

ISSUES IN TRANSMISSIVITY ESTIMATION

*G.N. Newsam***Abstract**

The dependence of transmissivity estimates on head data is both nonlinear and ill-posed, and so is difficult to analyse and solve. The paper looks at the setting of this problem, in particular in what spaces are the actual data and in what spaces can uniqueness be proven. The paper also looks at the problem of finding a discretization that has at least some of the useful properties found in discretizations of linear ill-posed problems based the singular value decomposition. As definitive answers have not yet been found to the many of the questions raised, the paper is intended to serve more as a platform for further work than as a report on results achieved.

1. Introduction

Water resource management is shaping up as a major issue for Australian communities. A succession of local crises (pollution of beaches and rivers, contaminated drinking water and land loss due to salinity) has dragged it into the limelight, and, in particular, has brought home the need for efficient management of what are quite limited resources [1]. Effective management requires good quantitative models of reality to resolve the many "What if?" scenarios that arise when a limited resource is to be distributed among many users. As is so often the case, the importance of the problem is reflected in the intrinsic interest and difficulty of the mathematical and numerical analysis needed to get reliable results from these models.

The particular mathematical problems considered here arise out of analysis of a model widely used in groundwater management: that is the modelling steady state flow in a confined aquifer as an elliptic p.d.e. The model assumes that the observable variables of piezometric head $\varphi(x)$ (i.e. water pressure in the aquifer) and recharge / discharge $q(x)$ of water in to / out of the aquifer may be reasonably related by a p.d.e. of the form:

$$\nabla \cdot (a(x) \nabla \varphi(x)) = q(x) \quad x \in \Omega \subseteq \mathfrak{R}^2 \quad (1)$$

where $a(x) > 0$ is the transmissivity of the aquifer and Ω is the region containing the aquifer. Effective management of groundwater requires repeated solution of this equation for φ under differing recharge regimes in order to explore the resulting changes in groundwater flows and

associated phenomena, such as the height of the water table and discharges at the margins of the aquifer.

Before such exploration can be carried out, however, the transmissivity a must be determined. Transmissivity essentially reflects the porosity of the aquifer and the ease with which water can flow through it. However, as the model is only valid on scales greater than the width of the aquifer, transmissivity is really a bulk property of the aquifer and includes the effects of large scale features such as cracks or gravel lenses as well as small scale pores. Thus transmissivity cannot be simply inferred from examination of rock cores from drills; indeed the only way to get "point" measurements of transmissivity is by what are known as pump tests (see, e.g., [6] and the references therein), and these are relatively costly to make on a large scale. Therefore the preferred method for determining transmissivity is to take measurements of recharge and piezometric head in the aquifer's existing equilibrium, and to use these and (1) to infer a .

This parameter identification problem is, however, an ill-posed inverse problem in that solutions for a can be arbitrarily sensitive to errors in measurements of ϕ , or to errors in the model. Therefore numerical solutions of (1) for a need to be preceded by a fairly rigorous mathematical analysis in order to ensure that they are reliable in some well-defined sense. This note briefly discusses the key issues in such an analysis: existence, uniqueness and stability. As transmissivity estimation is a difficult and at times frustrating problem, many of the points raised concern still open problems.

2. Appropriate mathematical settings for the model

Any rigorous analysis requires a well-defined setting for the model. Given the discontinuous nature of some of the variables (e.g. recharge), perhaps the most natural interpretation of (1) for scenario modelling is that it holds in some weak sense. No boundary conditions were given in (1) as in practice they are not usually known with confidence, so for convenience we assume here Dirichlet boundary data with $\phi(x) = 0$ on $\partial\Omega$. (This corresponds to maintaining a fixed pressure on the boundary, and would be true in practice if, for example, the boundary was a river). In this case (1) might be recast as:

$$\int_{\Omega} a \nabla \phi \cdot \nabla \phi = \int_{\Omega} q \phi \quad \forall \phi \in H_0^1(\Omega)$$

The theory of elliptic p.d.e.'s in weak form is very well developed; in it the most suitable spaces for the various functions would be: $a \in L^\infty(\Omega)$, $\phi \in H_0^1(\Omega)$ and $q \in H_0^{-1}(\Omega)$.

If a is known a priori, this setting is also convenient for numerical analysis; it is easiest to set up approximation schemes and derive error analyses for them in finite dimensional subspaces of Hilbert spaces. If, however, a is to be determined, then it would be more convenient that a also be in a Hilbert space, e.g. $L^2(\Omega)$ or $H_0^1(\Omega)$.

In opposition to these considerations is the fact that the data on φ and q available for identification of a usually consist of water pressures measured in a number of bore holes scattered over the aquifer, together with flow rates of any pumps sunk into the aquifer plus a (usually very rough) estimate of wide area recharge rates into the aquifer from above or below. Moreover any data on a is usually in the form of pump tests. Thus the data consists of the measurement sets:

$$\begin{aligned}
 a_m &= \int_{B_\varepsilon(x_m)} a(x) dx && \text{pump tests} \\
 \varphi_n &= \varphi(x_n) && \text{bore measurements} \\
 q_p &= \begin{cases} q_p \delta(x-x_p) \\ q_B(x) \end{cases} && \begin{array}{l} \text{pumps} \\ \text{background recharge} \end{array}
 \end{aligned}$$

where $B_\varepsilon(x)$ is the ball of radius ε around x . Thus translating error bars on the data set into error bounds on the functions suggests that the setting for the problem most consistent with the data is: $a \in L^1(\Omega)$, $\varphi \in C(\Omega)$ and that q consist of two components q_1 and q_2 with $q_1 \in C^*(\Omega)$ and $q_2 \in L^1(\Omega)$.

Finally, in transmissivity estimation (1) is viewed not as an elliptic p.d.e. for φ but as a first order p.d.e. for a . The standard theory for such an equation centres on the idea of characteristics along which the solution behaves like an o.d.e., and this theory essentially requires piecewise continuity of the variables in order for the characteristics to be well defined. As we shall see, this appears to be the only setting in which uniqueness can be easily proven.

3. Existence

We shall not examine the particular question of under what conditions a solution exists for the transmissivity estimation problem, but shall rather make a general point about the existence question: in a sense it may usually be reduced to questions of uniqueness or stability. To see this, consider the general linear problem:

$$\mathcal{K}f = g \quad \text{where } \mathcal{K}: \mathcal{X} \rightarrow \mathcal{Y} \quad (2)$$

If a solution f to (2) does not exist then g must be in \mathcal{Y} but not in the range $\mathcal{K}(\mathcal{X}) \subseteq \mathcal{Y}$. If $\mathcal{K}(\mathcal{X}) \neq \mathcal{Y}$ then there are two possibilities: that $\mathcal{K}(\mathcal{X})$ is a proper subspace of \mathcal{Y} , or that $\mathcal{K}(\mathcal{X})$ is dense in \mathcal{Y} . The first case might well be termed *strong non-existence* since it implies that there is data g such that:

$$\inf_{f \in \mathcal{X}} \|\mathcal{K}f - g\| > \varepsilon > 0$$

It immediately follows from this that the kernel of the adjoint operator $\mathcal{K}^*: \mathcal{Y}^* \rightarrow \mathcal{X}^*$ is non-empty, and that the equation $\mathcal{K}^*u = v$ will have multiple solutions. Thus in transmissivity estimation we could settle the question of strong non-existence of a solution a to $\nabla \cdot (a \nabla \varphi) = q$ by deciding whether the adjoint equation $\nabla \phi \cdot \nabla \varphi = 0$ has a nontrivial solution ϕ .

The second case can be termed *weak non-existence* since in this case there exists data g and a sequence f_k such that $\|\mathcal{K}f_k - g\| \downarrow 0$ but the sequence f_k does not converge in the given norm for \mathcal{X} . This is essentially a statement that the problem is unstable; under the given norms for \mathcal{X} and \mathcal{Y} , \mathcal{K} does not have a bounded inverse. If, however, \mathcal{X} (\mathcal{Y}) was enlarged (diminished) by appropriate re-norming (i.e. the problem was recast in a different setting) then in the new norms \mathcal{K} may have a bounded inverse, the problem would be stable and a solution would always exist. The relationship between the new norms and the old can then be used to characterize the degree of instability of the problem.

4. Uniqueness

Two general results on uniqueness of solutions to (1) for a have previously appeared. The first, due to Chicone and Gerlach [2], contains an elegant proof showing that if no characteristic crosses the aquifer then the solution must be unique. This condition applies in the particular problem considered here since the boundary essentially defines a closed contour for the head φ , and a characteristic cannot cross a closed contour twice. Their result requires, however, that φ be twice differentiable and does not hold out much promise of being generalized to prove uniqueness of weak solutions of (1).

The second, due to the author and Claude Dietrich [3], is based integration by parts, and so may still hold under weaker conditions than those of Chicone and Gerlach. To see if this is indeed possible, we look more closely at the result and its proof.

Theorem 1. *If $\nabla\varphi$ is continuously differentiable and vanishes only on a set of measure zero in Ω , then (1) coupled with the condition $\varphi = 0$ on $\partial\Omega$ has a unique solution among all continuously differentiable functions a .*

Proof: It suffices to show that $\nabla \cdot (a \nabla\varphi) = 0$ implies $a \equiv 0$, and this we shall prove by contradiction. In particular, assume that a non-zero solution does exist, let $\Omega^+ = \{x : a(x) > 0\}$ and let $\Omega^+ = \Omega \cap \Lambda^+$. Then w.l.o.g. we may assume that $a(x) > 0$ in some subset of Ω^+ with nonzero measure (if not we simply work with Ω^- in what follows). Now consider:

$$\int_{\Omega^+} \varphi \nabla \cdot (a \nabla\varphi) \quad (3)$$

Integrating by parts gives:

$$\int_{\Omega^+} \varphi \nabla \cdot (a \nabla\varphi) = \int_{\Omega^+} a \nabla\varphi \cdot \nabla\varphi + \int_{\partial\Omega^+} a \varphi \frac{\partial\varphi}{\partial n}$$

Since $\nabla \cdot (a \nabla\varphi) = 0$, the l.h.s. vanishes. By continuity and the construction of Ω^+ at any point $x \in \partial\Omega^+$ either $a(x) = 0$ or $\varphi(x) = 0$, so that the boundary integral also vanishes. But by assumption there is some subset of Ω^+ with nonzero measure such that $a \nabla\varphi \cdot \nabla\varphi$ is strictly positive. As the integrand is non-negative over the rest of Ω^+ it follows that the first term on the r.h.s. is strictly positive, which establishes the desired contradiction. Q.E.D.

The proof rests on the assumption that the functions φ , $\nabla \cdot (a \nabla\varphi)$ and the level set Ω^+ are sufficiently nice to permit integration by parts. It is known [5] that the class of sets for which the Gauss-Green identity:

$$\int_{\Lambda} \operatorname{div} g = \int_{\partial\Lambda} g \cdot n \quad \text{where} \quad \operatorname{div} g \equiv \sum_{i=1}^2 \frac{\partial g_i}{\partial x_i}$$

holds for every vector-valued continuously differentiable function $g : \Lambda \rightarrow \mathbb{R}^2$ are the so-called *Cacciopoli* sets. These sets can be characterized by the fact that their associated characteristic functions are in the space $BV(\Omega)$, where $\Lambda \subset\subset \Omega$ and $BV(\Omega)$ is the space of functions of bounded variation in Ω , i.e. the set of all functions $f \in L^1(\Omega)$ for which:

$$\sup \left\{ \int_{\Omega} f \operatorname{div} g : g_i \in C^1(\Omega), |g_i(x)| \leq 1 \right\} \quad (4)$$

is finite. Moreover it can be shown that if $f \in BV(\Omega)$ then almost all level sets of f are Cacciopoli sets.

These results indicate that the minimum requirement on a to ensure that integration by parts is permissible on the set Ω^+ is that $a \in BV(\Omega)$. Since $\Omega \subset \mathcal{R}^2$, the Sobolev inequalities show that this is roughly comparable to the condition that $a \in L^\infty(\Omega)$. However, with this restriction (3) should more properly be rewritten as

$$\int_{\Omega} (\varphi \chi_{\Omega^+}) \nabla \cdot (a \nabla \varphi)$$

Recognizing $\varphi \chi_{\Omega^+}$ as a function of bounded variation, in the worst case it follows from the definition (4) that integration by parts is valid only if the remainder of the integrand is continuous, and therefore that $a \in C^1(\Omega)$ and $\varphi \in C_0^2(\Omega)$.

This shows that striving for the most general level set Ω^+ does not actually result in a weakening of the conditions under which the theorem is valid. It may be possible, however, to get slightly weaker conditions on $\nabla \cdot (a \nabla \varphi)$ by tightening the class of permissible level sets. If a theory analogous to that of $BV(\Omega)$ could be developed by relaxing the class of functions g appearing in (4) to be, e.g., $g_i \in H_0^1(\Omega)$, $\|g_i\|_2 = 1$ (and so produce a new function space that was strictly contained in $BV(\Omega)$), then it might be that the existing two conditions ($a \in BV(\Omega)$ and $a \in C^1(\Omega)$, $\varphi \in C^2(\Omega)$) could be adjusted simultaneously with the first being strengthened while the second was relaxed, until ultimately some sort of optimal balance is reached.

Finally, the following example shows that a general uniqueness result for (1) cannot be established under the weaker conditions: $a \in L^\infty(\Omega)$, $\phi \in H_0^1(\Omega)$. Let $\Omega = [-1, 1]$ and let $\varphi(x) = 1 - |x|$. Now it is simple to show that if $a(x) = \text{sgn}(x)$ then

$$\int_{-1}^1 a(x) \frac{d\varphi}{dx} \frac{d\phi}{dx} dx = 0 \quad \forall \phi \in H_0^1(\Omega)$$

5. Stability

It is clear that a solution a to (1) depends linearly on q but nonlinearly on φ , and furthermore that a will be stable w.r.t. small perturbations in q (since these are essentially integrated and so smoothed out in recovering a) but the solution will be unstable w.r.t. small perturbations in φ (since these are differentiated to give the coefficients in the p.d.e. and are thus amplified). A rigorous stability analysis confirming this has been given by Richter [8] who showed that,

under some reasonable conditions needed to ensure uniqueness, given perturbations $\tilde{\varphi}, \tilde{q}$ of the data φ, q (due, e.g., to measurement errors), the induced perturbation in the transmissivity estimate is bounded above by:

$$\|a - \tilde{a}\|_{\infty} \leq c \|\varphi\|_{\infty} [\|a\|_{\infty} [\|\nabla(\varphi - \tilde{\varphi})\|_{\infty} + \|\Delta(\varphi - \tilde{\varphi})\|_{\infty}] + \|q - \tilde{q}\|_{\infty}]$$

Moreover Falk has given a finite element method for the numerical solution of (1) (again under certain side conditions necessary to ensure uniqueness) together with an error analysis consistent with Richter's. In particular, he showed that if $a \in H^{r+1}\Omega$ and \tilde{a}_h is a solution to a particular discretization of (1) using standard finite element spaces and with perturbed data $\tilde{\varphi}$, then:

$$\|a - \tilde{a}_h\|_2 \leq c [h^{-2} \|\varphi - \tilde{\varphi}\|_2 + h^r] \quad (5)$$

Unfortunately these results do not give much insight into exactly what sort of perturbations in φ cause instability in a , and thus how to construct a numerical solution that efficiently approximates only that component of a that is well determined by the model and the data. To make this point more clearly, consider again the model linear problem (2) with the extra assumptions that \mathcal{X} and \mathcal{Y} are both Hilbert spaces and that \mathcal{K} is a compact operator. For simplicity, consider the class of numerical solutions $\tilde{f}_{\mathcal{P}\mathcal{Q}}$ got by choosing two N dimensional subspaces $\mathcal{U} \subset \mathcal{X}, \mathcal{V} \subset \mathcal{Y}$ and then solving the reduced finite dimensional system:

$$Q\mathcal{K}\mathcal{P}\tilde{f}_{\mathcal{P}\mathcal{Q}} = Q\tilde{g}$$

where \mathcal{P}, \mathcal{Q} are the orthogonal projections onto \mathcal{U}, \mathcal{V} respectively and \tilde{g} is a perturbation of the data. After noting that the complete projection of the original system is:

$$Q\mathcal{K}\mathcal{P}f + Q\mathcal{K}\mathcal{P}^c f = Qg$$

where $\mathcal{P}^c = I - \mathcal{P}$ is the projection onto the complement of \mathcal{U} , it follows that

$$\begin{aligned} \|\tilde{f}_{\mathcal{P}\mathcal{Q}} - f\| &\leq \|(Q\mathcal{K}\mathcal{P})^{-1}\| [\|g - \tilde{g}\| + \|Q\mathcal{K}\mathcal{P}^c f\|] + \|\mathcal{P}^c f\| \\ &\leq \|(Q\mathcal{K}\mathcal{P})^{-1}\| \|g - \tilde{g}\| + [\|(Q\mathcal{K}\mathcal{P})^{-1}\| \|\mathcal{K}\| + 1] \|\mathcal{P}^c f\| \end{aligned} \quad (6)$$

The terms in Falk's error bound (5) can now be matched with those in (6).

Note in particular that there are two possible approaches to deriving error bounds from (6). The first, essentially that used by Falk, is take standard subspaces for \mathcal{U} and \mathcal{V} , use known results for these spaces to bound $\|(Q\mathcal{K}\mathcal{P})^{-1}\|$, and then to assume that f is such that as N increases $\|P^\epsilon\|$ goes to zero faster than $\|(Q\mathcal{K}\mathcal{P})^{-1}\|$ grows.

The second is instead to choose \mathcal{U} and \mathcal{V} so that $Q\mathcal{K}\mathcal{P}^\epsilon = 0$ and so remove this term from the error; this will hold if $\mathcal{U} = \mathcal{K}^*\mathcal{V}$ (see [7]). Next \mathcal{V} is chosen so as to minimize the remainder of the error bound, i.e. to minimize $\|(Q\mathcal{K}\mathcal{P})^{-1}\|$. It turns out that this is achieved if \mathcal{U} and \mathcal{V} are the subspaces spanned by the first N singular functions of \mathcal{K} . Moreover, this is an optimal discretization in that it minimizes the error over all discretizations of size N . Also, as $\|P^\epsilon\|$ may now tend to zero arbitrarily slowly, a broader class of solutions can be accurately approximated.

The singular value decomposition (SVD) is of course widely used to solve ill-posed inverse problems; the above analysis merely illustrates one of its many useful properties. It also answers for the linear problem the questions raised above: i.e. it demonstrates exactly how perturbations in g are magnified to give rise to increasing instability in f , and it shows that the most efficient discretization is one based on the SVD.

Unfortunately, as transmissivity estimation is nonlinear in the data φ , the SVD can no longer be used to construct optimal discretizations. Nevertheless it is still reasonable to ask if the above approach can still be applied to identify discretizations that are in some sense reliable. In particular, we may formally write (1) as:

$$\mathcal{B}(a, \varphi) = q$$

where $\mathcal{B} : \mathcal{X} \times \mathcal{Y} \rightarrow \mathcal{Z}$ is a bilinear operator. As before, let $\mathcal{U}, \mathcal{V}, \mathcal{W}$ be N dimensional subspaces of $\mathcal{X}, \mathcal{Y}, \mathcal{Z}$ with associated projection operators $\mathcal{P}, \mathcal{Q}, \mathcal{R}$ (but we shall no longer insist that the spaces be Hilbert and the projections orthogonal). Now consider the reduced system with perturbed data:

$$\mathcal{R}\mathcal{B}(\mathcal{P}a_{\mathcal{PQ}\mathcal{R}}, Q\varphi) = \mathcal{R}q$$

and again compare it with the correct projection of the complete system:

$$\begin{aligned} \mathcal{R}\mathcal{B}(\mathcal{P}a, Q\varphi) &= \mathcal{R}[q - \mathcal{B}(\mathcal{P}a, Q^\epsilon\varphi) - \mathcal{B}(\mathcal{P}^\epsilon a, Q\varphi) - \mathcal{B}(\mathcal{P}^\epsilon a, Q^\epsilon\varphi)] \\ &= \mathcal{R}[q - \mathcal{B}(\mathcal{P}a, Q^\epsilon\varphi) - \mathcal{B}(\mathcal{P}^\epsilon a, \varphi)] \end{aligned}$$

Any error analysis could be restricted solely to the operator $\mathcal{R}\mathcal{B}(\mathcal{P}, Q)$, and so be simplified, if the subspaces \mathcal{U}, \mathcal{V} and \mathcal{W} could be chosen so that the residual operators $\mathcal{R}\mathcal{B}(\mathcal{P}, Q^c)$ and $\mathcal{R}\mathcal{B}(\mathcal{P}^c, \cdot)$ all vanished identically. Moreover such an analysis would not have to make assumptions about the convergence rate of discrete approximations to the (unknown) solution in order to get stability bounds.

The following example shows that this is not a totally impossible request. Restricting for the moment our attention to one dimensional problems, let $\Omega = [-1, 1]$ and consider the simple multiplicative bilinear operator \mathcal{M} defined by:

$$\mathcal{M}(f, g)(x) \equiv f(x) g(x)$$

This operator encapsulates the underlying nonlinearity in \mathcal{B} . Now let the spaces $\mathcal{X}, \mathcal{Y}, \mathcal{Z}$ be the Hardy space \mathcal{H}^2 of analytic functions on Ω whose Taylor series have coefficients that are square summable; \mathcal{H}^2 is a Hilbert space under the l^2 norm on the coefficients. Next let the subspaces \mathcal{U}, \mathcal{V} and \mathcal{W} be the space $\mathcal{U}_N \equiv \text{span}\{x^n : n = 0, \dots, N-1\}$, and take for the associated projection operators the operator $\mathcal{P}_N : \mathcal{H}^2 \rightarrow \mathcal{U}_N$ defined by:

$$\mathcal{P}_N(f) = \mathcal{P}_N\left(\sum_{n=0}^{\infty} c_n x^n\right) = \sum_{n=0}^{N-1} c_n x^n$$

\mathcal{P}_N is an orthogonal projection under the \mathcal{H}^2 norm. Moreover the range of \mathcal{P}_N^c is the subspace $\mathcal{U}_N^c \equiv \text{span}\{x^n : n \geq N\}$, and if the product $\mathcal{U}_N \circ \mathcal{U}_N^c$ of \mathcal{U}_N and \mathcal{U}_N^c is defined by:

$$\mathcal{U}_N \circ \mathcal{U}_N^c \equiv \{f : f(x) = u(x)v(x), u \in \mathcal{U}_N, v \in \mathcal{U}_N^c\}$$

then $\mathcal{U}_N \circ \mathcal{U}_N^c \subseteq \mathcal{U}_N^c$, so that $\mathcal{P}_N \mathcal{B}(\mathcal{P}_N, \mathcal{P}_N^c \cdot) = \mathcal{P}_N \mathcal{B}(\mathcal{P}_N^c, \cdot) \equiv 0$.

This shows that there is at least one setting in which a stability analysis of a bilinear operator such as \mathcal{B} along the lines of the linear problem is possible. The setting is clearly unsatisfactory in practice, however, since the \mathcal{H}^2 norm is far removed from a standard error metric such as the L^2 norm and the mapping between point values of a function and the coefficients of the monomials in an approximating polynomial is well known to be numerically unstable. Unfortunately it may well be that \mathcal{U}_N and \mathcal{U}_N^c form the only family of finite dimensional subspaces and associated complements such that $\mathcal{U}_N \circ \mathcal{U}_N^c \subseteq \mathcal{U}_N^c$. Support for this rather gloomy conclusion comes from noting that an associated problem has essentially a unique solution: the only finite dimensional subspaces \mathcal{V}'_N for which $\mathcal{V}'_N \times \mathcal{V}'_N \subseteq \mathcal{V}'_N$ are spaces of

piecewise constant functions, so that essentially the only orthonormal basis that would generate a family of such subspaces are the Walsh functions.

6. Conclusion

In conclusion, despite the progress made on transmissivity estimation in the last decade there are still some important unanswered questions. First, it is still not clear exactly what the correct mathematical setting for the problem should be. Second, while a weak formulation is the preferred starting point for numerical solutions, the best results on uniqueness apply only for continuous functions. This leaves some uncertainty as to the performance of, e.g., finite element methods on the general problem with discontinuous data. It may be possible to extend the function spaces on which uniqueness holds by generalizing the idea of bounded variation, but this is a problem for a different discipline.

Finally, the numerical methods proposed for transmissivity estimation to date have used standard discretizations and have imposed a priori conditions on the solution in order to bound the residuals in the associated error analyses. The insight obtainable from these results does not yet match that available in the theory of linear ill-posed problems: in that theory optimal discretizations can be defined that separate out exactly that part of the problem for which a stable solution can be found. A similar approach can at least be formulated for transmissivity estimation, but a complete solution requires a better understanding of decompositions of bilinear operators.

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Information Technology Division,
Electronics Research Laboratory,
DSTO,
P.O. Box 1600,
Salisbury, S.A. 5108,
Australia.