A Posteriori Error Bounds for Meshless Methods

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Abstract

We show how to provide safe a–posteriori error bounds for numerical solutions of well-posed operator equations using kernel–based meshless trial spaces. The presentation is kept as simple as possible in order to address a larger community working on applications in Science and Engineering.

1 Operator Equations

Most contributions within application–oriented conferences only present numerical results without rigorous arguments concerning error bounds. Since *a–priori* error bounds are hard to find and to apply, we focus here on *a–posteriori* error bounds which are obtainable after a solution candidate is found.

In order to cover a fairly general range of partial differential equation (PDE) problems arising in Science and Technology, we do not want to confine ourselves here to elliptic problems. The crucial property replacing ellipticity is *well-posedness* of the problem, or *continuous dependence* of the *solution* on the *data*. In the context of a linear boundary–value problem

$$\begin{array}{rcll} Lu & = & f_\Omega & \text{in } \Omega \subset I\!\!R^d \\ Bu & = & f_\Gamma & \text{in } \Gamma \subset \partial\Omega \end{array} \tag{1}$$

on a domain Ω with a linear differential operator L and some linear boundary operator B, continuous dependence means existence of constants C_Ω, C_Γ such that

$$\|u\|_U \leq C_\Omega \|Lu\|_F + C_\Gamma \|Bu\|_G \text{ for all } u \in U \tag{2}$$

where we use suitable norms in the spaces U, F, G between which the differential operator L and the boundary operator B are defined:

$$\begin{array}{rcccl} L & : & U & \to & F, \\ B & : & U & \to & G. \end{array} \tag{3}$$

This easily generalizes to multiple differential or boundary operators. Note that the choice of spaces U, F, G usually is a mathematically hazardous problem in itself, even for fixed standard operators like $L = -\Delta$. A whole scale of *trace spaces* connected to *trace theorems* is possible, depending on the smoothness of the expected solution. For instance, a Poisson problem with Dirichlet data on a

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reasonable domain $\Omega \in I\!R^d$ allows either a scale of Hölder spaces [1] or a scale of Sobolev spaces [2]

$$U = W_2^m(\Omega),\ F = W_2^{m-2}(\Omega),\ F = W_2^{m-1/2}(\Gamma)$$

for arbitrary $m \in Z\!\!Z$. Another well–posed case arises whenever a maximum principle for homogeneous boundary value problems with Dirichlet data holds. In such a case we have

$$\|u\|_{\infty,\Omega} \leq \|Bu\|_{\infty,\Gamma},$$

but still the proper choice of spaces U and F must be done with care.

We do not describe details here, but we remind the application-oriented reader that the problem should have the property that small perturbations of the data lead only to small perturbations of the solution. Any uncontrolled blow-up effect will spoil continuous dependence. Note further that this is independent of numerical methods.

2 Residual Minimization

If continuous dependence holds in the sense of (2), a standard technique is to use the chosen space of trial functions to find an approximation $\tilde{u}$ for the exact solution u^* such that the *residuals* can be bounded a–posteriori by

$$\begin{array}{rcl} \|u^* - \tilde{u}\|_U & \leq & C_\Omega \|L(u^* - \tilde{u})\|_F \quad + \quad C_\Gamma \|B(u^* - \tilde{u})\|_G \\ & = & C_\Omega \|f_\Omega - L\tilde{u}\|_F \quad + \quad C_\Gamma \|f_\Gamma - B\tilde{u}\|_G. \end{array} \tag{4}$$

Many authors in application–oriented journals implicitly argue that way. The standard punchline is:

> If the differential equation and the boundary conditions are satisfied up to some “satisfactory” accuracy, the problem is solved to “satisfactory” accuracy.

Without additional information, the above statement is worthless. It makes sense only if there is continuous dependence in the above form, with known constants, and if residuals are small in the specific norms required there. Both facts are rarely checked correctly, and the literature does not supply handy references for continuous dependence inequalities as (2). Finally, when calculating residuals, authors usually only evaluate function values on fine discrete sets, but this does not guarantee small Sobolev norms of residuals as full functions. A graphic inspection of the full residuals at a fine resolution may convince the user at first sight, but since Sobolev norms blow up at hardly visible points where higher derivatives are singular, this is no reliable indication of a small error in the final solution.

However, the above approach via *residual minimization* is quite useful in theory and practice, because it is fairly general and since we shall show that the aforementioned problems can be overcome. But it cannot easily be used with trial functions of limited smoothness, e.g. for linear finite elements and differential operators of order two or more. However, for trial spaces generated by translates of smooth kernels like Gaussians or multiquadrics, and for problems with smooth solutions u^*, we can use standard high–order approximation error bounds [6] of the form

$$\|u^* - \tilde{u}\|_U \leq \epsilon$$

to guarantee small residuals via

$$\begin{array}{rcllcl} \|u^* - \tilde{u}\|_U & \leq & C_\Omega \|f_\Omega - L\tilde{u}\|_F & + & C_\Gamma \|f_\Gamma - B\tilde{u}\|_G \\ & \leq & C_\Omega \|L\| \|u^* - \tilde{u}\|_U & + & C_\Gamma \|B\| \|u^* \tilde{u}\|_G \\ & \leq & C_\Omega \|L\| \epsilon & + & C_\Gamma \|B\| \epsilon. \end{array}$$

This requires that the approximations are smooth enough to allow the operators L and B to act on them, but there are plenty of sufficiently smooth kernels. The same conclusion works for meshless trial spaces generated by moving least squares (MLS), but the operators will be less easy to apply.

However, the above argument is purely theoretic at this point, because it only proves that there are very useful meshless trial spaces which generate approximate solutions with arbitrarily small residuals. It does not indicate how to calculate them and how to evaluate the actual norms of the residuals.

3 Particular and Fundamental Solutions

The estimate (4) allows an easy analysis of the DRM, the MFS and the MPS. Assume first that there are trial functions u_j which provide particular solutions to the differential operator L via

$$f_j := Lu_j.$$

This is easy to do if the u_j are sufficiently smooth, and if the f_j are calculated from the u_j, not the other way round. Then, in order to solve

$$Lu = f_\Omega$$

without regard of boundary values, one would approximate f_Ω by a linear combination $\tilde{f}_\Omega$ of the f_j up to a small error $\epsilon_\Omega := \|f_\Omega - \tilde{f}_\Omega\|_F$. This sounds easy, but for a rigid theoretical analysis and an efficient numerical procedure one needs to have good approximation properties of the f_j. However, this can be done in all cases where the u_j have good approximation properties with respect to the real solution u^* and sufficient smoothness. In fact, if there is a good approximation $\tilde{u}$ to u^* with $\|u^* - \tilde{u}\|_U \leq \epsilon_U$, then there is a good approximation $\tilde{f}_\Omega = L\tilde{u}$ to $f_\Omega = Lu^*$ with

$$\|f_\Omega - \tilde{f}_\Omega\|_F = \|L(u^* - \tilde{u})\|_F \leq \|L\| \|u^* - \tilde{u}\|_U \leq \|L\| \epsilon_U.$$

If a suitable optimization routine is used to minimize residuals on Ω, it will in such cases be possible to have a small residual error $\|f_\Omega - \tilde{f}_\Omega\|_F$.

Again, we see that trial spaces of smooth functions with good approximation properties are of central importance. There is absolutely no need to link trial spaces to finely granulated space discretizations.

The next step in the DRM is to use the Method of Fundamental Solutions or a boundary integral method to solve the problem

$$\begin{array}{rcl} Lv & = & 0 \\ Bv & = & f_\Gamma - B\tilde{u} \end{array}$$

by some good candidate $\tilde{v}$ with $L\tilde{v} = 0$ and to use $\tilde{u} + \tilde{v}$ as the final candidate for an approximate solution of the full problem. Then (4) is a sum

$$\begin{array}{rcllll} \|u^* - (\tilde{u} + \tilde{v})\|_U & \leq & C_\Omega \|f_\Omega - L(\tilde{u} + \tilde{v})\|_F & + & C_\Gamma \|f_\Gamma - B(\tilde{u} + \tilde{v})\|_G \\ & \leq & C_\Omega \|f_\Omega - \tilde{f}_\Omega\|_F & + & C_\Gamma \|f_\Gamma - B\tilde{u} - B\tilde{v}\|_G \end{array}$$

of the two residuals of the MPS and the MFS, respectively. This simple and well-known argument yields a solid foundation for the DRM/MPS/MFS provided that the problem is well–posed and the residual norms are small. But it will be a problem to evaluate the norms involved here. We shall address this question now.

4 Residual Evaluation

In this paper, we do not want to go into the details of specific weak or strong testing strategies in the context of convergence analysis [4, 5]. Instead, we focus on safe ways of a–posteriori evaluation of residuals. Remember that we ended up at this question when looking at the error of the DRM/MPS/MFS. But we shall stay more general.

Assume that some method or other has produced a sufficiently smooth trial function $\tilde{u}$ which the user wants to insert into the inequality (4) in order to conclude that the problem is safely solved. The main problem is to get safe bounds of the norms $\|f_\Omega - L\tilde{u}\|_F$ and $\|f_\Gamma - B\tilde{u}\|_G$ where the norms can be quite exotic and numerically unavailable. Users will evaluate the residuals on sufficiently many points, find small absolute values there and be satisfied.

However, this is mathematically incorrect. If a function is small on a large but still finite point set, it is not necessarily small everywhere and in particular its derivatives may still be quite large. Typical examples are high–frequency sine and cosine functions as models of a "small" residual at many points. Weak testing will not overcome this problem, because highly oscillating residuals will have small integrals against plenty of test functions while not being small themselves.

Thus we need a good argument for concluding that a function is small in some norm provided that it is small on a large discrete set. There is a basic requirement for this: some higher derivative must be bounded.

Let us explain why. The simplest univariate case can be handled easily by Taylor's theorem. If u is continuously differentiable with $\|u'\|_\infty \leq C$ and if u takes values $|u(x)| \leq \epsilon$ on a discrete point set $X \subset \Omega := [a, b] \subset I\!R$ with *fill distance*

$$h = h(X, \Omega) := \sup_{y \in \Omega} \min_{x \in X} \|x - y\|_2,$$

one can bound $\|u\|_{\infty,[a,b]}$ via

$$|u(y)| = |u(y) - u(x) + u(x)| \le \left|\int_x^y u'(t)dt\right| + \epsilon \le Ch + \epsilon$$

where y is arbitrary and x is the point of X closest to y.

Models of such theorems holding in Sobolev spaces are *sampling inequalities* derived in [7, 3]. They roughly take the form [7]

$$\|u\|_{W_2^m(\Omega)} \quad \le \quad C\left(h^{M-m}\|u\|_{W_2^M(\Omega)} + h^{-m}\|u\|_{X,\infty}\right)$$

for all $u \in W_2^M(\Omega),\ 0 \le m < M - d/2$ or [3]

$$\|u\|_{L_2(\Omega)} \quad \le \quad C\left(h^M\|u\|_{W_2^M(\Omega)} + h^{d/2}\|u\|_{X,2}\right)$$

for all $u \in W_2^M(\Omega),\ d/2 < M$.

These tools would perfectly serve our purpose, if we had a grip on a high–level Sobolev norm like $\|u\|_{W_2^M(\Omega)}$ when applied to a residual. Such norms usually involve integrals over derivatives, and there is no known efficient way to evaluate or bound them in general.

But trial spaces made of meshless translates of positive definite kernels allow to evaluate bounds on high–level Sobolev norms efficiently and without any integration. The key fact is that they are reproducing kernels of Hilbert spaces H of smooth functions. If Φ is a positive definite kernel on $I\!R^d$ and if a linear combination

$$u(y) := \sum_{x_j \in X} \alpha_j \Phi(x_j, y) \tag{5}$$

of generalized "translates" of Φ is given, its Hilbert space norm is available via the quadratic form

$$\|u\|_H^2 = \sum_{x_j \in X}\sum_{x_k \in X} \alpha_j \alpha_k \Phi(x_j, x_k).$$

If the kernel is smooth enough, the above norm will be an upper bound for certain Sobolev norms, and it is easily available through the coefficients of the representation. We show some cases in Table 1, where we give the maximal order M of a Sobolev space $W_2^M(\Omega)$ on $\Omega \subset I\!R^d$ such that an inequality

$$\|u\|_{W_2^M(\Omega)} \le C(M, H, \Omega)\|u\|_H$$

holds for all $u \in H$, in particular those of the form (5). The case of conditionally positive definite kernels can be treated very similarly, but there is an additional condition on the coefficients of (5).

However, within the Method of Fundamental Solutions for second–order differential equations, things are not as simple. Fundamental solutions then are reproducing kernels of Sobolev spaces of rather low regularity, in particular without a

$\phi(r)$		M
$\exp(-r^2)$		∞
$(-1)^{\lceil\beta/2\rceil}(c^2+r^2)^\beta$	$\beta \in I\!R \setminus I\!N_0$	∞
$(-1)^{\lceil\beta/2\rceil}r^\beta$	$\beta > 0,\ \beta \notin 2I\!N$	$\frac{d+\beta}{2}$
$(-1)^{k+1}r^{2k}\log r$	$k \in I\!N$	$k+\frac{d}{2}$
$\phi_{d,k}(r)$ (Wendland[6])	$d \geq 1,\ k \geq 0$	$k+\frac{d+1}{2}$

Table 1: Maximal Sobolev Orders M

stable point evaluation. For instance, the fundamental solutions $\log r$ and $1/r$ of the Laplacian in $I\!R^2$ and $I\!R^3$, respectively, only reproduce W_2^1 spaces. In such cases users have to go back to the primitive and coarse technique to bound a linear combination via the triangle inequality, provided that the norms of each trial function can be evaluated.

Finally, note that the MFS also has problems with the approximation argument at the end of section 2, because there still is no sufficiently general theory for the approximation of given functions on domain boundaries by fundamental solutions from source points on an outside fictitious boundary. Using a single domain–based trial space for simultaneous minimization of both domain and boundary residuals avoids this problem.

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