A Posteriori Error Bounds for Two Point Boundary Value Problem with Uncertain Parameters

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Outline

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2. Uncertain Parameters
3. Error estimation
4. Computational method
5. Linearization-Based Algorithm
6. Conclusions
Errors in numerical calculations

Boundary value problem.

\[ L(u) = f, \quad u \in V \]

- exact solution, \( u_h \) - approximate solution.

Approximation error \( \| u - u_h \| = \| e \| \).

Parameter dependent boundary value problem.

\[ L(u, p) = f, \quad u \in V \]

- parameter dependent exact solution, \( u_h(p) \) - parameter dependent approximate solution.

Maximal approximation error

\[
\sup_{p \in P} \| u(p) - u_h(p) \|_E = \sup_{p \in P} \| e(p) \|_E = \| e \|_E
\]
Errors in numerical calculations

Uncertain Parameters

Error estimation

Computational method

Linearization-Based Algorithm

Conclusions

Extreme values of the solution

Parameter dependent boundary value problem.

$$L(u, p) = f, u \in V$$

Exact solution

$$u = \inf_{p \in P} u(p), \quad \bar{u} = \sup_{p \in P} u(p)$$

$$u(x, p) \in [u(x), \bar{u}(x)]$$

Approximate solution

$$u_h = \inf_{p \in P} u_h(p), \quad \bar{u}_h = \sup_{p \in P} u_h(p)$$

$$u_h(x, p) \in [u_h(x), \bar{u}_h(x)]$$
Solution of the equation with interval parameters for given $x$ can be defined as the following set:

$$[u(x), \bar{u}(x)] = \Diamond \{ u(x, p_1, ..., p_m) : p_1 \in [p_{1}, \bar{p}_1], ..., p_m \in [p_{m}, \bar{p}_m] \}$$

where $[p_{1}, \bar{p}_{1}], ..., [p_{m}, \bar{p}_{m}]$ are interval parameters (for example $E, A, n$ etc.) and $\Diamond B$ is the smallest interval that contains the set $B$. In presented example uncertain parameters may be $E, n, L$ etc.
Steepest Descent Method

In order to find maximum/minimum of the function \( u \) it is possible to apply a modified version of the steepest descent algorithm.

1. Given \( x_0 \), set \( k = 0 \).
2. \( d^k = -\nabla f(x_k) \). If \( d^k = 0 \) then stop.
3. Solve \( \min_\alpha f(x_k + \alpha d^k) \) for the step size \( \alpha_k \). If we know second derivative \( H \) then \( \alpha_k = \frac{d_k^T d_k}{d_k^T H(x_k) d_k} \).
4. Set \( x_{k+1} = x_k + \alpha_k d_k \), update \( k = k + 1 \). Go to step 1.
Two point boundary value problem

Sample problem

\[
\begin{cases}
    - (a(x)u'(x)) = f(x) \\
    u(0) = 0, u(1) = 0
\end{cases}
\]

and \( u_h(x) \) is finite element approximation given by a weak formulation

\[
\int_0^1 a(x)u'_h(x)v'(x)dx = \int_0^1 f(x)v(x)dx, \quad \forall v \in V_h^{(0)}
\]

or

\[
a(u_h, v) = l(v), \quad \forall v \in V_h^{(0)} \subset H_0^1
\]

where \( u_h(x) = \sum_{i=1}^n u_i \varphi_i(x) \) and \( \varphi_i(x_j) = \delta_{ij} \).
Example

Tension-compression problem

\[
\begin{aligned}
\begin{cases}
-(E(x)A(x)u'(x))' = n(x) \\
u(0) = 0, u(L) = 0
\end{cases}
\end{aligned}
\]

$E$ is a Young modulus and $A$ is an area of cross-section. $u_h(x)$ is finite element approximation given by a weak formulation.

\[
\int_0^L E(x)A(x)u_h'(x)v'(x)dx = \int_0^L n(x)v(x)dx, \forall v \in V_h^{(0)}
\]

or

\[
a(u_h, v) = l(v), \forall v \in V_h^{(0)} \subset H_0^1
\]
The Finite Element Method

Weak formulation

\[ \int_{0}^{1} a(x) u_h'(x) v'(x) \, dx = \int_{0}^{1} f(x) v(x) \, dx, \forall v \in V_h^{(0)} \]

Approximate solution

\[ u_h = \sum_{i=1}^{n} u_i \varphi_i(x), \quad v = \sum_{j=1}^{n} v_j \varphi_j(x) \]

\[ \frac{\partial u_h}{\partial x} = \sum_{i=1}^{n} u_i \frac{\partial \varphi_i(x)}{\partial x} \]

\[ \frac{\partial v}{\partial x} = \sum_{j=1}^{n} v_j \frac{\partial \varphi_j(x)}{\partial x} \]
The Finite Element Method

Approximate solution \[ \int_0^1 a(x)u'_h(x)v'(x)dx = \int_0^1 f(x)v(x)dx. \]

\[
\sum_{j=1}^{n} \left( \sum_{i=1}^{n} \int_0^1 a(x)\varphi_i(x)\varphi_j(x)dxu_i - \int_0^1 f(x)\varphi_j(x)dx \right) v_j = 0
\]

Final system of equations (for one element) \( Ku = q \) where

\[ K_{i,j} = \int_0^1 a(x)\varphi_i(x)\varphi_j(x)dx, \quad q_i = \int_0^1 f(x)\varphi_i(x)dx \]

Calculations of the local stiffness matrices can be done in parallel.
Global Stiffness Matrix

Global stiffness matrix

\[
\sum_{p=1}^{n} \left( \sum_{q=1}^{n} \sum_{e=1}^{n_e} \sum_{i=1}^{n_u^e} \sum_{j=1}^{n_u^e} U_{j,p}^e \int_{\Omega_e} a(x) \frac{\partial \varphi_i^e(x)}{\partial x} \frac{\partial \varphi_j^e(x)}{\partial x} \, dx U_{i,q}^e u_q - \right)
\]

\[
\sum_{q=1}^{n} \sum_{e=1}^{n_e} \sum_{i=1}^{n_u^e} \sum_{j=1}^{n_u^e} U_{j,p}^e \int_{\Omega_e} f(x) \varphi_i^e(x) \varphi_j^e(x) \, dx \right) v_p = 0
\]

Final system of equations

\[ Ku = q \]

Computations of the global stiffness matrix can be done in parallel.
The Gradient

After discretization

\[ Ku = q \]

Calculation of the gradient

\[ Kv = \frac{\partial}{\partial p_k} q - \frac{\partial}{\partial p_k} Ku \]

where \( v = \frac{\partial}{\partial p_k} u \).

Presented gradient can be used in the optimization process. Derivative with respect to different parameters \( p_k \) can be calculated simultaneously by using parallel computing.
The error of the solution can be approximated by the following inequality

\[ \| u - u_h \|_E \leq \| u - v \|_E, \forall v(x) \in V_h^{(0)} \subset H_0^1 \]

this means that the finite element solution \( u_h \in V_h^{(0)} \) is the best approximation of the solution \( u \) by the function in \( V_h^{(0)} \), where

\[ \| u - u_h \|_E^2 = \int_0^1 a(x) \left( u'(x) - u'_h(x) \right)^2 dx \]
(An apriori error estimate). Let $u$ and $u_h$ be the solutions of the Dirichlet problem (BVP) and the finite element problem (FEM), respectively. Then there exists an interpolation constant $C_i$, depending only on $a(x)$, such that

$$\| u - u_h \|_E \leq C_i \| hu'' \|_a$$

where

$$\| u \|_a^2 = \int_0^1 a(x) (u(x))^2 \, dx$$

This, however, requires that the exact solution $u(x)$ is known.
(a posteriori error estimate). There is an interpolation constant $C_i$ depending only on $a(x)$ such that the error in finite element approximation of the Dirichlet boundary value problem (BVP) satisfies

$$\|u - u_h\|_E \leq C_i \sqrt{\int_{0}^{1} \frac{1}{a(x)} h^2(x) R^2(u_h(x)) \, dx}$$

where $h(x)$ is some weight and

$$R_h(u_h(x)) = f(x) + (a(x)u'_h(x))'$$

is the residual error and $u_h$ is a solution of the Finite Element Method.
Adaptivity

Assume that one seeks an error bound less that a given error tolerance TOL:

\[ \|e(x)\|_E \leq TOL \]

Then one may use the following steps as a mesh refinement strategy:

(i) Make an initial partition of the interval.

(ii) Compute the corresponding FEM solution \( u_h(x) \) and residual \( R(u_h(x)) \).

(iii) If \( \|e(x)\|_E > TOL \) refine the mesh in the places for which \( \frac{1}{a(x)} R^2(u_h(x)) \) is large and perform the steps (ii) and (iii) again.
Adaptivity

**Figure:** Adaptive FEM.
Computational method

1. Set some initial grid points \( x_0, x_1, \ldots, x_n \) and set \( i = 0 \).

2. For given sets of grid points
   \( x_0^{\text{min},i}, x_1^{\text{min},i}, \ldots, x_n^{\text{min},i} \) for \( u_h \)
   \( x_0^{\text{max},i}, x_1^{\text{max},i}, \ldots, x_n^{\text{max},i} \) for \( \bar{u}_h \)

   find the approximate solutions
   \[ u_h^i = u_h(p_{\text{min}}^i), \quad \bar{u}_h^i = u_h(p_{\text{max}}^i). \]

3. If \( \| u_h^i - u_h^{i-1} \| < \varepsilon_1 \) and \( \| \bar{u}_h^i - \bar{u}_h^{i-1} \| < \varepsilon_2 \) then stop.
   The solution is \( u \approx u_h^i, \bar{u} \approx \bar{u}_h^i \).

4. If \( i > i_{\text{max}} \) then the method doesn’t converge and stop.

5. Find new sets of grid points
   \( x_0^{\text{min},i+1}, x_1^{\text{min},i+1}, \ldots, x_n^{\text{min},i+1} \) for \( u_h \)
   \( x_0^{\text{max},i+1}, x_1^{\text{max},i+1}, \ldots, x_n^{\text{max},i+1} \) for \( \bar{u}_h \)

   that minimize error estimator for \( \| e \|_E \) and compute new solutions
   \[ u_h^{i+1} = u_h(p_{\text{min}}^{i+1}), \quad \bar{u}_h^{i+1} = u_h(p_{\text{max}}^{i+1}) \]
   set \( i := i + 1 \) and go to the point 2.
KKT Conditions

Nonlinear optimization problem for $f(x) = x_i$

$$\begin{align*}
\min_{x} f(x) \\
h(x) &= 0 \\
g(x) &\geq 0
\end{align*}$$

Lagrange function $L(x, \lambda, \mu) = f(x) + \lambda^T h(x) - \mu^T g(x)$

Optimality conditions can be solved by the Newton method.

$$\begin{align*}
\nabla_x L &= 0 \\
\nabla_\lambda L &= 0 \\
\mu_i &\geq 0 \\
\mu_i g_i(x) &= 0 \\
h(x) &= 0 \\
g(x) &\geq 0
\end{align*}$$
Linearization-Based Algorithm

- **We know:** an algorithm $f(x_1, \ldots, x_n)$ and values $\tilde{y}_i$ and $\Delta_i$.

- **We need to find:** the range of values $f(x_1, \ldots, x_n)$ when $x_i \in [\tilde{x}_i - \Delta_i, \tilde{x}_i + \Delta_i]$.

- **Algorithm:**
  1) first, we compute $\tilde{y} = f(\tilde{x}_1, \ldots, \tilde{x}_n)$;
  2) then, for each $i$ from 1 to $n$, we compute
     
     $$y_i = f(\tilde{x}_1, \ldots, \tilde{x}_{i-1}, \tilde{x}_i + \Delta_i, \tilde{x}_{i+1}, \ldots, \tilde{x}_n);$$

  3) after that, we compute $\bar{y} = \tilde{y} + \sum_{i=1}^{n} |y_i - \tilde{y}|$ and

     $$\underline{y} = \tilde{y} - \sum_{i=1}^{n} |y_i - \tilde{y}|.$$
We rarely know the exact dependence \( y = f(x_1, \ldots, x_n) \).

We have an approx. model \( F(x_1, \ldots, x_n) \) w/known accuracy \( \varepsilon \): \[ |F(x_1, \ldots, x_n) - f(x_1, \ldots, x_n)| \leq \varepsilon. \]

We know: an algorithm \( F(x_1, \ldots, x_n) \), accuracy \( \varepsilon \), values \( \tilde{x}_i \) and \( \Delta_i \).

Find: the range \( \{ f(x_1, \ldots, x_n) : x_i \in [\tilde{x}_i - \Delta_i, \tilde{x}_i + \Delta_i] \} \).

If we use the approximate model in our estimate, we get

\[
\bar{Y} = \tilde{Y} + \sum_{i=1}^{n} |Y_i - \tilde{Y}|.
\]

Here, \( |\tilde{Y} - \tilde{y}| \leq \varepsilon \) and \( |Y_i - y_i| \leq \varepsilon \), so \( |\bar{y} - \bar{Y}| \leq (2n + 1) \cdot \varepsilon \).

Thus, we arrive at the following algorithm.
Resulting Algorithm

- We know: an algorithm $F(x_1,\ldots,x_n)$, accuracy $\varepsilon$, values $\tilde{x}_i$ and $\Delta_i$.
- Find: the range $\{f(x_1,\ldots,x_n): x_i \in [\tilde{x}_i - \Delta_i, \tilde{x}_i + \Delta_i]\}$.
- Algorithm:
  1) compute $\tilde{Y} = Y(\tilde{x}_1,\ldots,\tilde{x}_n)$ and
     $$Y_i = F(\tilde{x}_1,\ldots,\tilde{x}_{i-1},\tilde{x}_i + \Delta_i, \tilde{x}_{i+1},\ldots,\tilde{x}_n).$$
  2) compute $\bar{B} = \tilde{Y} + \sum_{i=1}^{n} |Y_i - \tilde{Y}| + (2n + 1) \cdot \varepsilon$ and
     $$\underline{B} = \tilde{Y} - \sum_{i=1}^{n} |Y_i - \tilde{Y}| - (2n + 1) \cdot \varepsilon.$$
- Problem: when $n$ is large, then, even for reasonably small inaccuracy $\varepsilon$, the value $(2n + 1) \cdot \varepsilon$ is large.
- What we do: we show how we can get better estimates for $\bar{Y}$. 
How to Get Better Estimates: Idea

- One possible source of model inaccuracy is discretization (e.g., FEM).
- When we select a different combination of parameters, we get an *unrelated* value of inaccuracy.
- So, let’s consider approx. errors
  \[ \Delta y \overset{\text{def}}{=} F(x_1, \ldots, x_n) - f(x_1, \ldots, x_n) \]
  as *independent* random variables.
- What is a probability distribution for these random variables? We know that \( \Delta y \in [-\varepsilon, \varepsilon] \).
- We do not have any reason to assume that some values from this interval are more probable than others.
- So, it is reasonable to assume that all the values are equally probable: a uniform distribution.
- For this uniform distribution, the mean is 0, and the standard deviation is \( \sigma = \frac{\varepsilon}{\sqrt{3}} \).
How to Get a Better Estimate for $\tilde{y}$

- In our main algorithm, we apply the computational model $F$ to $n + 1$ different tuples.
- Let’s also compute $M \overset{\text{def}}{=} F(\tilde{x}_1 - \Delta_1, \ldots, \tilde{x}_n - \Delta_n)$.
- In linearized case, $\tilde{y} + \sum_{i=1}^{n} y_i + m = (n + 2) \cdot \tilde{y}$, so
  $$\tilde{y} = \frac{1}{n + 2} \cdot \left( \tilde{y} + \sum_{i=1}^{n} y_i + m \right), \quad \text{and we can estimate } \tilde{y} \text{ as}$$
  $$\tilde{Y}_{\text{new}} = \frac{1}{n + 2} \cdot \left( \tilde{Y} + \sum_{i=1}^{n} Y_i + m \right).$$
- Here, $\Delta\tilde{y}_{\text{new}} = \frac{1}{n + 2} \cdot \left( \Delta\tilde{y} + \sum_{i=1}^{n} \Delta y_i + \Delta m \right)$, so its variance is
  $$\sigma^2 \left[ \tilde{Y}_{\text{new}} \right] = \frac{\varepsilon^2}{3 \cdot (n + 2)} \ll \frac{\varepsilon^2}{3} = \sigma^2 \left[ \tilde{Y} \right].$$


**Estimation of \( \sigma^2 \)**

- Let us compute \( Y_{\text{new}} = \tilde{Y}_{\text{new}} + \sum_{i=1}^{n} |Y_i - \tilde{Y}_{\text{new}}| \).
- Here, when \( s_i \in \{ -1, 1 \} \) are the signs of \( y_i - \tilde{y} \), we get:
  \[
  \bar{y} = \tilde{y} + \sum_{i=1}^{n} s_i \cdot (y_i - \tilde{y}) = \left( 1 - \sum_{i=1}^{n} s_i \right) \cdot \tilde{y} + \sum_{i=1}^{n} s_i \cdot y_i.
  \]
- Thus, \( \Delta \bar{y}_{\text{new}} = \left( 1 - \sum_{i=1}^{n} s_i \right) \cdot \Delta \tilde{y}_{\text{new}} + \sum_{i=1}^{n} s_i \cdot \Delta y_i \), so
  \[
  \sigma^2 = \left( 1 - \sum_{i=1}^{n} s_i \right)^2 \cdot \frac{\varepsilon^2}{3 \cdot (n+2)} + \sum_{i=1}^{n} \frac{\varepsilon^2}{3}.
  \]
- Here, \( |s_i| \leq 1 \), so \( \left| 1 - \sum_{i=1}^{n} s_i \right| \leq n + 1 \), and
  \[
  \sigma^2 \leq \frac{\varepsilon^2}{3} \cdot (2n + 1).
  \]
Using $\tilde{Y}_{\text{new}}$ (cont-d)

- We have $\Delta \tilde{y}_{\text{new}} = \left(1 - \sum_{i=1}^{n} s_i\right) \cdot \Delta \tilde{y}_{\text{new}} + \sum_{i=1}^{n} s_i \cdot \Delta y_i$.

- Due to the Central Limit Theorem, $\Delta \tilde{y}_{\text{new}}$ is $\approx$ normal.

- We know that $\sigma^2 \leq \frac{\varepsilon^2}{3} \cdot (2n + 1)$.

- Thus, with certainty depending on $k_0$, we have

  $$\bar{y} \leq \bar{Y}_{\text{new}} + k_0 \cdot \sigma \leq \bar{Y}_{\text{new}} + k_0 \cdot \frac{\varepsilon}{\sqrt{3}} \cdot \sqrt{2n + 1} :$$

  - with certainty 95% for $k_0 = 2$,
  - with certainty 99.9% for $k_0 = 3$, etc.

- Here, inaccuracy grows as $\sqrt{2n + 1}$.

- This is much better than in the traditional approach, where it grows $\sim 2n + 1$. 
We know: \( F(x_1, \ldots, x_n), \varepsilon, \tilde{x}_i \) and \( \Delta_i \).

We want: to find the range of \( f(x_1, \ldots, x_n) \) when \( x_i \in [\tilde{x}_i - \Delta_i, \tilde{x}_i + \Delta_i] \).

Algorithm:

1) compute \( \tilde{Y} = F(\tilde{x}_1, \ldots, \tilde{x}_n) \),
   
   \( M = F(\tilde{x}_1 - \Delta_1, \ldots, \tilde{x}_n - \Delta_n) \), and
   
   \( Y_i = F(\tilde{x}_1, \ldots, \tilde{x}_{i-1}, \tilde{x}_i + \Delta_i, \tilde{x}_{i+1}, \ldots, \tilde{x}_n) \);

2) compute \( \tilde{Y}_{\text{new}} = \frac{1}{n+2} \cdot \left( \tilde{Y} + \sum_{i=1}^{n} Y_i + M \right) \),

   \[ b = \tilde{Y}_{\text{new}} + \sum_{i=1}^{n} \left| Y_i - \tilde{Y}_{\text{new}} \right| + k_0 \cdot \sqrt{2n+1} \cdot \frac{\varepsilon}{\sqrt{3}}; \]

   \[ b = \tilde{Y}_{\text{new}} - \sum_{i=1}^{n} \left| Y_i - \tilde{Y}_{\text{new}} \right| - k_0 \cdot \sqrt{2n+1} \cdot \frac{\varepsilon}{\sqrt{3}}. \]
A Similar Improvement Is Possible for the Cauchy Method

- In the Cauchy method, we compute \( \tilde{Y} \) and the values

\[
Y^{(k)} = F(\tilde{x}_1 + \eta_1^{(k)}, \ldots, \tilde{x}_n + \eta_n^{(k)}).
\]

- We can then compute the improved estimate for \( \tilde{y} \), as:

\[
\tilde{Y}_{\text{new}} = \frac{1}{N + 1} \cdot \left( \tilde{Y} + \sum_{k=1}^{N} Y^{(k)} \right).
\]

- We can now use this improved estimate when estimating the differences \( \Delta y^{(k)} \): namely, we compute

\[
Y^{(k)} - \tilde{Y}_{\text{new}}.
\]
Conclusions

- Presented method allows to find the solution of the two point boundary value problem with uncertain parameters.
- The method takes into account two types of error in numerical solution: approximation errors and uncertainty in the initial data.
- In order to speed up the calculations parallel computing can be applied.
- Similar methodology can be applied for the solution of different types of differential equations.
- The method can be applied for the solution of large scale engineering (solid mechanics, oil engineering, CFM etc.) and scientific problems with uncertain parameters.