
Pollution Source Identification

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Outline

- 1 Introduction
 - Why do we care ?
 - Problem definition
- 2 Solving
 - A simple case : closed-form solution
 - A numerical method
- 3 Next Step

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Why is this problem interesting ?

- 300000 to 400000 contaminated sites



Figure: Water pollution

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- 300000 to 400000 contaminated sites
- Expected clean-up cost : 1 trillion \$ (4000\$ per US citizen)
- Chemical fingerprinting and records are seldom sufficient to determine the source.



Figure: Water pollution

Forward problem

Governing equation :

$$\begin{cases} \frac{\partial C}{\partial t} = \nabla [D \cdot \nabla C] - \nabla \cdot [v \cdot C] - \lambda C \\ C(x_1, t) = C_{in}(t) = 0 \leq t \leq T_{final} \\ C(x, 0) = C_0(x) \text{ initial concentration profile} \\ C(x_{sensor}, t) = f(t) \text{ measurements} \end{cases}$$

Some analytical (closed-form) solutions in simple cases. Solved numerically most of the time.

Inverse problem

- The problem of finding the source and possibly the time history of the pollution is a “time inversion” problem.
- Due to the irreversibility of diffusion it is fundamentally ill-posed. This means that we do not know in general :
 - ❶ if a solution exist
 - ❷ if it is unique
 - ❸ how much it is sensitive to the observed data.

⇒ Since the problem is severely underdetermined we have to make assumptions on the unknown function.

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Several methods are used

- Use of closed-form solutions
- Brute-force forward solving and optimization
- Probability and backward solving
- Statistical Estimation.

A groundwater model



Figure: Henri Darcy

$$\frac{\partial C}{\partial t} = D\Delta C + q$$

We can consider the equation far from the sources, and a decay rate for the contaminant :

$$\frac{\partial C}{\partial t} = D\Delta C - \lambda C$$

A groundwater model

We can add carefully chosen boundary conditions to the model :

$$\lim_{\|(\mathbf{x}, t)\| \rightarrow \infty} C(\mathbf{x}, t) = C_0$$

$$\int_{\mathbb{R}^n} [C(\mathbf{x}, t) - C_0] d\mathbf{x} = M_0 e^{-(t-t_0)}$$

$$\lim_{t \rightarrow t_0} [C(\mathbf{x}, t) - C_0] = 0$$

The solution to the direct problem is then :

$$C(\mathbf{x}, t) = \frac{M_0 e^{-(t-t_0)}}{\sqrt{[2\pi(t-t_0)]^n (2D)^n}} \exp\left(\frac{-\|\mathbf{x} - \mathbf{x}_0\|^2}{4D(t-t_0)}\right) + C_0$$

Identifying the source

We can take the log :

$$-\frac{\|\mathbf{x} - \mathbf{x}_0\|^2}{4D(t - t_0)} - \lambda(t - t_0) - \frac{n}{2} \ln(t - t_0) + \ln(M_0) - \frac{n}{2} \ln(4\pi D)$$

We also introduce additional parameters to simplify the notation : $\kappa = (2D)^{-1}$ and $\alpha = \ln(M_0) - \frac{n}{2} \ln(4\pi S)$ and consider the accordingly modified measurements $\ln(C(\mathbf{x}_j, t_k) - C_0) = \nu_{k,j}$. We thus have :

$$(k, j) \nu_{k,j} = -\frac{\|\mathbf{x}_j - \mathbf{x}_0\|^2 \kappa}{(t_k - t_0)} - \lambda(t_k - t_0) - \frac{n}{2} \ln(t_k - t_0) + \alpha$$

Theorem

For a space of any dimension \mathbb{R}^n , four measurements of $C(\mathbf{x}_j, t_k)$ at two different times $t_1 > t_0$ and $t_2 > t_0$ common at each to distinct locations \mathbf{x}_1 and \mathbf{x}_2 suffice to express t_0 in closed form :

$$t_0 = \frac{(\nu_{k+1,j+1} - \nu_{k+1,j})t_{k+1} - (\nu_{k,j+1} - \nu_{k,j})t_k}{(\nu_{k+1,j+1} - \nu_{k+1,j}) - (\nu_{k,j+1} - \nu_{k,j})}$$

Two additional measurements at the same locations at a third time lead to closed-form solution for the decay rate λ and for auxiliary parameter α (They are solutions of a system function of the t_k with a non-zero determinant)

With the condition that sensor locations $(x_l)_l$ are in general position

$\Leftrightarrow \forall m \in \{2, \dots, n+1\}$ no subset of m points is entirely included in an affine (hyper)plane of dimension $m-2$.

Theorem

For \mathbb{R}^n , $n+2$ measurements of $C(x_l, t_k)$ at the same time $t_k > t_0$ at each $n+2$ points $x_l \neq x_0$ in general position suffice to express the location of the source x_0 in closed form as well as parameter M_0 and D .

By using the previous equations and by substituting the values of t_0, α, λ in (k, l) we get

$$\kappa \|x_l - x_0\|^2 = -2(t_k - t_0) \left(\nu_{k,l} + \lambda(t_k - t_0) + \frac{n}{2} \ln(t_k - t_0) - \alpha \right)$$

By forming the ratio of the following form ($h \neq l$), we obtain $n+1$ independent equations :

$$\frac{\|x_h - x_0\|^2}{\|x_l - x_0\|^2} = r_{k,h,l}^2$$

Those are the equations of the median plane if $r_{k,h,l}^2 = 1$ or of a sphere which center is the centroid of $(x_h, 1)$ and $(x_l, -r_{k,h,l}^2)$. x_0 is the intersection of all these.

Probabilistic model

We define the probability density function F_q as $\frac{C(x, t)}{M_0}$ For a divergence-free flow and non-reactive transport :

$$\frac{\partial F_q}{\partial t} = -q \cdot \nabla F_q + \nabla [D \cdot \nabla F_q] \quad (1)$$

$$F_q(x_0, 0) = \delta(x - x_0) \quad (2)$$

The backward model :

$$\frac{\partial F_{-q}}{\partial t} = q \cdot \nabla F_{-q} + \nabla [D \cdot \nabla F_{-q}] \quad (3)$$

$$F_{-q}(x_1, 0) = \delta(x - x_1) \quad (4)$$

The boundary conditions are

$$\nabla F_{\pm q} = 0 \text{ on } \partial\Omega$$

Concept

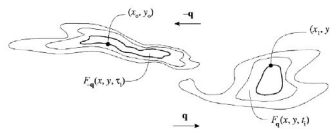


Figure: Backward model concept

$$F_q(x_1, t_i) = F_{-q}(x_0, \tau_i)$$

where $\tau_i = t_{detection} - t_i$

$$C_0(x_1, \tau_i) = \frac{1}{M_0} \cdot C(x_1, t_i)^2 dx_1$$

Solving

We can run the backward flow model and watch for the isocontour obtained by equation :

$$C_0(x_1, \tau_i) = \frac{1}{M_0} \cdot C(x_1, t_i)^2 dx_1$$

- Running this from a single point does not yield to a unique solution. But it can be done from several points, since the equations are true $\forall x_1$.
- Since the equation is linear we can use as initial condition for the backward model the whole concentration profile at $t_{detection}$. We can then backtrack it until it shrinks discovering the source.

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What to do next ?

For the project :

- Numerical example : Have the simulation working

After the project : Maybe investigating on other methods, there is still a lot to do.

Questions ?