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Optimal bounds in reaction diffusion problems with variable diffusion coefficient

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Abstract

A diffussion-reaction problem is considered involving a variable diffusion coefficient. A maximum principle for a functional of the solution is proven, which allows to derive bounds for various quantities of interest. The bounds are optimal in the sense that they become sharp if the domain is a slab or an N-sphere and the diffusion coefficient has an appropriate form.

1 Introduction

A chemical reaction diffusion process, with a single reactant of concentration $u(x)$, taking place in an inhomogeneous catalyst Ω is often modeled by

$$\begin{cases} \operatorname{div}(\sigma(x)\nabla u) + f(u) = 0 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega\,. \end{cases} \tag{1.1}$$

Here $\sigma(x)$ is the diffusion coefficient and $f(u)$ describes the kinetics of the reaction. There are of course numerous other possible backgrounds for problem (1.1).

In the case $\sigma(x) = \text{const.}$ there is a great amount of literature available on problem (1.1), dealing with many interesting phenomenae such as critical parameter values, dead cores and other features.

In this work bounds are derived with a modification of a method introduced by Payne & Stakgold [1] and extended by Schaefer & Sperb [2]. The bounds derived in these papers are optimal in the sense that they become sharp in the limit as the domain Ω degenerates into an infinite slab or strip. The bounds derived in this paper are also sharp if $\sigma = \text{const.}$ and Ω is a slab, but, in addition, there is a new situation here: if $\sigma = \sigma(r) = \frac{1}{r^{2(N-1)}}$ and Ω is a spherical shell $R_1 \leq r \leq R_2$ in N-dimensions, then the bounds are sharp. Though σ is singular at the origin there is still a bounded solution if $R_1 = 0$, such that the diffusion flux $|\sigma \cdot \nabla u|$ remains bounded for $r \to 0$.

2 Maximum principle for a functional of u

Our bounds will be derived from a maximum principle for the functional

$$P = \sigma \cdot |\nabla u|^2\, g(u) + h(u) \tag{2.1}$$

where u is the solution of (1.1) and $g(u), h(u)$ will be specified later on.

It is convenient to derive the main result from auxiliary results, starting with

Lemma 2.1. *Let Ω be a plane domain and choose $g(u) = e^{-\alpha\cdot u}$, $h(u) = 2\int_0^u e^{-\alpha\cdot v} f(v)\,dv$, $u =$ solution of (1.1). Then P satisfies the elliptic equation*

$$\begin{aligned} &\Delta P - \frac{1}{\sigma}\,\nabla\sigma\cdot\nabla P + \frac{\vec{W}\cdot\nabla P}{|\nabla u|^2} = e^{-\alpha u}\cdot|\nabla u|^2\{\Delta\sigma + 2\alpha\,\nabla\sigma\cdot\nabla u + \sigma f\} \\ &\vec{W} = \frac{2f}{\sigma}\,\nabla u - \frac{1}{\sigma}\,e^{\beta u}\,\nabla P - 2e^{-\alpha u}\sigma\cdot He[\nabla u,\nabla u]\,, \end{aligned} \tag{2.2}$$

where He denotes the Hessian of $\log\sigma$, i.e. $He[\nabla u,\nabla u] = (\log\sigma)_{/ik}\,u_{/i}\,u_{/k}$, where a subscript denotes a derivative and the summation convention is used.

Proof. Straightforward calculation gives

$$\nabla P = \nabla\sigma\cdot|\nabla u|^2\,g + 2\sigma g\,\nabla\nabla u\cdot\nabla u + \sigma|\nabla u|^2\,g'\nabla u + h'\cdot\nabla u \tag{2.3}$$

$$\begin{aligned} \Delta P = {} & \Delta\sigma\cdot|\nabla u|^2\,g + 2\sigma g(|\nabla\nabla u|^2 + \nabla(\Delta u)\cdot\nabla u) \\ & + \sigma|\nabla u|^2(g'\Delta u + g''|\nabla u|^2) + h'\Delta u + h''|\nabla u|^2 \\ & + 4\nabla\sigma(\nabla\nabla u\cdot\nabla u)g + 2\nabla\sigma\cdot\nabla u\cdot g'|\nabla u|^2 + 4\sigma(\nabla\nabla u\cdot\nabla u\cdot\nabla u)g'\,. \end{aligned} \tag{2.4}$$

Here the following notations have been used:

$$\nabla\nabla u\cdot\nabla u = u_{/ik}\,u_{/k}, \quad |\nabla\nabla u|^2 = u_{/ik}\,u_{/ik}\ .$$

We can now use the differential equation for u to express the third derivative term $\nabla(\Delta u)$ as follows:

$$\nabla(\Delta u) = -\frac{f}{\sigma}\,\nabla u + \frac{f}{\sigma^2}\,\nabla\sigma - \nabla\nabla(\log\sigma)\cdot\nabla u - \nabla(\log\sigma)\cdot\nabla\nabla u\,. \tag{2.5}$$

Furthermore, we use the identity (valid for any smooth function in $\mathbb{R}^2$)

$$|\nabla\nabla u|^2 = (\Delta u)^2 + \frac{2}{|\nabla u|^2}\,(|\nabla\nabla u\cdot\nabla u|^2 - \Delta u(\nabla\nabla u\cdot\nabla u)\cdot\nabla u)\,. \tag{2.6}$$

As another step we eliminate the terms $\nabla\nabla u\cdot\nabla u$ and $|\nabla\nabla u|^2$ through the relations (2.3), (2.6). After a considerable amount of algebra (which can easily be done e.g. by using "Mathematica") one finds, with our choice of $g(u)$ and $h(u)$, the equation (2.2).

In $N > 2$ dimensions we can derive an elliptic inequality. To this end we rewrite the relation (2.3) in the form

$$\frac{1}{2\sigma g}\,(\nabla P - \vec{A}) = \nabla\nabla u \cdot \nabla u\,, \tag{2.7}$$

with the obvious interpretation of the vector $\vec{A}$. Schwarz's inequality for vectors then tells us that

$$\frac{1}{4\sigma^2 g^2}\,(\nabla P - \vec{A})^2 \le |\nabla\nabla u|^2 \cdot |\nabla u|^2\,. \tag{2.8}$$

The relations (2.7) and (2.8) allow to eliminate all terms in (2.4) containing the expression $\nabla\nabla u$. □

The result is summarized in

Lemma 2.2. *For $N > 2$ the functional*

$$P = g(u)\cdot|\nabla u|^2 + 2\int_0^u g(v)\,f(v)\,dv \quad \textit{satisfies} \tag{2.9}$$

$$\begin{aligned}\Delta P - (\log g)'\nabla u\cdot\nabla P + \frac{\vec{B}\cdot\nabla P}{|\nabla u|^2} \ge & -2g\cdot\sigma\cdot(g^{-1/2})''\cdot|\nabla u|^4 \\ & + |\nabla u|^2\{-g'(f + \nabla u\cdot\nabla\sigma) + 2g\cdot\mu\sqrt{\sigma}\}\end{aligned} \tag{2.10}$$

where $\vec{B} = \frac{2f}{\sigma}\,\nabla u - \dfrac{1}{2g\sigma}\cdot\nabla P$ *and μ is the lowest eigenvalue of the matrix*

$$S_{ik} = \Delta(\sqrt{\sigma})\,\delta_{ik} - \sqrt{\sigma}\cdot(\ell u\,\sigma)_{/ik}\,.$$

The first result concerns the case $N = 2$. Let k denote the curvature of the boundary and set

$$\beta_2 = \min_{\partial\Omega}\left(\sigma^{-1/2}\cdot\frac{2\sigma}{\partial n} + 2\sigma^{1/2}\cdot k\right),\quad \frac{\partial}{\partial n}:\ \text{outward normal derivative} \tag{2.11}$$

$$\gamma = \max_{\Omega}(|\nabla\sigma|\,\sigma^{-1/2})\,, \tag{2.12}$$

$$\tau = \max_{\Omega}(\sqrt{\sigma}\cdot|\nabla u|)\,. \tag{2.13}$$

Theorem 2.3. a) *the matrix $M_{ik} = \Delta\sigma\cdot\delta_{ik} - 2\sigma(\log\sigma)_{/ik}$ has the lowest eigenvalue μ_2 and α can be chosen so that*

$$\mu_2 - 2\alpha\gamma + \alpha f(u) \ge 0 \quad \textit{for}\quad 0 \le u \le u_m\,.$$

b) $\beta_2 \ge \alpha\tau$. *Then the function*

$$P = e^{-\alpha u}\cdot\sigma\,|\nabla u|^2 + 2\int_0^u e^{-\alpha v} f(v)\,dv$$

takes its maximum at a point where $|\nabla u| = 0$.

Remark: In b) we need an upper bound for the quantity $\tau = \max_\Omega(\sqrt{\sigma}\cdot|\nabla u|)$ containing the gradient of the solution. We will see that Theorem 2.3 often allows to determine a bound for τ.

Proof. If condition a) is satisfied, P satisfies an elliptic inequality by (2.2). The maximum principle then tells us that maximum of P must occur on $\partial\Omega$ or at a point where a coefficient of ∇P becomes singular, i.e. where $\nabla u = 0$. We therefore check the normal derivative of P on $\partial\Omega$. Since $u = 0$ on $\partial\Omega$ we have

$$P = e^{-\alpha u}\cdot u_n^2 + 2\int_0^u e^{-\alpha u}\cdot f(v)\,dv, \quad u_n = \frac{\partial u}{\partial n}\,. \tag{2.14}$$

Hence

$$P_n = \sigma_n\cdot u_n^2 + 2\sigma\cdot u_{nn}\cdot u_n - H\alpha\sigma u_n^3 + 2f\,u_n\,. \tag{2.15}$$

□

We now use the facts that on $\partial\Omega$ we can write

$$\Delta u = u_{nn} + k u_n \tag{2.16}$$

and since $\partial\Omega \in C^{2+\varepsilon}$, the differential equation for u also is valid on $\partial\Omega$, that is

$$\sigma(u_{nn} + k u_n) + \sigma_n\cdot u_n = -f\,. \tag{2.17}$$

Elimination of u_{nn} in (2.15) allows to write

$$P_n = -u_n^2(\alpha\sigma u_n + \sigma_n + 2\sigma k) = -|\nabla u|^2\,\sqrt{\sigma}\,\left(\frac{\sigma_n}{\sqrt{\sigma}} + 2\sqrt{\sigma}\,k - \alpha\frac{|\nabla u|}{\sqrt{\sigma}}\right). \tag{2.18}$$

By condition b) we know that $P_n \le 0$. The boundary point lemma would be violated if the maximum were to occur on $\partial\Omega$. This proves the statement of Theorem 2.3.

In case of $N \ge 3$ dimensions we have the corresponding result. The quantity ω_2 defined in (2.11) is replaced now by

$$\beta_N = \frac{\sigma n}{\sqrt{\sigma}} + 2\sqrt{\sigma}\,(N-1)\,H, \quad H = \text{mean curvature of } \partial\Omega\,. \tag{2.19}$$

Then one has

Theorem 2.4. *Assume that $\partial\Omega \in C^{2+\varepsilon}$, $f \in C^1$ and*

a) *The matrix $\Delta(\sqrt{\sigma})\cdot\delta_{ik} - \sqrt{\sigma}(\log\sigma)_{/ik}$ has the lowest eigenvalue μ_N and for $0 \le u \le u_m$ one has*

$$\sqrt{\sigma}\cdot\mu_N + \frac{1}{1+u}\,f(u) \ge \frac{1}{1+u}\,\gamma\tau\,. \tag{2.20}$$

b) *$\beta_N \ge 2\alpha\tau$. Then*

$$P = \frac{\sigma\cdot|\nabla u|^2}{(1+\alpha u)^2} + 2\int_0^u \frac{f(v)}{(1+\alpha v)^2}\,dv$$

takes its maximum where $\nabla u = 0$.

Proof. The choice $g(u) = \frac{1}{(1+\alpha u)^2}$ makes the term containing $|\nabla u|^4$ in (2.10) vanish. Condition (2.20) ensures that P satisfies an elliptic inequality. The same calculation as in the foregoing proof shows that if b) holds then $\frac{\partial P}{\partial n} \leq 0$ on $\partial\Omega$, so that the boundary point lemma can be invoked again. This proves Theorem 2.4. □

Remarks:

(1) For $\sigma = \frac{1}{r^{2(N-1)}}$ and Ω a spherical shell in N-dimensions, a radially symmetric solution of (1.1) satisfies

$$\frac{1}{r^{N-1}} \left(r^{N-1}\sigma(r)\, u_r\right)_r + f(u) = 0 \;\; r \text{ in } (R_1, R_2)\,. \tag{2.21}$$

Taking the new variable $s = \frac{1}{N}\, r^N$ we find

$$\frac{1}{r^{N-1}} \left(r^{N-1} \cdot \frac{1}{r^{2(N-1)}}\, u_r\right)_r = u''(s)$$

hence (2.21) is equivalent to

$$u'' + f(u) = 0 \;\; \text{for} \;\; s\; in\left(\frac{R_1^N}{N}\,,\; \frac{R_2^N}{N}\right), \tag{2.22}$$

and then

$$u_s^2 + 2F(u) = \frac{1}{r^{2(N-1)}}\, u_r^2 + 2F(u) = \sigma|\nabla u|^2 + 2F(u) = \text{const.}\,. \tag{2.23}$$

This is the optimal case of Theorem 2.4 with $\alpha = 0$.

2) For $N = 2$ and $\sigma = \sigma(r)$ the eigenvalue μ_2 of the matrix M_{ik} is given by

$$\mu_2(r) = \frac{\sigma'^2}{\sigma} - \left|\frac{\sigma'^2}{\sigma} + \frac{\sigma'}{r} - \sigma''\right|.$$

In particular, if $\frac{\sigma'^2}{\sigma} + \frac{\sigma'}{r} - \sigma'' \geq 0$ then

$$\mu_2(r) = \sigma'' - \frac{\sigma'}{r} = r\left(\frac{\sigma'}{r}\right)', \tag{2.24}$$

3 Examples and applications

A. $f(u) = 1,\; N = 2$

We first consider the analog of the “torsion problem”, i.e.

$$\begin{cases} div(\sigma \cdot \nabla\psi) + 1 = 0 & \text{in } \Omega \\ \psi = 0 & \text{on } \partial\Omega\,. \end{cases} \tag{3.1}$$

In order to make the assumptions required in Theorem 2.4 explicit we need an upper bound for $\tau = \max_\Omega(\sqrt{\sigma} \cdot |\nabla u|)$: The lower eigenvalue μ_2 of the matrix

$$M_{iR} = \Delta\sigma \cdot \delta_{ik} - 2\sigma(\log\sigma)_{\prime ik} \quad \text{and} \quad \gamma = \max_{\overline{\Omega}} \frac{|\nabla\sigma|}{\sqrt{\sigma}}$$

must satisfy

$$\mu_2 - 2\alpha\gamma + \alpha \geq 0 \tag{3.2}$$

for some α which has to be determined. In addition we need to satisfy

$$\min_{\partial\Omega} \left(\frac{1}{\sqrt{\sigma}} \frac{\partial\sigma}{\partial n} + 2\sqrt{\sigma} \cdot k \right) \geq \alpha \cdot \tau\,. \tag{3.3}$$

If (3.2), (3.3) hold we know from Theorem 2.3 that

$$e^{-\alpha\psi}\sigma|\nabla\psi|^2 + 2\int_0^\psi e^{-\alpha v} dv \leq 2\int_0^\psi e^{-\alpha v}\, dv, \quad u_m = \max_\Omega u\,. \tag{3.4}$$

We rewrite (3.4) in the form

$$\sigma \cdot |\nabla\psi|^2 \leq \frac{2}{\alpha}\,(1 - e^{-\alpha(\psi_m - \psi)}\,. \tag{3.5}$$

Let x_m be a point in Ω where $u(x_m) = u_m$ and x_0 a point on $\partial\Omega$. Measuring the distance from x_m by r we use that

$$-\frac{d\psi}{dr} \leq |\nabla\psi| \leq \frac{1}{\sqrt{\sigma}} \sqrt{\frac{2}{\alpha}\,(1 - e^{-\alpha(\psi_m - \psi|}}\,. \tag{3.6}$$

Separation of variables and integration yields

$$\int_0^{\psi_m} \frac{du}{\sqrt{1 - e^{-\alpha(\psi_m - \psi)}}} \leq \sqrt{\frac{2}{\alpha}} \int_{x_m}^{x_0} \frac{1}{\sqrt{\sigma(r)}}\, dr = \sqrt{\frac{2}{\alpha}}\, d_\sigma\,, \tag{3.7}$$

with the obvious definition of d_σ. This is equivalent to the inequality

$$\psi_m \leq \frac{2}{\alpha}\, \log\left(\cosh\left(\sqrt{\frac{\alpha}{2}}\, d_\sigma\right)\right)\,. \tag{3.8}$$

We now combine (3.8) with inequality (3.5) evaluated on $\partial\Omega$. This gives after some simplification

$$\tau \leq \sqrt{\frac{2}{\alpha}} \cdot \tanh\left(\sqrt{\frac{2}{\alpha}}\, d_\sigma\right)\,. \tag{3.9}$$

Hence, for the validity of Theorem 2.3 it is sufficient to satisfy the set of inequalities

$$\begin{cases} \text{a)} \quad \mu_2 + \alpha \geq 2\alpha\gamma \\ \text{b)} \quad \beta_2 \geq \sqrt{2\alpha} \cdot \tanh\left(\sqrt{\frac{\alpha}{2}}\, d_\sigma\right) \end{cases} \tag{3.10}$$

for some $\alpha > 0$.

Numerical examples:

a) $\Omega =$ rectangle $(-1,1)\times(-2,2)$
$\sigma(x,y) = 1 + \frac{1}{4}\,(x^2+y^2)$.

One finds $\mu_2 = 0$, $\beta_2 \geq 0$ so that we can choose $\alpha = 0$. Then from (3.8) we get

$$\psi_m \leq 0.463 \quad (\text{exact: } \psi_m = 0.370)$$

and (3.9) yields

$$\tau \leq \delta_6 \leq 0.962 \quad (\text{exact: } \tau = 0.773)\,.$$

b) $\Omega =$ unit disk
$\sigma = e^{0\cdot 2\cdot r^2}$

$$\underline{\varphi(r)} = \frac{1}{2}\int_r^R t\cdot e^{-dk^2}dt = \underline{\frac{1}{4a}(e^{-\alpha r^2} - e^{-\alpha R^2})}\,.$$

One finds $\mu_2 = 0$, $\gamma_2 = 0.442$, $\beta_2 = 2.442$, $d_\sigma = 0.9676$, $\alpha = 4.4$ which leads to the bound $\psi_m \leq 0.362$. The exact value is $\psi_m = 0.227$.

f(u) = 1, N ¿2

If the assumptions of Theorem 2.4 are satisfied we have

$$\sigma\,\frac{|\nabla u|^2}{(\alpha u+1)^2} + 2\int_0^u \frac{dv}{(\alpha v + 1^2} \leq 2\int_0^{u_m}\frac{dv}{(\alpha v+1)^2}\,, \tag{3.11}$$

which can be rewritten as

$$\tau^2 \leq \max_{u\in(0,u_m)} \frac{2(u_m-u)(\alpha u+1)}{\alpha u_m + 1} = \frac{1+\alpha u_m}{2\alpha}\,. \tag{3.12}$$

In order to derive a bound for u_m we can use the same reasoning as the one following inequality (3.6), with $e^{-\alpha u}$ replaced by $\frac{1}{(\alpha u+1)^2}$.

After integration and some simplification one arrives at

$$\sqrt{\alpha u_m + 1}\cdot \arccos\Big(\frac{1}{\sqrt{\alpha u_m+1}}\Big) \leq \sqrt{\frac{\alpha}{2}}\,d_\sigma\,. \tag{3.13}$$

B. Applications of Bounds for ψ

The bounds for ψ derived in part 3.A are useful for the general problem (1.1) as the next result shows.

Theorem 3.1. *Assume that $\mu_N \geq 0$ and $\beta_N \geq 0$ and $f(0) > 0$ and $f' \geq 0$. Let ψ be the solution of* (3.1) *and $X(s)$ the solution of $X'' + f(X) = 0$ in $(0, s_0)$*

$$X'(0) = 0,\ X(s_0) = 0 \text{ with } s_0 = \sqrt{2\psi_m}\,.$$

Then $\overline{u}(x) = X(s(x))$ is a supersolution of problem (1.1). Here

$$s(x) = \sqrt{2(\psi_m - \psi(x))}\,.$$

Proof. By direct calculation one finds

$$\nabla s = -\frac{\nabla \psi}{s}$$

$$\Delta s = -\frac{\Delta \psi}{s} - \frac{|\nabla \psi|^2}{s^2} \,,$$

so that

$$\mathrm{div}(\sigma \cdot \nabla \psi) = \sigma \Delta \psi + \nabla \sigma \cdot \nabla s - \frac{1}{s}\left(1 - \frac{\sigma \cdot |\nabla \psi|^2}{s^2}\right)$$

Under the assumptions $\mu_N \geq 0$, $\beta_N \geq 0$ we can apply Theorem 2.4 which implies that

$$1 - \frac{\sigma \cdot |\nabla \psi|^2}{s^2} \geq 0 \,.$$

Setting now $\overline{u}(x) = X(s(x))$ we calculate

$$\Delta \overline{u} = X' \cdot \Delta s + X'' \cdot |\nabla s|^2$$

and

$$\sigma \cdot \Delta \overline{u} + \nabla \sigma \cdot \nabla \overline{u} = X' \, \frac{1}{s}\left(1 - \sigma \cdot \frac{|\nabla \psi|^2}{s^2}\right) + \sigma \cdot X'' \cdot \frac{|\nabla \psi|^2}{s^2} \,.$$

Therefore one has

$$\mathrm{div}(\sigma \cdot \nabla \overline{u}) + f(\overline{u}) = \left\{\frac{X'}{s} + f(X)\right\}\left[1 - \sigma \cdot \frac{|\nabla \psi|^2}{s^2}\right] \,.$$

To see the sign of the term in curly brackets we set

$$h(s) = X' + s f(X) \,.$$

We have $h(0) = 0$ and

$$h'(s) = X'' + f(x) + s f' \cdot X' \leq 0,$$

since $f' \geq 0$ and $X' \leq 0$ in $(0, s_0)$. Thus $\overline{u}$ satisfies

$$\mathrm{div}(\sigma \overline{u}) + f(\overline{u}) \leq 0 \text{ in } \Omega$$

and because of the definition s_0 we also have $\overline{u}(x) = 0$ for $x \in \partial\Omega$. This proves Theorem 3.1 □

Numerical example:

We take the same domain and σ as in Example a) before, and consider the Gelfand Problem

$$\begin{cases} \mathrm{div}(\sigma \nabla u) + \lambda e^u = 0 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \,. \end{cases} \tag{3.14}$$

A quantity of interest here (see also [3] is the critical value λ^*. For values $\lambda > \lambda^*$ problem (3.14) has no solution. The case $\sigma = 1$ has been discussed in [3] and it was shown that

$$\lambda^* \geq \frac{0.4392}{\psi_m} \tag{3.15}$$

with the exact value 0.3704 of ψ_m one finds in our case $\lambda^* \geq 1.186$ whereas the numerical solution of (3.14) gives $\lambda^* = 1.356$.

With the upper bound for ψ_m derived in example a) one would get the cruder bound

$$\lambda^* = 0.949\,.$$

Concluding Remark:

The methods developed in [3] can be combined with the results of this paper. This allows among other things an extension to parabolic problems of the form

$$\begin{cases} u_t = \operatorname{div}(\sigma \nabla u) + f(u) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \\ u(x,0) = u_0(x)\,. \end{cases} \tag{3.16}$$

References

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