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To cite this article: Xiao Liu & Kyongmin Yeo (2023) Inverse Models for Estimating the Initial Condition of Spatio-Temporal Advection-Diffusion Processes, *Technometrics*, 65:3, 432-445, DOI: [10.1080/00401706.2023.2181222](https://doi.org/10.1080/00401706.2023.2181222)

To link to this article: <https://doi.org/10.1080/00401706.2023.2181222>



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Inverse Models for Estimating the Initial Condition of Spatio-Temporal Advection-Diffusion Processes

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ABSTRACT

Inverse problems involve making inference about unknown parameters of a physical process using observational data. This article investigates an important class of inverse problems—the estimation of the initial condition of a spatio-temporal advection-diffusion process using spatially sparse data streams. Three spatial sampling schemes are considered, including irregular, nonuniform and shifted uniform sampling. The irregular sampling scheme is the general scenario, while computationally efficient solutions are available in the spectral domain for nonuniform and shifted uniform sampling. For each sampling scheme, the inverse problem is formulated as a regularized convex optimization problem that minimizes the distance between forward model outputs and observations. The optimization problem is solved by the Alternating Direction Method of Multipliers algorithm, which also handles the situation when a linear inequality constraint (e.g., non-negativity) is imposed on the model output. Numerical examples are presented, code is made available on GitHub, and discussions are provided to generate some useful insights of the proposed inverse modeling approaches.

ARTICLE HISTORY

Received November 2021
Accepted February 2023

KEYWORDS

Advection-diffusion processes; Alternating direction method of multipliers; Inverse models; Spatio-temporal processes

1. Introduction

1.1. Motivating Examples

Inverse problems involve making inference about unknown parameters of a physical process using observational data, and are widely found in scientific and engineering applications. For example, in urban air quality and environmental monitoring, inverse problems aim at quickly pinpointing the sources of instantaneous emissions of gaseous pollutants that cause public health concerns (Eckhardt et al. 2008; Martinez-Camara et al. 2014; Hwang et al. 2019), or detecting fugitive emissions due to accidental releases from industrial operations (Hosseini and Stockie 2016; Klein et al. 2016). In healthcare applications, inverse models have been employed to obtain heart-surface potentials from body-surface measurements, known as the inverse ECG problem (Yao and Yang 2021). In Seismology, inverse problems aim at getting information about the structure of the forces acting in the earthquake's focus from seismic waves at Earth's surface (Apostol 2019). Inverse modeling has also found its applications in detecting the impact location of the missing Malaysian Airlines MH370, using the drift of marine debris (Miron et al. 2019) or acoustic-gravity waves (Kadri 2019).

This article investigates an important class of statistical inverse problems—the estimation of the initial condition of a spatio-temporal advection-diffusion process using spatially sparse data streams. Consider the detection of accidental releases of fugitive emissions from industrial operations (Hosseini and Stockie 2016). Figure 1 shows a 2×2 km² spatial

area that includes a large lead-zinc smelter located in Trail, British Columbia, Canada. The four large red circles indicate the potential emission sources of Zinc Sulphate (ZnSO₄), while the small blue circles indicate the locations of nine receptors (i.e., sensors) deployed to detect accidental ZnSO₄ leak. The transport of ZnSO₄ is governed by an advection-diffusion equation in the form of a Partial Differential Equation (PDE). In case of accidental ZnSO₄ releases, sensor monitoring data are used to estimate probable emission locations. This inverse problem requires a statistical model that (i) establish the explicit and interpretable link between observations, emission sources, and process parameters (e.g., wind, diffusivity and decay) by integrating the underlying advection-diffusion physics, (ii) incorporate sensing data streams to estimate the initial condition when ZnSO₄ is released, and (iii) handle data arising from different sensor network layouts, such as irregular, uniform, nonuniform, nested, etc.

1.2. Statistical Inverse Models and Literature Review

An inverse model typically involves formulating an optimization problem that minimizes the distance between forward model output and observations (Constantinescu et al. 2019). Consider a physical process governed by an equation $F(\xi, 2) = 0$ with ξ and 2 respectively being the state and parameter (unknown). Because the state of the process ξ must depend on the parameter 2 following the governing equation, we may define a mapping from 2 to ξ , that is, $F(2) = \xi$, known as

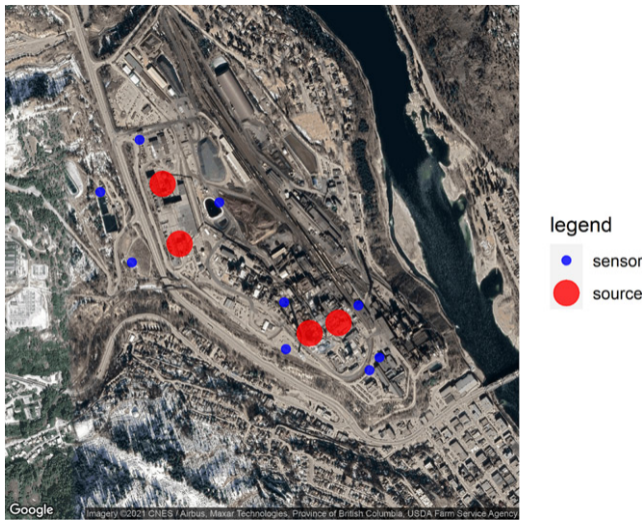


Figure 1. A spatial area that contains four potential ZnSO_4 emission sources (big red circles) and nine receptors for ground-level measurements (small blue circles).

the parameter-to-observable map. Once the observations \mathbf{Y} of the process are available, an inverse problem can be conceptually formulated as $\hat{\mathcal{Z}} = \arg\min_{\mathcal{Z}} L(F(\mathcal{Z}), \mathbf{Y})$ where L is some predefined loss function. For example, Hwang et al. (2019) proposed a Bayesian inverse model to estimate the two-dimensional source functions by exploiting the adjoint advection-diffusion operator. The authors used the finite difference method to solve both the forward and backward physics models, and constructed the likelihood function for the emission rate given observations. Oates et al. (2019) proposed an inverse model to estimate time-dependent parameters in an electrical potential model for industrial hydrocyclone equipment. Bayesian methods were employed to incorporate statistical models for the errors in the numerical solution of the physical equation. Yeo et al. (2019) proposed a spectral method for source detection of advection-diffusion processes. The authors used the Gaussian radial basis functions to approximate a smooth emission function over space, and the spectral coefficients are modeled by generalized polynomial chaos.

Note that, the physics model F is typically solved by converting the PDE to a large system of Ordinary Differential Equations (ODE) given a finite difference discretization of the physical domain. When the dimension of the discretization is high, it is often computationally expensive to obtain the forward model output by directly solving the governing equation F . Statistical surrogate modeling is thus used to construct the parameter-to-observable map F (Gul et al. 2018; Mak et al. 2018; Qian et al. 2019). For example, Gaussian Processes (GP) have been extensively investigated for constructing statistical surrogate models (Hung, Joseph, and Melkote 2015; Deng et al. 2017; Gramacy 2020; Zhang, Cole, and Gramacy 2021; Sauer, Gramacy, and Higdon 2021). For advection-diffusion processes, in particular, Sigrist, Kunsch, and Stahel (2015) obtained a GP by solving a PDE with an advection-diffusion operator that does not vary in space and time, and Liu, Yeo, and Lu (2022) extended this approach by considering spatially varying advection-diffusion. In recent years, physics-informed machine learning is rapidly emerging for data-driven discovery of governing physics and

state/parameter/operator inference which are physically meaningful. For example, Raissi, Perdikaris, and Karniadakis (2019) proposed a deep learning framework for solving both forward and inverse problems for nonlinear partial differential equations. Chen, Kang, and Lin (2021) proposed an active learning approach to estimate the unknown differential equations. An adaptive design criterion combining the D-optimality and the maximin space-filling criterion is used to reduce the experimental data size, where the D-optimality accounts for the unknown solution of the differential equations and its derivatives.

1.3. Problem Statement, Contributions and Overview

In this article, we investigate a statistical inverse model that aims to estimate the initial condition (over the entire spatial domain) of an advection-diffusion process from spatially sparse sensor measurements. The problem can be formally stated as follows:

Problem Statement. Let $\xi(t, \mathbf{s})$ be an advection-diffusion process monitored at M spatial locations for L discrete time periods, this article is concerned with an inverse problem that estimates $\xi(0, \mathbf{s})$ over the entire spatial domain using spatially sparse sensor data streams.

In particular, three important spatial sampling schemes (i.e., network layout) are considered: *irregular*, *nonuniform*, and *shifted uniform* sampling. Note that, (i) the irregular sampling (Figure 2(a)) is the general scenario that includes the nonuniform, shifted uniform, and uniform sampling as its special cases; (ii) the two special cases, that is, nonuniform and shifted uniform sampling (Figure 2(b) and (c)), are also investigated because computationally efficient solutions are available in the spectral domain for the two special schemes. In practice, nonuniform sampling is often used to minimize acquisition time, sensor installation cost and power consumption, and is particularly useful for monitoring low-activity signals (Venkataramani and Bresler 2001; Beyrouthy, Fesquet, and Roland 2015). Shifted uniform sampling (also known as the nested array or difference co-array) involves two nested uniform sensing networks, and significantly increases the degrees of freedom of linear arrays. By nesting two or more uniform linear arrays, shifted uniform sampling can provide $O(M^2)$ degrees of freedom using only M physical sensors, and thus mitigate the issue of spectral aliasing in spectral analysis (Pal and Vaidyanathan 2010; Qin and Amin 2021).

Contributions of this article are summarized as follows: (i) This article proposes the first inverse model based on a forward spatio-temporal model for advection-diffusion processes proposed in Liu, Yeo, and Lu (2022). This forward model, which provides the parameters-to-observables map F for our inverse model, decomposes a physical spatio-temporal process by the linear combination of spatial bases and a multivariate random process of spectral coefficients. The temporal dynamics of spectral coefficients is determined by the advection-diffusion equation so as to integrate the governing physics into statistical models; see Section 2.1. In this article, following the idea of spectrum decomposition, the estimation of $\xi(0, \mathbf{s})$ over the entire spatial domain can be performed by estimating the spectral

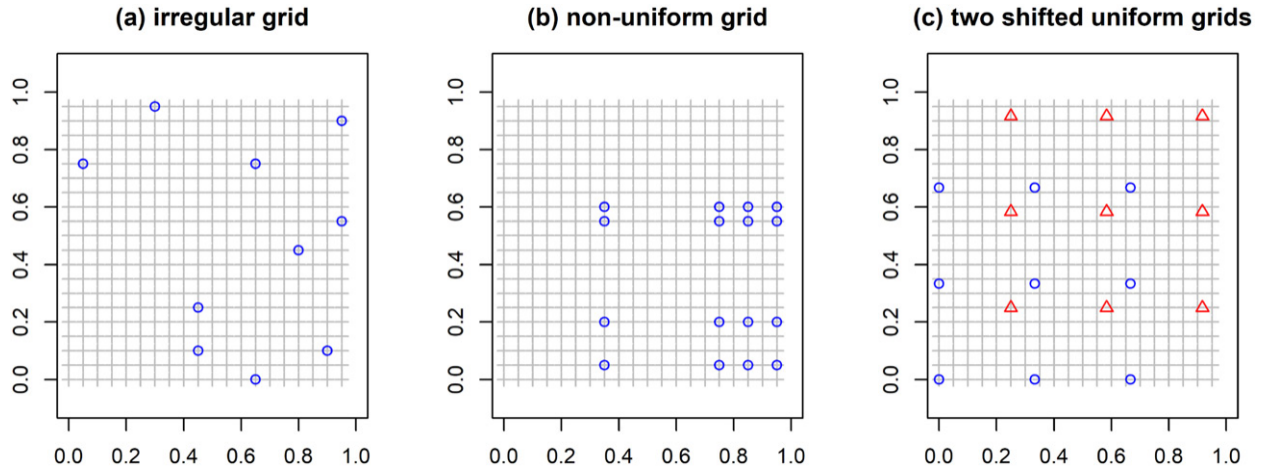


Figure 2. Illustrations of the three spatial sampling schemes considered in this article: (a) irregular grid, (b) nonuniform grid, and (c) shifted uniform grids (nested).

coefficients at time zero that determine $\xi(0, s)$. (ii) Because estimating the spectral coefficients at time zero requires sufficient observations over space and time given a sensor network layout, Section 2.2 performs theoretical investigations and obtains sufficient and necessary conditions for the spectral coefficients at time zero to be uniquely estimated. When such conditions are not met, spectral coefficients cannot be uniquely determined and this is known as spectral aliasing in signal processing. (iii) In Section 2.3, we further argue that it is not always possible to uniquely estimate all spectral coefficients at time zero. The sensor network layout and the number of observations in space and time are often subject to practical constraints. Hence, we often require the spectral coefficients to be estimated under the scenarios where neither the sufficient nor necessary conditions are met. It is also noted that, the spectral coefficients may rapidly decay at high-frequency modes if $\xi(0, s)$ is smooth. To cope with this issue, Section 2.3 presents a regularized inverse problem that estimates the spectral coefficients at time zero given any irregular sensor network layout. The regularization induces both the sparsity in spectral coefficients and the smoothness of neighboring spectral coefficients. Section 3 presents the special results when data are obtained from nonuniform and shifted uniform sampling, under which computationally efficient solutions are available in the spectral domain. (iv) Finally, Section 4 develops the Alternating Direction Method of Multipliers (ADMM) algorithm for efficiently solving the proposed regularized inverse problem. We then extend the proposed inverse model and the ADMM algorithm to handle nonnegativity constraint on $\xi(0, s)$, that is, $\xi(0, s) \geq 0$. Section 5 provides comprehensive numerical investigations. Sensitivity analysis is performed to demonstrate the robustness of the proposed method.

2. Inverse Modeling under General Irregular Sampling

2.1. Preliminaries

Consider a physical spatio-temporal advection-diffusion process $\xi(t, s)$ given by a PDE:

$$A\xi(t, s) = \varphi(t, s), \quad s \in S, t \geq 0 \quad (1)$$

where S is the spatial domain, $\varphi(t, s)$ is the source term, and the advection-diffusion operator A is given by $A\xi(t, s) = \xi_t(t, s) + \mathbf{v}^T \nabla \xi(t, s) - \nabla \cdot [\mathbf{D} \nabla \xi(t, s)] + \zeta \xi(t, s)$ with $\mathbf{v}, \mathbf{D}, \zeta, \nabla$ and $\nabla \cdot$ respectively being the velocity field, diffusion tensor, decay, gradient and divergence operator. The PDE (1) serves as the governing equation behind an extremely large class of physical phenomena where particles and energy are transferred inside a system.

In this article, the process $\xi(t, s)$ can only be observed by spatially distributed sensors at discrete times. Hence, the inverse problem is concerned with estimating the initial condition $\xi(0, s)$ over the entire spatial domain. Following Liu, Yeo, and Lu (2022), $\xi(0, s)$ is assumed to be spanned by a finite number of orthogonal spatial Fourier basis functions,

$$\xi(0, s) = \sum_{\mathbf{k} \in K} \eta(\mathbf{k}) f_{\mathbf{k}}(s) \quad (2)$$

where $\mathbf{k} = (k_1, k_2)^T \in K$ is the wavenumber, $f_{\mathbf{k}}(s) = e^{i2\pi s^T \mathbf{k}}$ is the Fourier basis function, $\eta(\mathbf{k})$ is the coefficient that determines the weight of each Fourier mode, and

$$K = \left\{ (k_1, k_2)^T; k_1 = -\frac{N_1}{2} + 1, -\frac{N_1}{2} + 2, \dots, \frac{N_1}{2}, k_2 = -\frac{N_2}{2} + 1, -\frac{N_2}{2} + 2, \dots, \frac{N_2}{2} \right\}. \quad (3)$$

Note that, the equality in (2) holds when the initial condition is band-limited with the high-frequency parts of its Fourier expansion decaying rapidly to exactly zero. Based on (2), it has been shown that the process $\xi(t, s)$ remains in S for $t \geq 0$ and also admits a spectral representation: $\xi(t, s) = \sum_{\mathbf{k} \in K} \alpha(t, \mathbf{k}) f_{\mathbf{k}}(s)$, where $\alpha(t, \mathbf{k})$ is the Fourier coefficient evolving over time, and $\alpha(0, \mathbf{k}) = \eta(\mathbf{k})$ (Sigrist, Kunsch, and Stahel 2015; Liu, Yeo, and Lu 2022).

Next, consider a sensor network with M sensors at spatial locations s_1, s_2, \dots, s_M . Let a column vector $\mathbf{Y}(l) = (Y(l, s_1), Y(l, s_2), \dots, Y(l, s_M))^T$ contain the observations arising from the advection-diffusion process (1) at time l ($l = 1, 2, \dots, L$), and let a $M \times L$ matrix \mathbf{Y} be a collection of the observations from the L time periods: $\mathbf{Y} = [\mathbf{Y}(1), \mathbf{Y}(2), \dots, \mathbf{Y}(L)]$.

Then, a spatio-temporal model based on the PDE (1) is proposed in Liu, Yeo, and Lu (2022):

$$\mathbf{Y} = \mathbf{F}\mathbf{E}\mathbf{G} + \mathbf{V}. \quad (4)$$

Here,

- \mathbf{F} is an $M \times N$ matrix of the Fourier basis functions ($N = N_1 \times N_2$), $\mathbf{F} = (\mathbf{f}_{k_1}, \mathbf{f}_{k_2}, \dots, \mathbf{f}_{k_N})$ where $\mathbf{f}_{k_i} = (e^{i2\pi s_1^T k_i}, e^{i2\pi s_2^T k_i}, \dots, e^{i2\pi s_M^T k_i})^T$ and i is the imaginary unit.
- $\mathbf{E} = \text{diag}(\alpha(0, \mathbf{k})) = \text{diag}(\eta)$ is a $N \times N$ matrix of the spectral coefficients at time 0, and η is a vector that contains $\eta(\mathbf{k})$ for all $\mathbf{k} \in K$.
- \mathbf{G} is a $N \times L$ matrix, $\mathbf{G} = (\mathbf{g}(1), \mathbf{g}(2), \dots, \mathbf{g}(L))$, which captures the temporal evolution of the elements in \mathbf{E} . Here, $\mathbf{g}(l) = (g_1(l), \dots, g_N(l))^T$ is a column vector where $g_j(l) = e^{\gamma_j(l-1)l}$, l is the sampling interval in time, and $\gamma_j = -\mathbf{k}_j^T \mathbf{D} \mathbf{k}_j - \zeta - i\mathbf{v}^T \mathbf{k}_j$ for $j = 1, 2, \dots, N$.
- $\mathbf{V} = (\mathbf{v}(1), \mathbf{v}(2), \dots, \mathbf{v}(L))$ is a $M \times L$ matrix that captures the measurement error, and $\mathbf{v}(l)$ is multivariate Gaussian, $N_M(0, \Sigma_v)$, for $l = 1, 2, \dots, L$.

Readers may refer to Sigrist, Kunsch, and Stahel (2015) and Liu, Yeo, and Lu (2022) for details of (4). The model (4) is based on the classical solution of nonlinear dynamical systems using the spectral theory and eigenfunction expansions, and serves as the foundation based on which the inverse models are to be established in this article.

2.2. The Inverse Problem and Its Basic Properties

In an inverse modeling problem considered in this article, \mathbf{Y} is the sensor observation, both \mathbf{F} and \mathbf{G} are pre-computed, and the goal is to estimate the coefficient vector η that determines the initial condition $\xi(0, s)$. Note that, the spectral coefficients η may not be uniquely determined given insufficient observations over space and time and particular sensor network layouts (known as spectral aliasing). Proposition 1 first establishes necessary conditions for all components in η to be uniquely estimated.

Proposition 1. Given the observations of the process (1) from M sensors and for L discrete time periods, all spectral coefficients in η can be uniquely estimated from the model (4) if at least one of the following two conditions is met:

Condition A: given the velocity \mathbf{v} and diffusivity \mathbf{D} , there exist no \mathbf{k}_{j_1} and \mathbf{k}_{j_2} ($\mathbf{k}_{j_1}, \mathbf{k}_{j_2} \in K$ and $j_1 \neq j_2$) such that

$$\mathbf{v}^T(\mathbf{k}_{j_1} - \mathbf{k}_{j_2}) = 0 \quad \text{and} \quad \mathbf{k}_{j_1}^T \mathbf{D} \mathbf{k}_{j_1} = \mathbf{k}_{j_2}^T \mathbf{D} \mathbf{k}_{j_2}. \quad (5)$$

Condition B: There exist at least two sampling locations s and s^0 such that neither of the following conditions holds:

$$2\mathbf{k}_{j_1}(s - s^0) \in Z^{(\text{odd})}, \quad 2\mathbf{k}_{j_2}(s - s^0) \in Z^{(\text{odd})} \quad (6a)$$

$$2\mathbf{k}_{j_1}(s - s^0) \in Z^{(\text{even})}, \quad 2\mathbf{k}_{j_2}(s - s^0) \in Z^{(\text{even})}. \quad (6b)$$

All proofs are presented in the supplemental materials. As shown by this proposition, whether all spectral coefficients in η can be uniquely estimated depends on key physical parameters of the underlying process, such as the velocity \mathbf{v} and diffusivity \mathbf{D} as one might naturally expect.

Next, we investigate the sufficient condition for all components in η to be uniquely estimated. In general, the sufficient condition requires either sufficiently large spatial observations (i.e., large M), or sufficiently large temporal observations (i.e., large L), or both. This is intuitively true and detailed discussions are presented as follows.

(When the spatial observations are large.) If $M \geq N$, the left inverse of \mathbf{F} exists. Let \mathbf{F}_L^{-1} be the left inverse of \mathbf{F} , (4) can be rewritten as $[\mathbf{F}_L^{-1} \mathbf{Y}]^T = \mathbf{G}^T \mathbf{E}^T + [\mathbf{F}_L^{-1} \mathbf{V}]^T$. Hence, let $\mathbf{G}_{\cdot j}^T$ be the j th column of \mathbf{G}^T , $j = 1, 2, \dots, N$, we have

$$\text{vec}([\mathbf{F}_L^{-1} \mathbf{Y}]^T) = \text{diag}(\{\mathbf{G}_{\cdot j}^T\}_{j=1}^N) \eta + \text{vec}([\mathbf{F}_L^{-1} \mathbf{V}]^T) \quad (7)$$

where $\text{vec}(\cdot)$ denotes matrix vectorization, and $\text{diag}(\{\mathbf{G}_{\cdot j}^T\}_{j=1}^N)$ is a block diagonal matrix with the column vector $\mathbf{G}_{\cdot j}^T$ being its j th block. The exponential structure of g_{ij} in \mathbf{G} guarantees that the $LN \times N$ matrix $\text{diag}(\{\mathbf{G}_{\cdot j}^T\}_{j=1}^N)$ is full column rank, and all elements in η can be uniquely determined. Note that, when $M \geq N$, the sampling frequency in space exceeds the Nyquist frequency—the largest bandwidth that can be sampled without aliasing.

(When the temporal observations are large.) A large value of L corresponds to another scenario where the temporal samples are abundant. By examining the expression of γ_j in (4), it is possible to find j and j^0 ($j \neq j^0$) such that $\gamma_j = \gamma_{j^0}$. In other words, it is possible that \mathbf{G} is row rank deficient with identical rows.

Let $\{1, 2, \dots, N\} \xrightarrow{M} \mathcal{G} = \{\mathcal{G}_1, \mathcal{G}_2, \dots, \mathcal{G}_{\tilde{N}}\}$ be a mapping where \mathcal{G}_i ($i = 1, 2, \dots, \tilde{N}$) is a set such that $\gamma_j = \gamma_{j^0}$ for $j, j^0 \in \mathcal{G}_i$. In other words, the mapping M defines a partition of \mathbf{G} where each partition contains identical rows, and the row rank of \mathbf{G} is given by \tilde{N} .

Proposition 2. If the number of temporal samples L is greater than the (row) rank of \mathbf{G} , that is, $L > \tilde{N}$, the sufficient condition for all components in η to be uniquely determined is

$$\text{rank}(\tilde{\mathbf{F}}_i) = |\mathcal{G}_i|, \quad i = 1, \dots, \tilde{N} \quad (8)$$

where $\tilde{\mathbf{F}}_i = \{\mathbf{f}_{m,j}\}_{m=1, \dots, M, j \in \mathcal{G}_i}$ is a $M \times |\mathcal{G}_i|$ matrix, and $|\mathcal{G}_i|$ represents the cardinality of the set \mathcal{G}_i for $i = 1, \dots, \tilde{N}$.

2.3. A Regularized Inverse Problem

Propositions 1 and 2 establish sufficient and necessary conditions for all components in η to be uniquely determined from spatially distributed sensor data streams. Despite the theoretical values rooted in the two propositions, real applications may not always require all components in η to be uniquely estimated. For example, the numbers of spatial/temporal samples as well as the locations where sensors can be deployed are always subject to practical constraints. Hence, we often require η to be estimated under the scenarios where neither sufficient nor necessary condition is met.

We first rewrite (4) and define \mathbf{Y}^E , $\mathbf{X}^{(P-L)}$, and $\mathbf{V}^E \in N(0, \Sigma)$ as follows:

$$\begin{aligned} \mathbf{Y}(1) &= \mathbf{F} \text{diag}(\{\mathbf{g}_j(1)\}_{j=1}^N) \eta + \mathbf{v}(1) \\ &\vdots \\ \mathbf{Y}(L) &= \mathbf{F} \text{diag}(\{\mathbf{g}_j(L)\}_{j=1}^N) \eta + \mathbf{v}(L) \end{aligned} \quad (9)$$

\mathbf{Y}^E

$\mathbf{X}^{(P-L)}$

\mathbf{V}^E

and consider a regularized inverse problem:

$$\text{Problem P-I:} \quad \min \quad \frac{1}{2} (\tilde{\mathbf{y}} - \mathbf{X}^{(P-1)} \eta)^T \mathbf{G}^{-1} (\tilde{\mathbf{y}} - \mathbf{X}^{(P-1)} \eta) + R(\eta). \quad (10)$$

Here, the choice of the regularization $R(\eta)$ is motivated by two considerations: (i) For smooth or band-limited initial condition (see (2)), the high-frequency modes decay rapidly, that is, the energy is concentrated in the low-frequency region. This motivates us to impose an L_1 -regularization to η (i.e., the *sparsity* of η). (ii) For smooth initial conditions, it is expected that the components in η gradually decay (not necessarily monotone). This motivates us to impose some level of *smoothness* among the *adjacent* components in η corresponding to adjacent frequencies to prevent sudden spikes of the estimated special coefficients. In particular, an L_2 -regularization is imposed on the difference between the connected components of η in both directions (horizontal and vertical) such that

$$\begin{aligned} \mathbf{J}_1 \eta \mathbf{J}_2^T &= \sum_{i,j \in K^{(h)}} (\eta(\mathbf{k}_i), \eta(\mathbf{k}_j))^2, \\ \mathbf{J}_2 \eta \mathbf{J}_1^T &= \sum_{i,j \in K^{(v)}} (\eta(\mathbf{k}_i), \eta(\mathbf{k}_j))^2 \end{aligned} \quad (11)$$

where \mathbf{J}_1 and \mathbf{J}_2 are the matrix difference operators in the horizontal and vertical directions, and the set $K^{(h)}$ and $K^{(v)}$ consist of all frequencies $\mathbf{k} \in K$ which are connected in the horizontal and vertical directions, that is, $K^{(h)} = \{\mathbf{k}_i, \mathbf{k}_j; k_{j,1} - k_{i,1} = 1, i < j\}$ and $K^{(v)} = \{\mathbf{k}_i, \mathbf{k}_j; k_{j,2} - k_{i,2} = 1, i < j\}$. Note that, (11) modifies the idea of Fused Lasso (Tibshirani et al. 2005). The difference is that, Fused Lasso involves an L_1 -regularization to the differences among the coefficients that leads to a sparse and piecewise constant solution, while it is appropriate for us to consider an L_2 -regularization such that the components in η can smoothly change between the high-frequency and low-frequency regions.

Finally, the regularization $R(\eta)$ in (10) is given by

$$R(\eta) = \lambda_1 \mathbf{J}_1 \eta \mathbf{J}_1^T + \lambda_2 \mathbf{J}_2 \eta \mathbf{J}_2^T \quad (12)$$

where $\mathbf{J} = (\mathbf{J}_1^T, \mathbf{J}_2^T)^T$ is a 2D difference operator, and λ_1 and λ_2 , respectively control the sparsity in η and the smoothness among the adjacent components in η . The inverse problem (10) can be solved by the Alternating Direction Method of Multipliers (ADMM) (Zou and Hastie 2005; Ramdas and Tibshirani 2016). Details of the ADMM algorithm for our problems are provided in Section 4.

3. Two Special Cases

In this section, we further investigate two special sampling schemes, that is, nonuniform sampling and shifted uniform sampling as discussed in Section 2.3, and show that computationally efficient solutions are possible in the spectral domain under the two special schemes.

3.1. Nonuniform Sampling

Consider a rectangular mesh system given by a tensor product of two one-dimensional collocation sets, $\tilde{\mathbf{M}} = \tilde{\mathbf{M}}_1 \boxtimes \tilde{\mathbf{M}}_2$, where $\tilde{\mathbf{M}}_1 = \{m_1; m_1 = 0, 1, \dots, \tilde{M}_1 - 1\}$ and $\tilde{\mathbf{M}}_2 = \{m_2; m_2 = 0, 1, \dots, \tilde{M}_2 - 1\}$ are the sets of collocation points. Here, $\tilde{\mathbf{M}}$ is a mesh system consisting of the candidate locations where sensors can potentially be deployed. Let $M_1 \boxtimes M_1$ and $M_2 \boxtimes M_2$, a nonuniform sampling grid is given by a mesh system $\mathbf{M} = M_1 \boxtimes M_2$ where $|M_1| = M_1$, $|M_2| = M_2$, and $|\cdot|$ represents the cardinality of a set. Let $y(l, \mathbf{m})$ represent the observation at time l and from location $\mathbf{m} \in \mathbf{M}$. Then, the nonuniform discrete Fourier transform of type II (NUDFT-II) of $y(l, \mathbf{m})$ is

$$\beta(l, \mathbf{q}) = \frac{1}{|\mathbf{M}|} \sum_{\mathbf{m} \in \mathbf{M}} y(l, \mathbf{m}) e^{-i2\pi \mathbf{m}^T \mathbf{q}}, \quad \text{for } \mathbf{q} \in \mathbf{Q}, \quad (13)$$

where $\mathbf{Q} = \{(q_1, q_2)^T; q_1 = -\frac{M_1}{2} + 1, -\frac{M_1}{2} + 2, \dots, \frac{M_1}{2}, q_2 = -\frac{M_2}{2} + 1, -\frac{M_2}{2} + 2, \dots, \frac{M_2}{2}\}$.

Replacing $y(l, \mathbf{m})$ in (13) by its discrete Fourier transform over the domain K , we have

$$\begin{aligned} \beta(l, \mathbf{q}) &= \frac{1}{|\mathbf{M}|} \sum_{\mathbf{m} \in \mathbf{M}} \sum_{\mathbf{k} \in K} [\alpha(l, \mathbf{k}) + \varepsilon(l, \mathbf{k})] e^{i2\pi \mathbf{m}^T \mathbf{k}} e^{-i2\pi \mathbf{m}^T \mathbf{q}} \\ &= \sum_{i \in I_q} \sum_{j \in J_q} \alpha(l, \mathbf{q} + (iM_1, jM_2)^T) + \varepsilon(l, \mathbf{q} + (iM_1, jM_2)^T) \end{aligned} \quad (14)$$

where ε is due to the observation error, and the sets I_q and J_q are respectively given by

$$\begin{aligned} I_q &= \left\{ i; -\frac{N_1}{2} + 1 \leq (q_1 + iM_1) \leq \frac{N_1}{2}, i \in \mathbb{Z} \right\} \\ J_q &= \left\{ j; -\frac{N_2}{2} + 1 \leq (q_2 + jM_2) \leq \frac{N_2}{2}, j \in \mathbb{Z} \right\}. \end{aligned} \quad (15)$$

Here, the first line of (14) is obtained by directly inserting the Fourier transform of $y(l, \mathbf{m})$ into (18). The second line of (14) is obtained by invoking the well-known orthogonal properties of Fourier bases, that is, $[\alpha(l, \mathbf{k}) + \varepsilon(l, \mathbf{k})] e^{i2\pi \mathbf{m}^T (\mathbf{k} - \mathbf{q})} = 1$ only when $\mathbf{k} = \mathbf{q} + (iM_1, jM_2)^T$ where $i \in I_q$ and $j \in J_q$; otherwise $[\alpha(l, \mathbf{k}) + \varepsilon(l, \mathbf{k})] e^{i2\pi \mathbf{m}^T (\mathbf{k} - \mathbf{q})} = 0$. Hence, given a mesh system \mathbf{M} (i.e., the spatial locations where data are collected), (14) implies that $\beta(l, \mathbf{q})$ is given by the sum of multiple Fourier coefficients $\alpha(l, \mathbf{q} + (iM_1, jM_2)^T)$ where $i \in I_q$ and $j \in J_q$. In other words, it is not possible to uniquely estimate $\alpha(l, \mathbf{q} + (iM_1, jM_2)^T)$ for all $i \in I_q$ and $j \in J_q$ from $\beta(l, \mathbf{q})$. This is known as *spectral aliasing*.

To reveal the spectral aliasing structure clearly, we introduce a set K_q

$$K_q = \{(k_1, k_2)^T; k_1 = q_1 + iM_1, k_2 = q_2 + jM_2, i \in I_q, j \in J_q\} \quad (16)$$

that consists of all wavenumbers in K corresponding to $\mathbf{q} \in \mathbf{Q}$. Obviously, the Fourier coefficients corresponding to wavenumbers in K_q are all confounded, and cannot be uniquely determined unless the number of temporal observations L is sufficient (see Proposition 2). Consider a simple illustrative example where $N_1 = N_2 = 4$ and $M_1 = M_2 = 2$, and define four sets: $K_{(0,0)^T} = \{(0,0)^T, (0,2)^T, (2,0)^T, (2,2)^T\}$,

$K_{(0,1)^T} = \{(0, 1)^T, (0, -1)^T, (2, 1)^T, (2, -1)^T\}$, $K_{(1,0)^T} = \{(1, 0)^T, (-1, 0)^T, (1, 2)^T, (-1, 2)^T\}$ and $K_{(1,1)^T} = \{(1, 1)^T, (-1, -1)^T, (-1, 1)^T, (1, -1)^T\}$ such that each set consists of the wavenumbers in K whose corresponding Fourier coefficients are confounded when the number of temporal samples is insufficient. Note that, $\sum_{q \in K_q} K_q = K$ and $K_q \cap K_{q^0} = \emptyset$ for $q \neq q^0$, that is, K_q are mutually exclusive and exhaustive.

Substituting the temporal dynamics of α in (4) into (14), we obtain

$$\beta(l, q) = \mathbf{1}^T \text{diag}(\eta_q) \mathbf{g}_q(l) + \mathbf{1}^T \varepsilon_q(l), \quad l = 1, 2, \dots, L, \quad (17)$$

where $\mathbf{1}$ is a column vector of ones, $\mathbf{g}_q(l)$, $\varepsilon_q(l)$ and η_q are respectively, the column vectors obtained from $\mathbf{g}(l)$, $\varepsilon(l)$ and η by keeping only the components corresponding to $k \in K_q$.

Combining $\beta(l, q)$ from all L sampling times, it follows from (17) that

$$\begin{bmatrix} \beta(1, q) \\ \vdots \\ \beta(L, q) \end{bmatrix} = \begin{bmatrix} \mathbf{1}^T \text{diag}(\mathbf{g}_q(1)) \\ \vdots \\ \mathbf{1}^T \text{diag}(\mathbf{g}_q(L)) \end{bmatrix} \eta_q + \begin{bmatrix} \mathbf{1}^T \varepsilon_q(1) \\ \vdots \\ \mathbf{1}^T \varepsilon_q(L) \end{bmatrix} \quad (18)$$

where β_q is a $L \times 1$ column vector, $\mathbf{B}_q = \text{diag}\{\mathbf{1}^T\}$ is a $L \times (L \times d_q)$ block diagonal matrix with $d_q = |K_q|$, and \mathbf{G}_q is a $(L \times d_q) \times d_q$ matrix. Hence, for any $q \in Q$, we obtain from (17) a linear model

$$\beta_q = \mathbf{B}_q \mathbf{G}_q \eta_q + \mathbf{B}_q \mathbf{W}_q, \quad \mathbf{B}_q \mathbf{W}_q \sim N(\mathbf{0}, \sigma^2 d_q \mathbf{I}). \quad (19)$$

Note that, several factors determine if the components in η_q can be uniquely determined from the linear model (19), including the sensor network layout M , the number of temporal samples L , as well as the parameters of the underlying physical process. The following proposition establishes the conditions for the components in η_q to be uniquely estimated.

Proposition 3. For $k_{j_1}, k_{j_2} \in K_q$ and $j_1 \neq j_2$, if (i) $L \geq d_q$, and (ii) at least one of the conditions, $\mathbf{v}^T(k_{j_1} - k_{j_2}) = 0$ and $k_{j_1}^T \mathbf{D} k_{j_1} - k_{j_2}^T \mathbf{D} k_{j_2} \neq 0$, does not hold, then, $\mathbf{B}_q \mathbf{G}_q$ is full column rank, and all spectral coefficients in η_q can be uniquely estimated from (19).

Although the Proposition 3 suggests that it is possible to estimate η_q from a system of linear models for all $q \in Q$, directly solving these individual linear models is rarely appropriate for the following reason: the matrix $\mathbf{B}_q \mathbf{G}_q$ can be easily ill-conditioned or computationally singular when both $\mathbf{v}^T(k_{j_1} - k_{j_2})$ and $k_{j_1}^T \mathbf{D} k_{j_1} - k_{j_2}^T \mathbf{D} k_{j_2}$ are close to zero. In other words, some columns in $\mathbf{B}_q \mathbf{G}_q$ can be near identical. Hence, we combine the

linear models (19) for all $q_1, q_2, \dots, q_{|Q|}$ and obtain

$$\begin{bmatrix} \beta_{q_1} \\ \vdots \\ \beta_{q_{|Q|}} \end{bmatrix} = \begin{bmatrix} \mathbf{B}_{q_1} \mathbf{G}_{q_1} & \cdots & \mathbf{B}_{q_{|Q|}} \mathbf{G}_{q_{|Q|}} \end{bmatrix} \begin{bmatrix} \eta_{q_1} \\ \vdots \\ \eta_{q_{|Q|}} \end{bmatrix} + \begin{bmatrix} \mathbf{B}_{q_1} \mathbf{W}_{q_1} \\ \vdots \\ \mathbf{B}_{q_{|Q|}} \mathbf{W}_{q_{|Q|}} \end{bmatrix} \quad (20)$$

where $\mathbf{y} \in^{(P-II)}$ is a $(|Q| \times L) \times 1$ column vector, $\mathbf{X} \in^{(P-II)}$ is a $(|Q| \times L) \times |K|$ matrix, η is a $|K| \times 1$ column vector, $\mathbf{V} \in^{(P-II)} \sim N(\mathbf{0}, \sigma^2 \text{diag}\{d_q \mathbf{I}_{|K|}\})$.

Similar to Problem P-I (10), we again obtain a regularized inverse problem as follows:

$$\text{Problem P-II: } \min \frac{1}{2} (\mathbf{y} \in^{(P-II)} - \mathbf{X} \in^{(P-II)} \eta)^T (\mathbf{G} \in^{(P-II)})^{-1} (\mathbf{y} \in^{(P-II)} - \mathbf{X} \in^{(P-II)} \eta) + R(\eta), \quad (21)$$

where $R(\eta)$ is defined in (12).

3.2. Shifted Uniform Sampling

Shifted uniform sensor arrays or platforms consists of two nested rectangular mesh systems (Figure 2(c)), $M^{(1)}$ and $M^{(2)}$, which are respectively defined by the tensor product of two one-dimensional collocation sets:

$$\begin{aligned} M^{(1)} &= \left(\frac{m_1}{M_1}; m_1 = 0, 1, \dots, M_1 - 1 \right) \\ &\quad \times \left(\frac{m_2}{M_2}; m_2 = 0, 1, \dots, M_2 - 1 \right) \end{aligned} \quad (22)$$

$$\begin{aligned} M^{(2)} &= \left(\frac{m_1}{M_1} + \delta_1; m_1 = 0, 1, \dots, M_1 - 1 \right) \\ &\quad \times \left(\frac{m_2}{M_2} + \delta_2; m_2 = 0, 1, \dots, M_2 - 1 \right) \end{aligned} \quad (23)$$

where $0 < \delta_1 < M_1^{-1}$ and $0 < \delta_2 < M_2^{-1}$, and $\delta = (\delta_1, \delta_2)^T$ is the spatial shift between the two sensor platforms. Let $y^{(1)}(l, \mathbf{m})$ represent the observation at time l and location \mathbf{m} from $M^{(1)}$, where $\mathbf{m} = (\frac{m_1}{M_1}, \frac{m_2}{M_2})^T$. For any $q = (q_1, q_2)^T \in Q$, the Fourier coefficient at $\beta^{(1)}(l, q)$ based on the observations from the first mesh system $M^{(1)}$ at time l is

$$\begin{aligned} \beta^{(1)}(l, q) &= \frac{1}{M_1 M_2} \sum_{\mathbf{m}} y^{(1)}(l, \mathbf{m}) e^{-i 2 \pi \mathbf{m}^T \mathbf{q}} \\ &= \frac{1}{M_1 M_2} \sum_{\mathbf{m}} \sum_{\mathbf{k} \in K} [\alpha(l, \mathbf{k}) + \varepsilon(l, \mathbf{k})] e^{i 2 \pi \mathbf{m}^T \mathbf{k}} e^{-i 2 \pi \mathbf{m}^T \mathbf{q}} \\ &= \sum_{i \in I_q} \sum_{j \in J_q} \alpha(l, \mathbf{q} + (i M_1, j M_2)^T) + \varepsilon(l, \mathbf{q} + (i M_1, j M_2)^T) \end{aligned} \quad (24)$$

where the sets I_q and J_q are defined in (15).

Because the second mesh system $M^{(2)}$ is obtained from the first mesh system $M^{(1)}$ given a shift δ in space, the Fourier

coefficient, $\beta^{(2)}(l, q)$, obtained from the data collected from $M^{(2)}$, can be immediately obtained:

$$\beta^{(2)}(l, q) = \begin{matrix} \mathbf{X} & \mathbf{X} \odot \\ i \mathbf{M}_1 \mathbf{q} & i \mathbf{M}_2 \mathbf{q} \end{matrix} \alpha(l, \mathbf{q} + (i \mathbf{M}_1, j \mathbf{M}_2)^T) + \varepsilon(l, \mathbf{q} + (i \mathbf{M}_1, j \mathbf{M}_2)^T) e^{i 2 \pi \delta^T (\mathbf{q} + (i \mathbf{M}_1, j \mathbf{M}_2)^T)} \quad (25)$$

where the last term $e^{i 2 \pi \delta^T (\mathbf{q} + (i \mathbf{M}_1, j \mathbf{M}_2)^T)}$ is due to the spatial shift from $M^{(1)}$ to $M^{(2)}$.

Hence, for $\mathbf{q} \in Q$, one may define a set

$$K_q = \{(k_1, k_2); k_1 = q_1 + i \mathbf{M}_1, k_2 = q_2 + j \mathbf{M}_2, i \in I_q, j \in J_q\}, \quad (26)$$

and for $\mathbf{k} \in K_q$, we have

$$\begin{matrix} \beta^{(1)}(l, \mathbf{q}) \\ \beta^{(2)}(l, \mathbf{q}) \end{matrix} = \begin{matrix} \mathbf{1}^T \\ \mathbf{b}_{\delta, q}^T \end{matrix} \text{diag}(\eta_q) \mathbf{g}_q(l) + \begin{matrix} \mathbf{1}^T \\ \mathbf{b}_{\delta, q}^T \end{matrix} \varepsilon_q(l) \quad (27)$$

for $l = 1, 2, \dots, L$. Here, $\mathbf{1}$ and $\mathbf{b}_{\delta, q}$ are column vectors of length $d_q = |I_q| |J_q|$, and $\mathbf{g}_q(l)$, $\varepsilon_q(l)$, and η_q are respectively the column vectors obtained from $\mathbf{g}(l)$, $\varepsilon(l)$ and η by keeping only the components corresponding to $\mathbf{k} \in K_q$. Similar to the discussions in Section 3.1, K_q consists of all wavenumbers in K corresponding to \mathbf{q} which are aliased and cannot be uniquely determined unless the number of temporal observations L is sufficiently large. Combining $\beta^{(1)}(l, \mathbf{q})$ and $\beta^{(2)}(l, \mathbf{q})$ from all sampling times, we have

$$\begin{matrix} \beta^{(1)}(1, \mathbf{q}) \\ \vdots \\ \beta^{(1)}(L, \mathbf{q}) \\ \beta^{(2)}(1, \mathbf{q}) \\ \vdots \\ \beta^{(2)}(L, \mathbf{q}) \end{matrix} = \begin{matrix} \mathbf{1}^T \\ \vdots \\ \mathbf{1}^T \\ \mathbf{b}_{\delta, q}^T \\ \vdots \\ \mathbf{b}_{\delta, q}^T \end{matrix} \begin{matrix} \text{diag}(\mathbf{g}_q(1)) \\ \vdots \\ \text{diag}(\mathbf{g}_q(L)) \\ \text{diag}(\mathbf{g}_q(1)) \\ \vdots \\ \text{diag}(\mathbf{g}_q(L)) \end{matrix} \eta_q + \begin{matrix} \mathbf{1}^T \\ \vdots \\ \mathbf{1}^T \\ \mathbf{b}_{\delta, q}^T \\ \vdots \\ \mathbf{b}_{\delta, q}^T \end{matrix} \begin{matrix} \varepsilon_q(1) \\ \vdots \\ \varepsilon_q(L) \\ \varepsilon_q(1) \\ \vdots \\ \varepsilon_q(L) \end{matrix} \quad (28)$$

where $\beta_q^{(P-III)}$ is a $2L \times 1$ column vector, $\mathbf{B}_{\delta, q} = \text{diag}\{\mathbf{1}, \mathbf{b}_{\delta, q}\}^T$ is a $2L \times (L \times d_q)$ block diagonal matrix with $d_q = |K_q|$, and \mathbf{G}_q is a $(L \times d_q) \times d_q$ matrix. For any $\mathbf{q} \in Q$, we have

$$\beta_q^{(P-III)} = \mathbf{B}_{\delta, q} \mathbf{G}_q \eta_q + \mathbf{B}_{\delta, q} \mathbf{W}_q \quad (29)$$

where $\mathbf{B}_{\delta, q} \mathbf{G}_q$ is a $2L \times d_q$ matrix. Because $0 < \delta_1 < M^{-1}$ and $0 < \delta_2 < M^{-1}$, the elements in $\mathbf{b}_{\delta, q}$ are identical, which immediately makes $2L \geq d_q$ the sufficient condition for $\mathbf{B}_{\delta, q} \mathbf{G}_q$ to be full column rank, that is,

$$L \geq \frac{d_q}{2} \geq \frac{1}{2} \left(\frac{N_1 - 1}{M_1} + 1 \right) + \frac{1}{2} \left(\frac{N_2 - 1}{M_2} + 1 \right). \quad (30)$$

As discussed in Section 3.1, directly solving the individual linear models in (29) is not an appropriate choice for ill-conditioned problems. Hence, combining the linear models (29) for all $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_{|Q|}$, we have

$$\begin{matrix} \beta_{q_1} \\ \vdots \\ \beta_{q_{|Q|}} \end{matrix} = \begin{matrix} \mathbf{B}_{\delta, q_1} \mathbf{G}_{q_1} \\ \vdots \\ \mathbf{B}_{\delta, q_{|Q|}} \mathbf{G}_{q_{|Q|}} \end{matrix} \begin{matrix} \eta_{q_1} \\ \vdots \\ \eta_{q_{|Q|}} \end{matrix} + \begin{matrix} \mathbf{B}_{\delta, q_1} \mathbf{W}_{q_1} \\ \vdots \\ \mathbf{B}_{\delta, q_{|Q|}} \mathbf{W}_{q_{|Q|}} \end{matrix} \quad (31)$$

where $\beta_q^{(P-III)}$ is a $(2|Q| \times L) \times 1$ column vector, $\mathbf{X}^{(P-III)}$ is a $(2|Q| \times L) \times |K|$ matrix, η is a $|K| \times 1$ column vector, $\mathbf{V}^{(P-III)} \sim N(\mathbf{0}, \mathbf{C}^{(P-III)})$, $\mathbf{C}^{(P-III)} = \sigma^2 \text{diag}\{\mathbf{S}_i\}^{|Q|}$ and $\mathbf{S}_i = \text{diag}(d_q \mathbf{I}, |\mathbf{b}_{\delta, q_i}|^2 \mathbf{I})$ for $i = 1, 2, \dots, |Q|$.

Similar to Problem P-II (21), we obtain a regularized inverse problem:

$$\text{Problem P-III: } \min_{\eta} \frac{1}{2} (\beta_q^{(P-III)} - \mathbf{X}^{(P-III)} \eta)^T (\mathbf{C}^{(P-III)})^{-1} (\beta_q^{(P-III)} - \mathbf{X}^{(P-III)} \eta) + R(\eta) \quad (32)$$

where $R(\eta)$ is defined in (12).

Remarks. Problem P-I estimates the special coefficients η by minimizing the squared distance between forward model outputs and observations in the space-time domain, while Problems P-II and P-III estimate the spectral coefficients η by minimizing the squared distance between the spectral coefficients of forward model outputs and that of observations in the spectral domain. For this reason, when we convert the optimal solution obtained by P-II and P-III from the spectral domain back to the space-time domain through the inverse Fourier transform, the solution is no longer optimal in the least squares sense (i.e., the squared distance between forward model outputs and observations is not minimized in the space-time domain). This is due to the fact that the least squares estimator is not invariant under transformation. If computational cost is not the primary concern, we recommend one to solve the inverse problem in the space-time domain using Problem P-I (10).

4. Solving the Problems P-I, P-II, and P-III using ADMM

This section provides the algorithm required to solve the inverse problems P-I, P-II and P-III (throughout this section, the superscripts, \cdot^{P-I} , \cdot^{P-II} , and \cdot^{P-III} , are dropped without causing ambiguity). Note that, the dimension of η in these three inverse problems is given by $|K| = N_1 \times N_2$. Hence, even for moderate size of N_1 and N_2 , the dimension of η can be large. The Alternating Direction Method of Multipliers (ADMM) for large-scale optimization problems becomes a sensible choice.

We first convert an unconstrained problem of the general form

$$\min_{\eta} \frac{1}{2} (\beta - \mathbf{X} \eta)^T \mathbf{C}^{-1} (\beta - \mathbf{X} \eta) + R(\eta) \quad (33)$$

to a constrained problem:

$$\min_{\eta, \psi} f(\eta) + R(\psi), \quad \text{s.t. } \eta = \psi \quad (34)$$

where $f(\eta) = \frac{1}{2}(\mathbf{\tilde{F}} - \mathbf{X} \eta)^T \mathbf{\tilde{G}}^{-1} (\mathbf{\tilde{F}} - \mathbf{X} \eta)$. For $\rho > 0$, the scaled form of the augmented Lagrangian is written as

$$f(\eta) + R(\psi) + \frac{\rho}{2} \|\eta - \psi + \mathbf{u}\|_2^2 + \frac{\rho}{2} \|\mathbf{u}\|_2^2. \quad (35)$$

Then, the ADMM solves the constrained problem (34) by repeating the following iterations (Zou and Hastie 2005; Ramdas and Tibshirani 2016):

$$\eta^{(i)} = \underset{\eta}{\operatorname{argmin}} f(\eta) + \frac{\rho}{2} \|\eta - \psi^{(i-1)} + \mathbf{u}^{(i-1)}\|_2^2 \quad (36a)$$

$$\psi^{(i)} = \underset{\psi}{\operatorname{argmin}} R(\psi) + \frac{\rho}{2} \|\eta^{(i)} - \psi + \mathbf{u}^{(i-1)}\|_2^2 \quad (36b)$$

$$\mathbf{u}^{(i)} = \mathbf{u}^{(i-1)} + \eta^{(i)} - \psi^{(i)} \quad (36c)$$

for $i = 1, 2, \dots$. The iterations satisfy: residual convergence (i.e., $\eta^{(i)} - \psi^{(i)} \rightarrow 0$ as $i \rightarrow \infty$), objective convergence (i.e., $f(\eta^{(i)}) + R(\psi^{(i)}) \rightarrow f^* + R^*$ where f^* and R^* are the primal optimal values), and dual convergence (i.e., $\mathbf{u}^{(i)} \rightarrow \mathbf{u}^*$ where \mathbf{u}^* is the dual solution). Algorithm 1 summarizes the ADMM algorithm developed for solving (33). In the supplemental materials, we provide technical details of how each step in Algorithm 1 is obtained.

Remarks. Although Problems P-I, P-II, and P-III can be solved by the ADMM algorithm, it is noted that Problem P-I is formulated in the space-time domain, while Problems P-II and P-III are constructed in the spectral domain. As a result, the design matrix $\mathbf{X}^{(P-I)}$ in (9) is a dense matrix, while the design matrices $\mathbf{X}^{(P-II)}$ and $\mathbf{X}^{(P-III)}$ in (20) and (31) are sparse (block diagonal), making the computation of $\mathbf{X}^T \mathbf{\tilde{G}}^{-1} \mathbf{X}$, $\mathbf{X}^T \mathbf{\tilde{G}}^{-1}$ and $\mathbf{\tilde{G}}^{-1} \mathbf{X}$ faster in the ADMM algorithm. In addition, Problems P-II and P-III enable one to truncate the high-frequency components because each block of \mathbf{X} , in both (20) and (31), corresponds to a frequency level. This further helps to reduce the computational time and details are provided in the supplemental materials.

In many applications, a nonnegativity constraint can be added to the output of the inverse model (e.g., the detected emissions or initial conditions need to be nonnegative). When a nonnegativity constraint is added, the inverse modeling problem (33) becomes:

$$\min_{\eta} \frac{1}{2} (\mathbf{\tilde{F}} - \mathbf{X} \eta)^T \mathbf{\tilde{G}}^{-1} (\mathbf{\tilde{F}} - \mathbf{X} \eta) + R(\eta), \quad \text{s.t. } \mathbf{X} \eta \geq 0. \quad (37)$$

In the supplemental materials, we show that the constrained problem (37) can be efficiently solved by modifying the ADMM algorithm described in Section 4, which expands the applicability of the proposed model for a wider range of problems.

5. Numerical Examples

This section presents two numerical examples to illustrate the application of the proposed inverse models and generate some useful insights of the approach.

Algorithm 1: ADMM for solving the Inverse Problems

Data: $\mathbf{\tilde{F}}, \mathbf{X}, \mathbf{\tilde{G}}, \lambda_1, \lambda_2$

$\eta^{(0)}, \psi^{(0)}, \mathbf{u}^{(0)}, \rho > 0, \omega > 0$ //initialize

$i \leftarrow 1$

(the outer loop)

while convergence criterion is not met **do**

$$\eta_n^{(i)} \leftarrow \mathbf{X}^T \mathbf{\tilde{G}}^{-1} \mathbf{X} + \frac{1}{2} \rho \mathbf{I}^{\zeta-1} \mathbf{X}^T \mathbf{\tilde{G}}^{-1} \mathbf{\tilde{F}} + \rho (\psi^{(i-1)} + \mathbf{u}^{(i-1)})$$

(the inner loop)

$\tilde{\psi}^{(0)}$ //initialization for the inner

loop $j \leftarrow 1$

while convergence criterion is not met **do**

$$\tilde{\psi}^{(j)} \leftarrow \frac{\rho}{2\lambda_2} \mathbf{J}^T \mathbf{J} + \frac{1}{2} (\rho + \omega) \mathbf{I}^{\zeta-1} (\eta^{(i)} + \mathbf{u}^{(i-1)} + \omega \theta^{(j-1)} - \omega \mathbf{v}^{(j-1)})$$

$$\theta^{(j)} \leftarrow S_{\lambda_1/\omega}(\tilde{\psi}^{(j)} + \mathbf{v}^{(j-1)}),$$

$$\mathbf{v}^{(j)} \leftarrow \mathbf{v}^{(j-1)} + \tilde{\psi}^{(j)} - \theta^{(j)}$$

$j \leftarrow j + 1$

$$\psi^{(i)} \leftarrow \tilde{\psi}^{(j)}, \mathbf{u}^{(i)} \leftarrow \mathbf{u}^{(i-1)} + \eta^{(i)} - \psi^{(i)}$$

$i \leftarrow i + 1$

5.1. Example I

We first simulate an advection-diffusion process from the PDE (1) on a 40×40 rectangular grid. The parameters of the advection-diffusion operator \mathbf{A} are chosen as: $\mathbf{v} = (0.5 \times 10^{-2}, 0.5 \times 10^{-2})^T$, $\mathbf{D} = \text{diag}\{0.25 \times 10^{-3}\}$ and $\zeta = 0$. The initial condition contains three spatially sparse instantaneous sources given by $g(t, s) = \delta(t - 0) \sum_{j=1}^3 \phi_j(s)$. Here, $\phi_j(s) = \phi_0 \exp\{-\frac{\|s - s_j^{(0)}\|_2}{0.0}\}$ where $\phi_0 = 300$, $s_0^{(1)} = (0.4, 0.2)^T$, $s_0^{(2)} = (0.2, 0.4)^T$ and $s_0^{(3)} = (0.5, 0.5)^T$.

Figure 3 (left panel) shows the initial condition, velocity field (indicated by arrows), and the locations of 64 randomly distributed sensors (indicated by small crosses). Figure 3 also highlights the locations of three selected sensors, “A”, “B”, and “C”, and the measurements over time are shown in the right panel of this figure. The measurement errors are iid samples from a Normal distribution with mean zero and standard deviation two. The strength of the signal from sensor “A” first increases when the process (primarily from source 1) quickly reaches location “A”. After that, the signal decreases as the process propagates away and diffuses. Sensor “B” gradually picks up the signal (first from source 3, and then, from the other two sources), while sensor “C” slowly picks up relatively weak signal because this sensor is far from all three sources. The goal is to estimate the initial condition in the absence of the “complete picture” of the spatio-temporal process over the entire spatial domain.

The first row of Figure 4 shows the snapshots of the process at times 2, 5, 10, 15, and 20. Solving the Inverse Problem P-I (10) for irregular sampling grid using Algorithm 1, the second row of Figure 4 shows the contour plots of the estimated initial

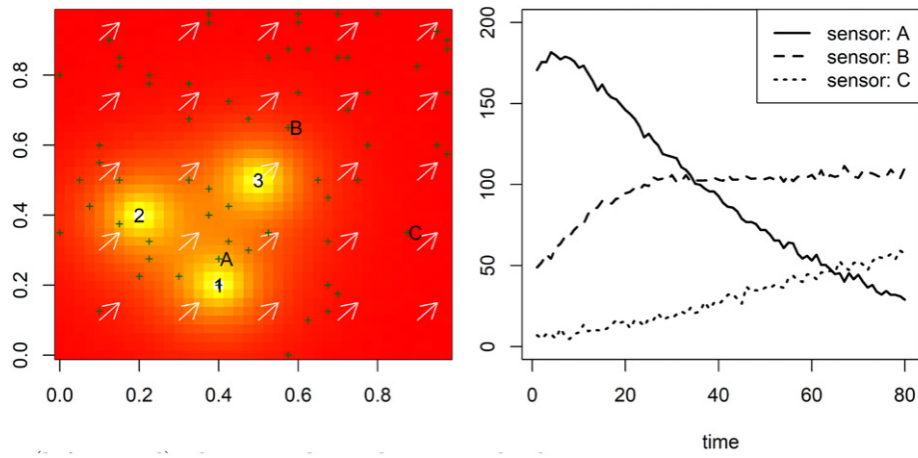


Figure 3. (Left panel) the initial condition with three instantaneous sources, velocity field (indicated by white arrows), and locations of 64 randomly distributed sensors; (right panel) noisy sensor measurements over time from three selected sensors, “A”, “B”, and “C”.

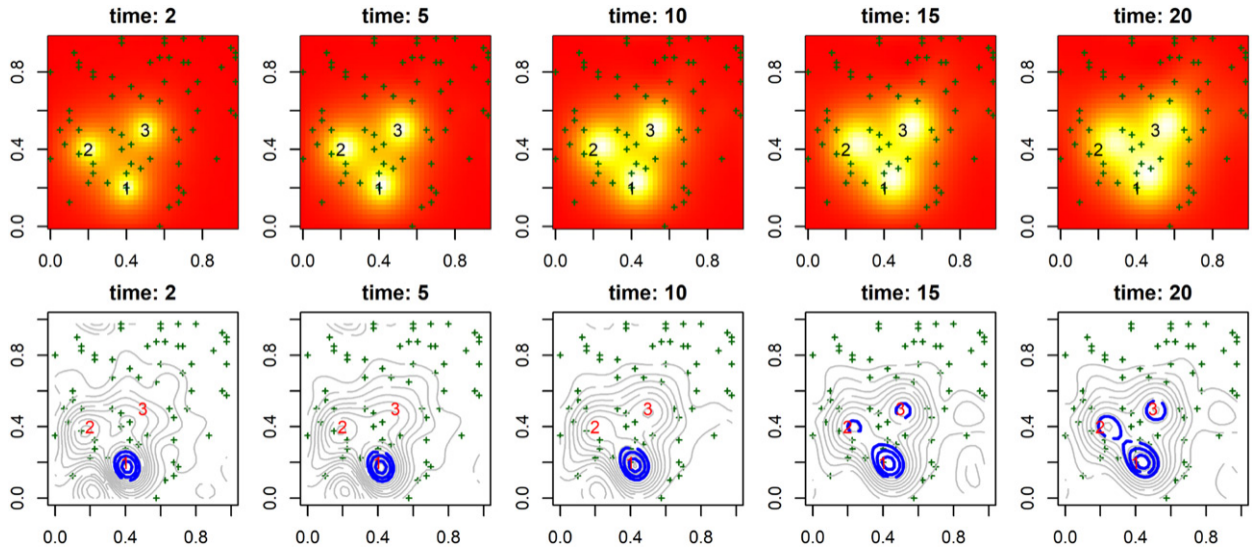


Figure 4. (Top row) snapshots of the advection-diffusion process at times 2, 5, 10, 15, and 20; (bottom row) detected spatial sources based on the streaming data from a network of 64 sensors up to times 2, 5, 10, 15, and 20.

condition using the sensor observations up to times 2, 5, 10, 15, and 20. The thick blue level sets are respectively the 75th, 85th, and 95th percentiles of the output generated by the inverse model. It is seen that, source 1 is quickly detected at time 2. This is only because there happens to be a sensor located near source 1. It is seen that source 2 might also have been detected (circled by a contour line). However, the estimated strength of source 2 is weaker than that of source 1. Source 3 cannot be detected at all at time 2 because most of the sensors have not yet picked up any signal from this source. At time 15, both sources 2 and 3 are clearly detected as the downstream sensors have picked up the signal from these two sources.

Expanding the size of the sensor network is expected to reduce the detection latency. We randomly add another 36 sensors to the existing sensor network (note that, only those sensors added to the downstream areas of the sources may help to reduce the detection latency). Figure 5 presents the updated results: with the additional 36 sensors, all three sources can be detected using the sensor data up to time 10. Figures 4 and 5 well

demonstrate the dynamic nature of the inverse problem based on spatially-distributed sensor data streams.

Next, we investigate the Inverse Problems P-II (21) and P-III (32) for nonuniform sampling grid and shifted sampling grids. Figure 6 shows the output of the Problem P-II based on the sensor data streams from a nonuniform sampling grid, which is given by a 10×10 mesh system generated from a 40×40 uniform mesh system as described in Section 3.1. Similar to Figure 4, the first row of Figure 6 shows the snapshots of the process at times 2, 5, 10, 15, and 20, while the second row shows the contour plots of the estimated initial condition using the streaming observations up to times 2, 5, 10, 15, and 20. The thick blue level sets are respectively the 75th, 85th, and 95th percentiles of the output generated by the inverse model. We see that, source 2 is almost immediately detected because of its proximity to nearby sensors. Sources 1 and 3 are detected later at times 10 and 15 only when sensors in the downstream areas have picked up the signal originated from these two sources.

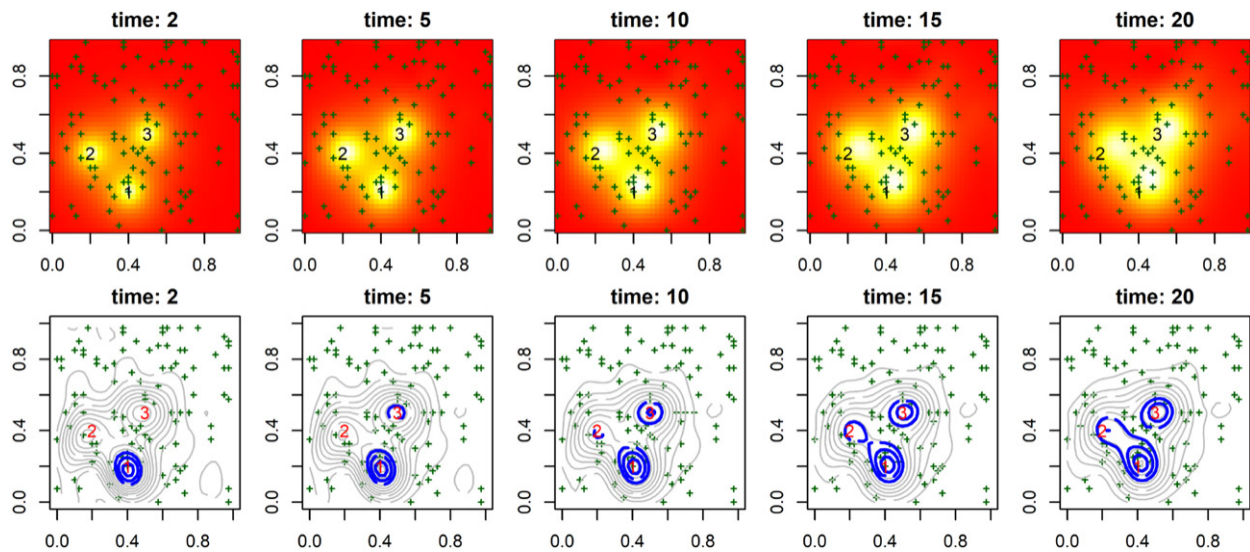


Figure 5. (Top row) snapshots of the advection-diffusion process at times 2, 5, 10, 15, and 20; (bottom row) detected spatial sources based on the streaming data from a network of 100 sensors up to times 2, 5, 10, 15, and 20.

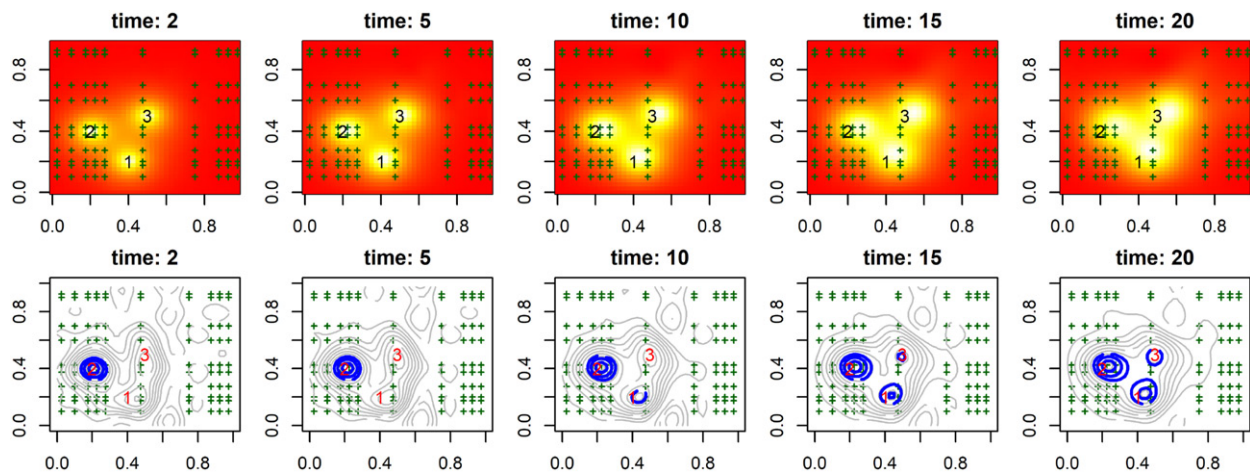


Figure 6. (Top row) snapshots of the simulated advection-diffusion process at times 2, 5, 10, 15, and 20; (bottom row) detected spatial sources based on the streaming data from a nonuniform sampling grid up to times 2, 5, 10, 15, and 20.

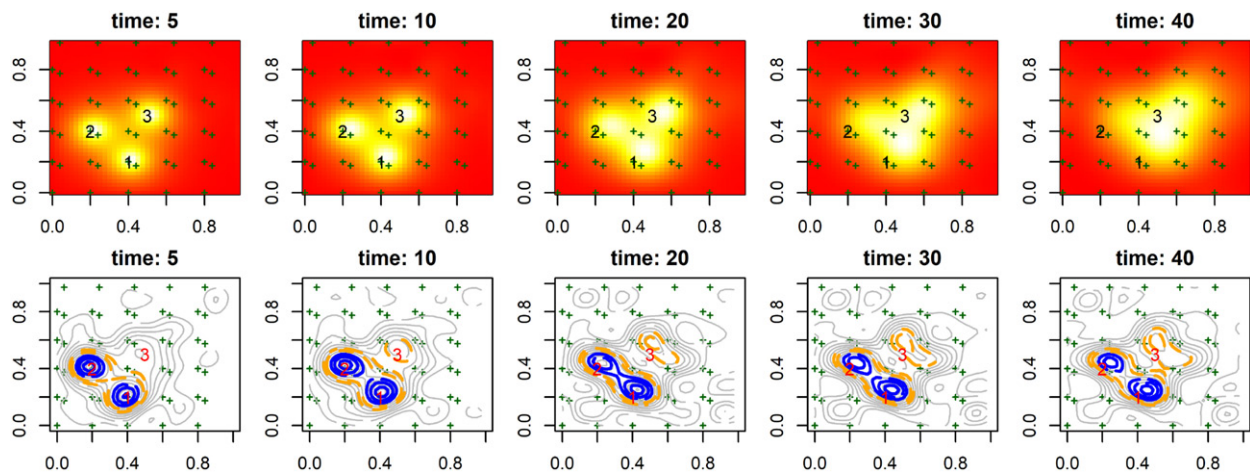


Figure 7. (Top row) snapshots of the simulated advection-diffusion process at times 5, 10, 20, 30, and 40; (bottom row) detected spatial sources based on the streaming data from two shifted uniform sampling grids up to times 5, 10, 20, 30, and 40.

Figure 7 shows the dynamic output from the Inverse Problem P-III based on the sensor data streams from two shifted sampling

grids. The first sampling grid is a 5×5 mesh system, while the second grid is obtained by shifting the first grid by $\delta =$

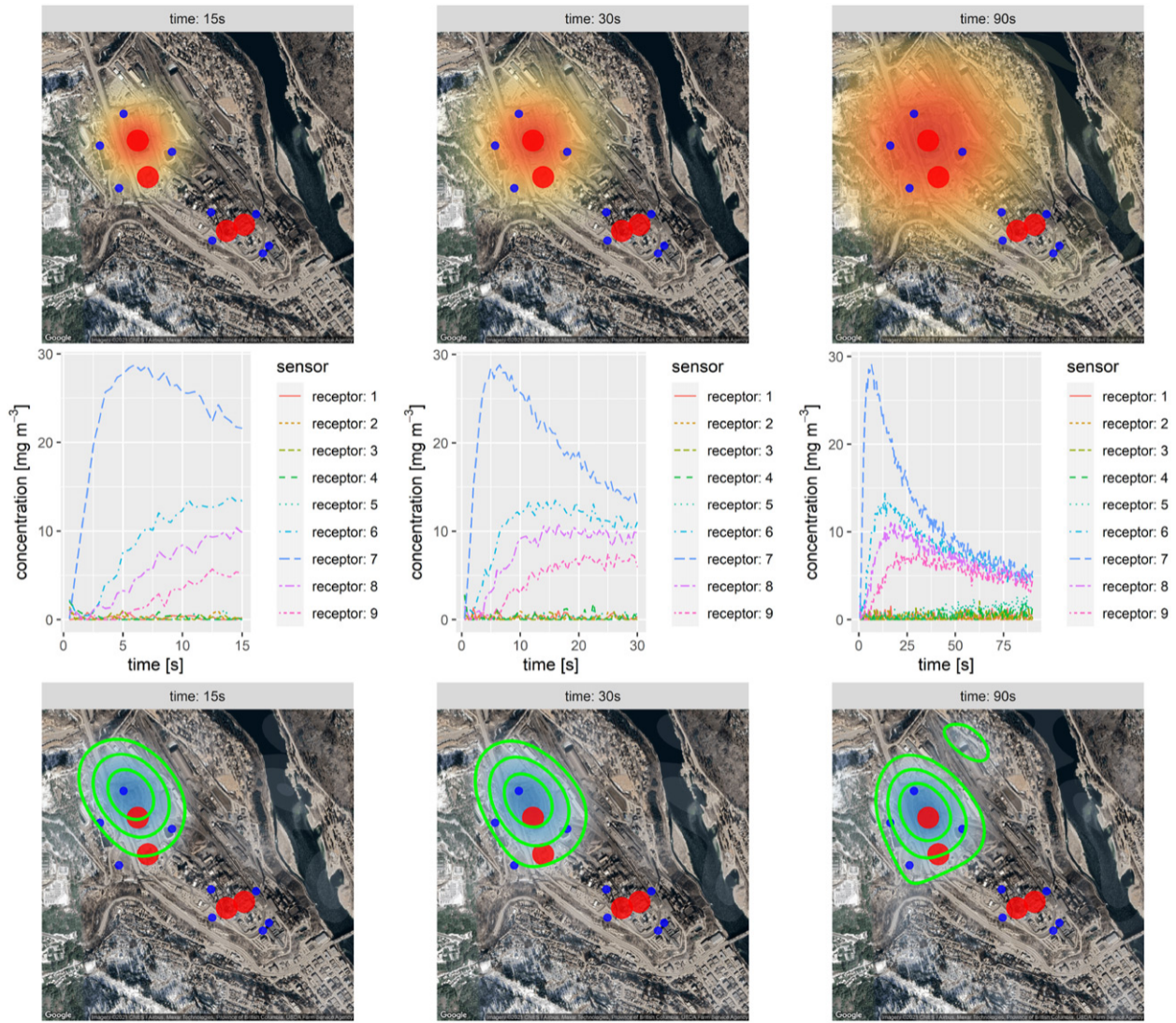


Figure 8. Inverse modeling for a pure diffusion process: (a) concentration of the pollutant 15, 30, and 90 sec after its release; (b) ground measurements by receptors; (c) contour plots of the output from the inverse model.

(0.04, 0.175). The first row of Figure 7 shows the process at times 5, 10, 20, 30, and 40, while the second row shows the model output up to times 5, 10, 20, 30, and 40. Similarly, the solid blue thick level sets are respectively the 75th, 85th, and 95th percentiles of the output generated by the model, while the dashed thick level sets are the 50th and 60th percentiles of the output generated by the inverse model. We see that, sources 1 and 2 are quickly detected at time 5 because of their proximity to nearby sensors. Source 3 is detected later when sensors in the downstream areas of source 3 have picked up the signal.

Example I generates useful insights on the proposed inverse models, and successfully reveals the dynamic nature of the inverse problem using spatially-distributed data streams. A source can be detected when sensors in the downstream areas (if there are any) pick up the signal originated from that source. In the supplemental materials, we compare the bias and Mean-Squared-Error (MSE) of the estimated initial condition $\hat{c}(0, s)$ for different choices of regularizations, including the proposed regularization, generalized Lasso, Elastic Net, L_1 and L_2 regularizations.

5.2. Example II

Example II revisits the motivating example described in Section 1.1. This example is concerned with the estimation of emission locations of accidental ZnSO_4 releases using sensor monitoring data; see Section 1.1 and Hosseini and Stockie (2016) for more details.

The release and transport of a single contaminant in the atmosphere can be well described by an advection-diffusion equation, $c(t, s) + \mathbf{v}^T \nabla c(t, s) - \nabla \cdot [\mathbf{D} \nabla c(t, s)] = \delta(t, s)$, where $c(t, s)$ is the contamination concentration [mg m^{-3}], \mathbf{v} is the wind vector [m s^{-1}], \mathbf{D} is the diffusivity [$\text{m}^2 \text{s}^{-1}$], and $\delta(t, s) = \delta(t - 0) \sum_{j=1}^4 \varphi_j(s)$ is the instantaneous emission source [$\text{mg m}^{-3} \text{s}^{-1}$]. This equation is a special case of the general form (1) in Section 2.

- Scenario 1: pure diffusion. We first consider the scenario where the propagation of ZnSO_4 , after its release, is driven by a pure diffusion process (i.e., the case when there is no wind). The first row of Figure 8 shows the concentration of the pollutant at times 15, 30, and 90 sec after its release. As shown by this figure,

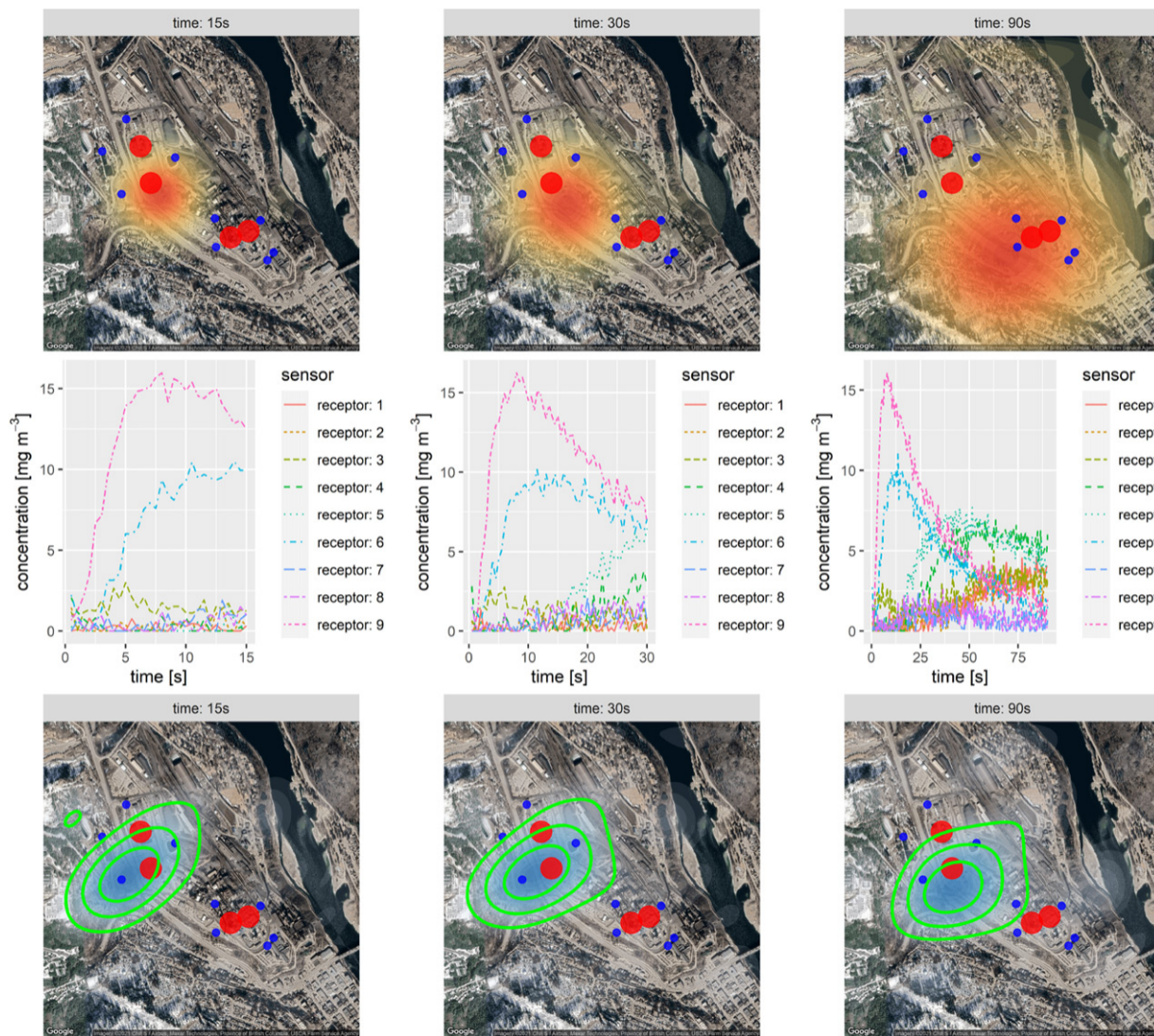


Figure 9. Inverse modeling for an advection-diffusion process: (a) concentration of the pollutant 15, 30, and 90 sec after its release; (b) ground measurements by receptors; (c) contour plots of the output from the inverse model.

the pollutant is released from the first source in the north, and propagates to all directions following a pure diffusion process. The second row of Figure 8 shows the noisy measurements over time. The third row of Figure 8 presents the contour plots of the output generated by the inverse model (10) using the streaming observations up to 15, 30, and 90 sec. As seen in the first and second rows of Figure 8, the sensor located to the north of the source first picks up signal. Hence, at times 15 and 30 sec, the peaks indicated by the contour plot are somewhere between that sensor and the actual source. As more data become available from the other three sensors located near the source (the second row of Figure 8), the peak moves closer to the actual source at time 90 and the emission source is successfully identified. Such observations rationalize the dynamic nature of the proposed inverse problems based on sensor data streams.

- **Scenario 2: advection and diffusion.** We now consider a more common scenario where the propagation of ZnSO₄, after its release, is driven by both advection and diffusion. The pollutant is released from the second source from the top of the spatial domain, and propagates to the southeast direction due to wind. The first row of Figure 9 shows the pollutant concentration at

times 15, 30, 90 sec after its release. The second row shows the noisy ground-level measurements. The third row of presents the contour plots of the output generated by the inverse model (10) based on the data up to 15, 30, and 90 sec. As seen in the first and second rows of Figure 9, the sensor located to the west of the source first picks up signal. Hence, at times 15 and 30 sec, the peaks indicated by the contour plot are somewhere between that sensor and the actual source. As more data become available

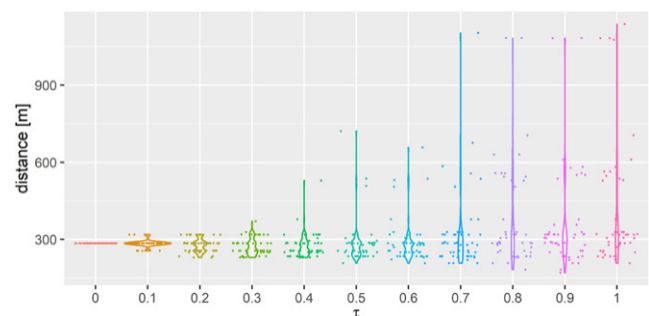


Figure 10. Sensitivity analysis against the misspecification of input velocity vector.

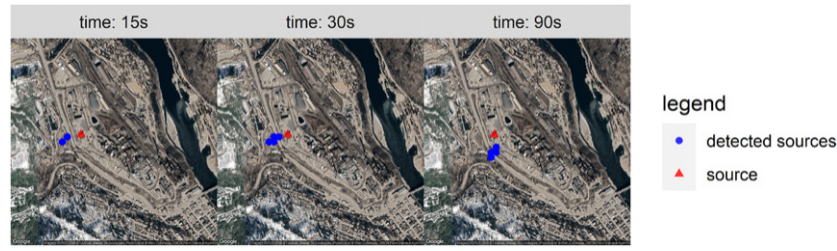


Figure 11. Sensitivity analysis of the detected sources, at times 15, 30, and 90 sec, for combinations of λ_1 and λ_2 taken from a mesh grid $\{5, 10, 15, \dots, 50\} \times \{5, 10, 15, \dots, 50\}$.

from the other sensors located near the source (shown in the second row of Figure 9), the peak moves closer to the actual source at time 90, accurately pinpointing the source of emission.

- **Sensitivity analysis.** The accuracy of the input velocity, that is, \mathbf{v} in the advection-diffusion operator A , significantly affects the performance of the inverse model. Imagine that, in the second scenario above, if the specified wind direction is far from the true direction, we no longer expect the model to yield accurate results. Hence, sensitivity analysis is performed to investigate the robustness of the model against the misspecification of the input velocity and the tuning parameters in the regularization, R . Let $\mathbf{p} = (v_x, v_y)^T = (10, -10)^T$ be the actual wind vector [ms^{-1}], and let $\mathbf{p}^{\text{input}} = (v_x + \frac{z^{\text{wind}}}{x}, v_y + \frac{z^{\text{wind}}}{y})^T$ be the input wind vector to the inverse model with random errors, $\frac{z^{\text{wind}}}{x} \sim N(0, |v_x|\tau)$ and $\frac{z^{\text{wind}}}{y} \sim N(0, |v_y|\tau)$, that is, the variance of the error is proportional to the magnitude of the wind vector given a factor τ .

Consider the second scenario above, Figure 10 shows the violin plot of the distance (in meters) between the detected source and the actual source for different values of τ ranging from 0.1 to 1. For each value of τ , the experiment is repeated by 50 times, and a new input wind vector is simulated for each run. It is seen that, the distance between the detected source and the actual source remains within the range from 225m to 380m when $\tau \leq 0.3$. In other words, the model performance appears to be robust when the input wind vector does not significantly deviate away from the actual wind vector. In the context of this problem, since the horizontal and vertical components of the actual wind vector are both 10 m s^{-1} , the standard deviation of the random error associated with input wind vector ranges from 1m to 3m in both the horizontal and vertical directions when $0.1 \leq \tau \leq 0.3$. Such a margin of specification error is reasonable and can be achieved in many applications where both wind speed and directions are observable (Ding et al. 2021). When $\tau \geq 0.4$, we note that the variance of the detection error dramatically increases, indicating a rapid performance deterioration of the inverse model, as expected.

The performance of the model also depends on the choice of the tuning parameters, λ_1 and λ_2 , in the regularization R . Note that, for many forward prediction problems, such as Lasso regression, Ridge regression, Elastic Net, etc., the tuning parameters can be chosen through cross-validation. However, the idea of cross-validation no longer applies to inverse problems because the true source is never known and it is impossible to establish the link between the tuning parameters and detection accuracy. Hence, it is more meaningful to investigate the robustness (sensitivity) of the proposed inverse model against

λ_1 and λ_2 . Figure 11 shows the detected sources, at 15, 30, and 90 sec, for combinations of λ_1 and λ_2 taken from a mesh grid $\{5, 10, 15, \dots, 50\} \times \{5, 10, 15, \dots, 50\}$. The figure shows that the detect sources are robust enough against the choices of the tuning parameters. In other words, the true source can be correctly identified for different combinations of λ_1 and λ_2 chosen from a relatively wide range, which is certainly desirable in practice.

Finally, it is worth noting that if the initial conditions are strictly modeled by delta functions (e.g., “point” sources), the Fourier series of the space-time process does not converge and the proposed approach may generate an oscillatory solution known as the Gibbs phenomenon (Gibbs 1898). Hence, the proposed approach works well if the initial condition is a smooth function, as seen in the numerical examples above. Even if the initial conditions consist of point sources, the model seeks a solution for a little bit later than the time of release when the point sources become smoother functions due to diffusion.

6. Conclusions

Based on a PDE-based statistical model for spatio-temporal data, this article proposed an inverse modeling approach for advection-diffusion processes using data streams generated by three spatial sampling schemes. The article obtained both necessary and sufficient conditions under which the Fourier coefficients of the initial condition of the advection-diffusion process can be uniquely estimated. Detailed iteration steps of the ADMM have been obtained, which solves the inverse problems in a computational efficient manner. The algorithm has also been extended for handling a linear inequality constraint on the model output. Numerical examples have been presented to demonstrate the robustness of the proposed inverse models against input model parameters, and reveal the dynamic nature of the inverse problem based on sensor data streams. Note that, the article considers data arising from a deterministic PDE. One critical future direction is to extend the proposed models for stochastic PDEs, which aim at minimizing the distance between the forward distribution and that of the observations. Computer code is available at <https://github.com/dnncode/inverse-model>.

Supplementary Materials

The supplementary materials provide (i) the proof of Propositions 1 and 2, (ii) derivation of the ADMM Algorithm 1, (iii) ADMM with non-negativity constraint, (iv) discussions on the computational time of Problems P-I, P-II, and P-III, and (v) Numerical comparison on different choices of regularizations.

Acknowledgments

We are grateful to two reviewers, the Associate Editor and the Editor for their constructive comments, which improved the quality of the article.

Funding

This material is based upon work supported by the National Science Foundation under grant no. 2143695.

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