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Reconstructing source terms from atmospheric concentration measurements: Optimality analysis of an inversion technique

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Key Points:

- A data assimilation technique (discrete renormalization technique) is proposed
- The renormalized solution can be computed using a generalized inverse operator
- This operator fulfils optimal properties for the localization of single sources

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Abstract

In the event of an accidental or intentional contaminant release in the atmosphere, it is imperative, for managing emergency response, to diagnose the release parameters of the source from measured data. Reconstruction of the source information exploiting measured data is called an inverse problem. To solve such a problem, several techniques are currently being developed. The first part of this paper provides a detailed description of one of them, known as the renormalization method. This technique, proposed by Issartel (2005), has been derived using an approach different from that of standard inversion methods and gives a linear solution to the continuous Source Term Estimation (STE) problem. In the second part of this paper, the discrete counterpart of this method is presented. By using matrix notation, common in data assimilation and suitable for numerical computing, it is shown that the discrete renormalized solution belongs to a family of well-known inverse solutions (minimum weighted norm solutions), which can be computed by using the concept of generalized inverse operator. It is shown that, when the weight matrix satisfies the renormalization condition, this operator satisfies the criteria used in geophysics to define good inverses. Notably, by means of the Model Resolution Matrix (MRM) formalism, we demonstrate that the renormalized solution fulfils optimal properties for the localization of single point sources. Throughout the article, the main concepts are illustrated with data from a wind tunnel experiment conducted at the Environmental Flow Research Centre at the University of Surrey, UK.

1. Introduction

In the specific context of emergency situations due to accidental or intentional releases of hazardous CBRN (Chemical, Biological, Radiological, and Nuclear) substances in the atmosphere, real-time concentrations and meteorological measurements are used, by authorities, to help to assess risks and to optimize response actions. Currently, at either local, continental, or global scales, these near-live measurements feed into models of atmospheric dispersion, to get a clear picture of the situation and provide basics for decisions. But, to obtain a reliable computation from these various models, a suitable description of the source strength and location is mandatory: if these source parameters are unreliable all the prediction of dispersion (and thus all the subsequent emergency response steps and management actions), quickly become questionable. Since, in most of the cases, an accurate description of the source is not available, source term estimation (STE) algorithms can be employed. These algorithms use data assimilation techniques to combine measured data with computer models for the purpose of determining the unknown source parameters. This task is called the STE inverse problem.

Recently developed assimilation techniques, used to solve the STE inverse problem, have been reviewed by different authors. *Liu and Zhai* [2007] divided the methods into three categories, i.e., forward, backward, and probability inverse modeling methods, and *Rao* [2007] into two parts, i.e., forward and backward transport modeling methods. *Yee* [2012] classifies the source estimation methods as deterministic optimization and stochastic Bayesian approaches just as *Zheng and Chen* [2011] who distinguish optimization modeling methods and probability modeling methods. These latter authors conclude with the observation that “as prior information about unknown parameters is lacking, probability modeling methods are insufficient in emergency situations.” In general, fast, safe, and reliable source estimates can be obtained from deterministic methods, associated with either forward or backward dispersion models, with minimum a priori information.

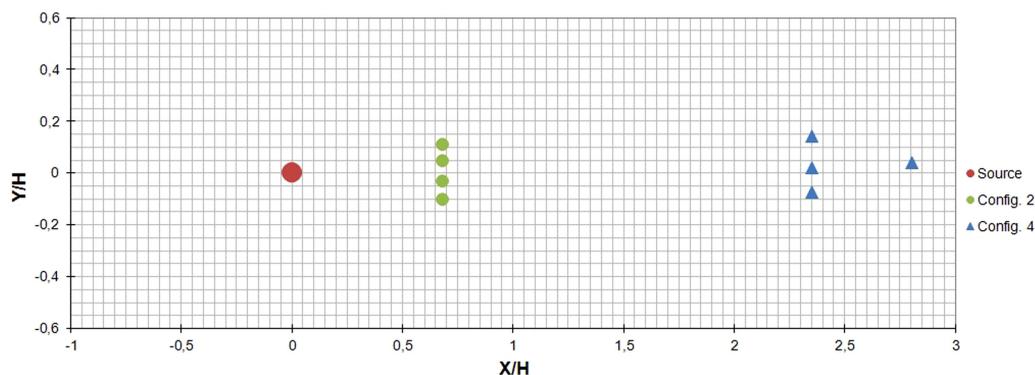


Figure 1. Arrangement of the EnFlo wind tunnel for the DYCE experiment [Rudd *et al.*, 2012]: source and receptors positions for configurations 2 and 4 (green filled circles and blue filled triangles). For determining the source characteristics, the full computational domain (not represented here) extends $-3H$ downstream from the actual source location.

In this paper, the deterministic assimilation strategy known as the renormalization method is reviewed and extended to discrete inverse problems. This approach has been defined by Issartel [2005] to reconstruct tracer source from air concentration measurements at continental scale only using measured data. It relies on the networking of several detectors, on the use of adjoint transport equations (inverse modeling methods) and on the computation of a renormalizing weight function (also referred to as the visibility function). It returns a continuous source estimate which is linear with respect to the observations and from which the origin of the contaminant can be appreciated. It has been used for the retrieval of distributed areal emissions at continental scale, from satellite measurements [Issartel *et al.*, 2007]. Sharan *et al.* [2009, 2012] and Issartel *et al.* [2011] extended it for the reconstruction of single ground-level point sources. They test it at local scale, especially during low wind speed conditions. Recently, Singh *et al.* [2013] used it for the identification of multiple-point sources releasing similar tracer, in which influences from the various emissions are merged in each detector’s measurement. In the first part of this article, the main results and physical interpretations of these previous works are summarized.

Then, the discrete counterpart of the renormalization method is presented. The linear relationship between the measured concentration data and the source, represented by an integral equation, is transformed into a system of discrete linear equations. The renormalized source estimate is then derived by using an appropriate weight matrix. It is shown that this estimate corresponds to a minimum weighted norm solution which can be expressed by using the concept of generalized inverse operator [Ben-Israel and Greville, 2003].

Moreover, it is shown that this inverse operator satisfies criteria used in geophysics to define a “good inverse” [Jackson, 1972] and that it fulfils several optimal properties for the localization of single point sources. This is demonstrated by using the so-called Model Resolution Matrix (MRM) formalism, initially defined for discrete geophysical data analysis by Menke [1984] and currently used to evaluate solutions to the neuroelectromagnetic inverse problem [Grave de Peralta *et al.*, 2009]. To the best of the authors’ knowledge, this is the first comprehensive Source Term Estimation study that investigates the properties of a method relative to the concept of MRM.

Throughout the paper, results computed from a series of dispersion experiments [Rudd *et al.*, 2012] conducted in a meteorological wind tunnel, under neutral condition, are provided for illustrative purposes. Those data were obtained at the Environmental Flow Research Centre (ENFLO), in the frame of the DYCE project [Lepley *et al.*, 2011]. In all the trials, a gas mixture of 1.5% propane in air was released as a tracer over a period of 15 min. The concentrations were measured by four fast-response flame ionization detectors (FFIDs) at the frequency response of 200 Hz. The height of the sources and of the samplers was $0.1H$, where H is the boundary layer height. Eleven different configurations for the position of the FFIDs were tested with the same wind speed ($U_H = 2.5 \text{ m s}^{-1}$) and direction (aligned with the x axis). For a representative purpose, only configurations 2 and 4, see Figure 1, have been used in this paper. The goal is not to analyze the data set but rather to highlight the optimal reconstruction features of the method.

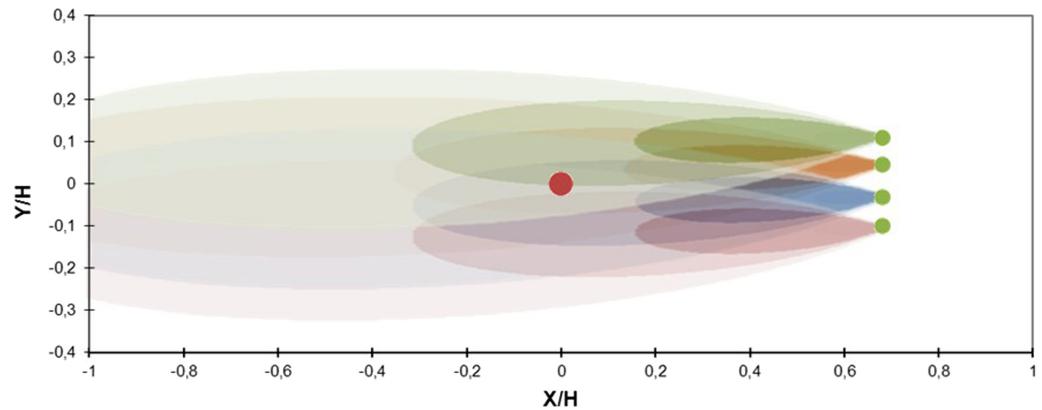


Figure 2. Steady retroplumes, drawn with four colors, for configuration 2 of DYCE experiment (focus around the source position). The Gaussian dispersion model proposed by *Sharan et al.* [1996] in the forward mode is utilized here for the computation of these sensitivity functions by rotating the wind direction by 180° and assuming an unit release at the FFIDs' locations [*Singh et al.*, 2013].

2. The Renormalization Method for Linear Inverse Problems

2.1. Inverse Problem Statement

Reconstruction of the release parameters exploiting data measured by a monitoring network is an inverse problem, called the Source Term Estimation (STE) problem. Such a problem is necessarily addressed by use of a model which describes our understanding of the relationship between the concentration measurements, the known parameters of the problem (meteorological data, variables characterizing the atmospheric domain and the receptors...), and the source parameters that we wish to estimate. In the approach proposed by *Issartel* [2005], a receptor oriented (also designated as backward) model is used to establish a mapping between the problem parameters and the measured data. The n actual measured concentrations are assembled into an observation vector $\boldsymbol{\mu} \in \mathbb{R}^n$ (bold-face, lower-case letters refer to vectors, and italic lower-case letters refer to vector components or scalar). The source parameters are represented, in the domain of interest Ω , by $\sigma(\mathbf{x}, t)$, a function of space $\mathbf{x} = (x, y, z)$ and time t , named the source function (or emission function) with an intensity proportional to the release rate.

The known parameters are taken into account through sensitivity functions, or adjoint functions, $r_i(\mathbf{x}, t)$ ($i = 1 \dots n$), which describe the sensitivity of the "receptors" with respect to the "emissions" in the various regions of Ω . Within the Eulerian framework, the functions r_i are solutions of adjoint transport equations and correspond to retroplumes scattered back in time upwind from detector locations [*Issartel and Baverel*, 2003]. They are obtained from physical modeling (backward dispersion models, see Figure 2) and assembled into an adjoint vector $\mathbf{r}(\mathbf{x}, t) \in \mathbb{R}^n$. In this paper, for a matter of simplicity, the renormalization technique is presented only for continuous releases and steady flow. For time varying releases, with time varying functions, the reader is referred to *Issartel et al.* [2007]. The relationship between the measurements μ_i ($i = 1 \dots n$), the source, and the sensitivity functions is expressed in a scalar form as:

$$\mu_i = \int_{\Omega} \sigma(\mathbf{x}) r_i(\mathbf{x}) d\mathbf{x} \tag{1}$$

2.2. Estimate of the Visible Part of the Source

The model (1) involves the scalar product $\langle \boldsymbol{\zeta}, \boldsymbol{\zeta} \rangle = \int_{\Omega} \boldsymbol{\zeta}(\mathbf{x}) \boldsymbol{\zeta}(\mathbf{x}) d\mathbf{x}$, so that the source term can be decomposed as $\sigma(\mathbf{x}) = \sigma_{\perp}(\mathbf{x}) + \sigma_{//}(\mathbf{x})$. $\sigma_{\perp}(\mathbf{x})$ is the source component orthogonal to the adjoint functions, $\langle \sigma_{\perp}, r_i \rangle = 0$, and $\sigma_{//}(\mathbf{x})$ is the parallel component, i.e., the "visible" component, which can be written as a linear combination of the $r_i(\mathbf{x})$

$$\sigma_{//}(\mathbf{x}) = \sum_{i=1}^N \lambda_i r_i(\mathbf{x}) \text{ or } \sigma_{//}(\mathbf{x}) = \boldsymbol{\lambda}^T \mathbf{r}(\mathbf{x}) \tag{2}$$

in which the superscript T denotes the transposition and where the coefficients λ_i are the elements of the vector $\boldsymbol{\lambda} \in \mathbb{R}^n$ obtained as

$$\lambda = \mathbf{H}^{-1} \boldsymbol{\mu} \tag{3}$$

$\mathbf{H} \in \mathbb{R}^{n \times n}$ is a positive definite, symmetric, Gram matrix of coefficients $H_{ij} = \langle r_i, r_j \rangle$ (bold-face, capital letters refer to matrices, italic capital letters refer to matrix elements). By reporting (3) in equation (2), the continuous source estimate is derived as

$$\sigma_{//}(\mathbf{x}) = \boldsymbol{\mu}^T \mathbf{H}^{-1} \mathbf{r}(\mathbf{x}) \tag{4}$$

We note that the source estimate given by (4) corresponds with a “normal solution” of an inverse problem as defined by *Bertero et al.* [1985].

2.3. An Appropriate Weight Function to Minimize Artificial Information

It has been shown by *Issartel et al.* [2007] that $\sigma_{//}(\mathbf{x})$ contains artifacts, in the form of peaks corresponding to a singularity of the adjoint functions associated with the points of measurement. These artifacts are removed through a process called renormalization, which minimizes the excess entropy corresponding to the artificial information unduly derived from the measurements. This is addressed by introducing, in the model, a weight function $f(\mathbf{x}) > 0$ such that $\int_{\Omega} f(\mathbf{x}) d\mathbf{x} = n$. The relationship between the measurements and the source function is modified as:

$$\mu_i = \int_{\Omega} \sigma(\mathbf{x}) r_{fi}(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} \quad \text{with} \quad r_{fi}(\mathbf{x}) = \frac{r_i(\mathbf{x})}{f(\mathbf{x})} \tag{5}$$

This expression involves a new weighted scalar product $\langle \zeta, \zeta \rangle_f = \int_{\Omega} \zeta(\mathbf{x}) \zeta(\mathbf{x}) f(\mathbf{x}) d\mathbf{x}$ and modified adjoint functions $r_{fi}(\mathbf{x})$ such that

$$\mu_i = \langle \sigma, r_{fi} \rangle_f \tag{6}$$

Following the scheme defined in section 2.2, the estimate of the visible part of the source at position \mathbf{x} is obtained as:

$$\sigma_{//f}(\mathbf{x}) = \boldsymbol{\mu}^T \mathbf{H}_f^{-1} \mathbf{r}_f(\mathbf{x}) \tag{7}$$

\mathbf{H}_f is the Gram matrix of the modified adjoint functions, with coefficients $\langle r_{fi}, r_{fj} \rangle_f$. *Issartel* [2005] showed that a unique weight function $f(\mathbf{x}) = \varphi(\mathbf{x})$ best avoiding inversion artifacts exists. This function is optimal in the sense that it minimizes the excess entropy. It satisfies the property as

$$\mathbf{r}_{\varphi}^T(\mathbf{x}) \mathbf{H}_{\varphi}^{-1} \mathbf{r}_{\varphi}(\mathbf{x}) \equiv 1 \tag{8}$$

From a practical point of view, the optimal weight function satisfying equation (8) is easily computed as the converged value of $\varphi_p(\mathbf{x})$ from the following iterative scheme [*Issartel et al.*, 2007]:

$$\varphi_{p+1}(\mathbf{x}) = \varphi_p(\mathbf{x}) \sqrt{\frac{\mathbf{r}_{\varphi_p}^T(\mathbf{x}) \mathbf{H}_{\varphi_p}^{-1} \mathbf{r}_{\varphi_p}(\mathbf{x})}{\varphi_p(\mathbf{x})}} \quad \text{with} \quad \varphi_0(\mathbf{x}) = 1 \tag{9}$$

This function is currently interpreted as the visibility of the monitoring network characterizing the regions well or poorly monitored. It is generally focused at the detectors locations and decreases with increasing downwind distance from the monitoring network. This focus is illustrated by Figure 3 for the DYCE experiment. If the value of the visibility function at a point is nearly zero, a source at that point will be hardly identified. That is to say, a source is detected with an enhanced probability if it falls in a high visibility region. Therefore, the visibility function has also been interpreted as the prior distribution of the emissions apparent to the monitoring system [*Issartel et al.*, 2011].

2.4. Best Weight Function for Single Point Source Localization

The weight function $\varphi(\mathbf{x})$ plays a key role in the renormalization theory especially when measurements are assumed to be generated from a single point source of unknown strength q and location \mathbf{x}_0 , i.e., when the source term may be written as $\sigma(\mathbf{x}) = q\delta(\mathbf{x} - \mathbf{x}_0)$. In this case, *Sharan et al.* [2009, 2012] and *Issartel et al.* [2011] have shown that equation (6) can be written as

$$\mu_i = q\varphi(\mathbf{x}_0) r_{\varphi i}(\mathbf{x}_0) \tag{10}$$

By applying equation (10) into the equation (7), we obtain

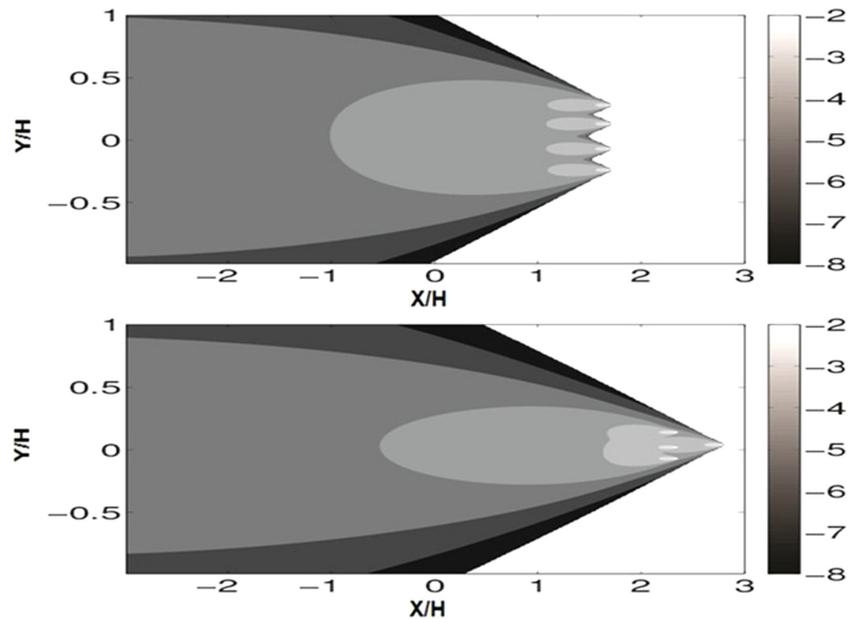


Figure 3. Classical black and white logarithmic representations of the visibility function $\varphi(\mathbf{x})$ for configurations 2 and 4. φ decays upwind of the monitoring network and becomes negligibly small after approximately $X/H = -1$ and $X/H = -0.5$, respectively, for configurations 2 and 4.

$$\sigma_{//\varphi}(\mathbf{x}) = q\varphi(\mathbf{x}_0)\mathbf{r}_\varphi^T(\mathbf{x}_0)\mathbf{H}_\varphi^{-1}\mathbf{r}_\varphi(\mathbf{x}) \quad (11)$$

Now, using Cauchy-Schwartz inequality in equation (11), it is elementary to show that with the renormalizing condition (8), the maximum of the source estimate will coincide with the location of the point source (since $\mathbf{r}_\varphi^T(\mathbf{x}_0)\mathbf{H}_\varphi^{-1}\mathbf{r}_\varphi(\mathbf{x}) \equiv 1$ only when $\mathbf{x} = \mathbf{x}_0$). Once the source location is identified, the source strength at source position \mathbf{x}_0 can be estimated as

$$q = \sigma_{//\varphi}(\mathbf{x}_0) / \varphi(\mathbf{x}_0) \quad (12)$$

To obtain this estimate, additional information, i.e., information not contained in the measurement vector, has been added to the problem. Here this “a priori information” quantifies an expectation about the character of the source (single point source). This assumption may not be based on the actual data and depends only on expert’s opinion. Since, in most of the cases, we are not able to identify reasonably a priori assumption, a more general method must be used to construct the source estimate.

3. The Discrete Renormalization Technique

3.1. Discrete Approach

In this part, a discrete approach to obtain a numerical solution of the inverse problem, defined in section 2.1, is presented. In this approach, common in data assimilation, the problem is reduced to determine the values of the source function on a grid of m points defined within the atmospheric domain. To that, the continuous source function $\sigma(\mathbf{x})$ is transformed into a source vector, taken as a column, and denoted as $\boldsymbol{\sigma} \in \mathbb{R}^m$. Assuming that the integral equation (1) can be represented by a discrete sum, the measurements are related to the source vector by a system of linear equations:

$$\boldsymbol{\mu} = \mathbf{R}\boldsymbol{\sigma} \quad (13)$$

In this model, the elements of the n lines of the retroplumes matrix $\mathbf{R} \in \mathbb{R}^{n \times m}$ correspond to the m discrete values of the n adjoint functions (retroplumes) obtained from physical modeling. This matrix is easily computed from analytical or numerical solutions of backward dispersion models as illustrated in Figure 2.

The estimation of the source from (1) is an ill-posed problem in the sense of *Hadamard* [1923]. As a consequence, the discrete problem (13) is highly underdetermined with m , the number of unknown components

of the source vector, always larger than n , the number of available concentration measurements. The underdetermination of (13) naturally implies the nonuniqueness of the inverse solution.

3.2. The Minimum Norm Solution (MNS) and the Moore-Penrose Inverse

Assuming, as proposed in section 2.2, that the source vector can be decomposed into two terms perpendicular to each other, $\sigma = \sigma_{\perp} + \sigma_{//}$ with

$$\sigma_{//} = \mathbf{R}^T \lambda \text{ and } \mathbf{R} \sigma_{\perp} = 0 \quad (14)$$

then the linear system (13) becomes

$$\mu = \mathbf{R}(\sigma_{\perp} + \sigma_{//}) = \mathbf{R} \mathbf{R}^T \lambda = \mathbf{H} \lambda \quad (15)$$

$\mathbf{H} = \mathbf{R} \mathbf{R}^T$ is the Gram matrix already defined for the continuous inverse problem. Substitution of λ , as described in (3), into (15) yields the following expression for the “visible” part of the source

$$\sigma_{//} = \mathbf{R}^T \mathbf{H}^{-1} \mu = \mathbf{R}^T (\mathbf{R} \mathbf{R}^T)^{-1} \mu = \mathbf{R}^+ \mu \quad (16)$$

The matrix $\mathbf{R}^T \mathbf{H}^{-1} \in \mathbb{R}^{m \times n}$, or $\mathbf{R}^T (\mathbf{R} \mathbf{R}^T)^{-1}$, corresponds with the standard definition for the Moore-Penrose pseudoinverse of the matrix \mathbf{R} usually denoted as \mathbf{R}^+ [Penrose, 1955]. For a given \mathbf{R} , this matrix is unique and verifies the four Penrose equations:

$$(a) \mathbf{R} \mathbf{R}^+ \mathbf{R} = \mathbf{R} \quad (b) \mathbf{R}^+ \mathbf{R} \mathbf{R}^+ = \mathbf{R}^+ \quad (c) (\mathbf{R} \mathbf{R}^+)^T = \mathbf{R} \mathbf{R}^+ \quad (d) (\mathbf{R}^+ \mathbf{R})^T = \mathbf{R}^+ \mathbf{R} \quad (17)$$

One of the principal applications of pseudoinverses is to compute Least Squares Solutions (LSS) of underdetermined systems of linear equations [Lewis et al., 2006]. The LSS of (13), i.e., σ which minimizes $\|\mu - \mathbf{R} \sigma\|$, where $\|\cdot\|$ denotes the Euclidean norm, is not unique (underdetermination of the system). Every LSS is obtained as:

$$\sigma = \mathbf{R}^+ \mu + (\mathbf{I}_m - \mathbf{R}^+ \mathbf{R}) \mathbf{s} \quad (18)$$

where \mathbf{s} is an arbitrary vector of \mathbb{R}^m and \mathbf{I}_m is the unit matrix of size m . It is obvious that $\sigma_{//} = \mathbf{R}^+ \mu$ also minimizes $\|\sigma\|$ among all the solutions given by (18). It can be concluded that the source estimate $\sigma_{//}$ given by equation (16) corresponds to the Minimum Norm (MN) solution of the system $\mu = \mathbf{R} \sigma$.

3.3. The Model Resolution Formalism

Equation (16) gives the discrete counterpart of the nonrenormalized source estimate (4). The inverse operator in it, \mathbf{R}^+ , is called the Moore-Penrose pseudoinverse. Several criteria can be used to measure the quality of an inverse operator: “an operator will be a good inverse” if it satisfies (i) $\mathbf{R} \mathbf{R}^+ \sim \mathbf{I}_n$, (ii) $\mathbf{R}^+ \mathbf{R} \sim \mathbf{I}_m$, and if (iii) “the uncertainties in the estimate are not too large, i.e., its variance is small” [Jackson, 1972]. The first criterion ensures, in case of noiseless data, that the measurements predicted with the source estimate ($\hat{\mu} = \mathbf{R} \sigma_{//} = \mathbf{R} \mathbf{R}^+ \mu$) correspond with the true measurements. The second one ensures that the solution is as close to unique as possible. Indeed, from equation (18), it is easily seen that if $\mathbf{R}^+ \mathbf{R}$ were equal to the identity matrix (which cannot occur in underdetermined inverse problems), we would have a unique estimate of the actual source. The third criterion, studied in section 3.7, is used to measure the stability of the solution, i.e., the variation of the estimate as the measurements vary within their measurements errors. It is obvious, from the definition of the Gram Matrix \mathbf{H} , that in the particular case of the minimum norm solution (16), the first criterion is exactly verified ($\mathbf{R} \mathbf{R}^+ = \mathbf{R} \mathbf{R}^T \mathbf{H}^{-1} = \mathbf{H} \mathbf{H}^{-1} = \mathbf{I}_n$). From a physical point of view, the second criterion is the most important: the matrix $\mathbf{P} = \mathbf{R}^+ \mathbf{R} \in \mathbb{R}^{m \times m}$ depends on \mathbf{R} and then includes all the substantial information used to define the inverse solution. It is an orthogonal projection matrix

$$(a) \mathbf{P}^T = \mathbf{P} \quad (b) \mathbf{P}^2 = \mathbf{P} \quad (c) \text{tr}(\mathbf{P}) = \text{rank}(\mathbf{R}) = n \quad (19)$$

\mathbf{P} constitutes the basic tool for the analysis of the quality of the estimated solution on each grid point and is often referred to as the Model Resolution Matrix (MRM) [Menke, 1984]. Substitution of the measurement vector, as described in (13), into (16) yields the following equation:

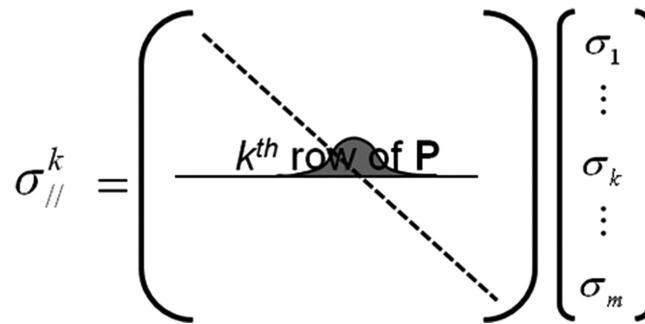


Figure 4. Plot of an ideal row of a MRM, adapted from Menke [1984].

$\sigma_{//}^k$, denoted as $\sigma_{//}^k$. A row of a MRM is known as a resolution kernel. It provides information on how other components of σ affect the reconstruction of the component associated to the row. An optimal resolution kernel exhibits a narrow peak near the main diagonal of the matrix, see Figure 4. In this case, $\sigma_{//}^k$ is obtained as a weighted sum of the nearby values σ_j of the true source vector with j near k . From the criterion proposed by Menke [1984], a resolution matrix with its largest elements near the main diagonal, i.e., a MRM close to an identity matrix, indicates that all the components of the true source can be independently identified.

Some authors [Grave de Peralta et al., 2009] prefer to center their attention on the columns of the matrix, also called the point spread functions (PSFs). Indeed, if the maximum value of the columns coincides with their diagonal element, the estimate shows optimal properties for single point source localization. By writing the j columns of \mathbf{P} as vectors \mathbf{p}_j ($j = 1 \dots m$), the estimate can be written as

$$\sigma_{//} = \mathbf{p}_1 \sigma_1 + \dots + \mathbf{p}_k \sigma_k + \dots + \mathbf{p}_m \sigma_m \quad (21)$$

Thus, $\sigma_{//}$ can be thought of as a weighted sum of the columns of \mathbf{P} , the weighting factors being the j components of the true source. For a single emission at the k th point of the domain, the source estimate is $\sigma_{//} = \mathbf{p}_k \sigma_k$. If \mathbf{p}_k exhibits a narrow peak at the main diagonal then the maximum component of the estimate corresponds to the location of the point source.

It can be concluded that an optimal MRM is a matrix close to an identity matrix, i.e., a symmetric matrix with columns (or rows) having a single sharp maximum centered about the main diagonal. Optimal rows indicate that each component of the true source is estimated independently of each other's. Optimal columns indicate that the location of all single point sources can be identified. Menke [1984] demonstrated that the Moore-Penrose pseudoinverse, used to define the minimum norm solution (16), is optimal in the sense that it minimizes the Dirichlet spread function, i.e., the difference between \mathbf{P} and \mathbf{I}_m in the least squares sense ($\text{spread}(\mathbf{P}) = \sum_{i=1}^m \sum_{j=1}^m (P_{ij} - I_{ij})^2$). However, the maxima for each row (or column, since \mathbf{P} is symmetric) are at the main diagonal only for points located very close to the receptors. Otherwise, the columns are peaked at points far from the actual source point. Thus, the minimum norm solution tends to force the solution as close as possible to the detectors' locations. This "bias" can be removed by a suitable weighting which causes the enhancement of some of the elements in \mathbf{P} .

3.4. The Minimum Weighted Norm Solution and the Weighted Generalized Inverse

Let the matrix $\mathbf{W}_f = \text{diag}(f_1, f_2, \dots, f_m) \in \mathbb{R}^{m \times m}$ be a diagonal weight matrix with components corresponding to the m discrete values of a weight function $f(\mathbf{x}) > 0$. The following change of variable can be applied to (13) leading to the following counterpart of equation (5):

$$\boldsymbol{\mu} = \mathbf{R} \mathbf{W}_f^{-1} \mathbf{W}_f \boldsymbol{\sigma} = \mathbf{R}_f \mathbf{W}_f \boldsymbol{\sigma} \quad (22)$$

where $\mathbf{R}_f = \mathbf{R} \mathbf{W}_f^{-1}$ is the modified retroplumes matrix. It can be verified that the weighted Gram matrix used in equation (7), can be written as

$$\mathbf{H}_f = \mathbf{R}_f \mathbf{W}_f \mathbf{R}_f^T \quad (23)$$

and that the "visible" part of the source, parallel to the adjoint function, is now represented as

$$\sigma_{//f} = \mathbf{R}_f^T \mathbf{H}_f^{-1} \boldsymbol{\mu} \tag{24}$$

This estimate is the discrete counterpart of the estimate given by equation (7). If \mathbf{H}_f is rewritten as $\mathbf{H}_f = \mathbf{R} \mathbf{W}_f^{-1} \mathbf{R}^T$, equation (24) becomes

$$\sigma_{//f} = \mathbf{W}_f^{-1} \mathbf{R}^T (\mathbf{R} \mathbf{W}_f^{-1} \mathbf{R}^T)^{-1} \boldsymbol{\mu} \tag{25}$$

The matrix $\mathbf{R}^{f+} = \mathbf{R}_f^T \mathbf{H}_f^{-1} = \mathbf{W}_f^{-1} \mathbf{R}^T (\mathbf{R} \mathbf{W}_f^{-1} \mathbf{R}^T)^{-1} \in \mathbb{R}^{m \times n}$ is referred to as the weighted pseudoinverse [Nakamura, 1991] or weighted generalized inverse [Ben-Israel and Greville, 2003] of \mathbf{R} . It verifies only three of the four Penrose equations (17)

$$(a) \mathbf{R} \mathbf{R}^{f+} \mathbf{R} = \mathbf{R} \quad (b) \mathbf{R}^{f+} \mathbf{R} \mathbf{R}^{f+} = \mathbf{R}^{f+} \quad (c) (\mathbf{R} \mathbf{R}^{f+})^T = \mathbf{R} \mathbf{R}^{f+} \tag{26}$$

but, instead of (d), it satisfies:

$$(d') (\mathbf{W}_f \mathbf{R}^{f+} \mathbf{R})^T = \mathbf{W}_f \mathbf{R}^{f+} \mathbf{R} \tag{27}$$

As a consequence of (27), \mathbf{R}^{f+} is also known as a \mathbf{W}_f weighted Moore-Penrose inverse, denoted by some authors as $\mathbf{R}_{\mathbf{W}_f}^+$ [Yang and Li, 2008].

Moreover, the two Hermitian positive definite matrices $\mathbf{W}_f \in \mathbb{R}^{m \times m}$ and $\mathbf{H}_f^{-1} \in \mathbb{R}^{n \times n}$ can be used to define weighted vector norms. Given two vectors $\boldsymbol{\xi} \in \mathbb{R}^m$ and $\boldsymbol{\zeta} \in \mathbb{R}^n$, the \mathbf{W}_f -weighted and \mathbf{H}_f^{-1} -weighted vector norms are, respectively, defined as

$$\|\boldsymbol{\xi}\|_{\mathbf{W}_f} = \sqrt{\boldsymbol{\xi}^T \mathbf{W}_f \boldsymbol{\xi}} = \|\mathbf{W}_f^{1/2} \boldsymbol{\xi}\| \quad \text{and} \quad \|\boldsymbol{\zeta}\|_{\mathbf{H}_f^{-1}} = \sqrt{\boldsymbol{\zeta}^T \mathbf{H}_f^{-1} \boldsymbol{\zeta}} = \|\mathbf{H}_f^{-1/2} \boldsymbol{\zeta}\| \tag{28}$$

where $\|\cdot\|$ is the Euclidian norm. It is easily seen that the problem

$$\text{minimize } \|\boldsymbol{\sigma}\|_{\mathbf{W}_f} \quad \text{subject to } \boldsymbol{\mu} = \mathbf{R} \boldsymbol{\sigma} \tag{29}$$

has the unique minimizer given by equation (25) with the minimum value

$$\|\sigma_{//f}\|_{\mathbf{W}_f} = \|\mathbf{R}^{f+} \boldsymbol{\mu}\|_{\mathbf{W}_f} = \sqrt{\boldsymbol{\mu}^T \mathbf{H}_f^{-1} \boldsymbol{\mu}} = \|\boldsymbol{\mu}\|_{\mathbf{H}_f^{-1}} \tag{30}$$

It can be concluded that the estimate given by equation (25) corresponds to the minimal \mathbf{W}_f -weighted norm solution of the system $\boldsymbol{\mu} = \mathbf{R} \boldsymbol{\sigma}$. It seems reasonable to use it as a source estimator since, in data interpretation, it attributes no possible role to $\sigma_{\perp f}$ about which nothing is known. But this raises the issue of determining a "best" weight matrix.

3.5. Optimal Weight Matrix for Single Point Source Localization

By substituting (22) in place of $\boldsymbol{\mu}$ in expression (24), the relationship between $\sigma_{//f}$ and $\boldsymbol{\sigma}$ is obtained as

$$\sigma_{//f} = \mathbf{R}_f^T \mathbf{H}_f^{-1} \mathbf{R}_f \mathbf{W}_f \boldsymbol{\sigma} = \mathbf{P}^f \boldsymbol{\sigma} \tag{31}$$

As explained in section 3.3, the nonsymmetric matrix $\mathbf{P}^f = \mathbf{R}_f^T \mathbf{H}_f^{-1} \mathbf{R}_f = \mathbf{R}^{f+} \mathbf{R} \in \mathbb{R}^{m \times m}$ is a Model Resolution Matrix. By writing the j columns of the matrices \mathbf{R} and \mathbf{R}_f as vectors, respectively, denoted as \mathbf{r}_j and $\mathbf{r}_{fj} = \mathbf{f}_j^{-1} \mathbf{r}_j$ ($j = 1 \dots m$) $\in \mathbb{R}^n$, the components of \mathbf{P}^f can be written as

$$P_{ij}^f = \mathbf{r}_{fi}^T \mathbf{H}_f^{-1} \mathbf{r}_j = \mathbf{f}_j \mathbf{r}_{fi}^T \mathbf{H}_f^{-1} \mathbf{r}_{fi} \tag{32}$$

If the elements of \mathbf{W}_f are chosen as the \mathbf{H}_f^{-1} -weighted norm of each column of \mathbf{R}

$$f_j = \sqrt{\mathbf{r}_j^T \mathbf{H}_f^{-1} \mathbf{r}_j} \quad \text{for } j = 1 \dots m \tag{33}$$

then the diagonal elements of \mathbf{P}^f are equal to the components of the weight matrix, i.e.,

$$P_{jj}^f = \mathbf{f}_j \mathbf{r}_{fi}^T \mathbf{H}_f^{-1} \mathbf{r}_{fi} = f_j \tag{34}$$

Since \mathbf{P}^f is a projection matrix, we have

$$\text{Tr}(\mathbf{P}^f) = \sum_{j=1}^m f_j = \text{rank}(\mathbf{R}) = n \tag{35}$$

We note that the conditions (33) or (34) can be rewritten as

$$\mathbf{r}_{fj}^T \mathbf{H}_f^{-1} \mathbf{r}_{fj} = 1 \quad \text{for } j=1 \dots m \tag{36}$$

which corresponds to the renormalization condition for discrete inverse problems. The weights $f_j = \varphi_j$ subject to this condition are called the renormalizing weights and are the m discrete values of the weight function $\varphi(\mathbf{x})$ defined by equation (8). By using those weights as components of the matrix \mathbf{W}_φ , the j columns of the MRM \mathbf{P}^φ , written as vectors \mathbf{p}_j^φ ($j = 1 \dots m$), are:

$$\mathbf{p}_j^\varphi = \varphi_j \begin{pmatrix} \mathbf{r}_{\varphi 1}^T \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi j} \\ \vdots \\ 1 \\ \vdots \\ \mathbf{r}_{\varphi m}^T \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi j} \end{pmatrix} \tag{37}$$

Since the Cauchy-Schwartz inequality yields

$$|\mathbf{r}_{\varphi i}^T \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi j}| \leq \sqrt{\mathbf{r}_{\varphi i}^T \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi i}} \sqrt{\mathbf{r}_{\varphi j}^T \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi j}} \tag{38}$$

from (36) we obtain:

$$|\mathbf{r}_{\varphi i}^T \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi j}| \leq 1 \quad \text{for all } i \text{ and } j=1 \dots m \tag{39}$$

With the renormalization condition (36), the columns of the resolution matrix \mathbf{P}^φ reach their maximum exactly at the main diagonal. This matrix is then close to an optimal resolution matrix described in section 3.3. In case of a single point source with an intensity q at the k th point of the domain, the source estimate will be

$$\boldsymbol{\sigma}_{//\varphi} = \mathbf{p}_k^\varphi q = \mathbf{R}_\varphi^T \mathbf{H}_\varphi^{-1} \mathbf{r}_k q \tag{40}$$

As a consequence, the maximum component of this vector, $\sigma_{//\varphi}^k = \varphi_k q$, will correspond to the location of the actual point source, as illustrated in Figure 5 for the dispersion experiment. In this case, the maximum value of the vector $\boldsymbol{\sigma}_{//\varphi} / \varphi_k$, i.e., $\sigma_{//\varphi}^k / \varphi_k$, will be taken as the source intensity. It can be concluded that the discrete renormalization technique is able to give a reliable estimate of the intensity and localization of any single point source. This good feature is due to the discrete renormalization condition (36) which confers optimal properties to the columns of the model resolution matrix.

3.6. Further Interpretations of the Method

The physical interpretation of the renormalizing weight function $\varphi(\mathbf{x})$ as a visibility function has already been discussed in section 2.3. The value of this function at a given point, which constitutes the diagonal element of both matrices \mathbf{W}_φ and \mathbf{P}^φ , quantifies the sensitivity of the receptors' configuration on a source located at this specific position. It decreases in the upwind direction and points out the lack of visibility for the most distant sources. By using equations (23) and (36), it can be easily verified that

$$\|\mathbf{p}_k^\varphi\|_{\mathbf{W}_\varphi} = \sqrt{\mathbf{p}_k^{\varphi T} \mathbf{W}_\varphi \mathbf{p}_k^\varphi} = \sqrt{\mathbf{r}_k^T \mathbf{H}_\varphi^{-1} \mathbf{r}_k} = P_{kk}^\varphi = \varphi_k \tag{41}$$

Thus, the norm of the estimate (40) is

$$\|\boldsymbol{\sigma}_{//\varphi}\|_{\mathbf{W}_\varphi} = q \|\mathbf{p}_k^\varphi\|_{\mathbf{W}_\varphi} = q \varphi_k \quad \text{and} \quad \varphi_k = \frac{\|\boldsymbol{\sigma}_{//\varphi}\|_{\mathbf{W}_\varphi}}{q} \tag{42}$$

This feature highlights another physical interpretation of the weight value at the source location as the ratio between the weighted strength of the "visible" part of a source (i.e., the \mathbf{W}_φ -weighted norm of $\boldsymbol{\sigma}_{//\varphi}$) and the real strength of the source q .

Moreover, from the definitions (28) and (37), the norm (41) can also be rewritten as

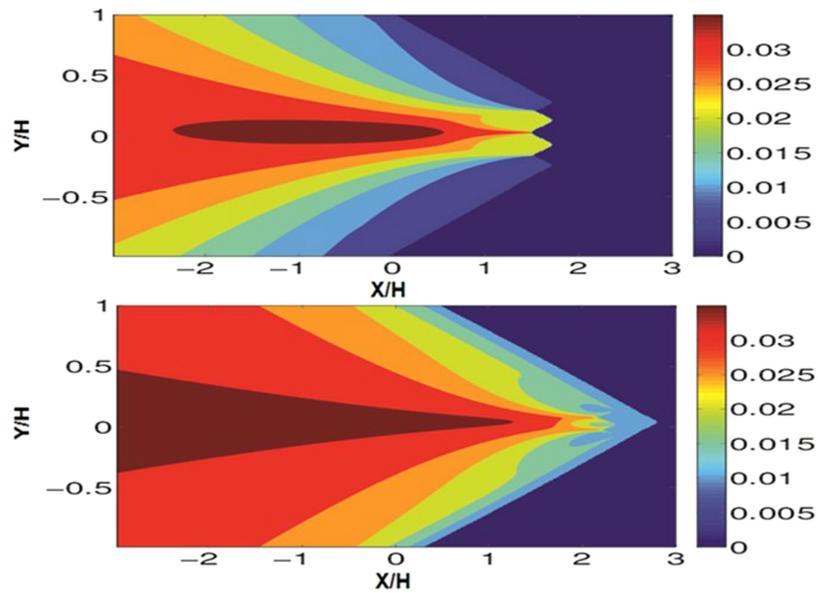


Figure 5. The renormalized estimate $\sigma_{j/\varphi}$ for configurations 2 and 4. The actual source is located at the center of the domain ($X_s = 0$ and $Y_s = 0$). In those two cases, the maximum of the source estimate is very close to that position (with a better estimate of Y_s due to the networks configurations). For configuration 4, the maximum values of the estimator are elongated along the mean wind direction indicating that the source is located in a region with less visibility.

$$\|\mathbf{p}_k^\varphi\|_{\mathbf{w}_\varphi} = \sqrt{\varphi_k^2 \sum_{j=1}^m (\mathbf{r}_{\varphi j}^\top \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi k})^2 \varphi_j} \quad (43)$$

which leads to the result that $\sum_{j=1}^m (\mathbf{r}_{\varphi j}^\top \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi k})^2 \varphi_j = 1$. This means either that a few of the terms $(\mathbf{r}_{\varphi j}^\top \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi k})^2 \varphi_j$ takes relatively large values or that a lot of them take smaller values. From (36) and (39), we, respectively, get $\mathbf{r}_{\varphi k}^\top \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi k} = 1$ and $|\mathbf{r}_{\varphi j}^\top \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi k}| \leq 1$ for all $j \neq k$, and thus, the following two situations are encountered: (i) if the value of φ_k is relatively small, i.e., in low visibility region, other components of \mathbf{p}_k^φ have the same order of magnitude and the maximum of the source estimate is flat, (ii) if the value of φ_k is relatively large, i.e., in high visibility region, the other components of \mathbf{p}_k^φ become relatively small and the maximum of the source estimate is sharp. This means that the value of the visibility function at the source location determines the sharpness of the maximum component of the source estimate: the maximum will be more flat in regions poorly monitored by the detectors, implying that the source identification of a single point source becomes ambiguous in that region.

3.7. Computation and Stability of the Solution

The renormalization condition expressed by equation (36) for discrete inverse problems can also be written in a matrix form as

$$\text{diag}(\mathbf{r}_{\varphi 1}^\top \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi 1}, \mathbf{r}_{\varphi 2}^\top \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi 2}, \dots, \mathbf{r}_{\varphi m}^\top \mathbf{H}_\varphi^{-1} \mathbf{r}_{\varphi m}) \equiv \mathbf{I}_m \quad (44)$$

i.e., the diagonal elements of the square symmetric matrix $\mathbf{P}^\varphi \mathbf{W}_\varphi^{-1}$ are equal to one. As a consequence, the computational algorithm (9) defined to compute the continuous weight function can be transformed to obtain the discrete values of the visibility function. The values φ_j ($j = 1 \dots m$) can be computed as the converged values of the components of the diagonal matrix \mathbf{W}_{f_p} (with $\mathbf{W}_{f_0} = \mathbf{I}_m$) obtained from the following iterative algorithm:

$$\mathbf{W}_{f_{p+1}} = \mathbf{W}_{f_p} \sqrt{\text{diag}(\mathbf{r}_{f_p 1}^\top \mathbf{H}_{f_p}^{-1} \mathbf{r}_{f_p 1}, \mathbf{r}_{f_p 2}^\top \mathbf{H}_{f_p}^{-1} \mathbf{r}_{f_p 2}, \dots, \mathbf{r}_{f_p m}^\top \mathbf{H}_{f_p}^{-1} \mathbf{r}_{f_p m})} \quad (45)$$

It has been observed that the matrix \mathbf{W}_{f_p} converges uniformly to the matrix \mathbf{W}_φ with components satisfying equation (36). The convergence of this algorithm has been proven by Issartel in an unpublished manuscript.

Once this optimum weight matrix has been obtained, the generalized inverse $\mathbf{R}^{\varphi+}$ can be computed and, for a given set of measurements, the source vector can be estimated as

$$\sigma_{//\varphi} = \mathbf{R}^{\varphi+} \boldsymbol{\mu} \text{ with } \mathbf{R}^{\varphi+} = \mathbf{R}_\varphi^T \mathbf{H}_\varphi^{-1} = \mathbf{W}_\varphi^{-1} \mathbf{R}_\varphi^T (\mathbf{R}_\varphi \mathbf{W}_\varphi^{-1} \mathbf{R}_\varphi^T)^{-1} \quad (46)$$

Moreover, it has already been shown, equation (30), that the \mathbf{W}_φ -norm of the estimate $\sigma_{//\varphi}$ is equal to the \mathbf{H}_φ^{-1} -norm of the measurement vector $\boldsymbol{\mu}$. Thus, $\mathbf{R}^{\varphi+}$ also corresponds with the standard definition for a weighted partial isometric matrix [Yang and Li, 2008]. This property is useful to study the stability of the method. Perturbing the observations with a noise vector $\Delta\boldsymbol{\mu}$, the estimate (46) is perturbed accordingly

$$\sigma_{//\varphi} + \Delta\sigma_{//\varphi} = \mathbf{R}^{\varphi+} (\boldsymbol{\mu} + \Delta\boldsymbol{\mu}) \quad (47)$$

From which we obtain

$$\Delta\sigma_{//\varphi} = \mathbf{R}^{\varphi+} \Delta\boldsymbol{\mu} \quad (48)$$

Any errors (noise) in the measurements will be mapped into errors in the source estimates. If small errors/changes in the inputs (measurements) result in large errors/changes in the estimate, the method is regarded as unstable. If small changes in the inputs lead to small changes in the results the method is called stable. By using the vector norms previously defined, a relation similar to equation (30) is obtained

$$\|\Delta\sigma_{//\varphi}\|_{\mathbf{W}_\varphi} = \|\mathbf{R}^{\varphi+} \Delta\boldsymbol{\mu}\|_{\mathbf{W}_\varphi} = \sqrt{\Delta\boldsymbol{\mu}^T \mathbf{H}_\varphi^{-1} \Delta\boldsymbol{\mu}} = \|\Delta\boldsymbol{\mu}\|_{\mathbf{H}_\varphi^{-1}} \quad (49)$$

In this case, the problem of computing $\sigma_{//\varphi}$ is said to be stable. Moreover, if the measurements have a distribution characterized by a covariance matrix $\mathbf{Var}(\Delta\boldsymbol{\mu})$, the covariance matrix of the source estimate can be calculated in a "straightforward fashion" by:

$$\mathbf{Var}(\sigma_{//\varphi}) = \mathbf{R}_\varphi^T \mathbf{H}_\varphi^{-1} \mathbf{Var}(\Delta\boldsymbol{\mu}) \mathbf{H}_\varphi^{-1} \mathbf{R}_\varphi \quad (50)$$

4. Conclusion

In this study, the discrete counterpart of the renormalization method has been presented. It has been shown that the source estimate $\sigma_{//\varphi}$ obtained by this approach represents the solution of the linear system $\boldsymbol{\mu} = \mathbf{R}\boldsymbol{\sigma}$ with the minimal \mathbf{W}_φ -weighted norm. As a consequence, $\sigma_{//\varphi}$ can be written in terms of a weighted generalized inverse (or weighted Moore-Penrose inverse) $\mathbf{R}^{\varphi+}$. Since most of the approaches used to solve the STE inverse problem give rise to solutions which can be expressed in terms of a generalized inverse operator, we are now able to conduct an objective theoretical comparison of those approaches with the discrete renormalization technique. Moreover, in recent years, the generalized inverse has become an important topic in the researches on matrix theory and has been widely applied to the area of geophysics, robotics, or neurosciences. Thus, existing numerical methods for an efficient computation of \mathbf{W}_φ and $\mathbf{R}^{\varphi+}$ should be evaluated and compared (it should be noted that the dimensions of those matrices are respectively $m \times m$ and $m \times n$ and the storage, and processing time, resources for computing them can rapidly become prohibitive as m increases).

It has also been shown that, when the components of the weight matrix \mathbf{W}_φ satisfy the renormalization condition, this inverse operator satisfies criteria used to define good inverses: the measurements are predicted exactly, the solution is as close to unique as possible and the solution is stable. Further, the reliability of the inverse solution has been investigated by using the Model Resolution Matrix (MRM) formalism. In case of noiseless observations generated from a point source, the maximum value of the source estimate corresponds to the location of the point source. It has been demonstrated here that this good feature is due to the discrete renormalization condition which gives optimal properties to the model resolution matrix. This highlights an important property of this condition which was interpreted, in the previous cited works, either as a minimum entropy criterion [Issartel et al., 2007] or as a condition to attribute a nonarbitrary statistical status to the measurements, irrespective of any error (having their own statistical status) and prior assumption [Issartel et al., 2011].

The renormalization technique has already been tested, and found to be working efficiently, with the concentration measurements obtained from dispersion experiments at local [Sharan et al., 2009, 2012] and continental [Issartel, 2005, Issartel et al., 2007] scales. Since the ultimate proof for any STE algorithms is the practical validation, the discrete renormalization method has to be "tested" and "validated" against new

Atmospheric and Tracer Data (ATD) sets or against data obtained from research studies from the past 50 years at local, regional, continental or global scale. In a future paper, the discrete renormalization technique will be evaluated against the results of the recent dispersion experiment "Fusion Field Trial 2007" [Storwald, 2007].

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