Sparse optimization for inverse problems in atmospheric modelling

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Abstract

We consider inverse problems in atmospheric modelling. Instead of using the ordinary least squares, we add a weighting matrix based on the topology of measurement points and show the connection with Bayesian modelling. Since the source–receptor sensitivity matrix is usually ill-conditioned, the problem is often regularized, either by perturbing the objective function or by modifying the sensitivity matrix. However, both these approaches may be heavily dependent on specified parameters. To ease this burden, we propose to use techniques looking for a sparse solution with a small number of positive elements. Finally, we compare all these methods on the European Tracer Experiment (ETEX) data where there is no apriori information apart from the release position.

Keywords: inverse modelling, sparse optimization, integer optimization, least squares, European tracer experiment, free Matlab codes.


1 Introduction

In the past decade, it often happened that a large amount of harmful substance was released into the atmosphere over a short period of time. As the probably most known examples we can mention the nuclear power accidents in Fukushima in 2011 and Chernobyl in 1986 or the Eyjafjallajökull volcanic eruption in 2010. When such an accident happens, there are two major questions to be asked. When is the substance going to be in a day or two? And how much of the substance was released into the atmosphere?

The problematic part is that in such cases only certain amount of measurements is known. And these two imposed questions have to be answered based only on this information from these measurements. The first question is usually simpler to answer: from the measurements we apply a model and observe in which direction and how fast the substance is transferred. The second question is generally more demanding, besides applying a model, one usually has to consider a certain optimization problem which needs to be solved. Since in this case we are interested in computation of a quantity which happened in the past, this field is often called inverse modelling. In this paper, we will focus purely on the second question.

There has been much progress in the field of inverse modelling. For a general introduction to inverse modelling in environmental modelling and protection, see books [4] and [29]. Furthermore, we mention works related to power plant accidents, for instance [15] and [26] focused on the Fukushima accident. Also volcanic ash, aerosol and gas emissions can influence climate significantly and pose hazards to human health and ocean productivity. Therefore, the impact of Eyjafjallajökull volcanic eruption was investigated

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by [25]. Another application of the inverse modelling lies in the monitoring of emission limits, e.g. [21] focused on the emission of carbon monoxide. [18] applied several inverse methods to US anthropogenic methane emissions modelling.

The problem described above gives rise to minimizing the discrepancy between the measurements and the model predictions. As we have already mentioned, one usually knows a vector of measurements \((y_1,\ldots,y_m)\in\mathbb{R}^m\) and tries to identify the unknown release profile \((x_1,\ldots,x_n)\in\mathbb{R}^n\). Both these vectors are aggregated over spatial and/or temporal domain. As an example, \((y_1,\ldots,y_m)\) consists of measurements at different places and times while \((x_1,\ldots,x_n)\) may represent release profile at one place but for different times.

To be able to identify the release profile, one has to know a mapping \(M: \mathbb{R}^n \to \mathbb{R}^m\) which assigns expected measurements to a release profile. In tracer transport modelling, this mapping is often linear, represented by a matrix \(M\in\mathbb{R}^{m\times n}\). This leads to an optimization problem

\[
\begin{aligned}
\text{minimize } & \|Mx-y\|_2^2 \\
\text{subject to } & x \geq 0,
\end{aligned}
\]

where \(\|\cdot\|_2\) is the Euclidean norm. In the objective, we minimize the discrepancy between the measured and predicted values. The constraint \(x \geq 0\) is natural here because release cannot be negative.

Matrix \(M\) is usually denoted as the source–receptor sensitivity matrix, see [22]. The reason for this is that element \(m_{ij}\) of matrix \(M\) represents the sensitivity of the measurement at point \(i\) to the release at point \(j\). Thus, in an ideal world where we know \(M\) precisely, we would obtain \(m_{ij}x_j = y_i\). This means that \(m_{ij}\) denotes the expected change in \(y_i\) upon a unit change in \(x_j\). For matrix \(M\), we will often use the shortened notation sensitivity matrix.

To obtain a column of the sensitivity matrix, one usually employs a transportation model and simulates a release of a large number of particles at the position corresponding to this column, see again [22]. After doing so, predicted values are computed at all places where a measurement is available. This means that the number of rows of \(M\) is fixed and is equal to the number of measurements. On the other hand, the number of columns of \(M\) may be chosen arbitrarily. For example, it may be increased by decreasing the time interval between two subsequent possible release instances. Since the computation of one column of \(M\) is very time consuming, \(M\) usually has much more rows than columns and thus the system is overdetermined.

There are two main approaches to finding a solution to (1). The first one is a deterministic approach and makes use directly of formulation (1) and tries to solve it by optimization techniques. Since the problem is often ill–conditioned, various regularizations are used to make the problem more tractable. This approach usually results in the necessity of solving a constrained quadratic program. The second approach is a stochastic one and instead of solving (1), it assumes that

\[
y = Mx + \epsilon,
\]

where \(\epsilon\) is a random vector. Provided that \(\epsilon\) has normal distribution with independent components having zero mean and the same variance, then applying the maximal likelihood estimate reduces precisely to solving (1). Naturally, this problem can be seen as ordinary least squares with nonnegativity constraint.

The main aim of this paper is twofold. The first goal is to propose a modification of the deterministic approach for solving problem (1) by adding nondiagonal weighting matrix \(W\). This approach is closely connected with Bayesian modelling, where the weighting matrix enters as a covariance matrix of the measurements. However, we base the weighting matrix purely on the topology of the measurement points and not on the measurement values as is the case of Bayesian modelling.

The second goal is to show a new approach of dealing with ill–conditioned sensitivity matrix \(M\). To the best of our knowledge, the usual approach is either to use some regularization or to ignore certain measurements, which reduces the number of rows in \(M\). This, however, may lead to a suboptimal solution when the solution of the reduced problem is not a solution to the original problem. Moreover, if this approach is applied, a certain parameter, such as the maximal matrix row norm, has to be specified. This parameter usually has huge impact on the optimal solution and thus, the problem is not very stable with respect to a choice of this parameter. This is especially true if the parameter takes form of apriori information.

We try to prevent this behaviour and suggest to look for a sparse solution \(x\), which means that \(x\) should contain as many zeros as possible. This problem may be formulated as a multiobjective optimization: we
try to minimize the measurement error $\|Mx - y\|_2$ and at the same time, we try to minimize the number of nonzeros, which is denoted by $\|x\|_0$. Using techniques from multiobjective optimization, we might rewrite the problem into another problem, in which one of the criteria is minimized while for the other one a maximal value is prescribed.

It is important to note that looking for a sparse solution has a natural effect of ignoring columns of $M$ with small norm, and thus only the goal value enters the problem as a parameter. This parameter prescribes the maximum number of nonzeros $\|x\|_0 \leq k_{tol}$. Note that the parameter $k_{tol}$ is an integer and has a natural explanation. Moreover, it is invariant to the scaling of variables, thus it is not necessary to rescale $k_{tol}$ whenever $y$ are measured in different units. As there are only finite number of possible values for $k_{tol}$, this parameter is relatively simple to choose. This is in contrast with most of the currently used regularization techniques.

The main assumption of following this approach is that the solution $x$ is indeed sparse. For example, it can be used for both problems of identification of the source location and of the time process of the source release. In the first case, it is usually assumed that there is only one or few release points and the task is to find them. In the second case, the considered time window is usually much longer than the duration of the actual release. In both cases, the optimal solution should contain a large number of zeros, justifying the use of sparsity techniques. Unfortunately, there are also instances where the sparse solution approach cannot be used. One example of this possibility is the CO$_2$ emission monitoring. This is caused by the fact that CO$_2$ is released globally and thus does not have a localized point source.

This paper is organized as follows: in Section 2 we comment on properties of $M$ and suggest a way of enhancing model (1) by multiplying both term in the objective $Mx$ and $y$ by a certain matrix $W$. Relations to stochastic Bayesian inverse modelling techniques are discussed. Section 3 summarizes the current state of the art for inverse modelling of tracer transport and proposes alternative approaches. After a short motivational part showing that the sensitivity matrix $M$ is often ill-conditioned, two subsections follow which present ways of solving problem (1) while dealing with this ill-conditioning. The first one summarizes the most widely used deterministic optimization techniques used for identifying point releases while the second one proposes a new way of handling the problem by looking for sparse solutions instead of regularizing the problem or modifying the sensitivity matrix.

In Section 4 we apply the described techniques to European Tracer Experiment (ETEX). After providing some information about the sensitivity matrix $M$, we show the validity of using the weight matrix $W$. After doing so, we depict both the known and the proposed solutions and compare them.

Finally, we would like to emphasize that all codes and data are available online.\footnote{http://staff.utia.cas.cz/adam/research.html}

## 2 Spatial and temporal locations weighting

In the introduction we have already described that the sensitivity matrix $M$ is obtained by repeatedly running an underlying tracer transport model. Unfortunately, it may happen that the model does not describe the real situation precisely because of certain reasons, be it using imprecise weather description, inability to incorporate mountain ranges, omitting some meteorological events or other reasons.

In this section, we introduce spatial and temporal location weighting to handle these possible deficiencies. We start with a simple example showing that relatively small changes in the sensitivity matrix $M$ can lead to big changes in solution $x$ of (1).

**Example 1.** Assume that we have the following data

$$M = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad y = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Thus, we have two measurements and only one potential release, leading to $m = 2$ and $n = 1$. By solving problem (1), we obtain trivial solution $x = 0$.

Matrix $M$ suggests that if a release occurred, all content of this release was transmitted to the second measurement point and nothing to the first one. Assume now that the locations of these two measurement
points are close to each other and that a wrong wind direction was considered and all release should have been transmitted to the first measurement point instead of the second one. This corresponds to using $M = (1, 0) \top$ instead of $M$. If we indeed consider $\tilde{M}$ instead of $M$, then we obtain optimal release $\hat{x} = 1$ instead of $x = 0$.

We can observe a highly undesirable situation when a small change in the real situation may cause a big change in the sensitivity matrix $M$ and in the obtained solution $x$. In the rest of this subsection, we will suggest a way of dealing with this problem. Unfortunately, this situation cannot be handled by adding a possibility to perturb $M$ with a penalization of such perturbation.

The potential problem with Example 1 is that model (1) may not be entirely suitable for modelling phenomena where additional information such as the spatial and temporal location of measurements is known. In our opinion, it could be advantageous not to compare $Mx$ and $y$ componentwise but to take into account their spatial and temporal locations and compare the sum on a neighborhood of every component. To present this idea in a more concise way, assume that for every measurement $y_j$ we know additional data $z_j = (z_{j1}, z_{j2}, z_{j3})$, where pair $(z_{j1}, z_{j2})$ represents the longitude and latitude of a measurement point and $z_{j3}$ the measurement time. We would like to define weights related to the distance between measurement points $z_i$ and $z_j$. First, we define the space and time weights as follows

$$w_S(z_i, z_j) := \begin{cases} \exp(-\alpha_S \|z_{ij} - z_{j}'\|) & \text{if } \|z_{ij} - z_{j}'\| \leq s_{\text{max}}, \\ 0 & \text{otherwise,} \end{cases}$$

$$w_T(z_i, z_j) := \begin{cases} \exp(-\alpha_T \|z_{ij}' - z_{j}'\|) & \text{if } \|z_{ij}' - z_{j}'\| \leq t_{\text{max}}, \\ 0 & \text{otherwise,} \end{cases}$$

where $\alpha_S \geq 0$, $\alpha_T \geq 0$ and $s_{\text{max}} \in [0, \infty]$, $t_{\text{max}} \in [0, \infty]$ are given parameters; the last two are known as cutoff distances. Since both quantities in (3) lie in interval $[0, 1]$, we may define the (non-normalized) weights related to the distance between $z_i$ and $z_j$ as

$$w(z_i, z_j) := w_S(z_i, z_j)w_T(z_i, z_j)$$

Note that this weight is zero if the measurements are performed at distant places (as specified by $s_{\text{max}}$) or at distant times (as specified by $t_{\text{max}}$). Moreover, the weight decreases with increasing spatial or temporal distance. This rate of decrease is determined by $\alpha_S$ and $\alpha_T$.

When considering ordinary least squares, we try to minimize for every $j = 1, \ldots, m$ the following discrepancy

$$(Mx)_j - y_j \right)^2$$

Following the idea from Example 1, instead of minimizing quantity (5) at given point $j$, we will minimize the difference between $Mx$ and $y$ on a neighborhood of point $j$. If we relate this neighborhood to weight $w$ defined in (4), for every measurement $j = 1, \ldots, m$ we try to minimize the following quantity

$$\left( \sum_{i=1}^{m} \frac{w(z_j, z_i)}{\sum_{k=1}^{m} w(z_j, z_k)} (Mx)_i - \sum_{i=1}^{m} \frac{w(z_j, z_i)}{\sum_{k=1}^{m} w(z_j, z_k)} y_i \right)^2,$$

where the denominator is used for weight normalization. Formula (6) corresponds precisely to (5) provided that $w(z_i, z_i) = 1$ and $w(z_i, z_j) = 0$ for $i \neq j$. When we combine components (6) into one vector, we arrive at minimizing

$$\sum_{j=1}^{m} \left( \sum_{i=1}^{m} \frac{w(z_j, z_i)}{\sum_{k=1}^{m} w(z_j, z_k)} ((Mx)_i - y_i) \right)^2,$$

which is equal to

$$\|W(Mx - y)\|_2^2,$$

where matrix $W$ consists of elements

$$w_{ij} = \frac{w(z_i, z_j)}{\sum_{k=1}^{m} w(z_i, z_k)}.$$
For other possibilities of choosing matrix $W$, we refer the reader to [10] or [12].

To conclude this approach, we propose to solve the (weighted least squares) problem
\[
\begin{align*}
\text{minimize} & \quad \|WMx - Wy\|_2^2 \\
\text{subject to} & \quad x \geq 0
\end{align*}
\] (9)

instead of the (ordinary least squares) problem (1), where matrix $W$ has been defined in (3), (4) and (8).

Now we present a continuation of Example 1 which strongly supports our arguments for using matrix $W$.

**Example 1 (continued).** Consider the same data as in Example 1. Denoting \( w := w(z_1, z_2) \), we have
\[
W = \frac{1}{1+w} \begin{pmatrix} 1 & w \\ w & 1 \end{pmatrix}, \quad WMx - Wy = \frac{1}{1+w} \begin{pmatrix} -1+wx \\ -w+x \end{pmatrix},
\]
and thus problem (9) reads
\[
\begin{align*}
\text{minimize} & \quad \frac{1}{(1+w)^2} [(1+w^2)x^2 - 4wx + 1 + w^2] \\
\text{subject to} & \quad x \geq 0.
\end{align*}
\]

Since \( w \geq 0 \), for the optimal solution we obtain
\[
x = \frac{2w}{1+w^2}.
\]

We note that for \( w = 0 \), matrix $W$ is equal to the identity matrix. Then problem (9) amounts to solving (1), and that the solution is indeed $x = 0$ for this case. However, if $w$ is close to 1, then the measurement points are at almost identical point, which means that they should not be distinguished as separate measurement points. Indeed, we obtain that $x$ is close to 1, which is in accordance to our expectation. \(\triangle\)

Even though this whole paper is based on deterministic formulation, problem (9) has close connection with stochastic (random) solution methods, where one make use of formula (2) and employs Bayesian modelling, see papers by [6], [20] with open source software package MAD# or [30], where Monte Carlo methods are proposed.

By computing the optimal solution to (9) without the nonnegativity constraint imposed on $x$, we obtain
\[
x = (M^TW^TW)^+ M^TW^Wy,
\]
where \( (M^TW^TW)^+ \) is a Moore–Penrose pseudoinverse matrix, see [2]. If the matrix in question is invertible, than the pseudoinverse reduces to the classical inverse matrix. If $W^TW$ is a regular matrix, then solution $x$ corresponds to the best linear unbiased estimator (BLUE) for model $y = Mx + \epsilon$, where $\epsilon$ is random vector with zero mean and covariance matrix $(W^TW)^{-1}$, see [23]. However, there is a major difference between our approach and the of Bayesian modelling. We show this in Example 1.

**Example 1 (continued).** It is not difficult to compute
\[
(W^TW)^{-1} = \frac{(1+w^2)}{(1-w^2)^2} \begin{pmatrix} 1+w^2 & -2w \\ -2w & 1+w^2 \end{pmatrix}.
\]
We return now back to the theoretical properties. \(\triangle\)

If we consider $(W^TW)^{-1}$ as a covariance matrix, there will be a strong negative correlation between close points, which may seem slightly counterintuitive. However, there is a simple explanation for such event. When the covariance matrix is not the identity matrix, the closeness of points is penalized to prevent similar measurements to have great impact on the solution. However, in our approach we want to perform a sum with respect to neighboring points, thus we want to promote and not penalize closeness of points.
3 Sparse optimization

In this section we first provide reasons why the sensitivity matrix $M$ may be ill-conditioned. The rest of the section is divided into two subsections and presents several possible ways of dealing with this problem. In the first one, we show several current methods and in the second one, we present the concept of sparse solution, thus a solution which contains many zero elements.

We are fully aware that the true release does not have to be sparse in general. In this case, our methods should not be used. However, looking for a sparse solution makes sense in the following widely used applications: identifying release points and identifying release time profile. When we know that the release was performed only from one or few places and the goal is to find these places, sparsity is naturally present. On the other hand, if we know the release place and want to identify the release time profile, the sparsity is present as well because the examined window of potential release is usually much longer than the true release window.

As we have mentioned in the introduction, the sensitivity matrix is computed by simulating a release of huge number of particles. Since the underlying model is stochastic, the trajectory of every particle is governed by a different realization of the random vector. Thus, every particle follows a different trajectory. The resulting concentration $y$ is then based on the number of particles in the vicinity of a measurement point.

To explain why the sensitivity matrix $M$ may be ill-conditioned, we consider identification of a time profile of a release where the true release point is known. Then $x_j$ denotes the released amount at some time $t_j$ and the sum of $j$-th column of $M$ denotes the total predicted sum of measurements at all measurement places per unit release at $t_j$. It is very likely that there will be some time instant $t_j$ which has no influence on the predicted values at the measurement places, for example if $t_j$ occurred much earlier than the first measurement was taken. But since the underlying process is stochastic and there is a large amount of considered particles, it may happen that some particles reached the measurement place. This would result in very small entries in the sensitivity matrix $M$. Unfortunately, this is a very unpleasant behavior as we show in the following example.

Example 2. Consider the following data

\[
M = \begin{pmatrix} 1 & 0 \\ 1 & 10^{-10} \end{pmatrix}, \quad y = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.
\]

Then it is clear that matrix $M$ is ill-conditioned and that the unique solution is equal to $x = (1, 0)$. However, if there is slight error in the measurements, for example if we consider $\tilde{y} = (1, 1 + 10^{-5})$, then the original solution $x$ changes by a big margin into $\tilde{x} = (1, 10^5)$.

Note that if we impose a requirement that at most one component of $x$ can be nonzero, then the solution is always $\tilde{x} = (1, 0)$ for any small perturbation of $y$. This is precisely the case of sparse optimization. △

There have been some attempts to deal with this problem. In [14] and [16] outliers were detected and removed from the model. In the first paper, an extension of the Random Sample Consensus (RANSAC) algorithm was proposed while in the second one, two matrices $M_1$ and $M_2$ were constructed and outliers were detected and removed based on differences in these matrices. Finally, in [15] it was suggested to keep removing rows from $M$ until the resulting matrix has a better condition number. However, we believe that the rows of $M$ should stay mostly untouched because removing rows of $M$ means ignoring valuable data (for example in the latter paper approximately 60% of all measurements were removed).

On the other hand, sparse optimization tries to find a sparse (approximate) solution of a linear system, where only a limited number of nonzero elements appears. There exist many underlying practical applications which make use of the developed theory. One of the well-known examples is the image compressing into special formats such as JPEG. During such compressing, the pixel information is transformed using special transforms such as Fourier transform. These transforms are constructed in such a way that only the first several coefficients are large (and thus important) and thus, the remaining ones can be ignored without losing much information. Hence, the image has a sparse representation. Another application from image processing is the image denoising of image deblurring. Applications from different fields amount for magnetic resonance imaging (MRI) or target location via radars. For more information about this field see [7].
and [9] for annotated bibliography and references, and [13] for implementation of selected algorithms in SparseLab or Sparse Modeling Software (SPAMS).

3.1 Traditional – approximate – approaches to inverse modelling

In this subsection, we formulate and shortly discuss methods which were already used for dealing with badly scaled matrices. These methods will be then compared with the sparse optimization technique in the empirical part in Section 4. In particular, we focus on removing low-influential columns of \( M \) and two traditional regularization techniques.

3.1.1 Columns removal

The most obvious strategy is to remove columns of the sensitivity matrix. We can imagine that we solve problem (9) where the components of \( x \) corresponding to the omitted columns are fixed to zero. However, it may happen that the optimal solution of this problem is far from an optimal solution to the original problem (9). Specifically, denoting all columns of \( M \) by \( m_j \), we remove all columns of \( M \) which satisfy

\[
\|m_j\|_2 \leq c_{\text{column}} \max_{k=1,\ldots,m} \|m_k\|_2,
\]

for some \( c_{\text{column}} > 0 \) is a given constant.

3.1.2 \( l_2 \)-regularization: Tikhonov approach

Another possibility is to use the Tikhonov regularization and to solve problem

\[
\begin{align*}
\text{minimize} & \quad \|WMx - Wy\|_2^2 + \alpha \|x\|_2^2 \\
\text{subject to} & \quad x \geq 0
\end{align*}
\]

with fixed penalization parameter \( \alpha > 0 \). The second term in the objective penalizes the Euclidean norm of the release. Note that the optimal solutions usually contain many small nonzero values, thus they are not sparse.

A similar approach was used in [26] where the following problem was solved: minimize \( x \geq 0 \quad \|W_1 (Mx - y)\|_2^2 + \|W_2 x\|_2^2 + \|W_3 Dx\|_2^2 \). Matrices \( W_1, W_2 \) and \( W_3 \) are diagonal with positive entries on their diagonal and thus allow for weighting of individual elements. Matrix \( D \) represents discretized differential operator, see Chapter 8 in [19], and thus the last term forces \( x \) to be as smooth as possible. Another possibility is to add term \( \|W_4 (x - x_a)\|_2^2 \) to the objective function, where \( x_a \) is either an expert or an a priori estimate. Since optimal solution \( x \) would strongly depend on the choice of \( x_a \) in this case, we try to avoid this possibility.

3.1.3 \( l_1 \)-regularization: LASSO

To the best of our knowledge, there have not been many attempts to use sparse optimization for atmospheric modelling. One of the attempts was performed in [15], where problem

\[
\begin{align*}
\text{minimize} & \quad \|WMx - Wy\|_2^2 + \alpha \|x\|_1 \\
\text{subject to} & \quad x \geq 0
\end{align*}
\]

was considered. This can be understood as the Least absolute shrinkage and selection operator (LASSO) method, which was introduced in [28] and later thoroughly studied in [8]. Compared with (11), this method penalizes \( l_1 \) norm of the release instead of \( l_2 \) norm. Since \( x \) is nonnegative, problem (12) is smooth.
3.2 Exact approaches to sparse optimization

All approaches from the previous subsection somehow regularized the problem and depended heavily on a real parameter. In this subsection we present another approach. Instead of modifying the objective or the data, it assumes that the solution is sparse and tries to search for a solution with only a limited number of nonzeros. Even though a (regularization) parameter is present as well in this case, it is an integer and thus much easier to select properly.

There are two possibilities in problem (9). Either system $M x = y$ is underdetermined, which usually corresponds to the case of $m < n$. Then there exist multiple solutions and the task of sparse optimization is to select the one with the lowest number of nonzero components. However, in our case it usually happens that the system is overdetermined, which usually corresponds to $m > n$. Then the solution of (9) is uniquely determined but the solution may be dense. In such cases it is possible to trade lower density for a slightly worse error $\|W M x - W y\|_2$. A big advantage of sparse solutions is that columns corresponding to zero components of a solution are ignored. This means that sparse solutions naturally deal with ill-conditioned matrices as described earlier in this section.

The basic concept used is the $l_0$ "norm", which is defined as

$$\|x\|_0 := \# \{ i \mid x_i \neq 0 \},$$

where $\#A$ denotes the number of elements in a set $A$. The term $l_0$ norm was coined because $\|x\|_0 = \lim_{p \to 0} \|x\|_p^p$, see Section 2.1 in [9]. Thus, sparse optimization tries to minimize $\|x\|_0$, together with criterion (7); a problem which can be understood as a multiobjective optimization, see [17]. This gives rise to problem

$$\begin{align*}
\text{minimize} & \quad \|W M x - W y\|_2^2 \\
\text{subject to} & \quad \|x\|_0 \leq k_{tol}, \\
& \quad x \geq 0,
\end{align*}
$$

(13)

where $k_{tol} \in \mathbb{N}$ is a natural number which denotes the maximal number of nonzeros in $x$.

Because the feasible set of problem (13) is highly nonconvex (for example for $n = 2$ and $k_{tol} = 1$ it consists of two halflines), this problem is usually very difficult to solve efficiently. One of the possibilities of handling these constraints is to use artificial binary variables $z_i \in \{0, 1\}$ such that

$$\begin{align*}
z_i = 0 & \iff x_i = 0, \\
z_i = 1 & \iff x_i > 0,
\end{align*}
$$

(14)

which leads to exact expression

$$\|x\|_0 = \sum_{i=1}^{n} z_i.$$

Relation (14) is equivalent to

$$0 \leq x_i \leq z_i \cdot u_{bi},$$

(15)

where $u_{bi} > 0$ is a given upper bound for the release (or a sufficiently large number). Instead of this relation, we will consider

$$z_i \cdot l_{bi} \leq x_i \leq z_i \cdot u_{bi},$$

(16)

where $l_{bi} \geq 0$ are lower bounds for release. Even though $l_{bi}$ and $u_{bi}$ may seem as additional penalization parameters, this is not the case. They serve only to improve the properties of the following integer programming. If $l_{bi} = 0$, then constraints (15) and (16) coincide. Moreover, if $u_{bi} = \infty$ then the upper bounds in (15) and (16) are eliminated from the system.

Concerning the interpretation of $l_{bi}$: if this constant is strictly positive, thus $l_{bi} > 0$, then either there is no release ($z_i = 0$ and $x_i = 0$) or if there is any positive release $x_i > 0$, then this release must be at least $l_{bi}$ ($z_i = 1$ and $x_i \geq l_{bi}$). Hence, this constraint basically says that if there is any release, then it has to be automatically greater than $l_{bi}$.
By the analysis in the previous paragraph, we have derived the following problem related to (13).

\[
\begin{align*}
\text{minimize} & \quad \|WMx - Wy\|_2^2 \\
\text{subject to} & \quad \sum_{i=1}^{n} z_i \leq k_{tol}, \\
& \quad z_i \cdot lb_i \leq x_i \leq z_i \cdot ub_i, \quad i = 1, \ldots, n, \\
& \quad z_i \in \{0, 1\}.
\end{align*}
\]

(17)

Note that the constraints imply \( x_i \geq 0 \) and thus, it is not necessary to state this constraint explicitly. For a solution \( x \) of this problem, we always have that at most \( k_{tol} \) components \( x_i \) are positive and if this is the case, then they are greater than \( lb_i \).

It is not difficult to see that problem (17) may be written in the following form

\[
\begin{align*}
\text{minimize} & \quad u^\top Hu + h^\top u \\
\text{subject to} & \quad Au \leq b, \\
& \quad u_z \in \{0, 1\},
\end{align*}
\]

(18)

where \( u = (x, z) \), \( u_z \) refers to the second part of \( u \) and the data read

\[
H = \begin{pmatrix}
M^\top W^\top W M & 0_{n \times n} \\
0_{n \times n} & 0_{n \times n}
\end{pmatrix}, \quad h = \begin{pmatrix}
-2M^\top W^\top Wy \\
0_{n \times 1}
\end{pmatrix}
\]

and

\[
A = \begin{pmatrix}
0_{1 \times n} & 1_{1 \times n} \\
-\text{diag}(1_{n \times 1}) & \text{diag}(lb) \\
\text{diag}(1_{1 \times n}) & -\text{diag}(ub)
\end{pmatrix}, \quad \begin{pmatrix}
k_{tol} \\
0_{n \times 1}
\end{pmatrix}.
\]

Here \( 0_{m \times n} \) stand for matrix (vector for \( n = 1 \) or \( m = 1 \)) of zeros, \( 1_{m \times 1} \) and \( 1_{1 \times n} \) stand for vectors of ones and \( \text{diag}(v) \) is a diagonal matrix formed from vector \( v \).

Thus, we managed to recast problem (13) into mixed-integer convex quadratic problem (18). Unfortunately, mixed–integer quadratic programming problems are highly computationally demanding. Thus, a special purpose software for solving such problems is necessary. Such software often works with a relaxed problem, where the integer requirements \( u_z \in \{0, 1\} \) are relaxed into simple box constraints \( u_z \in [0, 1] \).

Since the relaxed problem is convex, then the branch–and–bound algorithm, well known from mixed-integer linear problems, works well for such problems. Moreover, cutting planes can further improve its performance, see [5] and [27].

For the algorithmic implementation we have used one of the best available commercial solvers for mixed-integer linear and quadratic problems, CPLEX. \(^2\) Solver CPLEX is delivered with IBM ILOG CPLEX Optimization Studio,\(^3\) which is free for academic purposes and can be easily connected to Matlab. Other possibility is to employ the free optimization library OPTI Toolbox delivered together with noncommercial solver SCIP, see [1]. For the convex problems we have used CVX [11].

## 4 Application to ETEX

In this section we present numerical results and comparison of methods presented in this paper. The ETEX (European Tracer Experiment) is one of the few controlled tracer experiments with detailed information about the release. Similar experiments are for example CAPTEX (Cross–Appalachian Tracer Experiment), ANATEX (Across North America Tracer Experiment) or the not so well–known KATREX (Karlsruhe Tracer Experiment), see [3]. Among these three experiments, ETEX is the newest one and was performed in 1994 near Rennes in France. This experiment was performed twice, for the first time on 23 October 1994 and for the second time on 14 November 1994. Here, we will consider only the first experiment.

\(^2\)http://www-03.ibm.com/software/products/en/cpleoptiforzos

\(^3\)http://www-03.ibm.com/software/products/en/category/decision-optimization
A total mass of 340 kg of PMCH (Perfluoro-Methyl-Cyclo-Hexane) was released into the atmosphere during the course of 12 hours. After that, this substance got carried over Europe and its concentration was measured over the following several days. The sampling network consisted of 168 stations. The locations of these stations are depicted in Figure 1. Each station was supposed to sample over the period of 72 hours with the time difference between two subsequent measurements being 3 hours. The starting point for sampling was different for all stations: stations closest to the release point started to sample 3 hours before the release while the stations far away from the release ended their sampling activity 90 hours after the release had started. Unfortunately, large part of the data was either corrupted or not usable which resulted in having only 3104 instead of the intended number of 4032 measurements.

The sensitivity matrix was of dimension $3104 \times 112$, thus $m = 3104$ and $n = 112$ and the system was overdetermined. Every component of vector $x$ denoted a potential time when a release could have occurred. The time difference between two subsequent components was one hour. Since the true release was performed over 12 hours, the true solution had sparsity of 12, which is approximately 10% of the whole vector. The sensitivity matrix was generated by FLEXPART 9.2, see [24]. As we have mentioned several times, this matrix is badly scaled. This can be see at the ratio of the greatest and smallest nonzero element, which is equal to $5.41 \times 10^7$. For the sensitivity matrix from a different experiment in [15], this ratio was much worse and reached $8.16 \times 10^{14}$.

We have divided this section into three subsections. In the first one, we provide numerical justification for introducing the weighting matrix $W$. In the second part, we briefly comment on the dependence of optimal solutions on parameters. Finally, in the last part we summarize results obtained by different optimization methods and compare them with each other.

4.1 Justification of using weighting matrix $W$

Recall that the weighting matrix has been constructed via relations (3), (4) and (8). To obtain it, we need to specify parameters $\alpha_s$, $\alpha_T$, $s_{\text{max}}$ and $t_{\text{max}}$. We chose $t_{\text{max}} = 0$, which means that we allowed no measurement aggregation with respect to different times. In other words, we have $w_T(z_i, z_j) = 1$ when $z_i$ and $z_j$ were taken at the same time instants and 0 otherwise. This also made parameter $\alpha_T$ obsolete. The space distance $|| (z_i^x, z_i^y) - (z_j^x, z_j^y) ||$ was measured as the Euclidean norm applied on degrees of latitude and longitude. Parameter $s_{\text{max}}$ was chosen in such a way that we aggregated data from approximately 5% of all

\footnote{For plotting this and all further maps we have used package border, which is freely available at http://www.mathworks.com/matlabcentral/fileexchange/50390-borders}
stations. Having \( n = 3104 \) measurement, we chose \( s_{\text{max}} = 2.5 \) to obtain

\[
\frac{1}{n} \sum_{i=1}^{n} \chi_{w_{ij}>0} = 8.4626,
\]

where

\[
\chi_{w_{ij}>0} = \begin{cases} 
1 & \text{if } w_{ij} > 0 \\ 
0 & \text{otherwise},
\end{cases}
\]

stands for the characteristic function. This indeed forms approximately 5% from the 159 stations which were able to provide at least one measurement. For the remaining parameter, we have chosen \( \alpha_S = 1.15 \), which resulted in

\[
\frac{1}{n} \sum_{i=1}^{n} w_{ii} = 0.4951.
\]

In other words, since the sum of every row of \( W \) equals to 1, this means that approximately one half of the objective function of (9) is based on the distance between the measured value \( y_i \) and the predicted value \( (Mx)_i \) at the same point. On the other hand, the part consisting of the comparison of the measured value \( y_i \) at a point and the predicted values \( (Mx)_j \) at a neighborhood amounts approximately to the same amount of the objective. We find this to be a good balance between the ordinary least squares (which would correspond to only for the first part and none of the second one) and considering also some measurements on a neighborhood of every point.

In the rest of the text, we will denote the OLS (ordinary least squares) and WLS (weighted least squares) solution by the solutions of problems (1) and (9), respectively. In Figure 2 we show the relation between the predicted and actual measurements. Figure 2a shows the OLS solution and depicts the relation between \( y \) and \( Mx \). Similarly, Figure 2b shows that WLS solution and depicts the relation between \( Wy \) and \( WMx \). For the best fit, all data would have to lie on the central line. Even though the fit is not perfect, we see that Figure 2b shows better results that Figure 2a, and thus WLS solution has much better approximation capability than OLS solution. This is connected with the fact that adding weighting matrix \( W \) moves uncertainties from a point to its neighborhood. This visual hypothesis is supported by the \( R^2 \) variable, which tells how many percent of the measurements were explained by the model. We obtain the following data

\[
R^2_{\text{OLS}} := 1 - \frac{\|y - Mx\|^2}{\|y - \text{mean}(y)\|^2} = 0.5343,
\]

\[
R^2_{\text{WLS}} := 1 - \frac{\|Wy - WMx\|^2}{\|Wy - \text{mean}(Wy)\|^2} = 0.6092.
\]

In other words, by using the weighting matrix, we were able to explain approximately 7.5% more of the data.
4.2 Parameter dependence of current methods

In this subsection, we show that the dependence of the current methods, described in Subsection 3.1, on the involved parameters is rather strong. We can see the results in Figure 3, which where the x axis depicts

\[ \text{log}_{10}(\text{threshold}) \]

Figure 3: Dependence of the total release \( \sum_{i=1}^{n} x_i \) on parameters: either \( \log_{10}(c_{\text{column}}) \) (for matrix column reduction) or on \( \log_{10}(\alpha) \) (for Tikhonov regularization and LASSO)

parameter value, either \( \log_{10}(c_{\text{column}}) \) for column removal or \( \log_{10}(\alpha) \) for Tikhonov regularization and LASSO. The y axis then depicts the total release \( \sum_{i=1}^{n} x_i \) for the corresponding \( x \). The full line depicts the true release which is to be estimated, the dashed line corresponds to the solution where we removed certain amount of columns, the dash-dotted line to the Tikhonov regularization (11) and finally the dotted line to the LASSO (12). It can be seen that if the parameter is chosen in a bad way, either too small or too big, the computed solution is far off from the true solution. This shows the principal difficulty of the regularized ordinary least squared approach: it is not simple to choose the correct value of parameter \( \alpha \).

One of the possibilities is to choose the maximal \( \alpha \) such that the residual error \( \|WMx - Wy\|_2 \) stays rather constant. As we can see in Figure 4, this happened for approximately \( \alpha = 10^{-3} \). However, it may be difficult to find such \( \alpha \) because it is a real parameter. This may not be the case of sparse optimization and \( k_{\text{tol}} \) which may take only finite number of values. Moreover, in our opinion, it is much more meaningful to work with parameter \( k_{\text{tol}} \) rather than with \( \alpha \) or \( c_{\text{column}} \): while it is simple to explain the meaning of the former parameter, this is not the case of the latter two.

4.3 Sparse optimization and method comparison

We will start with Figure 5 which depicts variant of Figure 4 for sparse solutions and shows the dependence of error \( \|WMx - Wy\|_2 \) and the coefficient of determination \( R^2 \) on the solution sparsity, thus the number of nonzeros. For a good comparison, we have included \( l_2 \) and \( l_1 \) regularizations as well, thus solutions of problems (11) and (12), respectively. Constant \( \alpha \) was chosen as in the previous section, thus \( \alpha = 10^{-3} \). The remaining markers correspond to WLS solution and \( l_2 \) and \( l_1 \) regularizations. We see that for approximately \( k_{\text{tol}} = 11 \), the residual error got stable. For this reason, we would recommend this parameter.

In Figure 6 we plot comparison of selected solutions which were presented in this paper. In the left column, we can see the true release, the WLS solution and finally the LASSO regularization with \( \alpha = 10^{-3} \).
On the right hand side, we can see the sparse solution with $k_{tol} = 6$, $k_{tol} = 11$ and $k_{tol} = 16$, respectively. On the x axis the time scale is located. On the y axis we can see the release at the corresponding time instant. The gray dashed line on the background depicts the scaled column sum of $WM$. We did not include the Tikhonov regularization because it provided very similar results to LASSO.

All solutions provided rather good approximation of the true release. However, we may observe several interesting differences between various solution types. The WLS solution contains one huge element at time $t = 93$. Note that the corresponding column of $M$ contains only one nonzero element (out of 3104) and the corresponding column of $WM$ contains seven nonzero elements. What probably happened in this time is that the “best” approximation was found at the remaining coordinates and this coordinate provided only a small correction to the final solution. Unfortunately, this small correction in the residuals caused to increase the predicted total release by approximately 79%. Even the LASSO regularization seems that it is sparse, this is not true. From Figure 5 we can see that this solution contains 90 nonzero coordinates, many of them are very small. This raises a question whether these small elements should really be present in the solution or if they just provide some small corrections in the solution and are present only because of model or measurement errors.

This behavior is suppressed for the sparse solutions which are presented in the right column of Figure 6. We can see that the nonzero elements of the solution with $k_{tol} = 6$ are subset of nonzero elements of the
solution with $k_{tol} = 11$ and similarly when $k_{tol}$ is increased to 16. We would like to stress again that when using the sparse solutions, we do not have to perform any procedure of regularizing the sensitivity matrix or taking care of release elements with small or huge value.

<table>
<thead>
<tr>
<th></th>
<th>Total release</th>
<th>Mean square error</th>
<th>Coefficient of determination</th>
</tr>
</thead>
<tbody>
<tr>
<td>True</td>
<td>340.0000</td>
<td>47.0890</td>
<td>-102526</td>
</tr>
<tr>
<td>WLS</td>
<td>336.6389</td>
<td>8.7759</td>
<td>60.9167</td>
</tr>
<tr>
<td>LASSO</td>
<td>151.7701</td>
<td>8.7772</td>
<td>60.9049</td>
</tr>
<tr>
<td>Integer with $k_{tol} = 6$</td>
<td>134.9510</td>
<td>8.9540</td>
<td>59.3141</td>
</tr>
<tr>
<td>Integer with $k_{tol} = 11$</td>
<td>155.6267</td>
<td>8.7788</td>
<td>60.8903</td>
</tr>
<tr>
<td>Integer with $k_{tol} = 16$</td>
<td>185.6817</td>
<td>8.7760</td>
<td>60.9153</td>
</tr>
</tbody>
</table>

Table 1: Numerical evidence to Figure 6. The coefficient in determination is in percent. The negative value is possible because the coefficient of determination lies between 0% and 100% only for the optimal solution, thus WLS in this case. Even though it may seem that the model is inappropriate because of this value, based on Figure 7 we explain why this happened and that the model is still good.

We provide numerical summary to Figure 6 in Table 1. We can see that the release of the solutions of LASSO and all integer problems are very similar and approximately half the true release. The release of the WLS solution is almost exactly as the true solution but this is caused mainly by the huge release at one of the later time instant. Since the mean square error is reciprocal to the coefficient of determination $R^2$, we will comment only on the latter one. All the solutions besides the true was have very similar coefficient of determination around 60% or 61%. Based on the coefficient of determination for the true solution, one may think that the model is totally inappropriate. However, this is not true as we show in Figure 7.

Here, we depict the position of the plume (released substance) at one particular time instant. The plume is showed in gray scale. The crosses denote measurements with zero or negligible value. The circles denote measurements with positive values, the value is depicted by the circle color. In Figure 7a, we can find the plume corresponding to the true solution while in Figure 7b, we see plume corresponding to the solution of sparse optimization with $k_{tol} = 11$. Even though that this is a rather subjective feeling, we think that the location of the plume (but probably not the magnitude) is better for the true solution than for our computed solution. But the difference between the predicted and the observed value is huge for the true solution which means that the mean square error will be huge and the coefficient of determination extremely low.
Figure 7: The predicted plumes corresponding to the true release and the integer solution with $k_{tol} = 11$. The circles are the measurements with the value denoted by their color. Similarly, the crosses are zero (or very small) measurements.

5 Conclusion

In this paper, we have considered the identification of a source term in atmospheric modelling. First, we have mentioned the well-known technique of the ordinary least squares and showed the standard regularization techniques of the Tikhonov and LASSO regularization. After doing so, we have proposed to look for sparse solutions instead of using classical the above-mentioned methods. We can see the basic information about these methods in Table 2. As suggested in this table, all methods besides the sparse optimization are rather simple to perform and amount to solving a quadratic program. Besides suggesting to use the sparse optimization, we have also proposed to extend the model by adding a weighting matrix $W$ which is based purely on the topology of the measurements and not on the measurement values as is the case in Bayesian modelling.

To verify the proposed methods numerically, we have applied them on the European Tracer Experiment. The obtained results show good results of our techniques. Even though they are computationally more demanding, it is much simpler to choose the parameters in our case. Moreover, it is not necessary to deal with small or high values of the release vector.

For the future, we see several possible extensions. As we have already mentioned, the problem may be computationally demanding. Thus, instead of solving the the integer sparse problem, it may be possible to use its continuous approximations, which still provide a sparse solution and may be much more easier to solve. This holds true especially for large problems. For a second possible extension, we intend to add additional constraints into the model, which may represent for example the maximal ratio of two substances when there are more of them in the model.

<table>
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<th>Method</th>
<th>Solved problem</th>
<th>Variables</th>
<th>Optimization type</th>
</tr>
</thead>
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<tr>
<td>OLS</td>
<td>(1)</td>
<td>continuous only</td>
<td>continuous quadratic</td>
</tr>
<tr>
<td>WLS</td>
<td>(9)</td>
<td>continuous only</td>
<td>continuous quadratic</td>
</tr>
<tr>
<td>Tikhonov reg.</td>
<td>(11)</td>
<td>continuous only</td>
<td>continuous quadratic</td>
</tr>
<tr>
<td>LASSO</td>
<td>(12)</td>
<td>continuous only</td>
<td>continuous quadratic</td>
</tr>
<tr>
<td>Sparse opt.</td>
<td>(13)</td>
<td>integer and continuous</td>
<td>mixed-integer quadratic</td>
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Table 2: Review of models and optimization techniques
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