

# Spatial Localization of a Pollutant Point Source in Rivers via the Levenberg-Marquardt Algorithm within a Variable Projection Framework

Constance A. Ojwando<sup>1</sup>, Mark Kimathi<sup>2</sup>, John Awino<sup>3</sup>

<sup>1,3</sup>Department of Mathematics and Statistics, The Technical University of Kenya, Nairobi, Kenya

<sup>2</sup>Department of Mathematics and Statistics, Machakos University, Kenya

Corresponding author email: constanceatieno.tuk@gmail.com

**Abstract**—Determining the spatial location of an unknown pollutant point source from downstream concentration observations is an essential, yet challenging, inverse problem in river water-quality management. This paper develops and validates a method for recovering the location of a stationary point source in a river governed by a two-dimensional advection diffusion equation with temporally varying velocity and dispersion coefficients. Using the Green function method, the forward problem is expressed as a Volterra integral equation of the first kind and discretized into a separable non-linear least squares problem in which the source location appears as the non-linear parameter. By using Tikhonov regularization, the variable projection approach implicitly eliminates the linear parameter, which is independently recovered as the source intensity, resulting in a reduced functional that is only reliant on the source coordinates. The non-linear least squares functional is minimized using the Levenberg-Marquardt algorithm, whose damping parameter blends the global convergence of gradient descent with the local efficiency of the Gauss-Newton method and remedies rank deficiency of the Jacobian. The complete iterative scheme is derived from first principles. Numerical experiments on nine upstream source positions demonstrate accurate localization, with longitudinal coordinates recovered to within one part in a thousand. Convergence histories show stabilization within roughly one hundred iterations for all initial guesses tested. The results establish the Levenberg-Marquardt algorithm, embedded in the variable projection framework, as a reliable tool for non-intrusive source localization.

**Keywords**—Advection-diffusion equation: Inverse source problem: Levenberg-Marquardt algorithm: Separable nonlinear least squares: Source localization: Variable projection.

## I. INTRODUCTION

The contamination of rivers by point sources, such as industrial effluents and municipal sewage discharges at discrete locations, threatens human health, aquatic ecosystems, and the sustainable use of water resources. Knowing the precise location of pollution sources enables regulatory agencies to prioritize remediation, allocate limited resources efficiently, and enforce pollution-control regulations. Conventional detection methods, including water sampling, tracer studies, and remote sensing, are often invasive, costly, or limited in spatial and temporal coverage. Inverse modeling offers a non-intrusive and cost-effective alternative that recovers source characteristics directly from measured concentration data.

The inverse source problem is intrinsically ill-posed and, when both the intensity and the location of a source are sought, also non-linear. Prior studies typically assumed constant or spatially varying coefficients. El Badia and Ha-Duong localized a stationary source in an advection-diffusion-reaction equation with constant coefficients by a variational method [6]; Andrlé and El Badia treated moving sources with spatially dependent coefficients using functional-analytic tools [7]; Rap and others combined boundary element methods with sequential quadratic programming to recover both location and intensity [8]. Mazaheri and others formulated source identification as a linear least squares problem and recovered intensity via Tikhonov regularization, recommending extension to variable coefficients [9]. None of these works accounted for the temporal dependence of the velocity and dispersion

coefficients, nor did they exploit the separable structure of the joint intensity-location problem through variable projection.

This paper addresses the localization component of the inverse problem under temporally varying flow parameters. The joint issue is stated as a separable non-linear least squares problem; the source intensity, the linear parameter, is implicitly removed by the variable projection method, leaving a reduced functional that depends solely on the source location, the non-linear parameter. This functional is minimized by the Levenberg-Marquardt algorithm, whose damping parameter overcomes the rank deficiency of the Jacobian that defeats the plain Gauss-Newton method, while interpolating between gradient descent far from the optimum and Gauss-Newton near it.

The paper is organized as follows. Section II states the separable non-linear least squares formulation and variable projection. Section III derives the Gauss-Newton and Levenberg-Marquardt iterations and discusses the role of the damping parameter. Section IV presents identification and convergence results. Section V concludes.

## II. PROBLEM FORMULATION

### A. Forward Model and Integral Representation

The pollutant concentration in a river domain  $\Omega \subset \mathbb{R}^2$  with boundary  $\Gamma = \Gamma_{in} \cup \Gamma_L \cup \Gamma_{out}$ , shown schematically in Figure 1, obeys the two-dimensional advection-diffusion equation

$$\frac{\partial c}{\partial t} - \nabla \cdot (D^0 f^1(mt) \nabla c) + \nabla \cdot (V^0 f^2(mt) c) = \lambda(t) \delta(r - S), \quad (1)$$

where  $V_0$  and  $D_0$  are the initial velocity and dispersion coefficients,  $f_i(mt)$  encode the temporal dependence,  $S = (S_x, S_y)$  is the unknown source location, and  $\lambda(t)$  the source intensity. Equation (1) is solved with the homogeneous initial condition  $c(r,0) = 0$ , the inflow Dirichlet condition  $c = C_0$  on  $\Gamma_{in}$ , and homogeneous Neumann conditions on  $\Gamma_L \cup \Gamma_{out}$ .

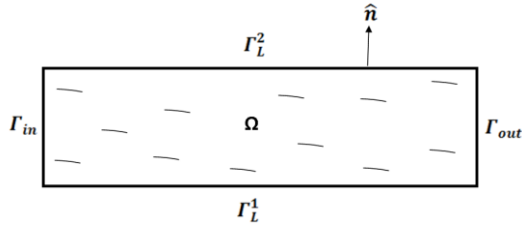


Fig. 1. The rectangular river domain  $\Omega$  with boundary  $\Gamma = \Gamma_{in} \cup \Gamma_L \cup \Gamma_{out}$ , where  $\Gamma_{in}$  is the inflow boundary,  $\Gamma_{out}$  the outflow boundary, and  $\Gamma_L = \Gamma_L^1 \cup \Gamma_L^2$  the lower and upper lateral boundaries;  $\hat{n}$  is the outward unit normal.

Applying the Green function method yields the Volterra integral equation of the first kind

$$c(r_j) = \int_0^{t_0^+} \lambda(\tau) \bar{G}[r, t; \vec{S}, \tau] d\tau \quad (2)$$

with the Green function

$$G(r, t; S, \tau^*) = \left( -\frac{4}{l \cdot h \cdot f(t)} \right) \sum_n \Psi_n^2(S) \exp[(\alpha + D^0 \Lambda_n)(\tau^* - t)], \quad (3)$$

where  $\Psi_n(\varepsilon, \eta) = \sin(\mu \varepsilon) \sin(\nu \eta)$ ,  $\Lambda_{mn} = \mu m^2 + \nu n^2$ , and  $\alpha = (u_0^2 + v_0^2)/(4D_0)$ . The dependence of  $G$  on  $S$  through  $\Psi_n^2(S)$  is what makes the localization problem non-linear.

### B. Separable Non-Linear Least Squares and Variable Projection

Discretizing (2) by Gauss-Legendre quadrature at observation points  $r_1, \dots, r_m$  gives, in matrix form,

$$c = G(S) \lambda, \quad (4)$$

a separable non-linear least squares problem with linear parameter  $\lambda$  and non-linear parameter  $S$ . The least squares estimate solves

$$(\hat{\lambda}, S) = \min \|G(S)\hat{\lambda} - c\|_2^2. \quad (5)$$

The variable projection method tends to converge in fewer iterations than the original joint minimization. Rather than separating the parameters explicitly, it implicitly eliminates the linear parameter: for fixed  $S$ ,

$$\hat{\lambda} = G(S)^\dagger c, \quad (6)$$

reducing (5) to the projected functional in  $S$  alone,

$$\min_s \rho(S) = \min_s \|G(S)\hat{\lambda} - c\|_2^2, \quad (7)$$

where  $\hat{\lambda}$  solves the linear sub-problem. The linear parameter is computed by Tikhonov regularization with generalized cross-validation, giving the filtered solution

$$\hat{\lambda} \alpha = \sum_i F_i (p_i^T c / \sigma_i) v_i, F_i = \sigma_i^2 / (\sigma_i^2 + \alpha^2). \quad (8)$$

with  $\hat{\lambda} \alpha$  available, the source location is obtained from

$$S = \min_s \frac{1}{2} \|G(S)\hat{\lambda} \alpha - c\|_2^2, \quad (9)$$

the non-linear least squares problem to which the Levenberg-Marquardt algorithm is applied.

## III. THE LEVENBERG-MARQUARDT ALGORITHM

### A. Gauss-Newton Iteration

Write the residual  $r(S) = G(S)\hat{\lambda} \alpha - c$ , so that

$$\rho(S) = \frac{1}{2} \|r(S)\|_2^2 = \frac{1}{2} r(S)^T r(S) = \frac{1}{2} \sum_i [r_i(S)]^2. \quad (10)$$

The gradient and the Gauss-Newton approximation of the Hessian are

$$\partial \rho / \partial S = J(S)^T r(S), \quad (11)$$

$$\partial^2 \rho / \partial S^2 \approx J(S)^T J(S), \quad (12)$$

where  $J(S) = \partial r_i / \partial S_j$  is the Jacobian, and the second-order term is dropped to obtain the Gauss-Newton method. Expanding  $\rho$  in a Taylor series about  $S_k$  and setting the derivative to zero yields the normal equations

$$J^T(S_k) r(S_k) + (S - S_k) J^T(S_k) J(S_k) = 0, \quad (13)$$

giving the Gauss-Newton update

$$S_{k+1} = S_k + dk, dk = -[J^T k J k]^{-1} J^T k r k. \quad (14)$$

The Gauss-Newton method avoids second-order derivatives and provides a descent direction provided the Jacobian has full column rank; it fails when  $J$  is rank-deficient, that is, has linearly dependent columns.

### B. Levenberg-Marquardt Modification

To remedy rank deficiency, Levenberg and Marquardt modify the search direction by adding a damping term  $\mu k$  to  $J^T J$ ,  $dk = -[J^T(S_k) J(S_k) + \mu k I]^{-1} J^T(S_k) r(S_k)$ , yielding the iterative scheme

$$S_{k+1} = S_k - [J^T k J k + \mu k I]^{-1} J^T k r k, k = 1, 2, \dots \quad (16)$$

The damping parameter  $\mu k$  has three principal effects. First, for all  $\mu > 0$  the coefficient matrix is positive definite, guaranteeing that  $dk$  is a descent direction. Second, for large  $\mu$  the step approaches  $dk \approx -\mu^{-1} r'(S)$ , a short step in the steepest-descent direction, appropriate when the current iterate is far from the solution. Third, for small  $\mu$  the scheme reduces to Gauss-Newton, giving fast quadratic-like convergence in the final iterations. Thus  $\mu k$  influences both the direction and the size of the step, so no separate line search is required. The Levenberg-Marquardt method behaves like gradient descent when parameters are far from optimal and like Gauss-Newton when they are close.

The complete identification procedure is as follows. Given the observations  $c$ , an initial guess  $S_0$ , a tolerance  $\varepsilon = 10^{-4}$ , and a maximum of  $K = 400$  iterations, the matrix  $G(S_k)$  is assembled from the Green function (3); the linear sub-problem is solved for  $\hat{\lambda} \alpha$  by Tikhonov regularization with generalized cross-validation (8); the residual  $r(S_k) = G(S_k)\hat{\lambda} \alpha - c$  and Jacobian  $J(S_k)$  are formed; the step  $dk$  is computed from (15) and the update  $S_{k+1} = S_k + dk$  applied; the damping  $\mu k$  is decreased if  $\rho$  decreases and increased otherwise; and the loop terminates when  $|dk| < \varepsilon$  or  $k \geq K$ , returning the identified source location  $S_k$ .

## IV. NUMERICAL RESULTS AND DISCUSSION

### A. Setup

The Levenberg-Marquardt algorithm (16) was applied with a maximum of 400 iterations and tolerance  $\varepsilon = 10^{-4}$ . Upstream source locations were used to generate the synthetic observations, a choice consistent with the zero concentration-gradient Neumann condition imposed at the outflow boundary. The velocity and dispersion coefficients increase exponentially with time,  $f_i(mt) = e^{mt}$  with  $m = 0.1$ , and the source intensity follows the Gaussian-sum profile  $\lambda(t) = \sum_i b_i e^{-u_i(t-q_i)^2}$ .

**B. Source Identification**

Table 1 lists nine used source locations together with the locations identified by the Levenberg-Marquardt algorithm.

TABLE 1. Used Versus Identified Source Locations

#	Used ( $S_x, S_y$ )	Identified ( $\hat{S}_x, \hat{S}_y$ )
1	(0.2500, 0.0069)	(0.2500, 0.0061)
2	(0.3000, 0.0069)	(0.3009, 0.0022)
3	(0.3500, 0.0069)	(0.3501, 0.0031)
4	(0.2500, 0.0241)	(0.2491, 0.0079)
5	(0.3000, 0.0241)	(0.2995, 0.0079)
6	(0.3500, 0.0241)	(0.3498, 0.0158)
7	(0.2500, 0.0414)	(0.2475, 0.0199)
8	(0.3000, 0.0414)	(0.3002, 0.0433)
9	(0.3500, 0.0414)	(0.3484, 0.0083)

The longitudinal coordinate  $S_x$  is recovered with excellent accuracy across all nine cases, typically to within one part in a thousand; for example, case 3 used 0.3500 and identified 0.3501, and case 5 used 0.3000 and identified 0.2995. The transverse coordinate  $S_y$  is recovered with somewhat larger discrepancies. The residual errors are attributable to errors carried forward from the concentration and Green function data used to assemble G. The established identification method localizes sources accurately, especially for sources situated upstream.

Once a source has been localized, the corresponding intensity recovered by Tikhonov regularization can be compared with the assumed profile. Figure 2 shows this comparison at the nine source locations, with the root-mean-square error (RMSE) reported for each case; the simulated intensity tracks the assumed intensity closely, the smallest error occurring for the most downstream transverse position.

**C. Convergence Behavior**

Table 2 traces the iteration history for three representative starting locations over one hundred iterations.

TABLE 2. Convergence of the Levenberg-Marquardt Iteration for Three Initial Locations

Iter.	(0.2500,0.0069)	(0.3000,0.0241)	(0.3500,0.0414)
1	(0.3329,0.3645)	(0.3577,0.3047)	(0.3500,0.0414)
2	(0.2503,0.0186)	(0.3040,0.0747)	(0.3500,0.0414)
3	(0.2501,0.0106)	(0.3005,0.0334)	(0.3733,0.2368)
4	(0.2501,0.0101)	(0.2999,0.0224)	(0.3546,0.0957)
⋮	⋮	⋮	⋮
97	(0.2500,0.0063)	(0.2995,0.0080)	(0.3484,0.0084)
98	(0.2500,0.0062)	(0.2995,0.0080)	(0.3484,0.0084)
99	(0.2500,0.0061)	(0.2995,0.0079)	(0.3484,0.0083)
100	(0.2500,0.0061)	(0.2995,0.0079)	(0.3484,0.0083)

All three trajectories stabilize by iteration 97, after which their values are essentially constant. The first set, starting at (0.2500, 0.0069), converges quickly to (0.2500, 0.0061), indicating early stabilization. The second, (0.3000, 0.0241), converges more slowly to (0.2995, 0.0079). The third, (0.3500, 0.0414), exhibits larger initial excursions before settling at (0.3484, 0.0083). The differences in convergence speed reflect the Levenberg-Marquardt mechanism: smaller steps are taken when the iterate is far from the optimum and larger steps as it approaches, with convergence speed depending on proximity of the initial guess to the true location.

**D. Discussion**

The results confirm three desirable properties of the combined Levenberg-Marquardt and variable projection approach. First, by damping the Gauss-Newton step, the algorithm remains well-defined even where the Jacobian is rank-deficient, as guaranteed by the positive definiteness of  $J^T J + \mu I$ . Second, the variable projection structure means that each Levenberg-Marquardt iteration solves only the low-dimensional non-linear problem in S, with the linear intensity recovered stably by Tikhonov regularization, reducing the effective dimensionality and improving robustness. Third, the upstream placement assumption is consistent with the Neumann outflow condition and yields the most accurate longitudinal localization. The transverse errors, larger in magnitude, indicate that observation networks should be designed to better resolve cross-channel position, a direction for future sensor-placement studies.

**V. CONCLUSION**

A method for non-intrusive localization of a stationary pollutant point source in a river with temporally varying flow parameters has been presented and validated. The forward advection-diffusion model was expressed as a Volterra integral equation via the Green function method and discretized into a separable non-linear least squares problem. Variable projection eliminated the linear intensity parameter, leaving a reduced functional in the source coordinates that was minimized by the Levenberg-Marquardt algorithm. The damping parameter was shown to guarantee descent directions, interpolate between gradient descent and Gauss-Newton, and overcome Jacobian rank deficiency. For all starting hypotheses evaluated, the

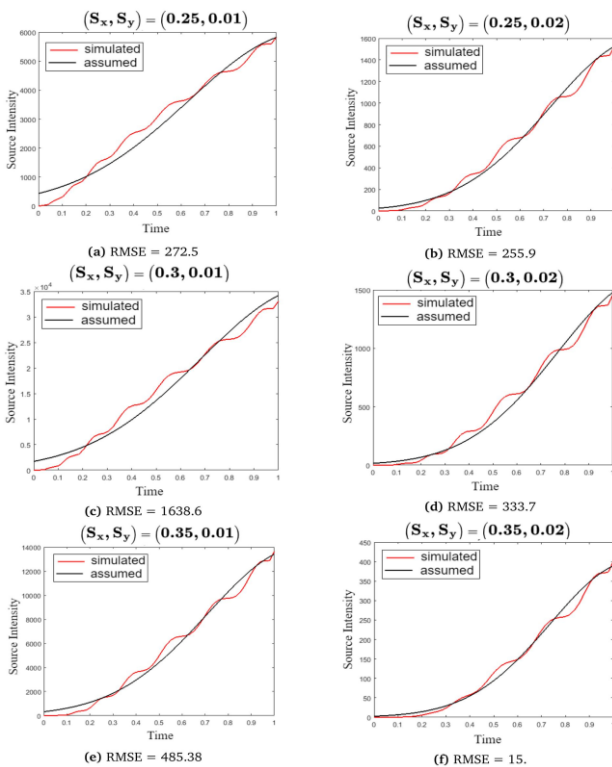


Fig. 2. Simulated versus assumed source intensity, with RMSE, for the nine source locations ( $S_x, S_y$ ) of Table 1.

method converged in approximately one hundred iterations and recovered the longitudinal coordinate to within one part in a thousand across nine upstream source locations. The method offers a robust, efficient route to source localization for water-quality monitoring. Future work will incorporate field concentration measurements, optimize observation-point placement to improve transverse localization, and extend the approach to curved meandering domains and reactive pollutants.

#### ACKNOWLEDGMENT

The authors thank the Department of Mathematics and Statistics, The Technical University of Kenya, and dedicate this work to the memory of the late Prof. Thomas Onyango.

#### REFERENCES

- [1] K. Levenberg, "A method for the solution of certain non-linear problems in least squares," *Quarterly of Applied Mathematics*, vol. 2, no. 2, pp. 164–168, 1944.
- [2] D. W. Marquardt, "An algorithm for least-squares estimation of nonlinear parameters," *SIAM Journal on Applied Mathematics*, vol. 11, no. 2, pp. 431–441, 1963.
- [3] K. Madsen, H. B. Nielsen, and O. Tingleff, *Methods for Non-Linear Least Squares Problems*, 2nd ed. Lyngby, Denmark: Technical University of Denmark, 2004.
- [4] G. H. Golub and V. Pereyra, "The differentiation of pseudo-inverses and nonlinear least squares problems whose variables separate," *SIAM Journal on Numerical Analysis*, vol. 10, no. 2, pp. 413–432, 1973.
- [5] J. Chung and J. G. Nagy, "An efficient iterative approach for large-scale separable nonlinear inverse problems," *SIAM Journal on Scientific Computing*, vol. 31, no. 6, pp. 4654–4674, 2010.
- [6] A. El Badia and T. Ha-Duong, "Identification of a point source in a linear advection-dispersion-reaction equation," *Inverse Problems*, vol. 21, no. 3, pp. 1121–1136, 2005.
- [7] M. Andrie and A. El Badia, "Identification of moving pointwise sources in an advection-dispersion-reaction equation," *Inverse Problems*, vol. 27, no. 2, p. 025007, 2011.
- [8] A. Rap, L. Elliott, and D. B. Ingham, "An inverse source problem for the convection-diffusion equation," *International Journal of Numerical Methods for Heat and Fluid Flow*, vol. 17, no. 6, pp. 547–565, 2007.
- [9] M. Mazaheri, J. M. V. Samani, and H. M. V. Samani, "Mathematical model for pollution source identification in rivers," *Environmental Forensics*, vol. 16, no. 4, pp. 310–321, 2015.
- [10] S. Shan, "Levenberg-Marquardt method for nonlinear least squares," M.S. thesis, Department of Mathematics, University of Tennessee, Knoxville, TN, 2008.
- [11] K. K. Lai, S. K. Mishra, and B. Ram, "On solving nonlinear least squares problems," *Journal of Computational and Applied Mathematics*, vol. 320, pp. 1–12, 2017.
- [12] R. C. Aster, B. Borchers, and C. H. Thurber, *Parameter Estimation and Inverse Problems*, 3rd ed. Amsterdam, Netherlands: Elsevier, 2018.