Towards Combining Interval and Probabilistic Uncertainty in Finite Element Methods

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1. Uncertainty in FEM: Probabilistic Approach

- **Traditional approach to FEM**: we know the exact equations and the exact values of the parameters $x_i$ of these equations.

- **In practice**: we only know the approximate values of the corresponding parameters.

- **Question**: estimate how the uncertainty in the parameters of the system can affect the result $y$ of applying the FEM techniques.

- **Probabilistic approach – assumption**: we know the exact probability distributions of all $x_i$.

- **Probabilistic approach – algorithm**: e.g., use Monte-Carlo simulations.
2. Uncertainty in FEM: Interval Approach and Remaining Problem

- *Interval approach – assumption:* sometimes, we only know the lower bounds $x_i$ and the upper bounds $\bar{x}_i$ on $x_i$.

- *Example:* the probabilities of different values of Young modulus may depend on the manufacturing process.

- *Interval approach – objective:* find the interval $[\tilde{y} - \Delta, \tilde{y} + \Delta]$ that contains $y$.

3. Uncertainty in FEM: Remaining Problem

• **In practice:** we sometimes have *both* interval and probabilistic uncertainty.

• **Example:**
  
  – for manufacturing-related parameters, we may only know intervals of possible values;
  
  – for weather-related parameters, we also know the probabilities of different values (e.g., from the weather records).

• **Objective:** for different $p \in [0, 1]$, find the value $\Delta(p)$ that bound $\Delta y$ with probability $p$. 
4. General Algorithm

• **Problem – reminder:**
  
  – for some $x_i$, we know intervals $[\underline{x}_i, \overline{x}_i]$;
  – for some $x_j$, we know the probability distribution;
  – we want to find the value $\Delta(p)$ that bound $\Delta y$ with probability $p$.

• **Algorithm:**
  
  – use Monte-Carlo techniques to simulate parameters $x_j$ with known probability distributions;
  – for each such simulation, use interval FEM techniques to get an upper bound $\Delta$ for $|y - \tilde{y}|$;
  – after several simulations, we get the resulting bounds distribution;
  – from this distribution, we can find the desired bound $\Delta(p)$. 


5. Case Study: Determining Earth Structure

- **Importance**: civilization greatly depends on the things we extract from the Earth: oil, gas, water.
- **Need**: is growing, so we must find new resources.
- **Problem**: most easy-to-access mineral resources have been discovered.
- **Example**: new oil fields are at large depths, under water, in remote areas – so drilling is very expensive.
- **Objective**: predict resources before we invest in drilling.
- **How**: we know what structures are promising.
- **Example**: oil and gas concentrate near the top of (natural) underground domal structures.
- **Conclusion**: to find mineral resources, we must determine the structure at different depths $z$ at different locations $(x, y)$. 
6. Data that We Can Use to Determine the Earth Structure

- **Available measurement results:** those obtained without drilling boreholes.

- **Examples:**
  - gravity and magnetic measurements;
  - travel-times $t_i$ of seismic ways through the earth.

- **Need for active seismic data:**
  - passive data from earthquakes are rare;
  - to get more information, we make explosions, and measure how the resulting seismic waves propagate.

- **Resulting seismic inverse problem:**
  - we know the travel times $t_i$;
  - we want to reconstruct velocities at different depths.
Hole Tomography Smashed Masked Velocity Models
7. Seismic Inverse Problem: Towards Mathematical Formulation

- **General description**: wave equation with unknown $v(x)$.
- **Difficulty**: due to noise, we only know $t_i$.
- **Ray approximation**: a seismic wave follows the shortest path $t = \int \frac{d\ell}{v} \rightarrow \min$; Eikonal equation $|\nabla t| = \frac{1}{v}$.
- **Discontinuity**: $v$ is only piece-wise continuous; Snell’s law describes the transition $\frac{\sin(\varphi)}{v} = \frac{\sin(\varphi')}{v'}$.
- **Ill-posed problem**: a change in $v$ outside paths does not affect observed travel-times $t_i$; hence, many drastically different $v(x)$ are consistent with observations.
- **Current solution**:
  - start with a meaningful first approximation;
  - use physically motivated iterations.
8. **Seismic Inverse Problem: FEM Approach**

- \( v(x) = v_j \) is constant within each element \( j \).
- **We know:** travel-times \( t_i \) between known points \( A_i, B_i \).
- **We want to find:** velocities \( v_j \) for which \( t_i = t_i(v) \overset{\text{def}}{=} \min \sum_j \frac{\ell_{ij}}{v_j} \), where:
  - \( \min \) is taken over all paths between \( A_i \) and \( B_i \), and
  - \( \ell_{ij} \) is the length of the part of \( i \)-th path within element \( j \).

- **Shortest path:** straight inside each element, Snell’s law on each border.

- **Simplification:** use slownesses \( s_j \overset{\text{def}}{=} \frac{1}{v_j} \); \( t_i = \sum_j \ell_{ij} \cdot s_j \).

- **Problem:** system is under-determined.
9. Existing Algorithm for the Seismic Inverse Problem: General Description

- **The most widely used**: John Hole’s iterative algorithm.
- **Starting point**: reasonable initial slownesses $s_j^{(0)}$.
- **Starting an iteration**: we use current (approximate) slownesses $s_j^{(k)}$ to:
  - find the shortest paths and
  - compute the corr. travel-times $t_i = \sum_j \ell_{ij} \cdot s_j^{(k)}$.
- **Fact**: measured travel-times $\tilde{t}_i$ are somewhat different: $\Delta t_i \overset{\text{def}}{=} \tilde{t}_i - t_i \neq 0$.
- **On each iteration**:
  - we find $\Delta s_j$ for which $\sum_j \ell_{ij} \cdot (s_j + \Delta s_j) = \tilde{t}_i$;
  - we take $s_j^{(k+1)} = s_j^{(k)} + \Delta s_j$. 

10. Algorithm for the Inverse Problem: Details

- **Objective (reminder):** find $\Delta s_j$ s.t. $\sum \ell_{ij} \cdot \Delta s_j = \Delta t_i$.
- **Simplest case:** one path.
- **Specifics:** under-determined system: 1 equation, many unknowns $\Delta s_j$.
- **Idea:** no reason for $\Delta s_j$ to be different: $\Delta s_j \approx \Delta s_{j'}$.
- **Formalization:** minimize $\sum_{j,j'} (\Delta s_j - \Delta s_{j'})^2$ under the constraint $\sum \ell_{ij} \cdot \Delta s_j = \Delta t_i$.
- **Solution:** $\Delta s_j = \frac{\Delta t_i}{L_i}$ for all $j$, where $L_i = \sum_j \ell_{ij}$.
- **Realistic case:** several paths; we have $\Delta s_{ij}$ for different paths $i$.
- **Idea:** least squares $\sum_i (\Delta s_j - \Delta s_{ij})^2 \rightarrow \min$.
- **Solution:** $\Delta s_j$ is the average of $\Delta s_{ij}$.
11. Successes, Limitations, Need for Prior Knowledge

- **Successes:** the algorithm usually leads to reasonable geophysical models.

- **Limitations:** often, the resulting velocity model is not geophysically meaningful.

- **Example:** resulting velocities outside of the range of reasonable velocities at this depth.

- **What is currently done:** trying different initial models (hacking).

- **Problem with this approach:** there is no algorithm for selecting a good starting model; often, dozens of tries are needed – and each try requires hours of computations.

- **It is desirable:** to incorporate the expert knowledge into the algorithm for solving the inverse problem.
12. Case of Interval Prior Knowledge

- **Additional information:** an interval \([s_j, \bar{s}_j]\) that contains the (unknown) actual value \(s_j\).

- **Problem:** for \(\Delta s_{ij} = \frac{\Delta t_i}{L_i}\), we may have \(s_j^{(k)} + \Delta s_{ij} \not\in [s_j, \bar{s}_j]\).

- **Idea:** as \(s_j^{(k+1)}\), take the value from \([s_j, \bar{s}_j]\) which is the closest to \(s_j^{(k)} + \Delta s_{ij}\), i.e., cut off at \(\bar{s}_j\) (or at \(s_j\)).

- **Problem:** since we decreased \(\Delta s_{ij}\), we have a remaining discrepancy \(\Delta t_i' \overset{\text{def}}{=} \Delta t_i - \sum_j \ell_{ij} \cdot \Delta s_{ij}\).

- **Solution:** repeat the same process for \(\Delta t_i'\), etc.

- **Problem:** many iterations instead of one – increase in computation time.

- **Our result:** a new linear time algorithm that computes the final result of these additional iterations.
13. A New Linear-Time Algorithm

- At each iteration, we have three sets:
  - $J^- = \{ j : \text{we know} \Delta s_{ij} = \Delta_j = \bar{s}_j - s_j^{(k)} \}$;
  - $J^+ = \{ j : \text{we know} \Delta s_{ij} < \Delta_j \}$,
  - $J = -(J^- \cup J^+)$. 

  and quantities $A^- \overset{\text{def}}{=} \sum_{j \in J^-} \ell_{ij} \cdot \Delta_j$ and $L^+ \overset{\text{def}}{=} \sum_{j \in J^+} \ell_{ij}$.

- We start with $J^- = J^+ = \emptyset$ and $J = \{1, \ldots, c\}$.

- At each iteration:
  - we compute the median $m$ of the set $J$ (median in terms of sorting by $\Delta_j$);
  - then, by analyzing the elements of the undecided set $J$ one by one, we divide them into subsets

$$P^- \overset{\text{def}}{=} \{ j : \Delta_j \leq \Delta_m \}, \quad P^+ \overset{\text{def}}{=} \{ j : \Delta_j > \Delta_m \}. $$
14. A New Linear-Time Algorithm (cont-d)

- we compute $a^- \overset{\text{def}}{=} A^- + \sum_{j \in P^-} \ell_{ij} \cdot \Delta_j$ and $\ell^+ \overset{\text{def}}{=} \mathcal{L}^+ + \sum_{j \in P^+} \ell_{ij}$;

- then, we compute $\Delta s = \frac{\Delta_i - a^-}{\ell^+}$; also, among all the values from $P^+$, we select the smallest value, which we will denote by $\Delta_{(p+1)}$;

- if $\Delta s > \Delta_{(p+1)}$, then we replace $J^-$ with $J^- \cup P^-$, $A^-$ with $a^-$, and $J$ with $P^+$;

- if $\Delta s \leq \Delta_m$, then we replace $J^+$ with $J^+ \cup P^+$, $\mathcal{L}^+$ with $\ell^+$, and $J$ with $P^-$;

- finally, if $\Delta_m < \Delta s \leq \Delta_{(p+1)}$, then we replace $J^-$ with $J^- \cup P^-$, $J^+$ with $J^+ \cup P^+$, and $J$ with $\emptyset$.

- Iterations continue until $J = \emptyset$.

- Return $\Delta s_{ij} = \Delta_j$ when $\Delta_j \leq \Delta_m$, else $\Delta s_{ij} = \Delta s$. 
15. Case of Probabilistic Prior Knowledge

- **Description:** from prior observations, we know $\tilde{s}_j \approx s_j$, and we know the st. dev. $\sigma_j$ of this value.

- **Minimize:**
  \[ \sum_{j,j'} (\Delta s_{ij} - \Delta s_{ij'})^2 \text{ s.t. } \sum_{j=1}^c \ell_{ij} \cdot \Delta s_{ij} = \Delta t_i \]
  \[ \frac{1}{n} \sum_{j=1}^c \frac{((s_j^{(k)} + \Delta s_{ij}) - \tilde{s}_j)^2}{\sigma_j^2} = 1. \]

- **Solution** (Lagrange multipliers):
  \[ \Delta s \overset{\text{def}}{=} \frac{1}{n} \sum_{j=1}^c \Delta s_{ij}, \]
  \[ \frac{2}{n} \cdot \Delta s_{ij} - \frac{2}{n} \cdot \Delta s + \lambda \cdot \ell_{ij} + \frac{2\mu}{n \cdot \sigma_j^2} \cdot (s_j^{(k)} + \Delta s_{ij} - \tilde{s}_j) = 0. \]

- **Fact:** $\Delta s_{ij}$ is an explicit function of $\lambda$, $\mu$, $\Delta s$.

- **Algorithm:** solve 3 non-linear equations (above one + 2 constraints) with unknowns $\lambda$, $\mu$, $\Delta s$. 
16. Combination of Different Types of Prior Knowledge

- **Need**: we often have both:
  
  - prior measurement results – i.e., *probabilistic* knowledge, and
  
  - expert estimates – i.e., *interval* knowledge.

- **Minimize**: \[
  \sum_{j,j'} (\Delta s_{ij} - \Delta s_{ij'})^2 \text{ s.t. } \sum_{j=1}^c \ell_{ij} \cdot \Delta s_{ij} = \Delta t_i,
  \]
  \[
  \frac{1}{n} \cdot \sum_{j=1}^c \frac{((s_j^{(k)} + \Delta s_{ij}) - \bar{s}_j)^2}{\sigma^2_j} \leq 1,
  \]
  
  and \( s_{j} \leq s_j^{(k)} + \Delta s_{ij} \leq \bar{s}_j \).

- **Idea**: we minimize a convex function under convex constraints; efficient algorithms are known.
17. Combination of Different Types of Prior Knowledge: Algorithm

- **Idea** – method of alternating projections:
  - first, add a correction that satisfy the first constraint,
  - then, the additional correction that satisfies the second constraint,
  - etc.

- **Specifics**: 
  - first, add equal values $\Delta s_{ij}$ to minimize $\Delta t_i$;
  - restrict the values to the nearest points from $[s_j, \bar{s}_j]$,
  - find the extra corrections that satisfy the probabilistic constraint,
  - repeat until converges.
18. Effects of Discretization: Technique

- **Worst-case bound:** $\infty$.

- **Geophysical approach** – “checkerboard” method:
  - add a doubly periodic function $\Delta v(x)$ to the solution $v(x)$;
  - compute corresponding $t'_i$;
  - reconstruct $v'(x)$ from $t'_i$;
  - compare $v'(x)$ with $v(x) + \Delta v(x)$.

- **Conclusion:**
  - For small-step $\Delta v(x)$, we will not see the difference
    - hence details of this size in $v(x)$ are not reliable.
  - If for some step $h$, we see the difference, this means
    that details of size $h$ are more reliable.
19. Effects of Discretization: Mathematical Results

- **Problem:** how to select functions $\Delta v_i(x)$?
- **Idea:** we want a shift-invariant process.
- **Analysis:** in linear approximation, what matters is the linear hull of the functions $\Delta v_i(x)$.
- **First result:** for bounded $\Delta v_i(x)$, we get
  \[ \Delta v_i(x_1, x_2) = \sin(a_1 \cdot x_1 + b_1) \cdot \sin(a_2 \cdot x_2 + b_2). \]
- **Alternative formulation:** we require that the family of functions $\{\Delta v_i(x)\}$ is optimal w.r.t. a shift-invariant optimality criterion.
- **Second result:** for each such criterion, we get the same functions
  \[ \Delta v_i(x_1, x_2) = \sin(a_1 \cdot x_1 + b_1) \cdot \sin(a_2 \cdot x_2 + b_2). \]
20. Acknowledgments

This work was supported in part by:

- NASA under cooperative agreement NCC5-209,
- NSF grants EAR-0225670 and DMS-0532645,
- Star Award from the University of Texas System, and
- Texas Department of Transportation grant No. 0-5453.