Methodology

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The forward model solves a depth-averaged advection-diffusion-reaction equation

$$\frac{\partial C}{\partial t} + \vec{\mathbf{v}} \cdot \nabla C - \frac{1}{H}\nabla \cdot (HK\nabla C) = R(x,y). \tag{1}$$

The inversion tends to minimize a cost function, which is a measurement of model-data misfit plus a smoothness regularization term

$$J = \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} \delta_M \frac{(C - C_{obs})^2}{\sigma^2} dxdydt + \int_{-L_x}^{L_x}\int_{-L_y}^{L_y} \frac{(\frac{\partial R}{\partial x})^2 + (\frac{\partial R}{\partial y})^2}{w} dxdy. \tag{2}$$

Here δ_M is a measurement functional which is equal to 1 where observations exist in space-time and 0 else where; L_x and L_y define the extend of the domain of interest; σ is set to 1; w is a weighting parameter for the smoothness term; t_0 and t_f are initial and terminal times. The optimization problem is to find a solution of the control vector $\mathbf{U}$, here the initial condition C(t=0) and R(x,y), such that J is minimized subject to the constraint of (1). The method used is that of Lagrange multipliers, sometimes known as the "adjoint method", because it uses the adjoint to (1) as an estimate of the derivatives of J. The Lagrange function is expressed as

$$\Psi = J + \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} \lambda\Big(\frac{\partial C}{\partial t} + \vec{\mathbf{v}} \cdot \nabla C - \frac{1}{H}\nabla \cdot (HK\nabla C) - R(x,y)\Big) dxdydt, \tag{3}$$

where λ are Lagrange multipliers. Because the forward model is satisfied, the second term is equal to zero. Therefore, the minimum point of Ψ is also the minimum point of J. Integrating by parts,

$$\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} \lambda \frac{\partial C}{\partial t} dxdydt = \int_{-L_x}^{L_x}\int_{-L_y}^{L_y} \lambda C|_{t_0}^{t_f} dxdy - \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} C\frac{\partial \lambda}{\partial t} dxdydt. \tag{4}$$

$$\begin{aligned}
\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} \lambda \vec{\mathbf{v}} \cdot \nabla C dxdydt &= \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} (\lambda u \frac{\partial C}{\partial x} + \lambda v \frac{\partial C}{\partial y}) dxdydt \\
&= \int_{-L_y}^{L_y}\int_{t_0}^{t_f} C\lambda u|_{-L_x}^{L_x} dydt - \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} C\frac{\partial \lambda u}{\partial x} dxdydt \\
&+ \int_{-L_x}^{L_x}\int_{t_0}^{t_f} C\lambda v|_{-L_y}^{L_y} dxdt - \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} C\frac{\partial \lambda v}{\partial x} dxdydt
\end{aligned}$$

where the zero concentration boundary condition of C and incompressibility of the fluid are used.

Similarly,

$$\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\frac{1}{H}\nabla\cdot(HK\nabla C)=\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\frac{C}{H}\nabla\cdot(HK\nabla\lambda)dxdydt. \tag{6}$$

The first variation in Ψ can be written as

$$\begin{aligned}\delta\Psi &= \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}2\delta_M\frac{(C-C_{obs})}{\sigma^2}\delta C dxdydt\\ &+ \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\frac{\frac{\partial}{\partial R}[(\frac{\partial R}{\partial x})^2+(\frac{\partial R}{\partial y})^2]}{w}\delta R dxdy\\ &+ \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}(\lambda_f\delta C_f-\lambda_0\delta C_0)dxdy-\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\delta C\frac{\partial\lambda}{\partial t}dxdydt\\ &- \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\delta C\vec{\mathbf{v}}\cdot\nabla\lambda dxdydt\\ &- \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\frac{\delta C}{H}\nabla\cdot(HK\nabla\lambda)dxdydt\\ &- \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\lambda\delta R dxdydt. \end{aligned}\tag{7}$$

Here subsripts 0 and f represent values at the initial and final times, respectively, and hereafter. By choosing λ such that $\partial\Psi/\partial C$=0, we get the adjoint equation

$$-\frac{\partial\lambda_i}{\partial t}-\vec{\mathbf{v}}\cdot\nabla\lambda_i-\frac{1}{H}\nabla\cdot(HK\nabla\lambda_i)=-2\delta_M(C-Cobs). \tag{8}$$

The lagrange multipliers are called the adjoint state variables, they can be obtained by integrating the adjoint equation (8) backward in time by choosing the terminal values λ_f=0.

Based on the choices of λ described above, equation (7) simplifies to

$$\begin{aligned}\delta\Psi &= \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\frac{\frac{\partial}{\partial R}[(\frac{\partial R}{\partial x})^2+(\frac{\partial R}{\partial y})^2]}{w}\delta R dxdy\\ &- \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\lambda_0\delta C_0 dxdy-\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\lambda\delta R dxdydt.\end{aligned}\tag{9}$$

Sensitivies are given by

$$\frac{\partial\Psi}{\partial R} = \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\frac{\frac{\partial}{\partial R}[(\frac{\partial R}{\partial x})^2+(\frac{\partial R}{\partial y})^2]}{w}dxdy-\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\lambda dxdydt \tag{10}$$

$$\frac{\partial\Psi}{\partial C_0} = -\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\lambda_0 dxdy \tag{11}$$

$$, \tag{12}$$

Sensitivies of J to the constrol variables are also given by (10) and (11), because the sencond term in (14) is zero, due to the constraint of the forward model.

nonlinear model

The forward model is

The cost function J is the same as (2).
The Lagrange function is expressed as

$$\Psi = J + \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} \lambda\Big(\frac{\partial C}{\partial t} + \vec{\mathbf{v}}\cdot\nabla C - \frac{1}{H}\nabla\cdot(HK\nabla C) - RC\Big)dxdydt, \tag{14}$$

Integrating by Parts, the first variation in Ψ can be written as

$$\begin{aligned}
\delta\Psi &= \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f} 2\delta_M\frac{(C-C_{obs})}{\sigma^2}\delta C dxdydt \\
&+ \int_{-L_x}^{L_x}\int_{-L_y}^{L_y} \frac{\frac{\partial}{\partial R}[(\frac{\partial R}{\partial x})^2 + (\frac{\partial R}{\partial y})^2]}{w}\delta R dxdy \\
&+ \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}(\lambda_f\delta C_f - \lambda_0\delta C_0)dxdy - \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\delta C\frac{\partial\lambda}{\partial t}dxdydt \\
&- \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\delta C\vec{\mathbf{v}}\cdot\nabla\lambda dxdydt \\
&- \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\frac{\delta C}{H}\nabla\cdot(HK\nabla\lambda)dxdydt \\
&- \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\lambda(C\delta R + R\delta C)dxdydt.
\end{aligned} \tag{15}$$

Take $\partial\Psi/\partial C$=0, we get the adjoint equation

$$-\frac{\partial\lambda_i}{\partial t} - \vec{\mathbf{v}}\cdot\nabla\lambda_i - \frac{1}{H}\nabla\cdot(HK\nabla\lambda_i) = -2\delta_M(C - Cobs) + R\lambda. \tag{16}$$

Sensitivies are given by

$$\frac{\partial\Psi}{\partial R} = \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\frac{\frac{\partial}{\partial R}[(\frac{\partial R}{\partial x})^2 + (\frac{\partial R}{\partial y})^2]}{w}dxdy - \int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{t_0}^{t_f}\lambda C dxdydt \tag{17}$$

$$\frac{\partial\Psi}{\partial C_0} = -\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\lambda_0 dxdy \tag{18}$$

$$, \tag{19}$$