1 Analytical solutions of transport equations

1.1 Notation

Let $\Omega \subseteq \mathbb{R}^n$ be open and connected, let $T \in \mathbb{R}^+$ and let $\Omega_T := \Omega \times (0, T)$. Furthermore we assume that $\Gamma \subseteq \overline{\Omega_T}$ is a n-dimensional manifold. We will later also need an unit normal vector to Γ at (x, t), which we will denote by $\nu(x, t)$. For existence of $\nu(x, t)$ see Remark 1. Furthermore, we define for two open and connected sets $V \subseteq \mathbb{R}^n$, $W \subseteq \mathbb{R}^m$ and a number $k \in \mathbb{N}$ the following functions-spaces :

$$C^0(V, W) := \{u : V \to W |\ u \text{ is continuous }\},$$
$$C^k(V, W) := \{u : V \to W |\ u \text{ is } k\text{-times differentiable }\}.$$

During the remarks, we will also occasionally need the following small balls:

$$B_\varepsilon(y) := \{x \in \mathbb{R}^n : \ \|x - y\| < \varepsilon\}.$$

as well as the characteristic function of a set $M \subseteq \mathbb{R}^n$

$$\chi_M(x) := \begin{cases} 1 & x \in M, \\ 0 & x \notin M. \end{cases}$$

Remark 1. A sufficient criterium that $\nu(x, t)$ is well defined is that „Γ is C^1" in (x, t). The condition „Γ is C^1" roughly means that Γ can locally be written as the graph of a C^1 function $\Psi : \mathbb{R}^n \to \mathbb{R}$ (for details see Appendix C.1 in [1]).

1.2 Problem Statement

For $\Omega \subseteq \mathbb{R}^2$ let Ω_T and Γ be as above (regularity on Γ will be imposed later). We will try to find a solution $c : \Omega_T \to \mathbb{R}$ for the following boundary-value problem:

$$c_t(x, t) + \nabla \cdot (c(x, t)\vec{q}(x)) = f(x, t), \qquad (x, t) \in \Omega_T, \tag{1a}$$
$$c(x, t) = c_0(x, t), \qquad (x, t) \in \Gamma \tag{1b}$$

where $\vec{q} \in C^1(\Omega, \mathbb{R}^2)$, $f \in C^0(\Omega_T, \mathbb{R}_0^+)$ and $c_0 \in C^0(\Gamma, \mathbb{R})$.

1.3 Selected Results

Lemma 1. *Equation* (1a) *is equivalent to the (fully) linear, inhomogeneous transport equation*

$$c_t + \vec{q} \cdot \nabla c + gc = f. \tag{2}$$

where (x, t) is dropped in the notation and $g = \nabla \cdot \vec{q}$.

Proof. Direct calculation. □

Lemma 2. *Assume that Γ is C^1 and that $\nu(x,t)\cdot\vec{q}(x)\neq 0$ on Γ (i.e. Γ is noncharacteristic, this meaning of this will be explained in the proof). Then there is a unique solution of (1) in a neighborhood of Γ.*

Proof. We follow Chapter 3 of [1] and apply the so-called *method of characteristics*: We assume that we start at an arbitrary point $(x_0,t_0)\in\Gamma$ and then „follow the flow". We parametrized the streamline emerging at (x_0,t_0) by $x=x(s)$ as well as $t=t(s)$ where $x(0)=x_0$ as well as $t(0)=t_0$ (here $s\in[0,\infty)$). If we define $C(s):=c(x(s),t(s))$, $F(s):=f(x(s),t(s))$ and $G(s):=g(x(s),y(s))$ this yields:

$$\frac{d}{ds}C=\dot{t}c_t+\dot{x}\cdot\nabla c.$$

Comparing this with (2) yields the following system of ODEs:

$$\dot{C}(s)+G(s)C(s)=F(s),\qquad C(0)=c_0(x_0,t_0) \tag{3a}$$
$$\dot{x}(s)=\vec{q}(x(s)),\qquad x(0)=x_0 \tag{3b}$$
$$\dot{t}(s)=1,\qquad t(0)=t_0 \tag{3c}$$

Since we assumed that $\vec{q}$ is Lipschitz-continuous, (3b) and (3c) have a unique solution due to the Picard-Lindelöf theorem. Having found solutions $x(s)$, $t(s)$ to these equations, we can solve (3a) in the same way.

In order to simplify notation, let us now combine the space and time variables and write $y_0:=(x_0,t_0)$. The domain Ω_T hence becomes a cylindrical subset of $\mathbb{R}^{n+1}$. Up to now, we found a way to construct a solution for any given point $y_0\in\Gamma$. Unfortunately it is still not clear, if the set of all these solution yields a well-defined solution to the problem. For example, characteristic curves may run inside of Γ and cause contradicting function values, or there might be points close to Γ, which are not hit by characteristic curves at all. This is, where the property of Γ to be *non-characteristic*, comes into play (i.e. $\nu(x,t)\cdot\vec{q}(x)\neq 0$). A more accessible formulation of this is: Γ does not follow the flow field. Let us denote by $X(s,y_0):=y(s)$ the characteristic curve starting at $y_0\in\Gamma$, i.e. $X(0,y_0)=y_0$. Keep in mind that from now on X is a function of s as well as of y_0, i.e. $X:[0,\infty)\times\Gamma\to\mathbb{R}^{n+1}$. We will now show that if Γ is non-characteristic at y_0, the function $X(s,y_0)$ is one-to-one in a neighborhood of y_0. It will then follow that indeed all points are hit by characteristic curves exactly one time and the solution will be well-defined in a neighborhood of Γ. To see this, we make use of the inverse-function theorem. Due to (3b), (3c) as well as the construction of Ω, the Jacobian of X at $(0,y_0)$ is given as follows:

$$\begin{aligned} JX|_{(0,y_0)} &= \begin{pmatrix} \frac{\partial X}{\partial s}(0,y_0) & \frac{\partial X}{\partial y_0}(0,y_0)\end{pmatrix} \\ &= \begin{pmatrix} \vec{q}(x_0) & \left(\frac{\partial X}{\partial y_0}(0,y_0)\right)_1 \\ 1 & \left(\frac{\partial X}{\partial y_0}(0,y_0)\right)_{n+1}\end{pmatrix}\in\mathbb{R}^{(n+1)\times(n+1)}.\end{aligned}$$

Now observe that since Γ is C^1, the columns of $\frac{\partial X}{\partial y_0}(0, y_0)$ form a basis of the n-dimensional tangential plane to Γ at y_0. Since we assumed that $\vec{q}(x_0) \cdot \nu(x_0, t_0) \neq 0$ (i.e. $\vec{q}(x_0)$ does not lie in the tangential plane), the matrix $JX|_{(0,y_0)}$ has full rank and we can apply the inverse-function theorem. Hence the is a local one-to-one mapping of characteristic curves and points, i.e. the constructed solution is well-defined. □

2 Remarks concerning out setting

Remark 2. In out setting we will consider the following problem: Let $\Omega := (0,1)^2$ and $\mu << 1$. Assume that there is a source around point $x_{\text{so}} := (\mu, 1-\mu)^\top \in \Omega$, namely in the area $I := B_\mu(x_{\text{so}})$. Furthermore assume that there is also a sink around point $x_{\text{si}} := (1-\mu, \mu)^\top \in \Omega$, namely in the area $O := B_\mu(x_{\text{si}})$. We will denote the source by $Q_{\text{so}}(x) := q_{\text{in}} \cdot \chi_I(x)$ and the sink by $Q_{\text{si}}(x) := q_{\text{in}} \cdot \chi_O(x)$ for some $q_{\text{in}} \in \mathbb{R}^+$. Following [2], will now try to describe the flow in $\Omega_T := \Omega \times (0,T)$ in the following way:

$$
\begin{aligned}
c_t(x,t) + \nabla \cdot (c(x,t)\vec{q}(x)) &= c_a(t)Q_{\text{so}}(x) - c(x,t)Q_{\text{si}}(x), \qquad (x,t) \in \Omega_T, && \text{(4a)}\\
c(x,t) &= c_0(x,t), \qquad (x,t) \in \Gamma, && \text{(4b)}
\end{aligned}
$$

where $c_a(t)$ denotes the arterial input function. This of course leaves the question where to put the $2D$ starting manifold $\Gamma \subseteq \overline{\Omega_T}$ and which boundary values $c_0(x,t)$ to prescribe on it. Since contrast-agent is brought into the system continuously within the area O, we define $\Gamma := \partial B_\varepsilon(x_{\text{so}}) \times [0,T)$ for $\varepsilon < \mu$. Since the contrast-agent is created by the source at I, we assume that $c_0(x,t) = 0$ on Γ. In order to analyze the contrast-agent flow, we will let $\varepsilon \to 0$. Unfortunately we run into problems for each nonzero ε, since there will be contrast-agent created within $B_\varepsilon(x_{\text{so}})$ which cannot exit the system. We will hence exclude $B_\varepsilon(x_{\text{so}})$ from our analysis. This brings us to the final problem formulation:

Let $\Omega^\varepsilon := \Omega \setminus \overline{B_\varepsilon(x_{\text{so}})}$ and let Ω^ε_T be as above. Let furthermore $\Gamma_\varepsilon := \partial B_\varepsilon(x_{\text{so}}) \times [0,T)$. We will study the following class of problems:

$$
\begin{aligned}
c^\varepsilon_t + \vec{q} \cdot \nabla c^\varepsilon + cQ_{\text{so}} &= c_a Q_{\text{so}}, \qquad (x,t) \in \Omega^\varepsilon_T, && \text{(5a)}\\
c^\varepsilon &= 0, \qquad (x,t) \in \Gamma_\varepsilon && \text{(5b)}
\end{aligned}
$$

CH: I am wondering: Where in (5) is the influence of the sink coming into play? Here the following situation is assumed

Here it is furthermore assumed, that $\vec{q}(x) = -\frac{K}{\mu}\nabla p(x)$ where p is the solution of the following (elliptic) boundary value problem:

$$
\left|
\begin{aligned}
\nabla \cdot \left(-\frac{K}{\mu}\nabla p(x)\right) &= Q_{\text{so}}(x) + Q_{\text{si}}(x), \qquad && x \in \Omega,\\
p_\nu(x) &= 0, && x \in \partial\Omega \setminus \{x_0\},\\
p(x_0) &= 0,
\end{aligned}
\right| \qquad (6)
$$

for some constants $K, \mu \in \mathbb{R}^+$ and $x_0 \in \partial\Omega$. The condition $p(x_0) = 0$ is necessary to make the elliptic problem well-posed. For a detailed explanation see [2].

Remark 3. We will now solve (5) using the method of characteristics. Substituting $x = x(s)$, $t = t(s)$ and denoting $C(s) := c^\varepsilon(x(s), t(s))$, $\tilde{Q}_{\mathrm{so}}(s) := Q_{\mathrm{so}}(x(s))$, $\tilde{Q}_{\mathrm{si}}(s) := Q_{\mathrm{si}}(x(s))$ and $C_a(s) := c_a(t(s))$ yields the following system of ODEs:

$$C'(s) + \tilde{Q}_{\mathrm{so}}(s)C(s) = C_a(s)\tilde{Q}_{\mathrm{so}}(s), \quad C(0) = 0 \tag{7a}$$

$$x'(s) = \vec{q}(s), \qquad x(0) = x_0 \tag{7b}$$

$$t'(s) = 1, \qquad t(0) = t_0, \tag{7c}$$

where $x_0 \in \partial B_\varepsilon(x_{\mathrm{so}})$.

In order to solve (7a), we use the method of *varying the constant*. First, we solve the homogenous ODE:

$$\dot{C}(s) = -\tilde{Q}_{\mathrm{so}}(s)C(s) \qquad \Longrightarrow \qquad C(s) = e^{-\int_0^s \tilde{Q}_{\mathrm{so}}(u)\,\mathrm{d}u}k, \qquad k \in \mathbb{R}$$

In order to simplify notation a bit, we define $R(s) := \int_0^s \tilde{Q}_{\mathrm{so}}(u)\,\mathrm{d}u$. We now assume that $k = k(s)$. A comparison of coefficients and use of the initial condition $C(0) = 0$ yields:

$$\dot{k}(s)e^{-R(s)} = C_a(s)\tilde{Q}_{\mathrm{so}}(s) \qquad \Longrightarrow \qquad k(s) = \int_0^s e^{R(v)}C_a(v)\tilde{Q}_{\mathrm{so}}(v)\,\mathrm{d}v.$$

This yields the following solution of (7a) originating at point $(x_0, t_0) \in \Omega$:

$$C(s) = \int_0^s e^{-(R(s)-R(v))}C_a(v)\tilde{Q}_{\mathrm{so}}(v)\,\mathrm{d}v$$

Also solving (7c) yields $t = s + t_0$ with $s \geq 0$ and hence $t \geq t_0$. Plugging this into the above equation yields:

$$C(t) = \int_{t_0}^t e^{-(R(t-t_0)-R(v-t_0))}c_a(v)\tilde{Q}_{\mathrm{so}}(v - t_0)\,\mathrm{d}v \tag{8}$$

where as above $R(v) = \int_0^v Q_{\mathrm{so}}(x(u))\,\mathrm{d}u$, $\tilde{Q}_{\mathrm{so}}(v) = Q_{\mathrm{so}}(x(v))$ and $C(t) = c(x(t - t_0), t)$. This is a (semi-)Lagrangian formulation of the flow. Going back to the Eulerian approach, we observe that since $\vec{q}$ is independent of t we can fix the position by assuming that $t - t_0 = k$ for constant $k \in \mathbb{R}^+$. For each starting timepoint t_0 the concentration at the location $x_k := x(k)$ is hence given by (8) in the following way:

$$c_{t_0}(x_k) = \int_{t_0}^{t_0+k} e^{-(R(k)-R(v-t_0))}c_a(v)\tilde{Q}_{\mathrm{so}}(v - t_0)\,\mathrm{d}v$$

Since the flow first arrives at location x_k at timepoint k, this yields CH: I'm not sure if it is allowed to change from Lagrangian t_0 to Eulerian t:

$$c(x_k, t) = \begin{cases} 0 & t < k \\ \int_t^{t+k} e^{-(R(k)-R(v-t))}c_a(v)\tilde{Q}_{\mathrm{so}}(v - t)\,\mathrm{d}v & t \geq k \end{cases}$$

Assuming that $Q_{\mathrm{so}}(x) = q_{\mathrm{in}}\delta_{x_{\mathrm{so}}}$ and hence $\tilde{Q}_{\mathrm{so}}(s) = 1$ for $s = 0$ and 0 elsewhere yields:

$$c(x_k, t) = \begin{cases} 0 & t < k \\ q_{\mathrm{in}}e^{-q_{\mathrm{in}}}c_a(t) & t \geq k \end{cases}$$

3 Deriving a PDE for the impuls-response functions

We will now try to derive an equation the impuls-response functions need to fulfill, if the functions are solution to the PDE (4). Let us assume that the solution can be represented in the following way:

$$c(x,t) = \int_0^t c_a(s) I(x, t-s)\,\mathrm{d}s.$$

If we want to use this relationship with (4), we will need to calculate the derivative w.r.t. t. This is done as follows:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t c_a(s) I(x,t-s)\,\mathrm{d}s &= \lim_{h\to 0} \frac{\int_0^{t+h} c_a(s) I(x,t+h-s)\,\mathrm{d}s - \int_0^t c_a(s) I(x,t-s)\,\mathrm{d}s}{h} \\
&= \lim_{h\to 0} \frac{\int_0^t c_a(s)\left(I(x,t+h-s) - I(x,t-s)\right)\mathrm{d}s}{h} \\
&\qquad + \frac{1}{h}\int_t^{t+h} c_a(s) I(x,t+h-s)\,\mathrm{d}s. \\
&= \int_0^t c_a(s) I_t(x,t-s)\,\mathrm{d}s + c_a(t) I(x,0).
\end{aligned}$$

CH: Assuming that $I(x,0) = 0$ (from the looks of the impuls-response functions obtained from the data this should hold), we obtain:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t c_a(s) I(x,t-s)\,\mathrm{d}s = \int_0^t c_a(s) I_t(x,t-s)\,\mathrm{d}s.$$

Combining this with (4) yields:

$$\begin{aligned}
\int_0^t c_a(s)\big[I_t(x,t-s) + \nabla\cdot(\vec{q}(x) I(x,t-s)) \\
+ I(x,t-s)Q_{\mathrm{si}}(x) - \delta_0(t-s)Q_{\mathrm{so}}(x)\big]\,\mathrm{d}s = 0.
\end{aligned}$$

where δ_0 is the delta-distribution with respect to time. Let us denote the term in squared brackets with $J(x,t)$, then we can write this equation as

$$\int_0^t c_a(s) J(x,t-s)\,\mathrm{d}s = 0 \quad \text{for all } x \in \Omega.$$

The following lemma shows that this implies that $J(x,t) = 0$ for all $x \in \Omega, t \in [0,\infty)$. We analyze the above equation for an arbitrary point in Ω.

Lemma 3. *Let $j, c_a : [0,\infty) \to \mathbb{R}$ be continuous and assume that $c_a \not\equiv 0$. If it holds for all $t > 0$ that*

$$\int_0^t c_a(s) j(t-s)\,\mathrm{d}s = 0$$

then $j \equiv 0$.

Proof. Assume that $j \neq 0$ and let t_j be the largest $t \in [0, \infty)$ such that $j(t_j) = 0$. Since we assumed that j is continuous, there is a small interval $(t_j, t_j + \beta)$ where either $j > 0$ or $j < 0$. For sake of simplicity assume that $j > 0$ on $(t_j, t_j + \beta)$, the case that $j(t_j) < 0$ will follow analogously. For c_a we analogously define the timepoint t_c and analogously assume that $c_a > 0$ on $(t_c, t_c + \delta)$. Let $\gamma := \min(\alpha, \delta)$. Then it holds for $t_0 := t_c + t_j + \gamma$ that

$$\int_0^{t_0} c_a(s) j(t - s)\,\mathrm{d}s = \int_{t_0-\gamma}^{t_0} c_a(s) j(t - s) > 0.$$

We can hence conclude the assertion. □

Next we observe that in our case Q_{so} and Q_{si} are both independent of time. As a consequence, one can see that if C has the above structure, $I(x, t)$ needs to fulfill the following equation:

$$I_t(x, t) - \nabla \cdot (\vec{q}(x) I(x, t)) = \delta_t Q_{\mathrm{so}}(x) - I(x, t) Q_{\mathrm{si}}(x)$$

Hence $I(x, t)$ can be regarded as a solution of a the transport equation with a Dirac-Delta as Arterial Input.

References

[1] L. C. Evans; *Partial Differential Equations*, American Mathematical Society, Providence, Rhode Island, 1998.

[2] Heck, Hodneland, Hanson, Lundervold, Modersitzki, Malyshev; *A one-compartment field model for perfusion*, work in progress, 2015.

Erlend Hodneland, Erik Hanson
University of Bergen

Constantin Heck
MIC, University of Lübeck
heck@mic.uni-luebeck.de
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