits of the estimation on a hybrid 3D MPI dataset.

2. System-Matrix-Based Reconstruction and Zero-Shot Plug-and-Play

In the measurement-based approach the scanning volume is subdivided into a grid and a known concentration of nanoparticles is scanned at each cell position. The scan at each grid cell position is collected to form a system matrix A which represents the response of the scanning system to delta impulses. Once the system matrix is collected, the specimen is inserted into the scanner and scanned; the scan f of the specimen is used to form the linear system $Au = f$ with u as the variable representing the unknown distribution, and the regularized inversion of the system yields the reconstructed concentration u_{rec} . In [24], we proposed to consider the following minimization problem:

$$u_{\text{rec}} = \arg \min_u \{ \|Au - f\|_2^2 + \lambda \mathcal{R}[u] + \alpha \|u\|_1 + \iota_+(u) \} \quad (1)$$

where $\mathcal{R}$ is a regularizer, ι_+ is the indicator function having value 0 if all entries of u are positive and infinity otherwise, and $\lambda, \alpha > 0$ are parameters. Using the half quadratic splitting scheme we proposed in [24], the ZeroShot- ℓ^1 -Plug-and-Play algorithm (ZeroShot- ℓ^1 -PnP from now on) is developed. More specifically, we considered the equivalent problem in consensus form and solved the new constrained minimization problem using half quadratic splitting, which yields a splitting scheme that involves iteratively a Tikhonov-type problem, Gaussian denoising and Soft-Thresholding (details can be found in [24]):

$$u_1^{k+1} = \arg \min_{u_1} \|f - Au_1\|_2^2 + \mu_k \left\| u_1 - \frac{u_2^k + u_3^k}{2} \right\|_2^2 \quad (2)$$

$$u_2^{k+1} = \arg \min_{u_2} \frac{1}{2(\lambda/\mu_k)} \|u_2 - u_1^{k+1}\|^2 + \mathcal{R}(u_2) + \iota_+(u_2) \quad (3)$$

$$u_3^{k+1} = \arg \min_{u_3} \frac{\alpha}{\mu_k} \|u_3\|_1 + \frac{1}{2} \|u_1^{k+1} - u_3\|_2^2. \quad (4)$$

The interesting aspect is that the subproblem in Equation (3) is a Gaussian denoising problem with regularizer $\mathcal{R}$ and Gaussian noise level $\sqrt{\lambda/\mu_k}$. In particular, we treat the problem in Equation (3) using the *deep denoiser prior* by Zhang et al. [25], which is publicly available and has been trained on a large dataset for the specific task of natural image denoising. We point out that no additional training has been done and the application of the denoiser is in a Zero-Shot fashion. The resulting algorithm is the following:

$$u_1^{k+1} = \arg \min_{u_1} \|f - Au_1\|_2^2 + \mu_k \left\| u_1 - \frac{u_2^k + u_3^k}{2} \right\|_2^2 \quad (5)$$

$$u_2^{k+1} = \text{Denoiser}\left(u_1^{k+1}, \sqrt{\lambda/\mu_k}\right) \quad (6)$$

$$u_3^{k+1} = \text{prox}_{\frac{\alpha}{\mu_k} \|\cdot\|_1}(u_1^{k+1}). \quad (7)$$

The fact that the denoiser we use can take the noise level maps as input allows us to couple the parameter μ_k in Equation (5) with the noise level $\sqrt{\lambda/\mu_k}$ in Equation (6). This relationship between the parameters allows for an automatic parameter update in each iteration: if σ_{k+1} is the estimated noise level of u_1^{k+1} , then σ_{k+1} and μ_k are in an inverse quadratic relationship mediated by λ , i.e., $\sigma_{k+1}^2 = \lambda/\mu_k$; moreover, initializing $u_0^2 = u_0^3 = 0$ and treating μ_0 as a hyperparameter, we can estimate σ_1 and fix $\lambda = \mu_0 \sigma_1^2$ for the next iterations. In particular, from iteration $k = 1$, λ is fixed and σ_{k+1} is estimated, providing a unique way to choose $\mu_k = \lambda/\sigma_{k+1}^2$. Therefore, if we can estimate the noise level σ_k and treat μ_0 as a hyperparameter, the parameter can be updated automatically, employing the only noise level estimations of the iterates u_1^{k+1} . In [24] we considered as proof of concept the simple estimation

$$\sigma_k^2 = \text{Var}(u_1^k) = \mathbb{E}[(u_1^k - \bar{u}_1^k)^2], \quad (8)$$

where $\bar{u}_1^k$ is the mean of the variable u_1^k . This worked in the experiments in [24] but the estimation in Equation (8) is only an upper bound on the noise level. In this work, we try a more precise noise level estimation technique to employ in the ZeroShot- ℓ^1 -PnP algorithm. The employed Laplacian-based estimation is explained in the following section.

3. Estimation of the Noise Level

In [26], the author observes that the structures and edges in an image have strong second-order differential components and consequently, if $I(x, y)$ is an image with coordinate x and y , with H, W its height and width, respectively, and if L is a mask representing an approximation of the 2D Laplacian, then the variance σ^2 of the noise of I can be estimated by

$$\sigma^2 = \frac{1}{\text{Var}(L)(W-2)(H-2)} \sum_{x,y} (I(x,y) * L)^2, \quad (9)$$

where $*$ represents convolution. In Equation (6) we use a 2D denoiser on 3D data by performing slice-wise denoising along each axis and averaging the results (as proposed

in [23]). One could think of estimating the noise level of each slice with the formula in Equation (9) and input it in the denoiser to have an optimal denoising effect; however, from this set of slicewise noise estimations one should distill one single parameter μ_k (and λ) for the Tikhonov problem in Equation (5), which is the regularization parameter needed at iteration $k + 1$ to reconstruct a 3D volume. We propose the following procedure: instead of using Equation (9) slicewise, we estimate the variance of the noise of the whole 3D array u_1^{k+1} using an analogous formula:

$$\sigma_{k+1}^2 = \frac{1}{\text{Var}(L_{3D})(W-2)(H-2)(D-2)} \|u_1^{k+1} * L_{3D}\|_2^2 \quad (10)$$

where L_{3D} is the standard seven-point stencil Laplacian and W, H, D are the width, height and depth of the array. Using Equation (10) to estimate the noise level of u_1^{k+1} we can input the estimation σ_{k+1} as constant noise level map for each slice and estimate λ and μ_k coherently to our automatic parameter update in the ZeroShot- ℓ^1 -PnP algorithm.

4. Numerical Experiments

We perform experiments to check if MPI reconstructions with the ZeroShot- ℓ^1 -PnP algorithm can benefit from the improved noise level estimation formula in Equation (10). To this aim, we fix $\alpha = 0.005$ and validate the parameters μ_0 and the number of iterations n_{it} on a hybrid dataset we created in [24]. We perform common MPI data preprocessing, i.e., we consider no Signal-to-Noise (SNR) thresholding, no whitening, and only frequencies between 80 and 625 kHz and perform a randomized SVD with rank 2000 (for more details we refer the interested reader to [27]).

Finally we compare the results on the validation set (see Table 1) for both the results with the variance estimation in Equation (8) (results from [24]) and with the Laplacian estimation in Equation (10). Moreover, we test the validated parameters on real data, in particular on the concentration phantom from the Open MPI Dataset [28]. The results on the Peak-Signal-to-Noise Ratio (PSNR) show the benefit of employing more sophisticated noise level estimations (see Table 2). In Figure 1 we also display a selected slice of the CAD ground truth, the reconstruction using the estimation in Equation (8) and the proposed estimation in Equation (10). Comparing the colorbars in Figure 1, one can observe that the reconstruction using the Laplace estimation in Figure 1c has a higher maximum and more particle mass around the lower left concentration dot in the phantom compared with Figure 1b. This shows that employing a more sophisticated noise level estimator is beneficial not only from a purely quantitative perspective but also from a visual qualitative perspective.

Table 1. Validation results on the hybrid dataset in [24]. We observe that employing the Laplace estimation in Equation (10) leads to a higher PSNR when compared to the results obtained using the variance estimation in Equation (8) proposed in [24].

	Variance Estimation [24]	Laplace Estimation Equation (10) (Proposed)
Param.	$\mu_0 = 3 \times 10^5$	$\mu_0 = 9 \times 10^4$
Iteration	$n_{it} = 5$	$n_{it} = 3$
PSNR	29.77 ± 5.82	29.94 ± 5.34
SSIM	0.794 ± 0.187	0.783 ± 0.189

Table 2. Results obtained with the ZeroShot- ℓ^1 -PnP, with the parameters in Table 1 on the concentration phantom in the 3D Open MPI Dataset [28]. We observe that for this particular phantom, the employment of the Laplace-based estimation of the noise level is beneficial and helps improve the PSNR and SSIM scores of the reconstruction.

Phantom	Metric	Variance Estimation [24]	Laplace Estimation Equation (10) (Proposed)
Concentration Phantom	PSNR	37.54	37.67
	SSIM	0.578	0.579

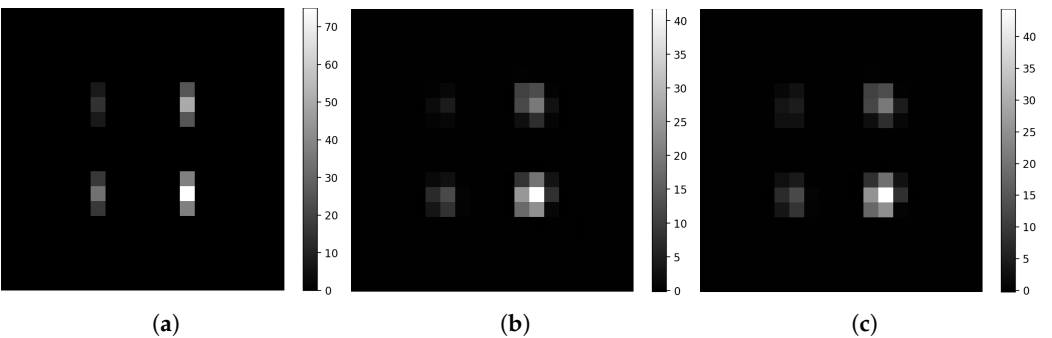


Figure 1. Reconstructions of the concentration phantom in the Open MPI Dataset [28]. We display here the 7-th xz-slice. Looking at the colorbars, we can see that Laplace estimation (Figure 1c) is able to yield a reconstruction with a higher maximum concentration level, which is closer to the ground truth (cf. with the colorbar in Figure 1b). (a) Concentration CAD reference used as ground truth. (b) Reconstruction using Variance estimation [24]. (c) Reconstruction using Laplace estimation in Equation (10).

5. Conclusions and Outlook

In this work we described the ZeroShot- ℓ^1 -PnP reconstruction algorithm proposed in [24] and described the automatic parameter update based on the noise level estimation of the reconstruction at each iteration. In [24] the noise level was estimated by simply considering the variance of the reconstruction, whereas in this work we propose to use convolution with a 3D Laplacian stencil to estimate the noise (a 3D variant of the Laplacian-based noise estimation proposed in [26]). We have shown that using more precise noise level estimators can improve the PSNR and SSIM scores of the reconstruction. However, the system matrix employed in the experiments is collected on a $19 \times 19 \times 19$ grid, leading to reconstruction of the same size and to 2D denoising of 19×19 pixel slices, which might be too small of a scale to observe substantial benefits of employing more sophisticated noise estimations. Future directions of our work include testing the ZeroShot- ℓ^1 -PnP algorithm with the Laplacian-based noise estimation, proposed here, on higher resolution MPI data, as well as testing even more sophisticated noise level estimation techniques.

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