Analysing and bounding error sources in numerical neural network simulations

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Numerical Error in Neural Networks

- Reproducibility is desirable, but tricky
- Different results with different compilers and architecture
- Even different in the same environment
- Need a way to measure how reproducible a simulation is...
Numerical Error in Neural Networks

Rounding error: \( x \text{ op } y = (x \hat{\text{ op }} y) (1 + \delta) \)

Nondeterminism: \( (x \hat{\text{ op }} y) \hat{\text{ op }} z \neq x \hat{\text{ op }} (y \hat{\text{ op }} z) \)

Truncation error: \( x_{t+h} = x_t + \left. \frac{dx}{dt} \right|_t h + O(h^2) \)

• Lots of nondeterminism in parallel hardware
• Errors quickly amplified in unstable systems
Interval Arithmetic (IA)

- Replace variables and operators with IA equivalents:

\[ x \in \bar{x}, \ y \in \bar{y}, \ z \in \bar{z} \]
\[ \bar{x} = [x_{lo}, x_{hi}] \]
\[ \bar{y} = [y_{lo}, y_{hi}] \]
\[ \bar{z} = \bar{x} - \bar{y} = [(x_{lo} - y_{hi}), (x_{hi} - y_{lo})] \]

- Cannot track correlations:

\[ p - p = 0 \]
\[ \bar{p} = [1, 2] \]
\[ \bar{p} - \bar{p} = [(1 - 2), (2 - 1)] = [-1, 1] \]

- Interval ‘explosion’ is an issue in long chained computations, such as numerical integration
Interval Arithmetic (IA)

- The ‘wrapping effect’

- IA tells us the axis-aligned white box is the reachable region

- If $m$ and $V$ are correlated, the real reachable region might in fact be the grey diamond
Affine Arithmetic (AA)

- Solution: encode correlations within representation

- Intervals are encoded as first-order polynomials with a centre: \( x_0 \), and \( n \) deviation terms: \( x_i \varepsilon_i \)

- All \( \varepsilon_i \) are unknown, shared amongst all affine intervals and represent the uncertainty from an error source

- \( x \) and \( y \) are correlated iff:

\[
\hat{x} = x_0 + x_1 \varepsilon_1 + \ldots + x_n \varepsilon_n
\]

\[
\varepsilon_i \in [-1,1]
\]

\[
\exists k > 0 : |x_k| \neq 0 \land y_k \neq 0
\]
Affine Arithmetic (AA)

- A convex hull ‘wraps’ the reachable region better
- Deviation terms correspond to edges

- Numerical error is placed in a new deviation term $x_k \varepsilon_k$

$$\hat{\chi} = x_0 + x_1 \varepsilon_1 + ... + x_n \varepsilon_n + x_k \varepsilon_k$$

- Nonlinear operations are approximated linearly (Chebyshev), and linearisation error is also added to $x_k \varepsilon_k$
Affine Arithmetic (AA)

**affine_1 (z, x, α, γ, δ)**

\[ z = (\alpha x_0 + \gamma) + (\alpha x_1)\varepsilon_1 + \ldots + (\alpha x_n)\varepsilon_n + (\delta)\varepsilon_{n+1} \]

**affine_2 (z, x, y, α, β, γ, δ)**

\[ z = (\alpha x_0 + \beta y_0 + \gamma) + (\alpha x_1 + \beta y_1)\varepsilon_1 + \ldots + (\alpha x_n + \beta y_n)\varepsilon_n + (\delta)\varepsilon_{n+1} \]
exp_cheb (z, x)

\[
\alpha = \frac{e^{x_{hi}} - e^{x_{lo}}}{x_{hi} - x_{lo}}
\]

\[
d_a = e^{x_{lo}} - \alpha x_{lo}
\]

\[
d_b = e^{x_{hi}} - \alpha x_{hi}
\]

\[
d_{\text{min}} = e^u - \alpha u
\]

\[
d_{\text{max}} = \max(d_a, d_b)
\]

\[
\gamma = \text{mid}([d_{\text{min}}, d_{\text{max}}])
\]

\[
\delta = \text{rad}([d_{\text{min}}, d_{\text{max}}])
\]

affine_1(z, x, \alpha, \gamma, \delta)
The MPFA Library

• Written in C
• Open Source (LGPLv3 license)
• Based on the GNU MPFR Library
• Link as a shared or static lib
• Uses the GNU Autotools, for simpler compilation, installation and portability
  
  ./configure && make && sudo make install

• Beta release very soon!

Available: www.github.com/jamesturner246/mpfa
The MPFA Library

• Benefits of MPFR
  - Results guaranteed to be correctly rounded
  - Support for IEEE-754-2008 rounding modes
  - Precision is adjustable at runtime
  - No opaque compiler optimisation
  - Extensive testing
  - All the above, for all functions
The MPFA Library

- Potentially lots of internal rounding error
- Centre and deviation terms are computed in working precision
- Intermediate variables and radius are computed in higher internal precision
Many new deviation terms: 1 per operation
Eventually need ‘garbage collection’

mpfa_condense_last_n (mpfa_t z, unsigned n)
- Condense the last \( n \) deviation terms
- Lossless (when used correctly)

mpfa_condense_small (mpfa_t z, double fraction)
- Condense terms smaller than some fraction of radius
- Lossy (some correlation information is lost)
The MPFA Library

mpfa_add and mpfi_add, 1,000,000 tests, 100 bins
Morris-Lecar Neuron Model

\[ C \frac{dV}{dt} = I - g_L(V - V_L) - g_{Ca} M_{ss}(V)(V - V_{Ca}) - g_K N(V - V_K) \]

\[ \frac{dN}{dt} = \frac{N_{ss}(V) - N}{\tau_N(V)} \]

\[ M_{ss}(V) = \frac{1}{2} (1 + \tanh\left( \frac{V - V_1}{V_2} \right)) \]

\[ N_{ss}(V) = \frac{1}{2} (1 + \tanh\left( \frac{V - V_3}{V_4} \right)) \]

\[ \tau_N(V) = \frac{1}{\phi \cosh\left( \frac{V - v_3}{2V_4} \right)} \]
Morris-Lecar Neuron Model

IA (top) and AA (bot). Iterations 1 to 83.
The MPFA Library
An arbitrary-precision affine arithmetic library based on GNU MPFR.

Open source permissive license (LGPLv3).

Download, contribute and give feedback at:
www.github.com/jamesturner246/mpfa