

## Article

# Sparse Ultrasound Imaging via Manifold Low-Rank Approximation and Non-Convex Greedy Pursuit

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**1** **Abstract:** Model-based image reconstruction has brought improvements in terms of contrast and  
**2** spatial resolution to imaging applications such as magnetic resonance imaging and emission  
**3** computed tomography. However, their use for pulse-echo techniques like ultrasound imaging  
**4** is limited by the fact that model-based algorithms assume a finite grid of possible locations of  
**5** scatterers in a medium – which does not reflect the continuous nature of real world objects and  
**6** creates a problem known as off-grid deviation. To cope with this problem, we present a method of  
**7** dictionary expansion and constrained reconstruction that approximates the continuous manifold  
**8** of all possible scatterer locations within a region of interest. The expanded dictionary is created  
**9** using a highly coherent sampling of the region of interest, followed by a rank reduction procedure  
**10** based on a truncated singular value decomposition. We develop a greedy algorithm, based on the  
**11** Orthogonal Matching Pursuit (OMP), that uses a correlation-based non-convex constraint set that  
**12** allows for the division of the region of interest into cells of any size. To evaluate the performance of  
**13** the method, we present results of 2-dimensional ultrasound image reconstructions with simulated  
**14** data in a nondestructive testing application. Our method succeeds in the reconstructions of sparse  
**15** images from noisy measurements, providing higher accuracy than previous approaches based on  
**16** regular discrete models.

**17** **Keywords:** ultrasound; nondestructive testing; manifolds; inverse problems; dictionary; rank  
**18** reduction.

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## 19 1. Introduction

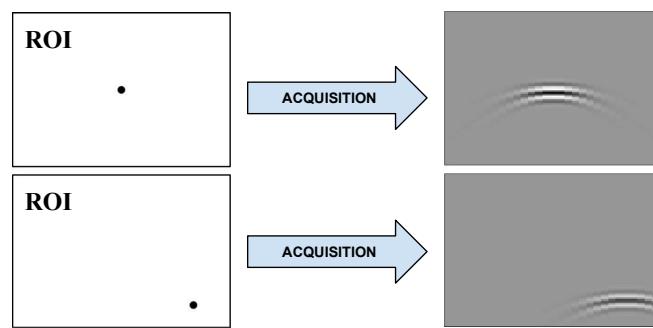
**20** Model-based image reconstruction methods provided important advances to imaging techniques  
**21** such as magnetic resonance imaging (MRI) [1] and emission computed tomography (ECT) [2] in the last  
**22** decades. These methods rely on a known model which results in the captured signal being represented  
**23** by a sum of  $N$  coefficient-weighted responses. These responses are usually point spread functions  
**24** (PSF), and coefficients are usually intensity of pixels at a modelled location. The discrete model is  
**25** then fed to regression algorithms along with a vector of acquired data, and the intensity on each  
**26** pixel is determined [3]. The use of model-based techniques in ultrasound imaging relies on a strong  
**27** assumption: that all reflectors (or scatterers) are located on any of a finite grid of  $N$  modelled positions  
**28** [4]. Naturally, real-world inspected objects easily break this assumption and many scatterers may be  
**29** located *off-grid*. Many previous studies with model-based algorithms for ultrasound imaging, including  
**30** but not limited to [4–11], have reported that resolution and contrast are substantially improved in  
**31** comparison to delay-and-sum (DAS) algorithms when data comes from simulations with scatterers  
**32** located strictly on a modelled grid. However, images are corrupted by artifacts when the grid is not  
**33** respected, which is typical in data acquired from real measurements. Consequently, DAS beamforming  
**34** algorithms remain as state-of-the-art for ultrasound imaging, despite having well understood physical  
**35** limitations regarding spatial resolution [12,13].

## 36 2. Model-based imaging and regularization

37 Let  $\mathbb{R}^M$  be the space of the data observed through an acquisition process. A single, unity amplitude  
 38 event located at position  $\tau \in \mathbb{R}^D$  (in the  $D$ -dimensional continuous space) causes the discrete acquired  
 39 signal  $\mathbf{y}(\tau) \in \mathbb{R}^M$ , known as the PSF. The physical meaning of such event depends on the type of  
 40 quantity being measured. In ultrasound imaging, the event denotes a point-like reflexivity (also called  
 41 a scatterer) [14,15], as represented in Fig. 1, and  $D$  typically equals 2 as the reflexivity is being mapped  
 42 over a 2-dimensional plane. The variation of the set of  $D$  parameters  $\tau$  within a region of interest  
 43 describes a  $D$ -dimensional manifold

$$\mathcal{M} := \{\mathbf{y}(\tau) : \tau \in \text{ROI}\} \quad (1)$$

44 of all possible PSFs on  $\mathbb{R}^M$ . We will develop our notation for the 2-dimensional case and consider the  
 45 two parameters  $\tau = [x, z]^T$  (where  $\cdot^T$  denotes the transpose) as the lateral and axial spatial dimensions  
 46 respectively.



47 **Figure 1.** Acquisition of the point spread function (PSF). For each position  $(x, z)$  of the unity amplitude  
 48 scatterer within the ROI (left side), an  $M$ -sample response  $\mathbf{y}(x, z) \in \mathbb{R}^M$  (arranged as an  $M$ -pixel image  
 on right side) is generated by the acquisition model. The set of all possible PSFs within the region of  
 interest form a manifold  $\mathcal{M}$  onto the data space. This example is taken from the pulse-echo ultrasound  
 model described in Section 6.1.

49 An acquired signal  $\mathbf{c} \in \mathbb{R}^M$  is assumed to be composed by a sum of individual contributions from  
 50  $N$  events, or  $N$  samples from the continuous PSF manifold

$$\mathbf{c} = \sum_{n=1}^N v_n \mathbf{y}(x_n, z_n) + \mathbf{w}, \quad (2)$$

51 where  $v_n$  is the amplitude of the  $n$ -th event and the vector  $\mathbf{w} \in \mathbb{R}^M$  accounts for acquisition noise,  
 52 which we will assume to be Gaussian white noise with variance  $\sigma^2$ .

53 In a pulse-echo image with  $N$  pixels,  $v_n$  in (2) encodes the reflexivity of the  $n$ -th scatterer, located  
 54 at position  $(x_n, z_n)$ , and is represented as the brightness of the corresponding pixel. This naturally  
 55 implies a sampling of the parameters  $(x, z)$  as a finite number  $N$  of possible scatterer locations (or  
 56 pixels) is assumed.

57 Once we have defined the  $N$  coordinate pairs  $(x_n, z_n)$  to be considered by the acquisition model,  
 58 we make  $\mathbf{h}_n = \mathbf{y}(x_n, z_n)$ ,  $n = 1, \dots, N$ , and define the model matrix  $\mathbf{H} = [\mathbf{h}_1, \dots, \mathbf{h}_N] \in \mathbb{R}^{M \times N}$ . Then  
 59 (2) can be written in compact form as

$$\mathbf{c} = \mathbf{H}\mathbf{v} + \mathbf{w}, \quad (3)$$

60 where  $\mathbf{v} = [v_1, \dots, v_N]^T$  is the vector of scatterer amplitudes. This model has been used in B-mode  
 61 (2-dimensional) [4–9], A-mode (1-dimensional) [16,17], and 3-dimensional [18] ultrasound imaging.

62 The reconstruction of the amplitudes vector  $\mathbf{v}$  from a given acquisition  $\mathbf{c}$  in (3) is based on the  
 63 minimization of a cost function, such as the LS problem

$$\hat{\mathbf{v}} = \arg \min_{\mathbf{v}} \|\mathbf{c} - \mathbf{Hv}\|_2^2, \quad (4)$$

62 which is linear and can be solved by well-known methods [19].

63 However, model matrices for real-world problems are often ill-conditioned, which causes artifacts  
 64 on the reconstructed signals in the presence of noise [20]. This is an issue even in reconstructions with  
 65 simulated data where all events are on grid, i.e., where the discrete acquisition model (3) is obeyed.  
 66 The specific problem of poor conditioning of the ultrasound acquisition model has been addressed  
 67 with linear regularization methods such as Truncated SVD (TSVD) [7] and Tikhonov regularization  
 68 [5,6,8], where the main goal is to stabilize the inverse operator.

69 Non-linear, sparsity-promoting regularization penalties such as  $\ell_p$ -(pseudo)norm minimization  
 70 with  $p \leq 1$  have shown successful results in ultrasound NDT, where the assumption of sparsity in the  
 71 space domain reflects the nature of discontinuities in observed materials [4,9,17,21].

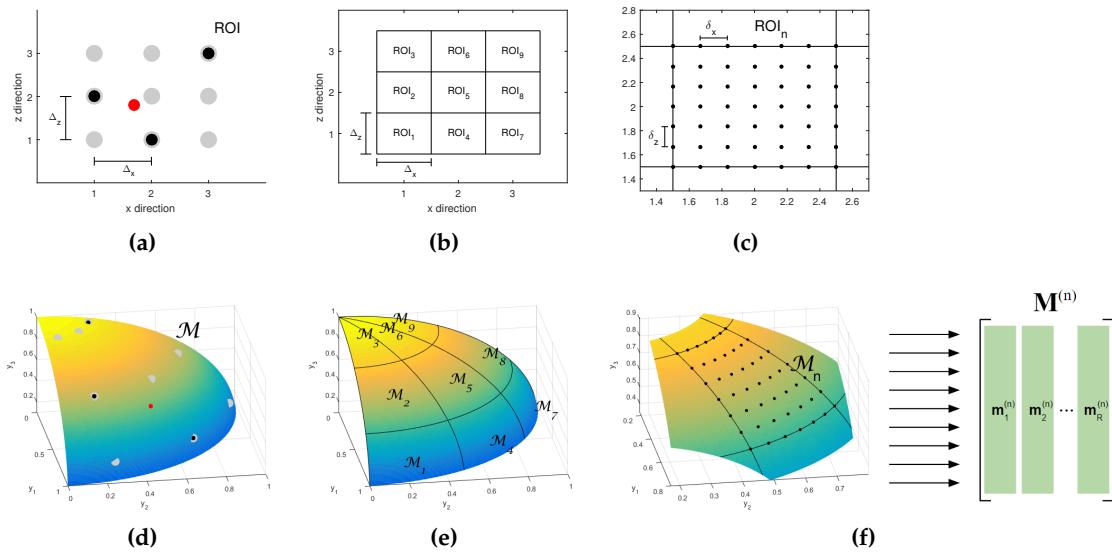
72 Greedy algorithms effectively solve reconstruction problems where the cost function involves  
 73 the  $\ell_0$  pseudonorm. In [10], sparsity is induced in the solution by the assumption that the presence of  
 74 scatterers can be modelled by a Bernoulli process with a low value for the probability parameter. The  
 75 problem is then solved with a greedy algorithm called Multiple Most Likely Replacement (MMLR)  
 76 [22]. In [16], a Gabor dictionary is used in the reconstruction of thickness with a Matching Pursuit  
 77 (MP)-based algorithm that penalizes a relaxed support measure corresponding to the  $\ell_p$ -pseudonorm  
 78 with  $0 < p < 1$ .

### 79 3. Off-grid events and dictionary expansion

80 Aside from poor matrix conditioning, another problem known as off-grid deviation [23] limits  
 81 the applicability of inverse-problem-based approaches on signal and image reconstruction. It derives  
 82 from the fact that, in many applications, the existing events may not be located strictly on the  $N$   
 83 positions modelled by (2) and (3), i.e., many events may be off-grid. Fig. 2a illustrates a grid of  $N = 9$   
 84 modelled positions, represented by gray dots. As three events (represented by black dots) are located  
 85 on modelled positions, the corresponding data vector  $\mathbf{c}$  can be synthesized according to the acquisition  
 86 models (2) and (3). The same does not hold when an off-grid event (represented by a red dot) is added:  
 87 attempts to reconstruct the locations and amplitudes for the corresponding events may fail, causing  
 88 artifacts and degradation on the reconstructed image.

89 Some formulations have been proposed for off-grid signal reconstruction, mainly within the  
 90 framework of Compressive Sensing. In [24], the acquisition model considers a perturbation matrix  
 91 summed column-wise to the (here referred to as  $\mathbf{H}$ ) regular discrete model matrix. The formulation  
 92 is applied to direction-of-arrival (DOA) estimation using the derivatives of the columns of  $\mathbf{H}$  with  
 93 respect to the sampled parameters as perturbation matrix. In [25], an adaptation of the OMP algorithm  
 94 is proposed where the columns of the model matrix are iteratively updated in order to accommodate  
 95 variations in the parameters of the PSFs. The algorithm is applied to pulse-Doppler radar. In [26]  
 96 the problem of continuous line spectral estimation is approached with an algorithm based on the  
 97 atomic norm minimization, which is solved via semi-definite programming. Similarly to the  $\ell_1$   
 98 minimization, the atomic norm minimization promotes sparse solutions. In [27], the regression  
 99 problem uses a Total Least Squares (TLS) penalization with sparsity constraints. The motivation is  
 100 that the "errors-in-variables" assumption of the TLS regression might be able to capture the mismatch  
 101 between the model matrix and the acquired data. The method is then applied to cognitive radio  
 102 sensing and DOA estimation.

103 Our approach relies on the framework of dictionary expansion, which has been firstly proposed  
 104 in [23] as a means to overcome the problem of off-grid deviation in neuron spike detection. Each  
 105 column  $\mathbf{h}_n$  of the discrete model  $\mathbf{H}$  of (3) is replaced by  $K$  columns  $[\mathbf{b}_1^{(n)}, \dots, \mathbf{b}_K^{(n)}] = \mathbf{B}^{(n)} \in \mathbb{R}^{(M \times K)}$  so  
 106 that a data vector  $\mathbf{c}$  resulting from the acquisition of an event located in the neighborhood of an  $n$ -th



**Figure 2.** (a) An illustrative discrete acquisition model with  $N = 3 \times 3 = 9$  modelled positions, represented by the gray dots. The black dots represent 3 well located events and the red dot represents an off-grid event. Because of the latter, the corresponding acquisition data vector  $\mathbf{c}$  cannot be synthesized as a linear combination of the columns of the discrete model matrix  $\mathbf{H}$ . (b) The ROI is divided into  $N$  local ROIs with area  $\Delta_x \times \Delta_z$ . (c) Each local ROI is sampled with a fine grid with lateral and axial distances  $\delta_x$  and  $\delta_z$ . (d) On the space  $\mathbb{R}^M$  of acquired data, the set of all possible PSFs within the ROI form a manifold  $\mathcal{M}$ . The gray dots are the PSFs of the modelled positions of Fig. 2a. The black dots are on the grid, while the red dot is off-grid. (e) As the ROI is divided into  $N$  local ROIs (Fig. 2b), the manifold is divided into  $N$  corresponding local manifolds. (f) The acquisitions over the fine grid on each  $n$ -th local ROI create  $R$  samples from the corresponding local manifold. Those samples compose matrix  $\mathbf{M}^{(n)} \in \mathbb{R}^{M \times R}$ .

modelled position can be approximated by some linear combination of  $\mathbf{B}^{(n)}$ , i.e., by  $\mathbf{B}^{(n)}\mathbf{x}^{(n)}$ , where  $\mathbf{x}^{(n)} \in \mathbb{R}^K$ . As a result, an arbitrarily acquired  $\mathbf{c}$  might be approximated as

$$\mathbf{c} \approx \sum_{n=1}^N \mathbf{B}^{(n)}\mathbf{x}^{(n)}. \quad (5)$$

In the 2-dimensional case, the neighborhood of the  $n$ -position is the region within  $(x_n \pm 0.5\Delta_x, z_n \pm 0.5\Delta_z)$ . This is represented in Fig. 2b, where the 9 modelled locations give place to 9 neighborhoods (local ROIs).

Two forms of approximation are proposed in [23] for 1-dimensional linear time-invariant (LTI) problems. The first one is the Taylor approximation, which relies on the fact that small shifts on a waveform can be well approximated by its Taylor expansion, i.e., by linearly combining the original waveform and its time derivatives. In this case, the column  $\mathbf{b}_1^{(n)}$  is identical to the original atom  $\mathbf{h}_n$  and the columns  $\mathbf{b}_k^{(n)}$  for  $k > 1$  correspond to its  $(k-1)$ -th time derivatives. The second is the Polar approximation, which is motivated by the fact that the continuous manifold  $\mathcal{M}$  of an LTI system lies over a hypersphere on the  $M$ -dimensional data space [23]. The PSFs of the neighborhood of each  $n$ -th modelled position are approximated by an arc of a circle and the the column  $\mathbf{h}_n$  is replaced by three normal vectors with the directions of the center ( $\mathbf{b}_1^{(n)}$ ) and the two trigonometric components ( $\mathbf{b}_2^{(n)}$  and  $\mathbf{b}_3^{(n)}$ ) of the circle. While the Taylor approximation can be done for any order  $K$ , in the Polar case  $K$  always equals 3.

123 An extension of the Basis Pursuit (BP) formulation [28], referred to as Continuous Basis Pursuit  
 124 (CBP), is proposed in [23] for the recovery of the expanded coefficients  $\{\mathbf{x}^{(n)}\}_{1 \leq n \leq N}$ . For the sake of  
 125 conciseness, from this point on we will represent sets  $\{\mathbf{x}^{(n)}\}_{1 \leq n \leq N}$  simply as  $\{\mathbf{x}^{(n)}\}$ . The formulation  
 126 of CBP is given by

$$\{\hat{\mathbf{x}}^{(n)}\} = \arg \min_{\{\mathbf{x}^{(n)}\}} \frac{1}{2\sigma^2} \|\mathbf{c} - \sum_{n=1}^N \mathbf{B}^{(n)} \mathbf{x}^{(n)}\|_2^2 + \lambda \sum_{n=1}^N |\mathbf{x}_1^{(n)}| \quad (6a)$$

$$\text{s.t. } \{\mathbf{x}^{(n)}\} \in \mathcal{C}, \quad (6b)$$

127 where the constraint set  $\mathcal{C}$  prevents recovered expanded coefficients from having any arbitrary values  
 128 that do not represent actual PSFs. The definition of the convex set  $\mathcal{C}$  varies according to the type of  
 129 approximation used. The  $\ell_1$  norm of a vector composed by the first element  $\mathbf{x}_1^{(n)}$  of each  $K$ -tuple  $\mathbf{x}^{(n)}$  is  
 130 used to obtain sparse solutions.

131 In [29], a low-rank approximation of the PSFs within the neighborhood of each  $n$ -th modelled  
 132 position is performed by means of a Singular Value Decomposition (SVD). The continuous manifold  
 133 drawn by  $\tau$  in a local ROI is sampled with a very fine grid of  $R$  locations, generating  $R$  columns that  
 134 form a matrix  $\mathbf{M}^{(n)} \in \mathbb{R}^{M \times R}$ , as represented in Fig. 2f. Each matrix  $\mathbf{M}^{(n)}$  then undergoes an SVD  
 135 decomposition and the  $K$  first left singular vectors compose the corresponding expanded coefficients  
 136  $\mathbf{B}^{(n)}$  for the  $n$ -th local ROI.

137 An adaptation of the Orthogonal Matching Pursuit (OMP) [30] algorithm, referred to as  
 138 Continuous OMP (COMP), is also presented in [29]. It aims at solving the  $\ell_2 - \ell_0$  problem

$$\{\hat{\mathbf{x}}^{(n)}\} = \arg \min_{\{\mathbf{x}^{(n)}\}} \|(x_1^{(1)}, \dots, x_1^{(N)})\|_0 \quad (7a)$$

$$\text{s.t. } \left\{ \begin{array}{l} \|\mathbf{c} - \sum_{n=1}^N \mathbf{B}^{(n)} \mathbf{x}^{(n)}\|_2^2 \leq \epsilon \\ \{\mathbf{x}^{(n)}\} \in \mathcal{C} \end{array} \right\}, \quad (7b)$$

139 where the symbol  $\|\cdot\|_0$  denotes the  $\ell_0$  pseudonorm, i.e., the cardinality (number of nonzero elements)  
 140 of a vector.

141 In [31], a minimize-maximum (Minimax) formulation is presented for the definition of the  
 142 expanded set  $\{\mathbf{B}^{(n)}\}$ . The resulting approximation minimizes the maximum residual within the  
 143 representation of each  $n$ -th local ROI. It is motivated by the assumption that the off-grid deviation  
 144 from a discrete grid follows a uniform distribution, therefore the off-grid error should be as constant  
 145 as possible, not privileging any distance from originally modelled positions.

#### 146 4. Rank-K approximation of local manifolds

147 The core idea of dictionary expansion is the substitution of each  $n$ -th column  $\mathbf{h}_n$  from the discrete  
 148 model  $\mathbf{H}$  by  $K$  basis vectors  $\mathbf{B}^{(n)}$  of which the column space approximates the  $n$ -th local PSF manifold  
 149  $\mathcal{M}_n$ . Our criterion to determine  $\mathbf{B}^{(n)}$  is based on the SVD expansion, which has been proposed for  
 150 1-dimensional, shift-invariant problems [29]. The extension to  $D$ -dimensional problems relies mainly  
 151 on the first step of the process, which is a fine sampling of each local manifold  $\mathcal{M}_n$ : here the regular,  
 152 fine grid is defined for all  $D$  dimensions. This extension is facilitated by the fact that the formulation  
 153 is non-parametric, i.e., the deviation from originally modelled positions is not mapped onto any  
 154 independent variable and does not play any role on the definition on the bases. On the other hand, in  
 155 the Taylor, Polar [23] and Minimax [31] expansions, the off-grid deviation is a parameter from which  
 156 the elements of the expanded dictionary are derived. Consequently, except for the Taylor expansion,  
 157 their extensions to 2 or higher dimensions are not promptly defined.

158 4.1. Highly coherent discrete local manifolds

159 Fig. 2d shows an illustrative example of a  $D$ -manifold embedded in an  $M$ -dimensional data space.  
 160 In this case,  $D = 2$  and  $M = 3$ . The 9  $D$ -dimensional modelled positions shown in Fig. 2a correspond  
 161 here to 9 samples of the  $M$ -dimensional manifold, as well represented by gray dots in Fig. 2d. The red  
 162 dot corresponds to the data caused by the off-grid reflector from Fig. 2a.

163 Fig. 2e shows the same manifold as Fig. 2d but, instead of having  $N$  modelled positions, it divides  
 164 the manifold into  $N$  local manifolds

$$\mathcal{M}_n := \{\mathbf{y}(x, z) : x \in [x_n - 0.5\Delta_x, x_n + 0.5\Delta_x], z \in [z_n - 0.5\Delta_z, z_n + 0.5\Delta_z]\}, \quad (8)$$

165 which correspond to the  $N$  local ROIs of Fig. 2b.

166 We start by performing a fine sampling on each local manifold  $\mathcal{M}_n$ , as represented in Fig. 2f. In  
 167 practice, this means acquiring the PSF of a set of points from a fine grid of  $R$  points defined for each  
 168 local ROI (Fig. 2c). The result is a matrix  $\mathbf{M}^{(n)} \in \mathbb{R}^{M \times R}$ , whose columns are local manifold samples.  
 169 The finer this grid is, the better the continuous local manifold is represented by the discrete dataset  
 170  $\mathbf{M}^{(n)}$ . For simplicity of notation, we keep regular spacing  $\delta_x$  and  $\delta_z$  for the lateral and axial directions  
 171 respectively. The number of sampled points is  $R = R_x \times R_z$ , where  $R_x$  and  $R_z$  are the number of  
 172 locations defined on the lateral and axial directions respectively. In the example of Fig. 2c,  $R_x = R_z = 7$ ,  
 173 thus  $R = 49$ .

174 Our sampling includes the boundaries of the local ROIs. For this reason, the relation between the  
 175 spacing and the number of locations on the lateral direction is given by

$$\delta_x = \frac{\Delta_x}{R_x - 1} \quad (9)$$

176 and the same holds for the axial direction.

177 Once we have the local matrices  $\{\mathbf{M}^{(n)}\}$ , we create a rank- $K$  approximation for each of them and  
 178 define the sets of  $K$  basis vectors  $\{\mathbf{B}^{(n)}\}$ , which form orthonormal bases for such approximations, to be  
 179 later used on inverse reconstruction problems such as (6b) and (7b).

180 4.2. SVD expansion

181 For each matrix  $\mathbf{M}^{(n)}$ , a rank- $K$  approximation  $\tilde{\mathbf{M}}^{(n)} \in \mathbb{R}^{M \times R}$  is to be defined and also factorized  
 182 in the form

$$\tilde{\mathbf{M}}^{(n)} = \mathbf{B}^{(n)} \mathbf{F}^{(n)}, \quad (10)$$

183 where  $\mathbf{B}^{(n)}$  is an orthonormal basis matrix and  $\mathbf{F}^{(n)} \in \mathbb{R}^{K \times R}$  modulates  $\mathbf{B}^{(n)}$  to form  $\tilde{\mathbf{M}}^{(n)}$ . Any  
 184 approximation creates a residual matrix  $\mathbf{R}^{(n)} \in \mathbb{R}^{M \times R}$  defined by the difference

$$\mathbf{R}^{(n)} = \mathbf{M}^{(n)} - \mathbf{B}^{(n)} \mathbf{F}^{(n)}. \quad (11)$$

185 The SVD expansion is defined by the minimization of the Frobenius norm [19] of  $\mathbf{R}^{(n)}$ :

$$\hat{\mathbf{B}}^{(n)}, \hat{\mathbf{F}}^{(n)} = \arg \min_{\mathbf{B}^{(n)}, \mathbf{F}^{(n)}} \|\mathbf{M}^{(n)} - \mathbf{B}^{(n)} \mathbf{F}^{(n)}\|_F. \quad (12)$$

186 According to the Eckart–Young theorem, a solution for (12) is achieved by a truncated SVD [32].  
 187 Consider the SVD of  $\mathbf{M}$

$$\mathbf{M}^{(n)} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T, \quad (13)$$

188 where  $\mathbf{U} \in \mathbb{R}^{M \times R}$  is the unitary matrix of left singular vectors,  $\mathbf{\Sigma} \in \mathbb{R}^{R \times R}$  is the diagonal matrix of  
 189 singular values and  $\mathbf{V} \in \mathbb{R}^{N \times R}$  is the unitary matrix of right singular vectors [19]. The rank- $K$  SVD

truncation is obtained by using only the  $K$  largest singular values from  $\Sigma$  and the  $K$  corresponding vectors from  $\mathbf{U}$  and  $\mathbf{V}$ . This low rank approximation is given by

$$\tilde{\mathbf{M}}^{(n)} = \tilde{\mathbf{U}}\tilde{\Sigma}\tilde{\mathbf{V}}^T, \quad (14)$$

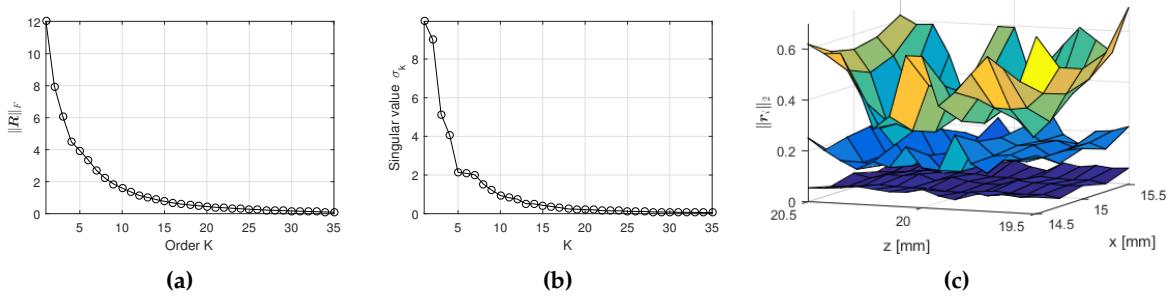
where  $\tilde{\mathbf{U}} \in \mathbb{R}^{M \times K}$ ,  $\tilde{\Sigma} \in \mathbb{R}^{K \times K}$  and  $\tilde{\mathbf{V}} \in \mathbb{R}^{R \times K}$ .

The  $K$  columns of  $\tilde{\mathbf{U}}$  form an orthonormal basis for  $\tilde{\mathbf{M}}^{(n)}$  and compose the expanded set  $\mathbf{B}^{(n)}$ , while the product  $\tilde{\Sigma}\tilde{\mathbf{V}}^T$  compose the modulating matrix  $\mathbf{F}^{(n)}$ :

$$\mathbf{B}^{(n)} = \tilde{\mathbf{U}}, \quad (15a)$$

$$\mathbf{F}^{(n)} = \tilde{\Sigma}\tilde{\mathbf{V}}^T. \quad (15b)$$

Naturally, large values for  $K$  mean more degrees of freedom in the approximation, which reduces the residuals. Fig. 3a shows how the value of  $K$  affects the Frobenius norm of  $\mathbf{R}^{(n)}$  for the center-most local ROI of the acquisition set presented in Section 6.1. The values of the 35 first singular values  $\sigma_k$  are shown in Fig. 3b. The 75 individual residual norms  $\|\mathbf{r}_i\|$  for  $K = 5, 10$  and  $20$  are shown in Fig. 3c.



**Figure 3.** Approximation metrics for the center-most local ROI of the ultrasound acquisition set described in Section 6.1, with  $R = 75$  ( $R_x = 5$  and  $R_z = 15$ ). (a) Frobenius norm  $\|\mathbf{R}^{(n)}\|_F$  of the residual matrix as a function of the order of approximation  $K$ . (b) 35 first singular values  $\sigma_k$  from the SVD of  $\mathbf{M}^{(n)}$ . (c) Individual residual norms  $\|\mathbf{r}_i^{(n)}\|_2$  (of columns of  $\mathbf{R}^{(n)}$ ), spatially arranged according to the corresponding positions on the local ROI. The three surfaces correspond to  $K = 5$  (top),  $K = 10$  (middle) and  $K = 20$  (bottom).

It shall be noted that the processes presented from (12) to (15b) have to be independently performed for every  $n$ -th local ROI. Although the construction of expanded dictionaries is computationally demanding, it is an offline procedure that is carried only once for each given acquisition set.

## 5. Reconstruction algorithm

### 5.1. Limitations of conic constraints

Two main algorithms were proposed to work with expanded dictionaries: the convex CBP [23] and the greedy COMP [29]. The first one aims at solving problem (6b) while the second attempts to solve problem (7b). A hybrid approach called Interpolating Band-excluded Orthogonal Matching Pursuit (IBOMP) was also proposed and applied to frequency estimation (FE) and time delay estimation (TDE) [33]. Basically, it performs a rough greedy estimation of the support of the solution, followed by a refining convex optimization.

In order to implement a constraint set  $\mathcal{C}$ , all the aforementioned algorithms have at least one step involving a constrained convex optimization where the constraints define either first-order (SVD,

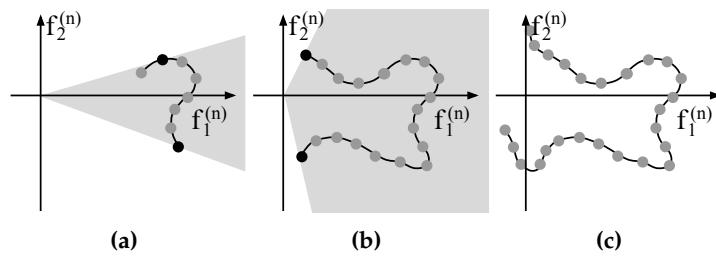
213 Minimax and Taylor) or second-order (Polar) cones. Fig. 4a illustrates an example of a first-order cone  
 214 for  $K = 2$ . The black curved line represents the projection onto the basis  $\mathbf{B}^{(n)}$  of a continuous  
 215 1-dimensional PSF manifold. The  $R$  vectors that compose a local manifold matrix  $\mathbf{M}^{(n)}$ , when  
 216 projected onto  $\mathbf{B}^{(n)}$ , result in vectors  $\mathbf{f}^{(n)}$ , represented by the dots, which compose the columns  
 217 of  $\mathbf{F}^{(n)}$ . When a reconstruction is performed, the recovered coefficients set  $\mathbf{x}^{(n)} \in \mathbb{R}^2$  for this  $n$ -th  
 218 local ROI is constrained to lie within a first-order cone, represented by the shadowed area (which  
 219 extends indefinitely to the right). This cone is defined by two linear constraints that impose an upper  
 220 and a lower bound for the relation  $x_2^{(n)} / x_1^{(n)}$ , combined with a non-negativity constraint for the first  
 221 component  $x_1^{(n)}$ . This constraint set aims to avoid arbitrary combinations for  $\mathbf{x}^{(n)}$  that do not represent  
 222 positively-weighted copies of actual manifold samples. The upper black dot defines the upper angle of  
 223 the cone, and is defined by the modulating matrix  $\mathbf{F}^{(n)}$  as  $\max_i(f_{2,i}^{(n)} / f_{1,i}^{(n)})$ , i.e., the maximum relation  
 224 between the first and second components found among the projections of  $\mathbf{M}^{(n)}$ . Similarly, the lower  
 225 black dot is defined by  $\min_i(f_{2,i}^{(n)} / f_{1,i}^{(n)})$ , and defines the lower angle of the cone. For higher orders of  
 226  $K$ , such a cone is defined for all  $K - 1$  relations between each  $k$ -th ( $k \geq 2$ ) component and the first one.  
 227 The resulting linear constraint set is defined as [29,31]

$$\min_{1 \leq i \leq R} \left( \frac{f_{k,i}^{(n)}}{f_{1,i}^{(n)}} \right) \leq \frac{x_k^{(n)}}{x_1^{(n)}} \leq \max_{1 \leq i \leq R} \left( \frac{f_{k,i}^{(n)}}{f_{1,i}^{(n)}} \right), \quad (16a)$$

$$f_{1,i}^{(n)} \geq 0 \quad (16b)$$

$$\forall k \in \{2, \dots, K\}, n \in \{1, 2, \dots, N\}, \quad (16c)$$

228 where  $f_{k,i}^{(n)}$  denotes the element on the  $k$ -th line and  $i$ -th column on  $\mathbf{F}^{(n)}$ . The principle is similar for the  
 229 Polar expansion, though in that case the cones are of second order [23].



**Figure 4.** (a) Illustrative case of projection of local manifold samples  $\mathbf{M}^{(n)}$  on a basis  $\mathbf{B}^{(n)}$ , for  $K = 2$ . The curved line represents the projection of a continuous 1-dimensional manifold, while the dots represent the projection of the samples (columns of  $\mathbf{M}^{(n)}$ ) on  $\mathbf{B}^{(n)}$ . When  $\Delta$  is sufficiently small, the projections have single-signed, relatively large values on the first component  $f_1^{(n)}$  and smaller values on the remaining components. In this case, the definition of a first-order cone (represented by the shadowed region) is possible and can be used in the reconstruction algorithm combined with a non-negativity constraint for the first component, ensuring that the recovered coefficients represent weighted copies of the local manifold, rather than other arbitrary combinations. The upper and lower angles of the cone depend on  $\max_i(f_{2,i}^{(n)} / f_{1,i}^{(n)})$  and  $\min_i(f_{2,i}^{(n)} / f_{1,i}^{(n)})$  respectively. (b) As  $\Delta$  increases, the angle of the cone may as well increase, making the constraint less effective, as a broader area is allowed for the recovered coefficients  $\mathbf{f}^{(n)}$ . (c) An example where the definition of a convex cone is no longer possible. This imposes a limit on the definition of  $\Delta$ .

230 Notice that the cone-based convex constraints assume that the projection of  $\mathbf{M}^{(n)}$  on the  $K$   
 231 components of  $\mathbf{B}^{(n)}$  yields relatively large, positive, small-variance values for the first component and  
 232 small values for the remaining, yielding relatively small values for minimum and maximum relations  
 233 of (16c). If this assumption is broken, the cone will span too large an area of the right half-plane, i.e.,

234 it will constrain less, being less effective, as represented in Fig. 4b. In some cases, defining the the cone  
 235 is not even possible, as depicted in Fig. 4c.

236 Assuring a well behaved relation between the first and the remaining components, as shown  
 237 in Fig. 4a, implies choosing considerably small values for  $\Delta_x$  and  $\Delta_z$ , what limits the applicability  
 238 of recovery algorithms based on conic constraints. For instance, on the simulated acquisition set of  
 239 Section 6.1, choosing  $\Delta_x = \Delta_z = 0.2\text{mm}$  still causes the first component to have both positive and  
 240 negative values on certain local manifolds, which makes the CBP [23], COMP [29] and IBOMP [33]  
 241 algorithms not applicable.

242 *5.2. Non-convex constraints*

243 The problem described in Section 5.1 is the main reason why our algorithm does not rely on conic  
 244 constraints. Instead, it attempts to constrain each  $K$ -tuple of recovered coefficients  $\mathbf{x}^{(n)}$  to be similar to  
 245 any column of the modulating matrix  $\mathbf{F}^{(n)}$ . We translate “similarity” as high correlation, as formalized  
 246 in the non-convex constraint set

$$\left( \max_{1 \leq i \leq R} \frac{\langle \mathbf{x}^{(n)}, \mathbf{f}_i^{(n)} \rangle}{\|\mathbf{x}^{(n)}\| \|\mathbf{f}_i^{(n)}\|} \right) \geq \mu_c, \quad \forall n \in \{1, 2, \dots, N\}, \quad (17a)$$

247 where  $\langle \mathbf{a}, \mathbf{b} \rangle = \mathbf{a}^T \mathbf{b}$  denotes the inner product of two vectors.

248 The minimum correlation parameter  $\mu_c$  controls how similar to any of the manifold samples on  
 249  $\mathbf{M}^{(n)}$  a recovered event must be. If a given  $\mathbf{x}^{(n)}$  passes the test (17a), proving to be sufficiently similar  
 250 to some  $i$ -th modulating vector  $\mathbf{f}_i^{(n)}$ , then the approximation

$$\tilde{\mathbf{m}}_i^{(n)} \frac{\|\mathbf{x}^{(n)}\|}{\|\mathbf{f}_i^{(n)}\|} = \mathbf{B}^{(n)} \mathbf{f}_i^{(n)} \frac{\|\mathbf{x}^{(n)}\|}{\|\mathbf{f}_i^{(n)}\|} \approx \mathbf{B}^{(n)} \mathbf{x}^{(n)} \quad (18)$$

251 is assumed and the product  $\mathbf{B}^{(n)} \mathbf{x}^{(n)}$  is considered as a valid weighted copy of a PSF within the  $n$ -th  
 252 local ROI, rather than an arbitrary combination of the  $n$ -th basis vectors. This constraint is imposed by  
 253 our greedy algorithm on the decision of which expanded set  $\mathbf{B}^{(n)}$  will be added to the reconstruction  
 254 problem at each iteration.

255 *5.3. OMP for Expanded Dictionaries*

256 The proposed algorithm, summarized in Algorithm 1, is an extension of the OMP algorithm,  
 257 referred to as OMP for Expanded Dictionaries (OMPED). It attempts to solve a problem similar to (7b)  
 258 (i.e., to explain an acquired data vector  $\mathbf{c}$  with the expanded dictionary  $\{\mathbf{B}^{(n)}\}$ ) with the non-convex  
 259 constraint set  $\mathcal{C}$  defined in (17a). The stop criterion is based on the residual yielded by the LS solution  
 260 with a given cardinality, yet instead of comparing the residual to a fixed parameter  $\epsilon$ , we compare it  
 261 to an estimate of the current residual that takes into account the expected acquisition noise and the  
 262 estimated residuals resulting from the reduced-rank approximation.

263 The input parameter  $e_{\text{noise}}$  contains the expected  $\ell_2$  norm of the acquisition noise. In practice, this  
 264 value can be obtained from acquisitions with samples of the inspected material known to have neither  
 265 discontinuities nor other sort of scatterers. For our simulations, we use the relation

$$e_{\text{noise}}^2 = \|\mathbf{w}\|_2^2 \approx M\sigma^2, \quad (19)$$

266 which holds if the noise vector  $\mathbf{w}$  contains white Gaussian noise with variance  $\sigma^2$ . The approximation  
 267 of (19) becomes an equality as  $M \rightarrow \infty$ . We assume the equality and use  $e_{\text{noise}} = \sqrt{M\sigma^2}$ .

268 We define the support  $S$  of the solution, which is initialized as the empty set, and its complement  
 269  $S^c = \{1, \dots, N\} \setminus S$ . The solution residual  $\mathbf{e} \in \mathbb{R}^M$  is initialized with the vector of acquired data  $\mathbf{c}$  on  
 270 line 2.

**Algorithm 1** OMP for Expanded Dictionaries (OMPED)**Input:**  $\{\mathbf{B}^{(n)}\}, \{\mathbf{F}^{(n)}\}, \{\mathbf{R}^{(n)}\}, \mathbf{c}, e_{\text{noise}}, \mu_c, \Delta_\mu$ 1:  $S \leftarrow \emptyset$ 2:  $\mathbf{e} \leftarrow \mathbf{c}$ 3: **repeat**4:    $j \leftarrow$  Compute from (21)5:   **while**  $j = \emptyset$  **do**6:      $\mu_c \leftarrow \mu_c - \Delta_\mu$ 7:      $j \leftarrow$  Compute from (21)8:     **end while**9:      $S \leftarrow S \cup \{j\}$ 10:    $\{\mathbf{x}^{(n)}\} \leftarrow$  Compute from (22b)11:    $\mathbf{e} \leftarrow$  Compute from (23)12:    $\mathbf{e}_{\text{rank}} \leftarrow$  Compute from (24)13:    $e_{\text{est}} \leftarrow$  Compute from (25)14: **until**  $e_{\text{est}} \geq \|\mathbf{e}\|_2$  or  $S^c = \emptyset$ **Output:**  $S, \{\mathbf{x}^{(n)}\}_{n \in S}$ 

271 At each iteration, an index  $j \in S^c$  is added to  $S$  as we choose the expanded set  $\mathbf{B}^{(j)}$  which is  
 272 capable of causing the maximal decrease on the energy of the residual, as represented on the left side  
 273 of (20). Since the columns of each  $\mathbf{B}^{(n)}$  are orthonormal, the identity

$$\hat{j} = \arg \min_j \|\mathbf{e} - \mathbf{B}^{(j)} \mathbf{B}^{(j)T} \mathbf{e}\|_2 = \arg \max_j \|\mathbf{B}^{(j)T} \mathbf{e}\|_2 \quad (20)$$

274 holds as a consequence of Parseval's relation [34], which allows us to perform the simpler operation of  
 275 taking the norm of each product  $\mathbf{B}^{(j)T} \mathbf{e}$ .

276 This operation is a generalization of the measurement of maximum correlation on the original  
 277 OMP [30]. A constraint based on (17a) is imposed to prune candidates that do not accomplish the  
 278 minimum correlation required. The resulting criterion is formalized as

$$\hat{j} = \arg \max_{j \in S^c} \|\mathbf{B}^{(j)T} \mathbf{e}\|_2 \text{ s.t. } \max_{1 \leq i \leq R} \frac{\langle \mathbf{B}^{(j)T} \mathbf{e}, \mathbf{f}_i^{(j)} \rangle}{\|\mathbf{B}^{(j)T} \mathbf{e}\| \|\mathbf{f}_i^{(j)}\|} \geq \mu_c. \quad (21)$$

279 The constraint in (21) allows for the recovery of only positive-amplitude events. It can be adapted  
 280 to consider both positive and negative amplitudes by simply replacing the inner product by its absolute  
 281 value  $|\langle \mathbf{B}^{(j)T} \mathbf{e}, \mathbf{f}_i^{(j)} \rangle|$ .

282 The algorithm must consider the case where no index meets the correlation criterion of (21). This  
 283 case is treated from line 5 to line 8: while problem (11) remains infeasible, a decrease of  $\Delta_\mu$  is made on  
 284 the parameter  $\mu_c$  and a new attempt to compute the index  $j$  is performed.

285 The support  $S$  is then updated to include the new index  $j$  (line 9) and is used to compute the  
 286 coefficients

$$\{\hat{\mathbf{x}}^{(n)}\} = \arg \min_{\{\mathbf{x}^{(n)}\}} \left\| \mathbf{c} - \sum_{n=1}^N \mathbf{B}^{(n)} \mathbf{x}^{(n)} \right\|_2^2 \quad (22a)$$

$$\text{s.t. } \mathbf{x}^{(n)} = \mathbf{0}, \forall n \in S^c \quad (22b)$$

287 (where  $\mathbf{0} \in \mathbb{R}^K$  is the zero vector), which then yield a residual

$$\mathbf{e} = \mathbf{c} - \sum_{n \in S} \mathbf{B}^{(n)} \mathbf{x}^{(n)}. \quad (23)$$

288 Were the manifold approximation exact,  $\mathbf{e}$  in (23) would be composed strictly of: 1) PSFs located  
 289 at local ROIs with the corresponding indices not yet added to the support  $S$  and 2) additive noise. In  
 290 that case, we could use the widespread stop criterion that compares  $\|\mathbf{e}\|_2$  to the expected noise power.  
 291 However, our residual estimate must take into account the rank- $K$  approximation. This estimate is  
 292 computed on vector  $\mathbf{e}_{\text{rank}} \in \mathbb{R}^M$  as

$$\mathbf{e}_{\text{rank}} = \sum_{n \in S} \mathbf{r}_{\hat{i}}^{(n)} \frac{\|\mathbf{x}^{(n)}\|}{\|\mathbf{f}_{\hat{i}}^{(n)}\|}, \quad (24a)$$

$$\text{where } \hat{i} = \arg \max_{1 \leq i \leq R} \frac{\langle \mathbf{x}^{(n)}, \mathbf{f}_i^{(n)} \rangle}{\|\mathbf{x}^{(n)}\| \|\mathbf{f}_i^{(n)}\|} \quad (24b)$$

293 and  $\mathbf{r}_i^{(n)}$  denotes the  $i$ -th column from  $\mathbf{R}^{(n)}$ . Based on (17a), the index  $i$  in (24b) is a function of  $n$ : for  
 294 every index  $n$  in the current support  $S$ , the correlations performed in (24b) estimate which  $i$ -th PSF  
 295 within the  $n$ -th local manifold best explains the recovered coefficients  $\mathbf{x}^{(n)}$  (see Figs. 2c and 2f). The  
 296 residual  $\mathbf{r}_i^{(n)}$ , from the dictionary low-rank approximation, is then used as template for the estimation  
 297 of the current approximation residual. The amplitude estimate is taken from the ratio between the  
 298 norms of the recovered coefficients  $\mathbf{x}^{(n)}$  and of the similar modulating vector  $\mathbf{f}_i^{(n)}$ .

299 The current total residual norm is estimated as

$$e_{\text{est}} = (\|\mathbf{e}_{\text{rank}}\|_2^2 + e_{\text{noise}}^2)^{\frac{1}{2}}, \quad (25)$$

300 where the summation is performed under the assumption that the acquisition noise and the vector  
 301  $\mathbf{e}_{\text{rank}}$  have negligible correlation.

302 The algorithm greedily increases the support until the estimated residual norm  $e_{\text{est}}$  reaches the  
 303 norm  $\|\mathbf{e}\|$  of the actual residual yielded by the LS or all indices  $n = 1, \dots, N$  have been added to the  
 304 support  $S$ .

#### 305 5.4. Recovery of locations and amplitudes

306 OMPED yields a support  $S$  as well as the sets of expanded coefficients  $\{\mathbf{x}^{(n)}\}_{n \in S}$ . The computation  
 307 of the locations and amplitudes follows the same principle used on (24a) and (24b): each event is  
 308 located inside an  $n$ -th local ROI; its high resolution location is assigned the same as that of the  $i$ -th  
 309 response  $\mathbf{m}_i^{(n)}$  within the  $R$  responses of the fine grid (Fig. 2c) which most correlates to  $\mathbf{x}^{(n)}$ . Recalling  
 310 the approximation  $\mathbf{m}_i^{(n)} \approx \mathbf{B}^{(n)} \mathbf{f}_i^{(n)}$ , we determine  $i$  by finding out which  $\mathbf{f}_i^{(n)}$  most correlates to  $\mathbf{x}^{(n)}$ :

$$\hat{i}(n) = \arg \max_{1 \leq i \leq R} \frac{\langle \mathbf{x}^{(n)}, \mathbf{f}_i^{(n)} \rangle}{\|\mathbf{x}^{(n)}\| \|\mathbf{f}_i^{(n)}\|}, \quad \forall n \in S. \quad (26)$$

311 The amplitude estimations  $v_n$  result from the ratios between the norms of  $\mathbf{x}^{(n)}$  and of the chosen  
 312 template  $\mathbf{f}_i^{(n)}$ :

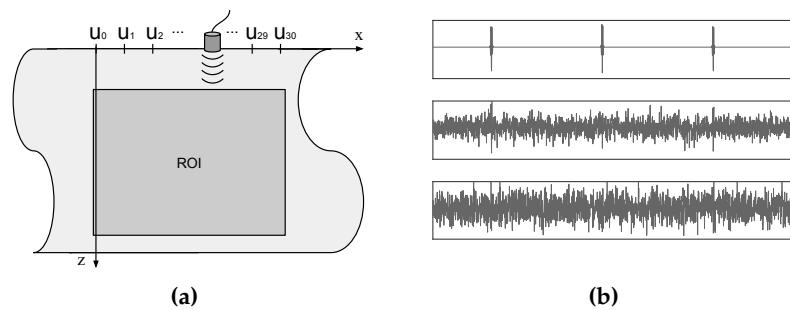
$$v_n = \frac{\|\mathbf{x}^{(n)}\|}{\|\mathbf{f}_i^{(n)}\|}, \quad \forall n \in S, i \text{ as in (26)}. \quad (27)$$

313 As consequence, the spatial resolution of the reconstructed events equals the fine sampling  
 314 represented in Fig. 2c, i.e.,  $\delta_x$  and  $\delta_z$  for the lateral and axial axes respectively.

## 315 6. Empirical results

### 316 6.1. Simulated acquisition set

317 To simulate the ultrasound NDT acquisition set from [21], represented in Fig. 5a, we used Field II  
 318 package for Matlab [15]. A piston transducer with 3mm radius (125 $\mu$ m mathematical element size)  
 319 interrogates a steel sample object (sound speed  $c = 5680\text{m/s}$ ). The excitation pulse has center frequency  
 320  $f_c = 5\text{MHz}$  and 6dB fractional bandwidth of 100%. The simulated transducer slides horizontally  
 321 along the surface of the object, acquiring scanlines from 31 lateral positions  $u_i$ , from  $u_0 = 0\text{mm}$  to  
 322  $u_{30} = 30\text{mm}$  (center of transducer), with a distance of 1mm between consecutive lateral positions. The  
 323 31 scanlines are sampled with sampling rate  $f_s = 25\text{MHz}$  and concatenated to form the acquisition  
 324 vector  $\mathbf{c}$ .



325 **Figure 5.** (a) Simulated set (figure adapted from [21]). The transducer, fixed vertically at  $z = 0$ ,  
 326 slides horizontally over the surface of the interrogated object, acquiring scanlines at 31 positions  
 327  $x = \{u_0, \dots, u_{30}\}$ , corresponding to 0mm up to 31mm with 1mm step. The scanlines are concatenated  
 328 to form the acquired vector  $\mathbf{c}$ . A PSF  $y(x, z)$  is determined by placing a unity amplitude scatterer on  
 329 position  $(x, z)$  and acquiring the corresponding  $\mathbf{c}$ . (b) Extracts from the acquired data for the three  
 330 center-most transducer positions, with a unity amplitude scatterer located at the center of the ROI.  
 331 White Gaussian noise was added with  $\sigma = 0$  (up),  $\sigma = 0.08$  (middle) and  $\sigma = 0.12$  (bottom).

332 Following [21], the model grid has  $31 \times 41 = 1271$  modelled locations distributed with regular  
 333 spacing of 1mm on both  $x$  and  $z$  directions. On  $x$  direction, the locations are the same as the transducer  
 334 positions, i.e.  $x = 0, 1\text{mm}, \dots, 30\text{mm}$ . On  $z$  direction, 41 locations are modelled regularly between  
 335 18mm and 58mm, i.e.,  $z = 18\text{mm}, 19\text{mm}, \dots, 58\text{mm}$ .

336 As explained in Section 4.1, in the expanded acquisition model, the grid locations give place to  
 337 local ROIs. Our expanded model has 1271 local ROIs with  $\Delta_x = \Delta_z = 1\text{mm}$ , with centers corresponding  
 338 to the modelled locations of the regular model. Consequently, our ROI extends from  $x = -0.5\text{mm}$  to  
 339  $x = 30.5\text{mm}$  and from  $z = 17.5\text{mm}$  to  $z = 58.5\text{mm}$ . The highly coherent local manifolds were created  
 340 with  $R_x = 5$  and  $R_z = 15$ , thus  $R = 75$ . Therefore,  $\delta_x = 250\mu\text{m}$  and  $\delta_z = 71.4\mu\text{m}$ .

341 We simulated the acquisition for 200 cases of 5 unity amplitude scatterers randomly distributed  
 342 over the ROI. The scatterers positions were not forced over any kind of grid. White Gaussian noise  
 343 with three different levels ( $\sigma = 0, 0.08, 0.12$ ) was added to each simulated acquisition. Since the energy  
 344 of the acquired signal (without noise) varies according to factors such as distance to transducer and  
 345 constructive/destructive interference, we consider that the parametrization of noise in terms of its  
 346 standard deviation  $\sigma$  is more appropriate than signal-to-noise ratio (SNR). To provide a visual notion of  
 347 the noise levels, Fig. 5b shows an extract of acquired data for the three noise levels from an acquisition  
 348 where a single scatterer was placed on the center of the ROI. Scanlines from the three center-most  
 349 positions of the transducer are concatenated.

## 343 6.2. Recovery accuracy

344 To compute the accuracy on the recovery of scatterers, we ran OMPED with a fixed number of  
 345 5 iterations, with  $\mu_c = 0.8$ ,  $\Delta_\mu = 0.1$  and  $K$  varying from 2 to 10 for the 200 simulated acquisitions  
 346 with the three levels of noise. Each recovered scatterer distant less than 0.5mm in both axial and  
 347 lateral directions from the closest original simulated scatterer was computed as a hit – otherwise it  
 348 was computed as a miss. Fig. 6a shows the percentage of misses from 1000 recovered scatterers for  
 349 all 9 values of  $K$  and 3 noise levels. Even for the highest level of noise, misses kept below 10% for  
 350  $6 \leq K \leq 10$ . For comparison, we ran OMP with the regular dictionary  $\mathbf{H}$  on the same set of simulated  
 351 acquisitions. The resulting percentages of misses were 38.9%, 42.4% and 45.2% for the noise levels  
 352  $\sigma = 0, 0.08$  and 0.12 respectively.

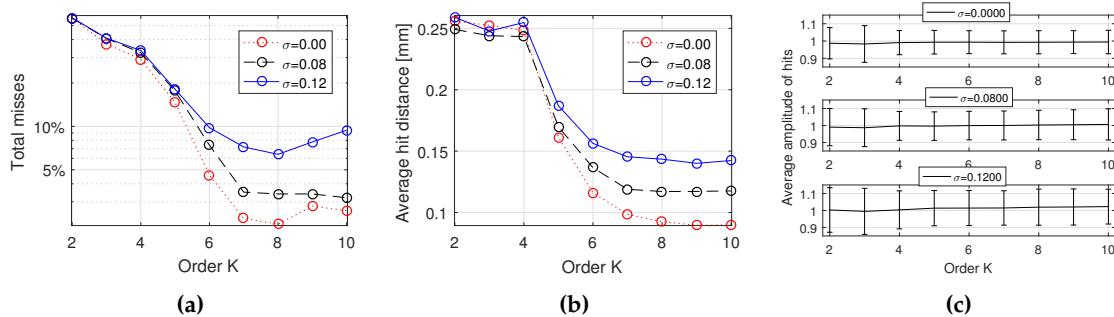


Figure 6. (a) Percentage of misses (from 1000 simulated events) as a function of  $K$ , for three levels of noise, with OMPED running with a fixed number of 5 iterations (each of the 200 simulated acquisition had 5 scatterers). Each recovered scatterer distant more than 0.5mm in any direction (axial or lateral) from the closest original simulated scatterer was computed as a miss. A minimum in the global number of misses is found at  $K = 8$ . For  $K > 8$ , few useful information is added to the dictionary at the expense of increased coherence. (b) Distance between recovered events (hits) and their corresponding simulated true event. (c) Average amplitude of the events computed as hits, for noise levels  $\sigma = 0$  (up),  $\sigma = 0.08$  (middle) and  $\sigma = 0.12$  (bottom). The bars indicate one standard deviation above and below the average. All simulated events have unity amplitude.

353 A small increase in the count of misses is observed for values of  $K \geq 8$ . This is possibly explained  
 354 by the fact that, for  $K \geq 8$ , increasing  $K$  adds few useful information to the dictionary at the cost of  
 355 increasing coherence. For the SVD basis, the value of the singular values  $\sigma_k$  can be used as a measure  
 356 of useful information. Fig. 3b shows how  $\sigma_k$  behaves for the center-most local manifold  $\mathbf{M}$ <sup>(636)</sup>. Notice  
 357 that values of  $\sigma_k$  for  $k \geq 8$  are significantly smaller than the previous ones.

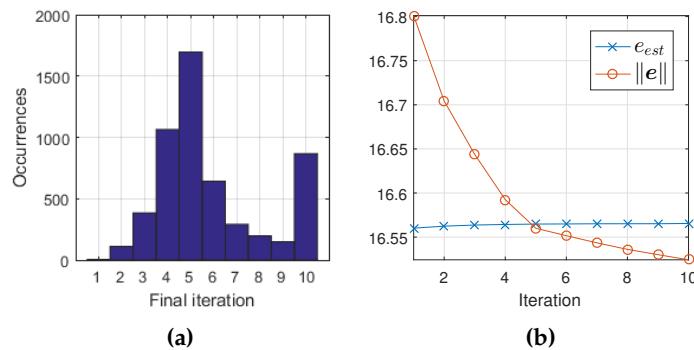
358 For every hit, the distance between the original and the recovered scatterers was computed. The  
 359 average distances are shown in Fig. 6b.

360 The computation of hits and misses does not take into account the amplitude of recovered  
 361 scatterers, i.e., recovered scatterers are implicitly considered as having unity amplitude. To endorse  
 362 this assumption, the average amplitudes of recovered events are shown in fig. 6c, where the bars  
 363 indicate one standard deviation above and below the average. Notice that, for all cases, the average  
 364 amplitudes are between 0.98 and 1.01, i.e., the average amplitude error is less than 2%. The average  
 365 absolute amplitude resulting from the reconstructions with OMP using the regular dictionary  $\mathbf{H}$  were  
 366 0.70, 0.70 and 0.71 for the noise levels  $\sigma = 0, 0.08$  and 0.12 respectively.

## 367 6.3. Estimation of residual and stop criterion

368 To assess the accuracy of the stop criterion, OMPED was executed one more time on the 5-scatterer  
 369 dataset of Section 6.1, this time with the residual-based stop criterion defined on line 14 of Algorithm 1,  
 370 with a maximum of 10 iterations. Because all images contained 5 scatterers, the algorithm was expected

371 to stop at the 5-th iteration. The histogram of Fig. 7a shows this outcome: the peak of occurrences is on  
 372 iteration 5. The frequencies on the neighboring final iterations 4 and 6 are also sensibly greater than  
 373 on the remaining iterations (except for the maximum 10). The maximum iteration allowed was 10, at  
 374 which the algorithm stopped when  $e_{\text{est}}$  failed to reach  $\|\mathbf{e}\|$ . The results for values of  $K$  from 2 to 10 are  
 375 summed on the histogram of Fig. 7a. A total of 5400 reconstruction (3 noise levels  $\times$  200 images  $\times$  9  
 376 orders  $K$ ) are computed.



**Figure 7.** (a) Histogram of final iteration (when  $e_{\text{est}} \geq \|\mathbf{e}\|$  for the first time) for OMPED running with the SVD dictionary, for  $K$  varying from 2 to 10. Results from all values of  $K$  are summed. The total number of reconstructions is 5400. The 5th iteration was more frequently identified as final iteration, which is correct since all simulated acquisitions contained 5 scatterers. (b) Example of evolution of  $e_{\text{est}}$  and  $\|\mathbf{e}\|$  along the iterations of OMPED. In this case,  $e_{\text{est}}$  dropped below  $\|\mathbf{e}\|$  at the 5th iteration, which was correctly identified as the final iteration. The simulated object contained 5 scatterers. White Gaussian noise with  $\sigma = 0.12$  was added to the acquired data. OMPED was ran with the SVD dictionary with  $K = 8$ .

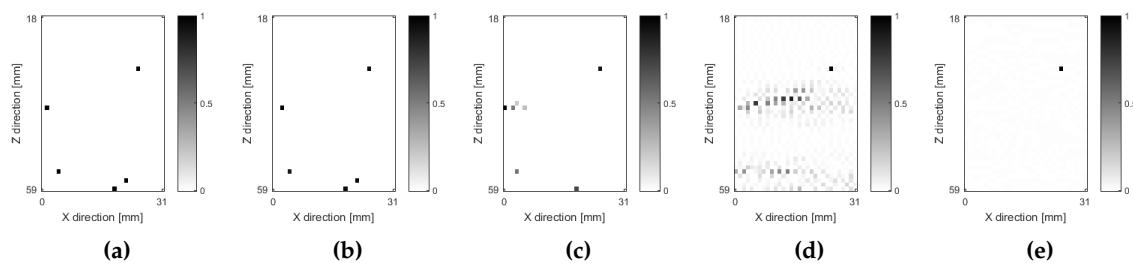
377 Fig. 7b shows an example of the evolution of the regression residual norm  $\|\mathbf{e}\|$  and the estimated  
 378 residual norm  $e_{\text{est}}$ . As new events are iteratively added to the solution, the latter decreases while the  
 379 former increases. On iteration 5,  $\|\mathbf{e}\|$  drops below  $e_{\text{est}}$  and OMPED correctly meets the stop criterion,  
 380 yielding a final solution with cardinality 5. White Gaussian noise with  $\sigma = 0.12$  was added to the data.  
 381 OMPED was ran with SVD ( $K = 8$ ) dictionary.

#### 382 6.4. Reconstructed images: examples

383 Fig. 8a shows the ground truth for a simulation from the dataset of Section 6.1. Gaussian noise was  
 384 added to the acquired data with  $\sigma = 0.08$ . The reconstructed image using OMPED with SVD dictionary  
 385 ( $K = 8$ ) is shown in Fig. 8b. No limit was imposed on the number of iterations, i.e., the algorithm  
 386 correctly stopped at the 5th iteration based on the values of the estimated and actual residuals. The  
 387 activated pixels are the same on the ground truth of Fig. 8a and on the OMPED result of Fig. 8b. While  
 388 all simulated scatterers had unity amplitude, the recovered amplitudes ranged from 0.9398 to 1.0387.  
 389 Both Figs. 8a and 8b have  $41 \times 31$  pixels corresponding to the local ROIs of the expanded model.

390 The result of the reconstruction using OMP with the regular dictionary model  $\mathbf{H}$  is shown in Fig. 8c.  
 391 We ran 7 iterations of the algorithm in order to show that, beyond iteration 4, the algorithm created  
 392 artifacts around the left-most scatterer instead of identifying the bottom-right scatterer. The recovered  
 393 amplitudes also display small and even negative values (the image shows absolute, normalized values).  
 394 Moreover, the bottom-left scatterer is displaced one pixel to the left on the reconstructed image.

395 Fig. 8d shows the image yielded by the LS (unregularized) solution of (4). As is common in  
 396 unregularized model-based solutions, the image is dominated by noise [35]. We also applied  $\ell_1$   
 397 regularization to the LS problem, which corresponds to the BP formulation [28]



**Figure 8.** Example of image simulated and reconstructed, from the dataset described in Section 6.1. The simulated data contains 5 scatterers and white Gaussian noise with  $\sigma = 0.08$ . All images are normalized by the maximum absolute pixel value. (a) Ground truth, with 5 unity amplitude scatterers randomly distributed over the ROI. (b) Result from OMPEd with the SVD dictionary ( $K = 8$ ). The algorithm correctly identified the 5th iteration as the final one. (c) Result from OMP with regular model H. 7 iterations were run to show that, after the 4th iteration, the algorithm creates artifacts on the neighborhood of the left-most scatterer instead of identifying the bottom-right scatterer present on the ground truth image. (d) Solution of the unregularized LS problem (4). The image is dominated by artifacts. (e) Solution of the  $\ell_1$ -regularized problem (28). The penalization of the recovered amplitudes causes the suppression of most points on the resulting image. The chosen regularization parameter  $\lambda = 2.0691$  minimizes the norm  $\|\mathbf{v} - \hat{\mathbf{v}}\|$ , where  $\mathbf{v}$  is the ground truth.

$$\hat{\mathbf{v}} = \arg \min_{\mathbf{v}} \|\mathbf{c} - \mathbf{Hv}\|_2^2 + \lambda \|\mathbf{v}\|_1. \quad (28)$$

398 The  $\ell_1$ -regularized formulation was solved with L1\_LS package for Matlab [36]. The resulting image is  
 399 shown in Fig. 8e. While a small value for  $\lambda$  yields an image dominated by noise, such as that of Fig. 8d,  
 400 larger values cause the image to be too sparse, suppressing some features. This is a consequence of  
 401 the penalization of recovered amplitudes on (28). The chosen regularization parameter  $\lambda = 2.0691$   
 402 minimizes the norm  $\|\mathbf{v} - \hat{\mathbf{v}}\|_2$ , where  $\mathbf{v}$  is the ground truth and  $\hat{\mathbf{v}}$  is the BP result.

## 403 7. Discussion

404 To cope with the problem of off-grid deviation in image reconstruction from pulse-echo ultrasound  
 405 data, we developed a technique of dictionary expansion based on a highly coherent sampling of the  
 406 PSF manifold followed by a rank reduction procedure, as well as a generalization of the OMP algorithm  
 407 with non-convex constraints. Based on [29], the criterion for the rank reduction is the minimization of  
 408 the Frobenius norm of the resulting residuals.

409 Since no assumption is made regarding the geometry of the continuous PSF manifold, our  
 410 expansion formulation is applicable to both shift-invariant and shift-variant problems. On the other  
 411 hand, for instance, the Polar expansion [23] is conceived based on the fact that the PSF manifold of  
 412 any shift-invariant system lies over a hypersphere. In 2-dimensional ultrasound (our main motivating  
 413 application), the fact that the Spatial Impulse Response (SIR) is spatially variant [15,37] puts the direct  
 414 acquisition model in the class of shift-variant systems.

415 The criterion for definition of the order  $K$  of expansion may vary according to each application. In  
 416 cases where it is possible to carry out simulations (as presented here) or a relevant amount of data  
 417 with accessible ground truth is available,  $K$  can be determined empirically. Moreover, in our case,  
 418 a minimum in the number of misses is identifiable and lies near to a transition on the baseline of  
 419 singular values shown in Fig. 3b. A suggestion for future studies is the development of a generalized  
 420 criterion for the definition of  $K$ . The behavior of the singular values yielded by an SVD decomposition  
 421 of matrices  $\mathbf{M}^{(n)}$  is potentially a starting point for such investigation.

422 The original OMP algorithm [30] is a particular case of OMPED where  $K = 1$  and the parameter  
423  $\mu_c$  (Eqs. (17a) and (21)) is set to an arbitrarily large negative value. In both OMP and OMPED, the  
424 residual vector  $\mathbf{e}$  on each iteration is orthogonal to all active elements of the dictionary, what places  
425 OMPED in the family of *Orthogonal* Matching Pursuit algorithms. The same does not hold for the  
426 COMP algorithm presented in [29]: the fact that the LS regression performed at each iteration contains  
427 linear constraints may result in eventual coherence between the residual and the active atoms.

428 Another particularity of OMPED in regard to previously proposed algorithms for expanded  
429 dictionaries [23,29,33] is that it is not based on conic constraints, which removes any restrictions on the  
430 choice of the sizes  $\Delta_x$  and  $\Delta_z$  (and further dimensions if that is the case) for the division of the ROI into  
431 local ROIs.

432 The adaptation of OMP into OMPED, with a constraint imposed on the selection of the index  
433 added the support at each iteration, might be replicable to other greedy search algorithms. The class of  
434 forward-backward algorithms is of special interest in signal and image recovery because of its capacity  
435 of later “correction” of “wrong” choices made on the selection of indices to add to the support [38,39],  
436 what constitutes a motivation for future investigation.

437 The computation of the estimated residual  $e_{\text{est}}$  on OMPED may be subject to improvement in  
438 order to increase the accuracy of the stop criterion (see Fig. 7a). Decreasing the variance of the residuals  
439  $\mathbf{r}_i^{(n)}$  caused by the low-rank approximation inside each local ROI (i.e. flattening the surfaces of Fig. 3c)  
440 would cause the inaccuracies on the computation of high resolution locations to have a smaller impact  
441 on the computation of  $e_{\text{est}}$ . This may be achieved with a different criterion for the rank reduction than  
442 the LS. For instance, an extension of the Minimax dictionary expansion [31].

443 One limitation of our technique is that one single point-like event is identifiable inside each local  
444 ROI. The search for a means to overcome this limitation, allowing for the recovery of several scatterers  
445 inside the same local ROI is a relevant topic for further investigation and may broaden the applicability  
446 of the proposed technique.

447 Finally, our simulated data considered point-like reflectors, with spatial coordinates  $(x, z)$  as the  
448 only nonlinear parameters. The ultrasound NDT literature contains parametric reflection models for  
449 more complex discontinuity structures, such as spherical voids and circular cracks, where the distortion  
450 of ultrasound waves is modelled as a nonlinear function of parameters like diameter and angle to  
451 the surface [40,41]. The proposed method is applicable to those cases as long as those parameters  
452 are comprised in the parameter set  $\tau$  in (1) and sampled like the parameters of spatial location. In  
453 this case, characterization of discontinuities could be performed along with location. Classification of  
454 discontinuities could also be jointly performed if dictionaries for several types of discontinuities are  
455 combined. An equivalent principle has been used in the joint detection and identification of neuron  
456 activity using SVD [29] and Taylor [42] expanded dictionaries.

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458 *Reconstruction* (LIPRO) at the Graduate Program in Electrical and Computer Engineering (CPGEI), at the Federal  
459 University of Technology-Paraná (UTFPR), Brazil. T.A.R.P. is responsible for generating the datasets, writing and  
460 running the MATLAB codes, and describing the models and methods. M.V.W.Z. and D.R.P. are responsible for  
461 reviewing the mathematical accuracy of methods, organizing the paper argument and reviewing the ultrasonic  
462 model accuracy.

463 **Conflicts of Interest:** The authors declare no conflict of interest.

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