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An inverse problem in biology: Estimating microbial production rates from nutrient concentration profiles in sea water

An inverse problem in biology: Estimating microbial production rates from nutrient concentration profiles in sea water

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1 Description of the Problem

Biologists are interested in the biological activity in sea-floor sediment. Nutrients, for example Nitrogen and Oxygen, in the sediment are consumed by various organisms that live there. Thus we define biological activity as the rate of consumption of nutrients in the sea-floor sediment. In this report we are concerned with determining the rate at which organisms in the sediment consume nutrients. Biologists can measure the concentration of nutrients in the sea water and the sea-floor sediment. However, it is quite difficult to experimentally measure the rate of consumption of nutrients by organisms in the sediment. In this report we pose a model to determine the consumption rate of a given nutrient in the sediment by two biological organisms, sea-worms and microbes.

Sediment is a porous medium consisting of impermeable rock and water. The sediment lies on-top of a layer of impermeable rock. Nutrients can dissolve in water but not rock. The microbes can move only through the water and they consume nutrients. The sea-worms are found to inhabit canals channeled vertically through the sediment. The worms irrigate the sea-floor sediment i.e. they control the ammount of nutrient in the sediment. They do this by a pumping mechanism; they pump water into the sediment if the concentration at the sediment-sea interface is above the concentration of nutrient at the bottom of their canals and they pump water out of the sediment if the concentrations are reversed. This mechanism is called bio-irrigation [6]. A schematic diagram for this system is shown in Figure 1.

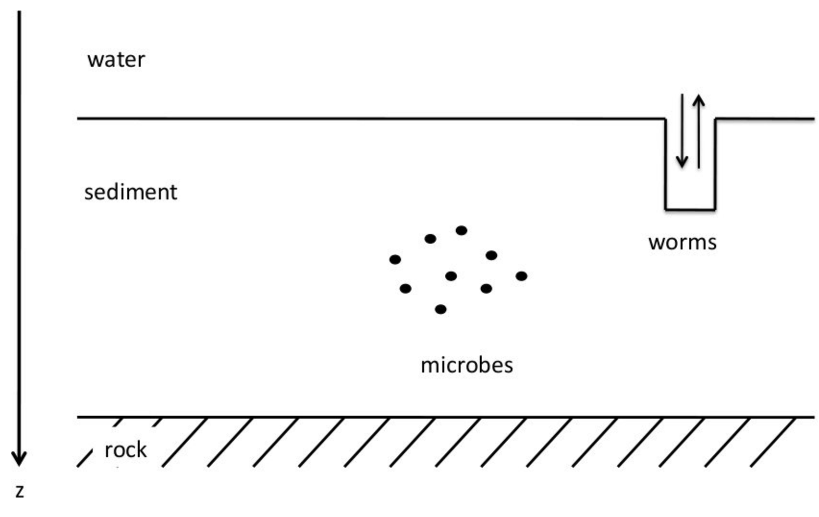


Figure 1: Schematic diagram

2 Derivation of the Model

We consider a simple one dimensional model for the concentration of nutrient in both the water and sediment. We set the z-axis pointing vertically downwards into the water-sediment-rock layers as shown in Figure 1. The sediment water interface is at $z = 0$ and the sediment-rock interface is at $z = L$ where L is the known depth of the sediment in m. We denote the concentration of nutrient in the sediment and water by $C(z,t)$ and $C_w(z,t)$ respectively. Both have dimensions mol m^{-3} (or M). We assume that the nutrient can diffuse through the water and we write down the diffusion equation for $C_w(z,t)$,

$$\frac{\partial C_w}{\partial t} = D_w \frac{\partial^2 C_w}{\partial z^2} \quad \text{in} \quad z < 0, \tag{1}$$

where D_w is the constant diffusion coefficient of nutrient in the water with dimension m^{2}s^{-1}. Both the microbes and worms in the sediment consume nutrient and we assume they do so at an unknown rate $R(z,t)$ with dimension mol m^{-3} s^{-1}. Once the model has been derived we will try to determine the form of $R(z,t)$ using both analytical and numerical approaches. We assume that the worms irrigate the sediment (i.e. they control the level of nutrient concentration in the sediment) by the following mechanism;

- if $C < C_{\text{crit}}$ then the worms pump water into the sediment to increase the total concentration of nutrient in the sediment,
- if $C > C_{\text{crit}}$ then the worms pump water out of the sediment to lower the total concentration of nutrient in the sediment.

Where C_{crit} is the known critical concentration of nutrient in the sediment. We define C_{crit} to be the concentration of nutrient in a small boundary region of $O(\epsilon)$ near the sediment-water interface i.e. $C_{\text{crit}} = C_w(\epsilon, t)$. Thus we mathematically model this process as a source/sink term,

$$k\left(C_{\text{crit}} - C(z,t)\right), \tag{2}$$

where k is the irrigation constant. It is worth noting here that biologists are still unsure as to why the worms use this mechanism for irrigation. The sediment is a porous medium in order to model this we introduce a porosity function, $a(z)$, which we assume to be independent of time and dependent on depth only. We also assume that the nutrient can diffuse through the sediment with a constant diffusion coefficient D. We now write down the diffusion equation for $C(z,t)$ in the sediment with contribution terms for the consumption rate and irrigation,

$$\frac{\partial C}{\partial t} = D\frac{\partial}{\partial z}\left(a(z)\frac{\partial C}{\partial z}\right) - R(z,t) + ka(z)\left(C_{\text{crit}} - C\right) \quad \text{in} \quad 0 < z < L. \tag{3}$$

At the sediment-water interface we assume that the nutrient concentration is equal and also that the flux of nutrients through the interface is conserved. Thus,

$$C_w = C \quad \text{and} \quad D_w \frac{\partial C_w}{\partial z} = D \frac{\partial C}{\partial z} \quad \text{on} \quad z = 0. \tag{4}$$

The rock is assumed to be impermeable so we have no flux of nutrient through the sediment-rock interface. We also assume that the concentration at the sediment-rock interface is a constant and from experiment this constant is taken to be zero, [1]. Thus,

$$C = 0 \quad \text{and} \quad D \frac{\partial C}{\partial z} = 0 \quad \text{on} \quad z = L. \tag{5}$$

Given experimental data for the nutrient concentration in the sediment we wish to determine a model for the consumtion rate $R(z,t)$. The experimental data we will use in this report was obtained from a system in steady state. Thus, we drop the time-dependence from equations (1)–(5) and obtain the reduced model for the system,

$$\frac{\mathrm{d}^2 C_w}{\mathrm{d}z^2} = 0 \qquad \text{in} \quad z > 0, \tag{6}$$

$$D \frac{\mathrm{d}}{\mathrm{d}z}(a(z) \frac{\mathrm{d}C}{\mathrm{d}z}) = R(z) - k a(z) \left(C_{\text{crit}} - C\right) \qquad \text{in} \quad 0 < z < L, \tag{7}$$

with boundary conditions

$$C_w = C \quad \text{and} \quad D_w \frac{\mathrm{d}C_w}{\mathrm{d}z} = D \frac{\mathrm{d}C}{\mathrm{d}z} \quad \text{on} \quad z = 0, \tag{8}$$

$$C = 0 \quad \text{and} \quad D \frac{\mathrm{d}C}{\mathrm{d}z} = 0 \quad \text{on} \quad z = L. \tag{9}$$

We leave the equations in dimensionless form for this report.

To simplify the numerical computation we later ignore the water concentration C_w and simply assume that the concentration at the sediment-water interface is known and given. Together with Neumann boundary condition at $z = L$ this yields the simpler model equation (8) plus

$$D \frac{\mathrm{d}C}{\mathrm{d}z} = 0 \quad \text{at} \quad z = L \quad \text{and} \quad C = C_{\text{crit}} \quad \text{at} \quad z = 0. \tag{10}$$

3 Analytical Solution

For simplicity, we consider an experiment with constant porosity, we take $a(z) = 1$ (w.lo.g). Then equation (6) and equation (7) can be integrated analytically. The solutions for $C_w(z)$ and $C(z)$ for are given by,

$$C_w(z) = A_1 + B_1 z, \tag{11}$$

$$\begin{aligned} C(z) &= \mathrm{e}^{\sqrt{K/D}z}\left(A_2 + \int_0^z \frac{1}{\sqrt{Dk}}\mathrm{e}^{-\sqrt{k/D}s}\left(R(s) - kC_{\text{crit}}\right)ds\right) \\ &+ \mathrm{e}^{-\sqrt{k/D}z}\left(B_2 - \int_0^z \frac{1}{\sqrt{Dk}}\mathrm{e}^{\sqrt{K/D}s}\left(R(t) - kC_{\text{crit}}\right)ds\right), \end{aligned} \tag{12}$$

where A_1, A_2, B_1, B_2 are constants determined by boundary conditions (8) and (9). To do this we must know the form of the consumption rate, $R(z)$. In order to determine the consumption rate we could make an ansatz for the form of $R(z)$ and see whether the function $C(z)$ produced matches with the experimental data. From experiments we know that the concentration profile of the nutrient in the sediment decreases monotonically with depth so it is logical to assume $R(z)$ is a decreasing function also. We consider a gaussian of the form $R(z) = R_0\mathrm{e}^{-\gamma z^2}$. Where R_0 and γ are the fitting parameters. We omit the full analytical solution for the case $R(z) = R_0\mathrm{e}^{-\gamma z^2}$ as it is a trivial exercise to do. Instead we plot the solution for $C(z)$ and $C_w(z)$ in Figure 2.

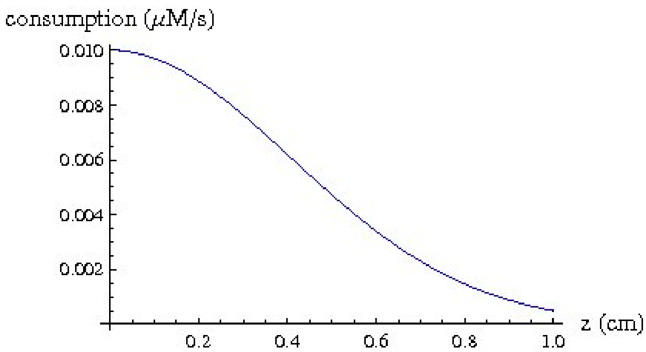


Figure 2: Plot of nutrient consumption rate $R(z) = R_0\mathrm{e}^{-\gamma z^2}$ against depth. The parameters values used were, $D_w = 1.2 \times 10^{-5}\mathrm{cm}^2\ \mathrm{s}^{-1}$, $D = 9 \times 10^{-6}\ \mathrm{cm}^2\ \mathrm{s}^{-1}$, $L = 1\mathrm{cm}$, $\epsilon = -0.05$ cm, $k = 3.75 \times 10^{-6}$ s−1, $\gamma = 3\ \mathrm{cm}^{-1/2}$, $R_0 = 0.01\mu\mathrm{M\ s}^{-1}$.

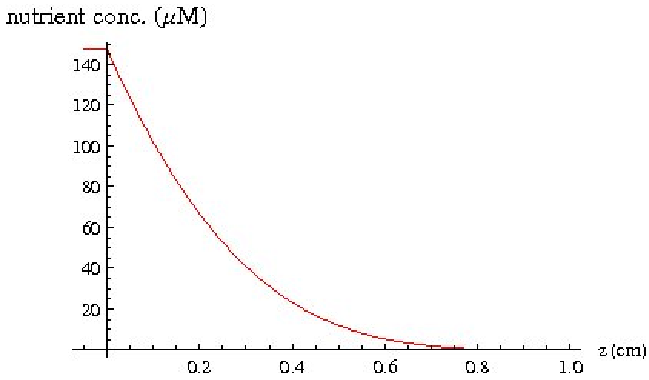


Figure 3: Plot of nutrient concentration in the water ($z < 0$) and the sediment ($0 < z < 1$) against depth. Nutrient consumption rate is given by $R(z) = R_0 \mathrm{e}^{-\gamma z^2}$. The parameters values used were, $D_w = 1.2 \times 10^{-5}$cm^2 s^{-1}, $D = 9 \times 10^{-6}$ cm^2 s^{-1}, $L = 1$cm, $\epsilon = -0.05$ cm, $k = 3.75 \times 10^{-6}$ s-1, $\gamma = 3$ cm$^{-1/2}$, $R_0 = 0.01\mu$M s^{-1}.

Figure 3 shows the qualitative behaviour observed in experiments for the concentration of nutrient in the water and the sediment. With this choice of $R(z)$ we have two degrees of freedom to enable us to fit the analytical solutions $C_w(z)$ and $C(z)$ to some given data. This report does not compare actual experimental data with the analytical solutions but it would be an interesting extension of the work to do.

4 Numerical Simulation

We discretize our model using a finite difference method with a central difference scheme. We define the grid points:

$$z_j = (j-1)\triangle z, \qquad \text{at } j = 1, 2, ..., M \tag{13}$$

where $\triangle z = \frac{1}{M-1} = h$. Let $C(z_j) = C_j$, and let $\underline{C} = (C_2, C_3, ..., C_M)^T$ be the nutrient concentration vector by excluding the first entry into the calculation since it is already known and let $\underline{R} = (R_2, R_3, ..., R_M)^T$ be the consumption rate at the same grid points. From now on we also assume that $C_w = C_{\text{crit}}$.

4.1 Discretization with constant diffusion and irrigation coefficients

First we assume constant constant porosity i.e. $a(z) = 1$. The model now simply becomes

$$D\frac{\mathrm{d}^2 C}{\mathrm{d}z^2} + k(C_{\text{crit}} - C(z)) - R(z) = 0 \tag{14}$$

The central difference scheme of this model is

$$\begin{aligned}\frac{D}{h^2}\left(C_{j-1}-2C_j+C_{j+1}\right)+k\left(C_{\text{crit}}-C_j\right)-R_j &= 0\\ \frac{D}{h^2}\left(C_{j-1}-\left(2+k\frac{h^2}{D}\right)C_j+C_{j+1}\right) &= R_j-kC_{\text{crit}}, \qquad \text{for } j=2,3,...,M\end{aligned} \tag{15}$$

By applying the boundary condition to the scheme (15), we have:

$$\begin{aligned}\tfrac{D}{h^2}\left(-\left(2+k\tfrac{h^2}{D}\right)C_2+C_3\right) &= R_2-\left(k+\tfrac{D}{h^2}\right)C_{\text{crit}},\\ \tfrac{D}{h^2}\left(C_{j-1}-\left(2+k\tfrac{h^2}{D}\right)C_j+C_{j+1}\right) &= R_j-kC_{\text{crit}}, \qquad \text{for } j=3,...,M-1\\ \tfrac{D}{h^2}\left(2C_{M-1}-\left(2+k\tfrac{h^2}{D}\right)C_M\right) &= R_M-kC_{\text{crit}},\end{aligned}$$

where $C_1 = C_{\text{crit}}$, from the Dirichlet boundary condition of equation (8), and the Neumann boundary condition of equation (9), gives us $C_{M+1} = C_{M-1}$. This system of equations can be written in the matrix form as follows:

$$A\,\underline{C} = \underline{R} - \underline{P}$$

where:

$$A = \tfrac{D}{h^2}\begin{bmatrix} -\left(2+k\frac{h^2}{D}\right) & 1 & & & \\ 1 & -\left(2+k\frac{h^2}{D}\right) & 1 & & \\ \ddots & \ddots & \ddots & & \\ & & 1 & -\left(2+k\frac{h^2}{D}\right) & 1 \\ & & & 2 & -\left(2+k\frac{h^2}{D}\right)\end{bmatrix},$$

$$\underline{C} = \begin{bmatrix} C_2 \\ C_3 \\ \vdots \\ \\ C_M\end{bmatrix}, \underline{R} = \begin{bmatrix} R_2 \\ R_3 \\ \vdots \\ \\ R_M\end{bmatrix}, \text{ and } \underline{P} = \begin{bmatrix} \left(k+\frac{D}{h^2}\right)C_{\text{crit}} \\ kC_{\text{crit}} \\ \vdots \\ \\ kC_{\text{crit}}\end{bmatrix}$$

4.2 Discretization with general diffusion and irrigation functions

We now consider a system with non-constant porosity, $a(z)$. We are now looking at equation (7). We will now discretize it. Again we apply finite difference methods and get

$$\frac{D}{h^2}\left(a(z+\frac{h}{2})(C(z+h)-C(z))-a(z-\frac{h}{2})(C(z)-C(z-h))\right)$$
$$+ka(z)(C_{\text{crit}}-C(z))-R(z)=0 \tag{16}$$

Finally the boundary conditions give us the system of equations

$$\begin{aligned}
&\frac{D}{h^2}\left(-(a_{2+\frac{1}{2}}+a_{2-\frac{1}{2}}+\frac{h^2}{D}ka_2)C_2+a_{2+\frac{1}{2}}C_3\right)= \\
&R_2-ka_2C_{\text{crit}}-\frac{D}{h^2}a_{2-\frac{1}{2}}C_{\text{crit}} \\
&\frac{D}{h^2}\left(-(a_{j+\frac{1}{2}}+a_{j-\frac{1}{2}}+\frac{h^2}{D}ka_j)C_j+a_{j+\frac{1}{2}}C_{j+1}+a_{j-\frac{1}{2}}C_{j-1}\right)= \\
&R_j-ka_jC_{\text{crit}} \qquad \text{for} j=3...M-1 \\
&\frac{D}{h^2}\left(-(a_{M+\frac{1}{2}}+a_{M-\frac{1}{2}}+\frac{h^2}{D}ka_M)C_M+(a_{M+\frac{1}{2}}+a_{j-\frac{1}{2}})C_{M-1}\right)= \\
&R_M-ka_MC_{\text{crit}}
\end{aligned} \tag{17}$$

If we define $\alpha_j = a_{j+\frac{1}{2}}+a_{j-\frac{1}{2}}+\frac{D}{h^2}ka_j$ and again write (17) in the form of $A\underline{C}=\underline{R}-\underline{P}$ we get

$$A=\frac{D}{h^2}\begin{bmatrix} -\alpha_2 & a_{2+\frac{1}{2}} & & & \\ a_{3-\frac{1}{2}} & -\alpha_3 & a_{3+\frac{1}{2}} & & \\ & \ddots & \ddots & \ddots & \\ & & a_{M-1-\frac{1}{2}} & \alpha_{M-1} & a_{M-1+\frac{1}{2}} \\ & & & a_{M-\frac{1}{2}}+a_{M+\frac{1}{2}} & \alpha_M \end{bmatrix},$$

$$\underline{C}=\begin{bmatrix} C_2 \\ C_3 \\ \vdots \\ C_M \end{bmatrix} \text{ and } \underline{R}-\underline{P}=\begin{bmatrix} R_2 \\ R_3 \\ \vdots \\ R_M \end{bmatrix}-\begin{bmatrix} ka_2C_{\text{crit}}+\frac{D}{h^2}a_{2-\frac{1}{2}}C_{\text{crit}} \\ ka_3C_{\text{crit}} \\ \vdots \\ ka_MC_{\text{crit}} \end{bmatrix}.$$

5 Inverse problem

A mathematical model is a mapping

$$A: X \longrightarrow Y$$

from the set of causes X to the set of effects Y. So, the inverse problem is when the values of some model parameter must be obtained from the observed data. We can formulate it as follows

$$\text{Data} \longrightarrow \text{Model parameter}$$

Inverse problems are typically ill-posed (in the sense of Hadamard). It means that if the solution exist we don't know if it is unique. It also could be that the solution depends not continuously on the data. The inverse problems are often formulated in infinite dimensional spaces and they are typically ill-conditioned. We have to solve

$$B \cdot R = C_{noise}$$

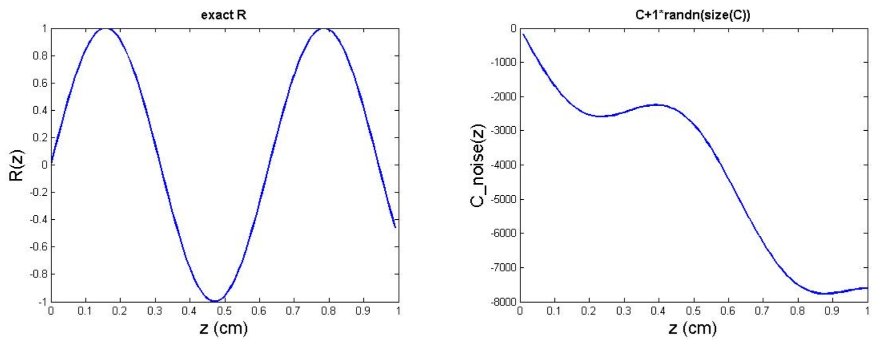
where C_{noise} is given. Perhaps $C_{noise} \notin Im(B)$ That's why we reformulate our problem to

$$R = \underset{T}{\operatorname{argmin}} ||B \cdot T - C_{noise}||$$

It is equivalent to solve the following system

$$B^T B \cdot R = B^T \cdot C_{noise}$$

This equation is ill-conditioned. As shown in Figure 4a we have chosen exact R. With this we derive an "exact" concentration, C, with the direct solver.



(a) Exact R (b) C noisy

Figure 4: $R(z) = sin(10z)$ and the solution for C using the direct solver. Small noise is added to the solution of C

Then we put noise on C. C_{noise} is now simulated data with noise and shown in Figure 4b. Figure 5 shows the solution of $B^T B \cdot R = B^T \cdot C_{noise}$. We can now easily see that if we slightly disturb C we get huge oscillations in the solution.

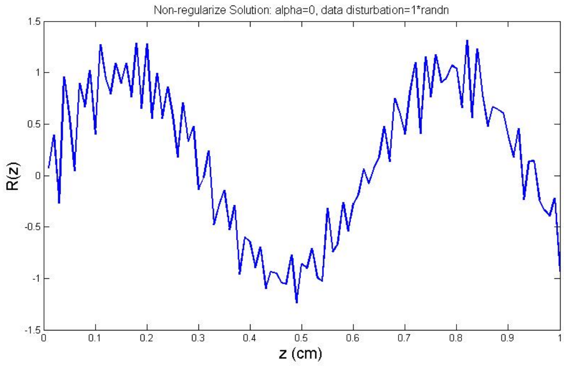


Figure 5: Solution of $B^T B \cdot R = B^T \cdot C_{noise}$

This is why we need to use regularization methods like Tikhonov or Landweber to solve the inverse problems.

5.1 Regularisation by Tikhonov-Method

In the Tikhonov-Regularization we solve instead of

$$\min_R ||\mathbb{B}R - C||^2$$

a slightly disturbed problem [5], namely

$$\min_R ||\mathbb{B}R - C||^2 + \alpha ||MR||^2 \tag{18}$$

where

C	discretised concentration of nutrients depending on the depth z
R	discretised consumption rate depending on the depth z
$\mathbb{B}$	operator which maps R to C. Has the form $\mathbb{B}R = B \cdot (R - P) = C$
B	matrix
P	constant vector
α	Regularization Parameter
M	Tikhonov-Matrix

Solving equation (18) is equivalent to solve

$$\begin{aligned} (\mathbb{B}^\star \mathbb{B} + \alpha M^\star M) R_\alpha &= \mathbb{B}^\star C \\ \Leftrightarrow (B^T B + \alpha M^T M) \cdot R_\alpha &= B^T \cdot (C + B \cdot P) \end{aligned}$$

The choice of the parameter α is really important for the regularized solution. If you choose a very small α the truncated problem is almost the original problem, but errors in the data are amplified. The bigger the parameter is chosen, the fewer are the two problems comparable, but the fewer is the influence of the data error. If the data error is known ($||R_{exact} - R_{measured}|| < \epsilon$) the apriori parameter choice has to fulfill:

$$\begin{aligned} \alpha(\epsilon) &\longrightarrow 0 \quad \text{for} \quad \epsilon \to 0 \quad \text{and} \\ \epsilon/\sqrt{\alpha(\epsilon)} &\longrightarrow 0 \quad \text{for} \quad \epsilon \to 0. \end{aligned}$$

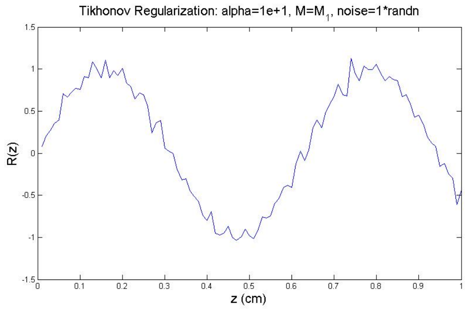
With this parameter choice the regularized solution converges to the exact solution as $\epsilon \to 0$ [5]. The matrix M has essential influence on the shape of the solution. Putting just $M = Id$ we are looking for a solution with minimal norm. There are also other choices for M. We will use the two matrices M_1 and M_2 defines as

$$M_1 = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}$$

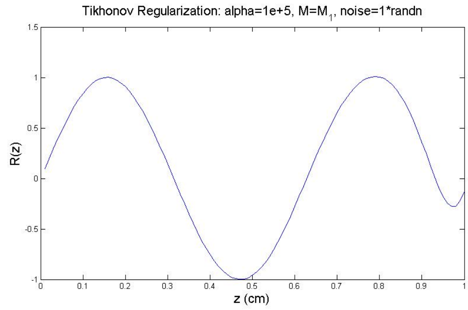
and

$$M_2 = \begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}.$$

M_1 minimizes the second derivative of the solution. If you desire additionally that the derivative on the boundarie(s) is zero you have to change the first and/or last entry to 1. We call the matrix with 1 in the first diagonal entry M_2. We tested this method with the same consumption rate as for Landweber iteration, $R(z) = \sin(10z)$. To regularize the solution, we need to have some number of non-zero α. Its value is defined by simulation which depends on the solution we would like to have. As examples, we gave two different values of $\alpha = 10^{-3}, 10^{+3}$. Figures 6a and 6a show the results for these choices of α.



(a) Tikhonov-regularize solution with $\alpha = 10$, $M = M_1$ and simulated noise on output from direct problem



(b) Tikhonov-regularize solution with $\alpha = 10^{+5}$, $M = M_1$ and simulated noise on output from direct problem

Figure 6: Results of the Tikhonov method

With a α small and $\alpha = 10$, we get a disturbed sinusoidal profile. This means that we are in the right way, only need to define the most suitable Tikhonov parameter α. Once we apply a bigger parameter, $\alpha = 10^{+5}$, then we get smoother sinusoidal graph but with some error in its boundaries. This happens since we know that the bigger Tiknonov parameter the further the problem is from the original problem. Hence, smoothness and exactness compensate each other.

5.2 Regularisation by Landweber-Method

The Landweber-Method is an iteration to find the solution of an inverse problem. It needs the operator $\mathbb{B}$ of the direct problem, that means

$$C = \mathbb{B} \cdot R$$

where

C discretised concentration of nutrients depending on the depth z
R discretised consumption rate depending on the depth z
$\mathbb{B}$ operator which maps R to C. Has the form $\mathbb{B}R = B \cdot (R - P) = C$
B matrix
P constant vector

Solving the inverse problem means looking for a solution of the normal equations

$$\mathbb{B}^{\star}\mathbb{B} \cdot R = \mathbb{B}^{\star} \cdot C$$

or here

$$B^T B \cdot R = B^T \cdot (C + B \cdot P)$$

To regularize we use the Richardson-Method for this equation [5]($\cong$ Landweber-Method):

$$R_{n+1} = (Id - \omega B^T B) \cdot R_n + \omega B^T \cdot (C + B \cdot P)$$

For convergence we require that ω as $0 < \omega < \frac{2}{||B||^2}$. You can change the method (and the result) by some wishes on the shape of the solution. It is expressed in terms of a matrix M with which we change the iteration. The changed Landweber method is then:

$$R_{n+1} = (Id - \omega M^{-1} B^T B) \cdot R_n + \omega M^{-1} B^T \cdot (C + B \cdot P)$$

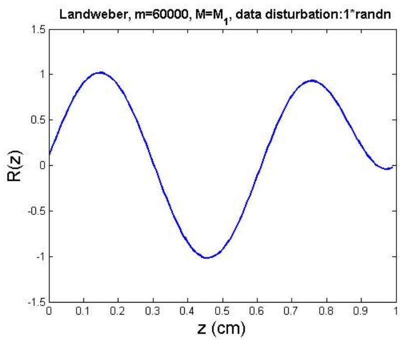
For some choices of M it is not possible to compute the inverse, so you have to change it slightly. We now require that $0 < \omega < \frac{2}{||M^{-1}B^T B||}$ to guarantee convergence. Like in the method of Tikhonov there is also a regularization parameter which you have to choose well-thought-out. Here the number of iterations plays the role of this parameter. If you do many steps the stabilized problem will be near the original one, but the noise will be amplified. If you do few iterations noise is not amplified but perhaps you solve a problem that is too far away from the original. So you have to find the right one. For example, if you know the noise level ϵ ($||R_{exact} - R_{measured}|| < \epsilon$) then your stopping rule has to behave in the following way:

$$\begin{aligned} m(\epsilon) &\longrightarrow \infty \quad \text{for} \quad \epsilon \to 0 \quad \text{and} \\ \epsilon\sqrt{m(\epsilon)} &\longrightarrow 0 \quad \text{for} \quad \epsilon \to 0 \end{aligned}$$

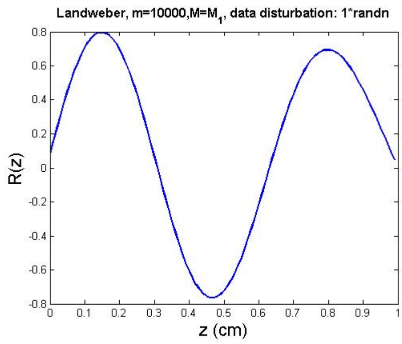
where $m(\epsilon)$ is the number of iterations where we stop (apriori). Another way to find the right stopping is discrepancy principle. It is an aposteriori parameter choice because it uses the given data. It says: stop at iteration $m^\star$ if it fulfills

$$||\mathbb{B}R_{m^\star} - C_{measured}|| < \tau\epsilon < ||\mathbb{B}R_m - C_{measured}|| \qquad \forall \quad m \leq m^\star \quad \text{with} \quad \tau > 1$$

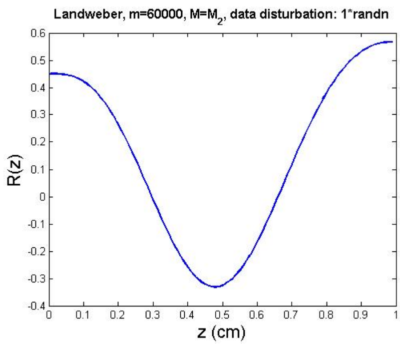
For testing the programm `Landweber_fd`, we use the same example as in Figure 4. We gave an exact $R(z) = \sin(10 \cdot z)$ and with the direct solver we computed an exact $C(z)$, and then disturbed it by $C_{noise} = C + 1*$`randn(size(C))`. In Figure 7 show results of the Landweber method with different numbers or iterations m and different choices of M.



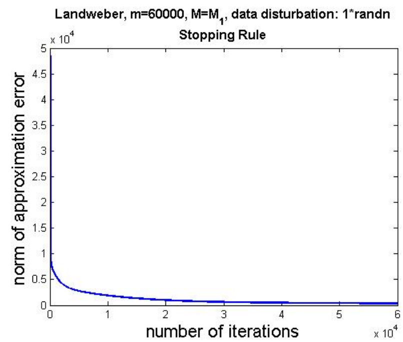
(a) Landweber Method with 60000 Iterations an $M = M_1$



(b) Landweber Method with 10000 Iterations an $M = M_1$



(c) Landweber Method with 60000 Iterations an $M = M_2$



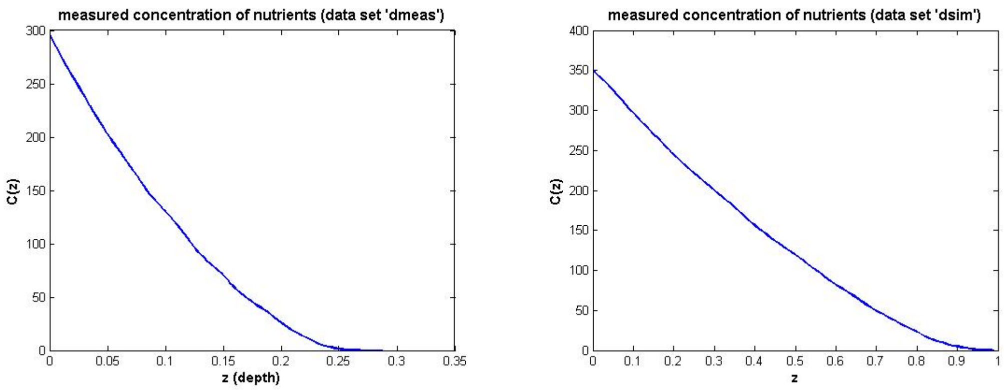
(d) Behavior of the approximation error, that decides when to stop the iteration, Landweber Method with 60000 Iterations an $M = M_1$

Figure 7: Results of the Landweber method

Figure 7a that with 60000 iterations and $M = M_1$ the Landweber method almost finds the exact solution. The 2-norm of the error is 1.01. 10000 iterations are too few to find the right solution (error is 2.175). The problem we solve is too far away from the original problem. If you would take much more iterations you would amplify the data error. The choice of M depends on the result which you expect. In this case it is better to choose $M = M_1$ because 2-norm of the error with M_1 is 1.01 and with M_2 is 5.011. In the Landweber method we use as stopping rule the discrepancy principle. In picture 7d you see that this error goes to zero but very slowly. The methods never stopped because of the discrepancy principle, because this would mean to do much more than 60000 iterations, and this takes too long. That's why the error of the Landweber-solutions is bigger than the solution to the non-regularized problem. We should have to do more iterations. We have seen that choosing 60000 iterations leads to good-agreement in the results. So truly the slow computational time of the Landweber-method is a disadvantage.

6 Results

Now we will use the method on two given data sets 'dmeas' and 'dsim', shown in Figure 8. The paramater values we used were obtained from [1]. They are D= 9×10^{-6} cm^2 s^{-1}, k= 3.75×10^{-6} s^{-1}, $C_s = 1.8 \times 10^{-7}$ mol cm^{-3}. We are assuming $a(z) = Ae^{-\beta z}$ according to [2]. In the function $a(z)$ we used $\beta = 0.98$ [3] and the value of A was chosen from [4].

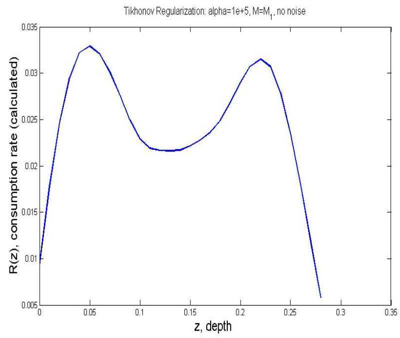


(a) Data Set 'dmeas'

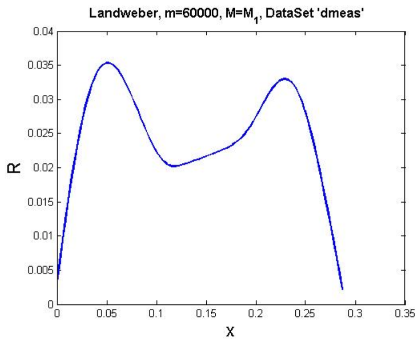
(b) Data Set 'dsim'

Figure 8: The two datasets

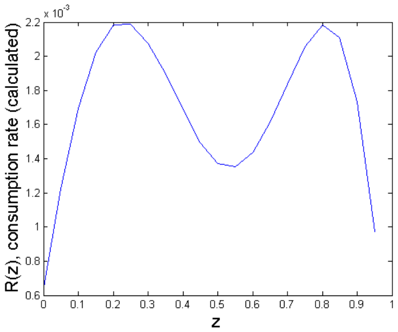
In Figure 9 we observe that if we use matrix M_1 in Tikhonov- as well as in Landweber-Method then the consumption rate at the top and the bottom goes to zero for both the datasets.



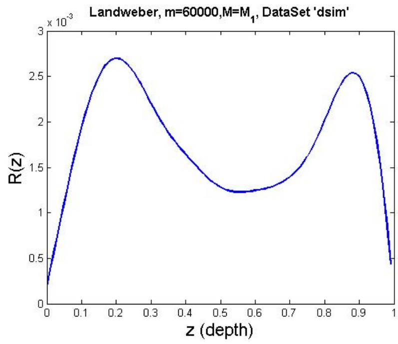
(a) Tikhonov-regularize solution with $\alpha = 10^{+5}$ on 'dmeas'



(b) Landweber on 'dmeas'



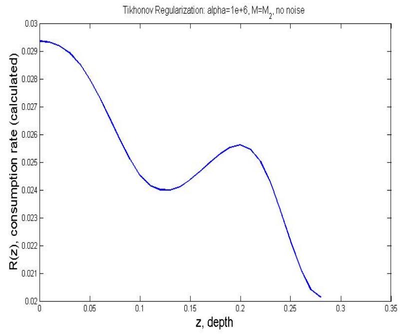
(c) Tikhonov-regularize solution with $\alpha = 10^{+8}$ on 'dsim'



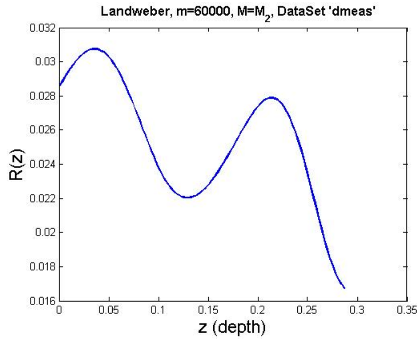
(d) Landweber on 'dsim'

Figure 9: Results on the two data sets using $M = M_1$

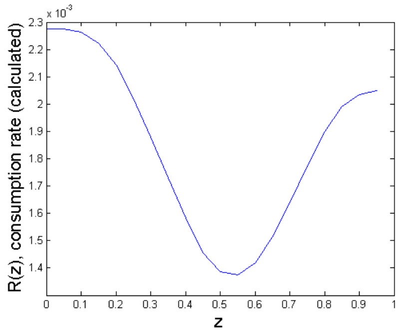
This result was for us unreal. That's why we decided to change the matrix and use Neumann's boundary conditions, that is use $M = M_2$. In Figure 10 we see the results.



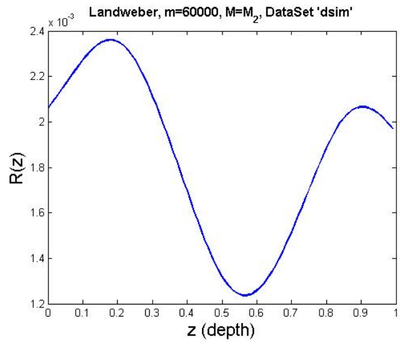
(a) Tikhonov-regularize solution with $\alpha = 10^{+6}$ on 'dmeas'



(b) Landweber on 'dmeas'



(c) Tikhonov-regularize solution with $\alpha = 10^{+8}$ on 'dsim'



(d) Landweber on 'dsim'

Figure 10: Results on the two data sets using $M = M_2$

We notice the difference between results with matrix M_1 and M_2. We think that the solution derived with M_2 are those which agree best with reality.

7 Conclusion

In this report we have looked at solving an inverse problem applied to a biological system. In the sediment there are nutrients such as Nitrogen and Oxygen that are consumed by organisms. In this report we proposed models to estimate the rate of consumption of nutrients by organisms in the sediment. First we predicted a form of the consumption rate so that we could then use this to determine the concentration of nutrient in the sediement. Although we did not match the results directly with experimentla data in this report we have shown that is possible to do so. The second method we applied to determine the consumption rate lead us to solving an inverse problem numerically. We modelled the biological system as a PDE and showed how it could be discretized using finite difference methods.

Due to the ill-posedness of the inverse problem we needed to use regularization methods to get a good solution. We implemented both Tikhonov and Landweber and compared this results. Landweber seems to give the most accurate results, but Tikhonov is by far the most computational efficient method.

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