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Non-Intrusive Estimation of a Time-Dependent Pollutant Source Intensity in Rivers Using a Variable Projection–Tikhonov Regularization Framework

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Abstract: **The identification of pollutant source characteristics from downstream concentration measurements is an inverse source problem of central importance for non-intrusive water-quality monitoring. This paper presents a mathematical framework for estimating the time-dependent intensity of an unknown point source in a river governed by an advection–diffusion equation (ADE) with temporally varying velocity and dispersion coefficients. The forward problem is recast in integral form using Green's function method, yielding a linear Volterra integral equation of the first kind which, upon discretization by Gauss–Legendre quadrature, reduces to a separable non-linear least squares (SNLLS) problem in a linear parameter (the source intensity) and a non-linear parameter (the source location). The variable projection (VP) method is employed to implicitly eliminate the linear parameter. The resulting linear sub-problem is severely ill-conditioned (condition number $\kappa(\mathcal{G}) \gg 10^4$), and is stabilized by Tikhonov regularization, with the regularization parameter selected via Generalized Cross-Validation (GCV). Convergence and stability of the regularized solution are established theoretically. Numerical experiments over nine candidate source positions show that the reconstructed intensity grows exponentially in time and that the root-mean-square error (RMSE) between assumed and recovered intensities is consistently low, reaching values as small as 0.4. The results confirm that Tikhonov regularization, coupled with VP and GCV, provides an accurate and stable means of recovering source intensity for non-intrusive pollution monitoring.**

Keywords: **Inverse source problem, Tikhonov regularization, Variable projection, Generalized cross-validation, Advection–diffusion equation, Water pollution.**

1. INTRODUCTION

Water pollution caused by anthropogenic activities such as industrialization, urbanization, and poor waste management constitutes a pressing environmental concern, particularly in developing countries. While the total quantity of water on Earth remains constant, its quality changes in time and space, with rivers acting as major recipients of heavy metals, pathogens, and nutrient-rich waste. Pollutants enter water bodies either from point sources, such as industrial effluents and municipal sewage treatment plants discharging at discrete locations, or from diffuse (non-point) sources distributed over a range of river extent. Identifying point sources, in particular, is essential for effective mitigation: knowing the precise intensity and location of pollution sources allows regulatory agencies to prioritize efforts and allocate limited resources efficiently.

A range of techniques have been used to characterize pollutant sources, including water sampling and analysis, tracer studies, hydrodynamic and water-quality modeling, and remote sensing combined with Geographic Information System (GIS) analysis. Each suffers limitations in spatial and temporal coverage, cost, complexity, or accuracy. Among the alternatives, mathematical modeling combined with inverse techniques is especially promising for pinpointing the location of point sources and quantifying their pollutant loading at a fraction of the cost of full-scale experimental investigation.

Inverse modeling is the estimation of unknown parameters in a model from a set of observed data. When the unknown is the source term, the problem is an inverse source problem. Such problems are characteristically ill-posed: the analytical solution is highly sensitive to the manner in which data are acquired and to the errors they contain, so that any perturbation in the input acts as a perturbation that can produce arbitrarily large variations in the recovered solution. Stability is restored by incorporating additional information that restricts the class of admissible solutions; the deterministic version of this idea is regularization, in which a parameter handling noise in an optimal fashion produces stable solutions, provided the regularization parameter is chosen successfully.

Earlier studies on pollution source identification predominantly assumed constant or spatially varying dispersion and velocity coefficients. El Badia and Ha-Duong identified a stationary point source in a one-dimensional advection–diffusion–reaction equation (ADRE) with constant coefficients using a variational method without iteration. Hamdi treated spatially varying coefficients and transformed the problem into a generalized Sturm–Liouville eigenvalue problem. Rap et al. combined the dual reciprocity boundary element method with a sequential quadratic programming procedure to recover both location and intensity. Mazaheri et al. used an ADE with constant velocity and diffusion coefficients, formulated the inverse problem as a linear least squares problem, and applied Tikhonov regularization to estimate the source intensity, recommending the extension to variable coefficients. None of these studies accounted for the temporal dependence of the flow parameters.

The present work addresses this gap by considering an ADE with temporally varying velocity and dispersion coefficients, and by formulating the source-identification problem as a separable non-linear least squares problem solved via the variable projection method. This paper focuses on the first stage of the identification process: recovery of the time-dependent source intensity (the linear parameter) using Tikhonov regularization with the regularization parameter selected by Generalized Cross-Validation. The companion problem of source localization (the non-linear parameter) is treated separately.

The remainder of this paper is organized as follows. Section 2 formulates the forward model and its Green's function integral representation. Section 3 introduces the SNLLS formulation and the variable projection method. Section 4 develops the Tikhonov regularization framework, the SVD analysis, and the GCV parameter-choice rule, and establishes convergence and stability. Section 5 presents numerical results. Section 6 concludes.

2. FORWARD MODEL AND GREEN'S FUNCTION REPRESENTATION

2.1 Governing equation

We consider a river occupying a bounded, open, connected domain $\Omega \subset \mathbb{R}^2$ with sufficiently smooth boundary $\Gamma = \partial\Omega = \Gamma_{in} \cup \Gamma_L \cup \Gamma_{out}$, where Γ_{in}, Γ_{out}, and Γ_L denote the inflow, outflow, and lateral boundaries respectively. The transport of a conservative pollutant is described by the two-dimensional advection–diffusion equation

$$\frac{\partial c(\vec{r},t)}{\partial t} - \nabla \cdot (\vec{D}_0 f_1(mt)\ \nabla c(\vec{r},t)) + \nabla \cdot (\vec{V}_0 f_2(mt)\ c(\vec{r},t)) = Q(\vec{r},t), \tag{1}$$

where $c(\vec{r},t)$ $[M/L^3]$ is the pollutant concentration at position $\vec{r} = (x,y)$ and time t, $\vec{V}_0 = (u_0, v_0)$ $[L/T]$ and $\vec{D}_0 = (D_{x_0}, D_{y_0})$ $[L^2/T]$ are the initial velocity and dispersion coefficients, $f_i(mt)$ $(i = 1,2)$ describe the temporal dependence of the coefficients, and m is an unsteadiness parameter with dimension of inverse time. The source term for a single stationary point source with time-dependent intensity is

$$Q(\vec{r},t) = \lambda(t)\ \ \delta(\vec{r} - \vec{S}), \tag{2}$$

where $\vec{S}$ is the source location and $\lambda(t)$ is the time-dependent intensity. Equation (1) is solved subject to

$$c(\vec{r},0) = 0 \qquad \text{in}\Omega, \tag{3}$$

$$c(\vec{r},t) = C_0 \qquad \text{on}\Gamma_{in} \times (0,t), \tag{4}$$

$$\nabla c(\vec{r},t) = 0 \qquad \text{on}(\Gamma_L \cup \Gamma_{out}) \times (0,t). \tag{5}$$

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2.2 Uniqueness of the weak solution

The forward problem possesses a unique weak solution.

Theorem 1 *The solution of the ADE (1) subject to the initial condition (3) is unique.*

Sketch. Write (1) as $\partial_t c + P[c] = Q$ with the second-order linear operator $P = -\vec{D}_0 f_1(mt)\nabla^2 + \vec{V}_0 f_2(mt)\nabla$, where the coefficients lie in $L^\infty(\Omega)$ and $Q \in L^2$. Multiplying by a test function $q \in H_0^1$ and integrating over Ω yields the weak form $\langle c_t, q\rangle_{L^2} + M[c, q; t] = \langle Q, q\rangle_{L^2}$, $0 \le t \le T$, with $M[\cdot,\cdot; t]$ the time-dependent bilinear form associated with P. Taking $q = c$ and $Q = 0$ gives $\frac{1}{2}\frac{d}{dt} \parallel c \parallel_{L^2}^2 + M[c, c; t] = 0$. Since the coefficients are uniformly bounded in time, the coercivity estimate $M[c, c; t] \ge \beta \parallel c \parallel_{H_0^1}^2 - \gamma \parallel c \parallel_{L^2}^2$ holds for constants $\beta, \gamma \ge 0$, whence $\frac{1}{2}\frac{d}{dt} \parallel c \parallel_{L^2}^2 \le \gamma \parallel c \parallel_{L^2}^2$. Gronwall's inequality with $\parallel c(0) \parallel_{L^2} = 0$ from (3) forces $\parallel c(t) \parallel_{L^2} = 0$ for all $t \ge 0$, i.e. $c \equiv 0$. Linearity then yields uniqueness.

2.3 Integral representation via Green's function

Introducing the time transformation $T(t) = \int_0^t f(m\tau)\ d\tau$ converts (1) into an ADE with constant coefficients in the new time variable. Applying Green's function method (with the adjoint operator $\mathcal{L}^* = -\partial_T - \vec{V}_0 \cdot \nabla - \vec{D}_0 \nabla^2$), together with the homogeneous initial and boundary conditions (3)–(5) and the causality principle, the concentration at a downstream point reduces to a convolution against the source intensity. For a k-th source located at $\vec{S}$,

$$c(\vec{r}, t) = \int_0^{t_{0^+}} \frac{\lambda(\tau)}{f(\tau)}\ G[\vec{S}, \tau;\ \vec{r}, t]\ d\tau, \qquad 0 \le \tau \le t_{0^+} \le \infty, \tag{6}$$

which is a linear Volterra integral equation of the first kind for the unknown intensity λ. The Green's function, obtained by eigenfunction expansion after elimination of the advection term, is

$$G(\vec{r}, t; \vec{S}, \tau^*) = \frac{-4}{l\ \ h\ \ f(t)} \sum_{n=1}^{\infty} \{\Psi_n^2(\vec{S}) \exp[(\alpha + D_0 \Lambda_n)(\tau^* - t)]\}, \tag{7}$$

with eigenfunctions $\Psi_n(\varepsilon, \eta) = \sin(\mu_m \varepsilon)\sin(\nu_n \eta)$, eigenvalues $\Lambda_{mn} = \mu_m^2 + \nu_n^2$, and $\alpha = \frac{1}{4D_0}(u_0^2 + v_0^2)$. Here l and h denote the longitudinal and transverse extents of the domain.

3. SEPARABLE NON-LINEAR LEAST SQUARES AND VARIABLE PROJECTION

3.1 Discretization

Equation (6) is discretized by Gauss–Legendre quadrature, which yields very high-order accuracy for few points and is numerically stable because all quadrature nodes lie inside the integration interval and all weights are positive. Assuming concentration data are available at finite points $r_1, \ldots, r_m$ at a later time t_{0^+}, a linear mapping $\tau = \frac{t_{0^+}}{2}(\tau' + 1)$ sends $[0, t_{0^+}]$ to $[-1, 1]$ and gives

$$c_j = \sum_{k=1}^{n} \lambda_k^*\ \ w_k^*\ \ \bar{G}_k^*(r_j, t_{0^+}; \vec{S}), \qquad j = 1, \ldots, m, \tag{8}$$

where $w_k^* = \frac{t_{0^+}}{2} w_k$, $\lambda_k^* = \lambda[\frac{t_{0^+}}{2}(\tau'_k + 1)]$, and $\bar{G}_k^* = \frac{1}{f(\tau)} G$. In matrix form,

$$\mathbf{c} = \mathcal{G}(\vec{S})\ \ \boldsymbol{\lambda}, \tag{9}$$

with $\mathbf{c} = [c_1, \ldots, c_m]^T$ and $\boldsymbol{\lambda} = [\lambda_1^*, \ldots, \lambda_n^*]^T$. This is a separable non-linear least squares problem: $\bar{G}_k^*(\vec{S})$ and c_j are known, while $\boldsymbol{\lambda}$ (linear) and $\vec{S}$ (non-linear) are to be estimated.

3.2 Variable projection

Since the elements of $\mathbf{c}$ are computed numerically, the system is generally inconsistent; the least squares estimate solves

$$(\hat{\boldsymbol{\lambda}}, \vec{S}) = \min_{\lambda, \vec{S}} \parallel \mathcal{G}(\vec{S})\ \ \hat{\boldsymbol{\lambda}} - \mathbf{c} \parallel_2^2. \tag{10}$$

The variable projection method exploits separability: rather than separating the parameters explicitly, it implicitly eliminates the linear parameter. For fixed $\vec{S}$,

$$\hat{\boldsymbol{\lambda}} = \mathcal{G}(\vec{S})^{\dagger} \ \mathbf{c}, \tag{11}$$

where $\mathcal{G}(\vec{S})^{\dagger}$ is the pseudo-inverse, reducing (10) to the projected non-linear functional

$$\min_{\vec{S}} \| [\mathcal{G}(\vec{S})\mathcal{G}(\vec{S})^{\dagger} - I]\mathbf{c} \|_2^2. \tag{12}$$

The present article concentrates on the linear sub-problem (11), which determines the source intensity once $\vec{S}$ is fixed.

4. TIKHONOV REGULARIZATION OF THE LINEAR SUB-PROBLEM

4.1 Ill-posedness

The least squares solution minimizing $\| \mathcal{G}\hat{\boldsymbol{\lambda}} - \mathbf{c} \|_2^2$ satisfies the normal equations

$$\mathcal{G}^T\mathcal{G} \ \ \boldsymbol{\lambda} = \mathcal{G}^T\mathbf{c} \qquad \Longrightarrow \qquad \hat{\boldsymbol{\lambda}} = (\mathcal{G}^T\mathcal{G})^{-1}\mathcal{G}^T\mathbf{c} = \mathcal{G}^{\dagger}\mathbf{c}. \tag{13}$$

In practice only noisy data $\mathbf{c}^{\delta} = \mathbf{c} + \delta$ are available, giving $\hat{\boldsymbol{\lambda}}^{\delta} = \mathcal{G}^{\dagger}\mathbf{c}^{\delta}$. The ill-posedness is governed by the condition number $\kappa(\mathcal{G})$, the ratio of the largest to smallest singular value; values $\kappa(\mathcal{G}) > 10^4$ indicate ill-conditioning. In the present problem $\kappa(\mathcal{G}) \gg 10^4$, so $\mathcal{G}$ is severely ill-conditioned.

The singular value decomposition (SVD) $\mathcal{G} = PBV^T$ expresses the noisy solution as

$$\hat{\boldsymbol{\lambda}}^{\delta} = \sum_{i=1}^{r} \frac{p_i^T\mathbf{c}^{\delta}}{\sigma_i} \ \ v_i = \hat{\boldsymbol{\lambda}} + \sum_{i=1}^{r} \frac{p_i^T\delta}{\sigma_i} \ \ v_i, \tag{14}$$

where $\sigma_1 \geq \cdots \geq \sigma_r > 0$. Because the small singular values decay gradually toward zero and their associated right singular vectors are increasingly oscillatory, division by small σ_i amplifies high-frequency noise components, rendering the naive inverse useless.

4.2 Regularized solution

Following Hadamard, a problem is ill-posed if existence, uniqueness, or stability fails; the stability deficiency is remedied by regularization, the approximation of an ill-posed problem by a family of neighboring well-posed problems through a regularized operator R_{α}, $\alpha > 0$. Tikhonov regularization adds a stabilizing penalty to the residual:

$$\hat{\boldsymbol{\lambda}}_{\alpha} = \min_{\hat{\boldsymbol{\lambda}}} J_{\alpha}[\hat{\boldsymbol{\lambda}}] = \min_{\hat{\boldsymbol{\lambda}}}(\| \mathcal{G}\hat{\boldsymbol{\lambda}} - \mathbf{c} \|_2^2 + \alpha^2 \| \hat{\boldsymbol{\lambda}} \|_2^2). \tag{15}$$

The minimizer satisfies the modified normal equations

$$(\mathcal{G}^T\mathcal{G} + \alpha^2 I) \ \ \hat{\boldsymbol{\lambda}}_{\alpha}^{\delta} = \mathcal{G}^T\mathbf{c}^{\delta}, \tag{16}$$

so that the Tikhonov regularization operator is $R_{\alpha} = (\mathcal{G}^T\mathcal{G} + \alpha^2 I)^{-1}$. Adding the diagonal perturbation $\alpha^2 I$ converts the singular matrix $\mathcal{G}^T\mathcal{G}$ into the invertible $\mathcal{G}^T\mathcal{G} + \alpha^2 I$.

Theorem 2 *Let $\mathcal{G}: X \to Y$ be a compact linear operator. Then $\mathcal{G}^T\mathcal{G} + \alpha^2 I$ has a bounded inverse, and $\hat{\boldsymbol{\lambda}}_{\alpha}^{\delta} = (\mathcal{G}^T\mathcal{G} + \alpha^2 I)^{-1}\mathcal{G}^T\boldsymbol{c}^{\delta}$ is the unique minimizer of the Tikhonov functional J_{α}.*

In terms of the SVD, the regularized solution reads

$$\hat{\boldsymbol{\lambda}}_{\alpha} = \sum_{i=1}^{r} F_i \ \frac{p_i^T\mathbf{c}}{\sigma_i} \ \ v_i, \qquad\qquad F_i = \frac{\sigma_i^2}{\sigma_i^2 + \alpha^2}, \tag{17}$$

where the F_i are the Tikhonov filter factors: contributions from singular values large relative to α are retained essentially unchanged, while those from small singular values are damped, thereby suppressing amplified noise.

4.3 Convergence and stability

Theorem 3 (Convergence) *Let $\{R_{\alpha}\}_{\alpha>0}$ be a family of continuous functions on L^2 with $lim_{\alpha\to 0}R_{\alpha} = (\mathcal{G}^T\mathcal{G})^{-1}$. If $\boldsymbol{c} \in D(\mathcal{G}^{\dagger})$, $\alpha(\delta) \to 0$, and $\delta^2 r(\alpha(\delta)) \to 0$ as $\delta \to 0$, then $lim_{\delta\to 0}\hat{\boldsymbol{\lambda}}_{\alpha(\delta)}^{\delta} = \hat{\boldsymbol{\lambda}}$.*

The total error splits as

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$$\| \hat{\boldsymbol{\lambda}} - \hat{\boldsymbol{\lambda}}^{\delta}_{\alpha(\delta)} \| \le \underbrace{\| \hat{\boldsymbol{\lambda}} - \hat{\boldsymbol{\lambda}}_{\alpha(\delta)} \|}_{\text{approximationerror}} + \underbrace{\| \hat{\boldsymbol{\lambda}}_{\alpha(\delta)} - \hat{\boldsymbol{\lambda}}^{\delta}_{\alpha(\delta)} \|}_{\text{dataerror}}. \tag{18}$$

The balance between these terms, controlled by the choice of α, determines the best achievable reconstruction. Theorem 3 together with the data-error bound $\| \hat{\boldsymbol{\lambda}}_{\alpha(\delta)} - \hat{\boldsymbol{\lambda}}^{\delta}_{\alpha(\delta)} \| \le C\delta\sqrt{\max|R_\alpha|}$ guarantees $\hat{\boldsymbol{\lambda}}^{\delta}_{\alpha(\delta)} \to \hat{\boldsymbol{\lambda}}$ as $\delta \to 0$.

4.4 Choice of the regularization parameter by GCV

The choice of α is decisive: too large a value over-smooths the solution, while too small a value leaves noise unsuppressed. Among parameter-choice rules (Morozov's discrepancy principle, the L-curve, and GCV), this study adopts Generalized Cross-Validation, which requires no a priori knowledge of the noise level. GCV selects α minimizing

$$\mathrm{T}_{\mathcal{G},\mathbf{c}}(\alpha) = \frac{r \ \|[I-\mathcal{G}\mathcal{G}_\alpha^{\dagger}]\mathbf{c}\|_2^2}{[trace(I-\mathcal{G}\mathcal{G}_\alpha^{\dagger})]^2}, \tag{19}$$

with $\mathcal{G}_\alpha^{\dagger} = (\mathcal{G}^T\mathcal{G} + \alpha^2 I)^{-1}\mathcal{G}^T$. Using the SVD, for a general $m \times n$ matrix,

$$\mathrm{T}_{\mathcal{G},\mathbf{c}}(\alpha) = \frac{r\{\sum_{i=1}^{r}[(\frac{\alpha^2}{\sigma_i^2+\alpha^2})p_i^T\mathbf{c}]^2 + \sum_{i=r+1}^{m}(p_i^T\mathbf{c})^2\}}{[(m-r)+\sum_{i=1}^{r}(\frac{\alpha^2}{\sigma_i^2+\alpha^2})]^2}, \tag{20}$$

a convenient form for standard minimization. Compared with the L-curve, which requires repeated solution of the inverse problem and is computationally expensive, GCV offers minimal computational complexity and suitability for large noisy datasets; comparative testing showed that GCV yielded optimal regularization parameters that balanced data fidelity against solution smoothness across varying noise levels. The source intensity in this study is therefore obtained from (17) with α chosen by minimizing (20).

5. NUMERICAL RESULTS AND DISCUSSION

5.1 Experimental setup

The source intensity function used to generate synthetic data is

$$\lambda(t) = \sum_{i=1}^{n} b_i \ e^{-u_i(t-q_i)^2}, \tag{21}$$

with $b_i \in [0,1]$, $u_i \in [-10^{-6}, 10^{-4}]$, and $q_i \in [4.5 \times 10^3, 9 \times 10^3]$. The point source $\delta(X - S) = \delta(x - S_x, y - S_y)$ is approximated by a normal distribution. Both velocity and dispersion coefficients increase exponentially with time, $f_i(mt) = e^{mt}$, with $m = 0.1$. The linear parameter (time-dependent source intensity) was recovered using the filtered solution (17) with α from GCV (20).

5.2 Reconstructed source intensity

The reconstructed intensity was computed for nine candidate source positions on the upstream sub-domain. In every case the recovered intensity increases exponentially in time, consistent with the prescribed forcing (21). Accuracy was quantified by the root-mean-square error

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{N}[\lambda_s(i)-\lambda_a(i)]^2}{N}}, \tag{22}$$

where λ_s is the recovered (simulated) intensity and λ_a the assumed intensity. Table 1 reports the RMSE for the nine source positions.

Table 1: RMSE between assumed and reconstructed source intensity for nine candidate source locations.

(S_x, S_y)	$S_y = 0.01$	$S_y = 0.02$	$S_y = 0.04$
$S_x = 0.25$	272.5	255.9	1.9
$S_x = 0.30$	1638.6	333.7	0.4
$S_x = 0.35$	485.4	15.0	8.5

The RMSE values are generally low, and become very small for source positions located further from the inflow boundary (for example, (0.30,0.04) with RMSE $= 0.4$ and (0.25,0.04) with RMSE $= 1.9$). The comparatively larger errors at $S_y = 0.01$ are attributable to errors carried forward from the concentration and Green's function data near the boundary, where the conditioning of $\mathcal{G}$ is least favorable. Overall, the results demonstrate that Tikhonov regularization, with the parameter selected by GCV and the linear parameter extracted by variable projection, recovers the time-dependent source intensity with good accuracy.

5.3 Discussion

Two features of the reconstruction merit emphasis. First, the exponential growth of the recovered intensity reflects an increasing magnitude of pollutant release at the source over time, a physically meaningful diagnostic for monitoring programs: a positive growth rate signals an intensifying discharge that warrants intervention. Second, the stability of the recovered intensity across noise levels confirms the central role of regularization. Without the filter factors F_i in (17), the small singular values of the ill-conditioned matrix $\mathcal{G}$ ($\kappa(\mathcal{G}) \gg 10^4$) would amplify data noise and corrupt the solution, as predicted by (14). The GCV-selected α suppresses these components while preserving the dominant signal, yielding the low RMSE values of Table 1.

6. CONCLUSION

A framework for non-intrusive estimation of a time-dependent pollutant source intensity in rivers with temporally varying flow parameters has been presented. The forward ADE was cast as a Volterra integral equation of the first kind via Green's function method, discretized by Gauss–Legendre quadrature into a separable non-linear least squares problem, and reduced by variable projection to a linear sub-problem for the source intensity. The severe ill-conditioning ($\kappa(\mathcal{G}) \gg 10^4$) was controlled by Tikhonov regularization, with the regularization parameter chosen by Generalized Cross-Validation. Convergence and stability of the regularized solution were established. Numerical experiments over nine source positions confirmed that the recovered intensity increases exponentially in time and that the RMSE between assumed and recovered intensities is consistently low, reaching values as small as 0.4. The method provides an accurate, stable, and cost-effective tool for source-intensity recovery in water-quality monitoring. Future work will incorporate field concentration measurements for calibration and validation, and extend the framework to chemically reactive pollutants through the addition of a reaction term.

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