DETECTION AND ESTIMATION OF BIOCHEMICAL SOURCES IN ARBITRARY 2D ENVIRONMENTS

Aleksandar Jeremić

Dept. of Electrical and Computer Engineering McMaster University, Hamilton, Canada

ABSTRACT

We develop algorithms for biochemical detection and estimation in arbitrary two-dimensional (2D) environments using integrated sensor arrays. The development of biochemical sensors techniques has been a subject of considerable research interest in recent years. In this paper we propose statistical algorithms for automatic monitoring of biochemical agents in a realistically shaped 2D environments using multi-sensor measurements. We derive models for the concentration distribution using the diffusion equation and finite element approximations. Using these results we develop parametric statistical models and maximum likelihood estimation algorithm to find the parameters of the biochemical agent. To detect a presence of the source, we develop a generalized likelihood ratio test. We demonstrate the applicability of our techniques through numerical examples. Our results are potentially useful for national security, environmental engineering, food industry, oil industry etc.

1. INTRODUCTION

The possibility of an adversarial biochemical attack is currently considered serious and presents a real danger. Biochemical weapons are inexpensive to produce, yet powerful enough to potentially harm thousands of people. A necessary condition in fighting against such an attack is the development of biochemical sensors which can quickly detect the presence of toxic agents. The sensor design has been a subject of enormous interest and various techniques have been recently proposed (for a detailed list of existing technologies see [1], [2].) However, early and reliable decision making (to minimize the damage) after the toxins are detected requires additional information such as the size of the affected region(s), biochemical spread trends, i.e., direction and speed in which the toxins are moving, etc. The answer to these questions can be given only by appropriate data processing (estimation) algorithms including the source localization. Once the attack has occurred, the source transforms into a biochemical cloud dispersing through the space and the term "source" can be misinterpreted. Estimating the location and time at which the source was introduced into the environment as well as its intensity, enables predicting the dispersion of the toxins in time

Arye Nehorai*

Dept. of Electrical and Computer Engineering The University of Illinois at Chicago

and space, and consequently, taking appropriate countermeasures (decontamination).

In our previous work we presented algorithms for chemical source localization and detection [3]-[7] for various scenarios using regular geometries. However, there is an obvious need for signal processing algorithms which can deal with realistic geometries such as buildings, tunnels, moving sources, etc. In this paper we present signal processing algorithms for biochemical detection and estimation in a realistic 2D environment. We first develop physical models for the transport of the diffused biochemical agents from a point source in an arbitrarily shaped environment using the diffusion equation, which is useful to model various propagation phenomena (toxins, bacteria, species, etc.) In many of these applications estimating the diffusion parameters may be crucial (for example, propagation trends of toxins or bacteria.) The first challenge in estimating the unknown parameters from a diffusion model is obtaining a so-called *inverse model*. We develop an inverse model by applying a finite element (FE) method in which the spatial and temporal derivatives are linearized. Using these results we develop parametric statistical models and derive signal processing algorithms for the biochemical detection and estimation. We demonstrate the applicability of our results through numerical examples. In addition to security, the proposed algorithms are directly applicable to a variety of applications, such as detection and localization of oil leakage, automatic monitoring of air pollution, bio-process monitoring in food industry, etc.

2. PHYSICAL MODELS

We present the physical models for the concentration distribution of biochemical agents emitted from a fixed point source. To simplify the FE meshing, we assume that the problem can be reduced to a 2D Cartesian space, i.e., we consider the diffusion in the (x, y) plane only. We assume a realistic geometry consisting of a rectangular domain with multiple subdomains (of polygonal shapes) being removed from it. Such a scenario represents the most general constructive solid geometry description for 2D problems. We then solve the diffusion equation using an FE method in terms of the biochemical source location, intensity and environment parameters (geometry and diffusivity.)

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2.1. The Diffusion Equation

Let $c(\mathbf{r}, t)$ denote the biochemical agent concentration at a location $\mathbf{r} = (x, y)$ and time t. The transport of biochemical agents follows the well-known diffusion equation [8]

$$\frac{\partial c(\boldsymbol{r},t)}{\partial t} = \operatorname{div}(\kappa \nabla \cdot c(\boldsymbol{r},t)), \qquad (1)$$

where c is the substance concentration in units of kg/m³, and κ is a diffusivity coefficient in units of m²/s. Observe that in equation (1) we omit the effects of wind since it is irrelevant to our FE approach and can be easily included.

To uniquely define the concentration distribution, we also need to specify the boundary and initial conditions. The most important issue of the boundary conditions is the permeability of the boundaries. In practice, the substance cannot be totally reflected by the boundary surface. In [7] the authors demonstrated how to solve one-dimensional equations with permeable surfaces. For simplicity, in the remainder of the paper we will assume that all the boundaries are impermeable i.e., $\nabla c(\mathbf{r}, t) = 0$ for $\mathbf{r} \in \mathcal{G}$ where \mathcal{G} denotes a boundary.

We assume an instantaneous source located at an arbitrary location r_0 . Under this assumption and the above boundary conditions the Green function is uniquely determined. In complex geometries, we can compute the Green function only numerically or approximately using some discretization techniques such as finite difference or finite element methods [8].

2.2. Finite Element Approximation

The finite element approximation consists of two steps. First, we present a geometrically complex domain of the problem as a collection of geometrically simple subdomains called finite elements. Then, the concentration distribution is approximated over each finite element by a set of algebraic polynomials.

In our case, the domain of interest is infinite i.e., the biochemical agents disperse in open space. Observe that equation (1) assumes infinitely fast propagation of biochemical agents i.e., $c(\mathbf{r}, 0+) > 0$ for $|\mathbf{r}| \gg 0$. In practice, the dispersion of the biochemical agents cannot be infinitely fast since the source particles have a finite propagation speed. Therefore, we can reduce our domain to a reasonably large, but finite, area and impose boundary condition $c(\mathbf{r}, t) = 0$ on the border of the domain.

As a first step, we perform a finite element discretization. Let S_i , $i = 1, ..., n_e$ denote subdomains with geometrically regular shapes (triangles). The collection of all subdomains is called a mesh (see Figure 1). For a particular domain, the meshing can be done in advance using any of the existing FE software tools (PDE toolbox MATLAB, Ansoft, FEMLAB, etc.) To achieve better performance we can use a non-uniform mesh (different sizes of triangles) and adaptive remeshing in which the size of the elements is iterated until we reach the desired approximation error.

We then derive the element equations, i.e., interpolate the concentration distribution over the triangles. It can be shown that



Fig. 1. Finite element mesh of the domain after refinement.

a for a particular S_i the concentration distribution is

$$c^{(i)}(\mathbf{r},t) = \sum_{l=1}^{3} c_{l}^{(i)}(t)\psi_{l}^{(i)}(\mathbf{r}), \quad \mathbf{r} \in S_{i}$$
(2)

where $c_l^{(i)}(t)$ denotes the concentration at the *l*th node of the element S_i , and $\psi_l^{(i)}(\mathbf{r})$ are linear interpolation functions for the triangular elements, see [9]. Using the (known) interpolation functions we can compute the spatial derivatives over single subdomains and apply assembly procedures to compute the spatial derivatives over the whole domain.

The time derivatives can be also approximated using various finite difference techniques (forward, backward, or central.) In addition, similar to the *spatial elements* we can use temporal elements and approximate time derivatives using the FE method. As a result we obtain the well-known FE approximation of the transient problems [9]

$$C\dot{\boldsymbol{c}}_{\mathrm{m}}(t) + K\boldsymbol{c}_{\mathrm{m}}(t) = \boldsymbol{f}(\boldsymbol{r}_{0}, t), \qquad (3)$$

where K is so called global "stiffness matrix," C is the "damping matrix," $f(r_0, t)$ is the load vector, $c_m(t)$ is the nodal vector, and r_0 is the location of the source. This terminology comes from strain-stress analysis in which the FE method has been historically often used [10]. The global nodal vector $c_{\rm m}(t)$ represents the concentration distribution at the nodal points. The stiffness matrix is computed by applying spatial derivatives and assembling local matrices $K^{(i)}$ corresponding to subdomains S_i into the global matrix K. Similarly the damping matrix is computed by applying time derivatives to temporal interpolation functions. The load vector $f(r_0, t)$ is computed from the initial conditions and continuous sources. The details of computing the above matrices and vectors can be found in [9]. Before solving (3) we need to incorporate the boundary conditions. The permeability related boundary conditions for a particular element i can be written as $B^{(i)} c^{(i)} = 0$ where $B^{(i)}$ is the spatial gradient of the interpolation functions (flux) defined over subdomain S_i , and $\boldsymbol{c}^{(i)}$ is the nodal vector for the *i*the element. The modified stiffness matrix \overline{K} is then given by

$$K = K + B \tag{4}$$

where B is assembled from $B^{(i)}$ matrices. It can be shown that the solution to (3) is then given by

$$\boldsymbol{c}_{\mathrm{m}}(t) = \mathrm{e}^{-\tilde{K}t} \boldsymbol{f}(\boldsymbol{r}_0, 0).$$
 (5)

The $c(\mathbf{r}, t)$ can then be interpolated using the nodal vectors and the appropriate interpolation functions.

3. SOURCE ESTIMATION AND DETECTION

We describe the measurement model and develop the signal processing algorithms for biochemical detection and estimation.

3.1. Measurement Model

We assume a spatially distributed array of p selective biochemical sensors located at known locations $r_i, i = 1, ..., p$ taking concentration measurements at times $t_j, j = 1, ..., q$ where p and q denote the number of sensors and time samples, respectively. The measurement model for a sensor located at r_i and time t_j is

$$y_{ij} = c(\boldsymbol{r}_i, t_j) + e_{ij}, \tag{6}$$

where e_{ij} is the measurement noise assumed to be zero-mean Gaussian uncorrelated in space and time. The model predicted concentration $c(\mathbf{r}_i, t_j)$ is computed using the FE approximation from Section 2. For example, assuming that at time t = 0 a biochemical agent of intensity μ is released at a location \mathbf{r}_0 we obtain

$$c(\boldsymbol{r}_i, t_j) = \mu \boldsymbol{w}_i^T \mathrm{e}^{-Kt_j} \boldsymbol{f}(\boldsymbol{r}_0, 0), \qquad (7)$$

where w is the interpolation vector. We can further lump the measurements in a vector form

$$\boldsymbol{y} = \mu A \boldsymbol{a}(\boldsymbol{r}_0) + \boldsymbol{e}, \qquad \boldsymbol{a}(\boldsymbol{r}_0) \equiv \boldsymbol{f}(\boldsymbol{r}_0, 0), \qquad (8)$$

where y is a (pq)-dimensional vector whose (q(j-1)+i) component is y_{ij} and similarly for e. The matrix A is a known spatial interpolation matrix defined by the FE approximation. We assume that the time of release can be estimated using the approach presented in [3] and thus, without loss of generality, we can assume that the time of release is set to $t_0 = 0$.

3.2. Parameter Estimation

To estimate the unknown parameters $\boldsymbol{\theta} = [\mu, \boldsymbol{r}_0, \sigma^2]^T$ we use the maximum likelihood (ML) estimator. We first define the likelihood function

$$l(\boldsymbol{y},\boldsymbol{\theta}) = \frac{1}{\sigma^2} [\boldsymbol{y} - \mu A \boldsymbol{a}(\boldsymbol{r}_0)]^T [\boldsymbol{y} - \mu A \boldsymbol{a}(\boldsymbol{r}_0)].$$
(9)

Then the ML estimate of the unknown parameters is given by

$$\hat{\boldsymbol{\theta}} = \arg \max_{\boldsymbol{\theta}} [l(\boldsymbol{y}, \boldsymbol{\theta})].$$
(10)

Solving the above optimization directly would be computationally expensive since it would require computation of the concentration distribution at each iteration step. Therefore, we propose to estimate the source location by searching over a discrete set of points. Let r_i^m , i = 1, ..., n be the locations of mesh points and let $\mathcal{R} = \{r_1^m, \dots, r_n^m\}$. We estimate the parameters using

$$\hat{\boldsymbol{r}}_{0} = \arg \max_{\boldsymbol{r} \in \mathcal{R}} \left\{ [\boldsymbol{y} - \hat{\mu} A \boldsymbol{a}(\boldsymbol{r})]^{T} [\boldsymbol{y} - \hat{\mu} A \boldsymbol{a}(\boldsymbol{r})] \right\},$$
$$\hat{\mu} = \boldsymbol{y}^{T} A \boldsymbol{a}(\hat{\boldsymbol{r}}_{0}) / \|A \boldsymbol{a}(\hat{\boldsymbol{r}}_{0})\|^{2}$$
(11)

Observe that we can compute Aa(r) before the actual detection/estimation and thus significantly reduce the computational time. The variance estimate is then given by

$$\hat{\sigma}^2 = \frac{1}{pq} [\boldsymbol{y} - \hat{\mu} A \boldsymbol{a}(\boldsymbol{r}_0)]^T [\boldsymbol{y} - \hat{\mu} A \boldsymbol{a}(\boldsymbol{r}_0)].$$
(12)

Computing \hat{r}_0 is extremely important for predicting the trends in concentration distribution. For example, in urban environments, densely populated with buildings, it is very likely that the biochemical agents can get "trapped" within certain regions. In that case computing the predicted concentration distribution using \hat{r}_0 is an irreplaceable tool for determining which regions will be affected. In addition, we can use the predicted concentration distribution to optimally select sensor locations with respect to estimation accuracy.

3.3. Source Detection

The detection of the biochemical agents is a binary decision: H_0 :, only the noise is present, and H_1 :, the source is present as well, i.e. the biochemical agents are being released from the unknown location r_0 . We consider the generalized likelihood ratio test (GLRT) which is a commonly used technique for hypothesis testing [11]. This detector is based on the assumption that the solution (5) approximates the physical processes reasonably well.

The GLR test is given by the ratio

$$GLR = \frac{\sup_{\mu \ge 0, \sigma^2 > 0} \{l(\boldsymbol{y}, \boldsymbol{\theta})\}}{\sup_{\mu = 0, \sigma^2 > 0} \{l(\boldsymbol{y}, \boldsymbol{\theta})\}},$$
(13)

where the numerator (denominator) on the r.h.s. corresponds to the likelihood function under H₁ (H₀). The detection decision is then made by comparing the GLR in (13) with a threshold τ : if GLR > τ accept H₁, otherwise H₀. The computation of τ requires knowledge of the probability distribution of GLR under H₀. Due to the nonlinear dependence on r_0 this distribution requires computationally expensive Monte Carlo simulations. Instead we propose to test for the presence of the source at *a priori* known locations, i.e., mesh nodes. We formulate the multiple hypotheses test as (hypothesis H₀ remains unchanged)

$$H_i: \quad \boldsymbol{y} = \mu A \boldsymbol{a}(\boldsymbol{r}_i) + \boldsymbol{e}, \qquad i = 1, \dots n.$$

The problem of the source detection can now be viewed as a classification into one of several multivariate normal populations, see [11]. To classify the measurement y we fist compute the random variables

$$\lambda_{ij} = \left[\boldsymbol{y} - \frac{\mu}{2} A \left(\boldsymbol{a} (\boldsymbol{r}_i + \boldsymbol{r}_j) \right) \right]^T \left[\boldsymbol{y} - \frac{\mu}{2} A \left(\boldsymbol{a} (\boldsymbol{r}_i + \boldsymbol{r}_j) \right) \right]$$
(14)



Fig. 2. Concentration distribution at t = 600s.



Fig. 3. Probability of detection vs. number of time samples.

where $\lambda_{ij} = -\lambda_{ji}$. As a result we obtain n(n + 1)/2 classification functions. The detailed classification algorithm and expressions for performance measures, probabilities of false alarm $P_{\rm fa}$ and detection $P_{\rm d}$ are given in [11].

4. NUMERICAL EXAMPLES

We present numerical examples to demonstrate the applicability of the proposed algorithms. We consider rather general 2D scenario in which the objects have arbitrary shapes (see Figure 1). We define the domain of interest to be square shaped with side length of 500m. The diffusivity coefficient is set to $\kappa = 120m^2/s$. We assume uniformly spaced grid of sensors with 10m distance in the x and y directions. The measurements are taken every 10 seconds.We assume a unit source intensity located at (-5, 0)m with release time $t_0 = 0s$.

In Figure 2 we illustrate the concentration distribution at t = 600s. It is seen that the biochemical agent is mainly contained within the four objects and thus our detection time could be significantly improved by placing the sensors on a non-uniform grid with most of the sensors being located in the space between these objects. In Figure 3 we illustrate the probability of detection (we assume $\sigma = 1 \times 10^{-6} \text{Kg/m}^3$ and $P_{\text{fa}} = 0.05$) as a function of the number of time samples for both uniform and non-uniform grid. In the non-uniform case we placed 10% of the sensors outside of the contaminated area while other 90% are uniformly placed within the area.

5. CONCLUSIONS

We addressed the problem of detecting and estimating biochemical agents in a realistic two-dimensional environments using sensor array measurements. To model the biochemical dispersion we considered 2D diffusion in a domain consisting of an arbitrary 2D constructive solid geometry description. This approach can be easily extended to various scenarios such as urban environment consisting of buildings, complex tunnel structures, etc. We assumed a fixed point source and derived the physical model by solving the diffusion equation using an FE approximation. Using adaptive refinement procedures, we constructed the FE mesh and linearized the spatial and temporal derivatives in the diffusion equation. We used the maximum likelihood method to estimate the unknown parameters and the generalized likelihood ratio test to detect the presence of the biochemical agents. Numerical examples were used to illustrate the applicability of the proposed algorithms.

Future research will extend these techniques to 3D scenarios. We will investigate the possibility of incorporating finite particle speed effects. We will also address the issue of computational complexity and develop sub-optimal algorithms using mesh nodes as potential source locations.

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