Bounds from Slopes

David M. Gay
dmg@ampl.com
http://www.ampl.com

Why bound computations?

- Global optimization
- Assess effects of input uncertainty
- Design – avoid failures

DMG work done at Sandia National Laboratories in Albuquerque, NM, building on work of others cited in the paper:
http://www.sandia.gov/~dmgay/bounds10.pdf
Original motivation for this work: assess utility of "uncertainty compiler".

Computation Strategies

- Compile, link, execute
  - *Only choice for large scale?*
- Interpret
  - *E.g., python, awk, perl, ...*
- Mixture
  - *E.g., Java, AMPL, ...*

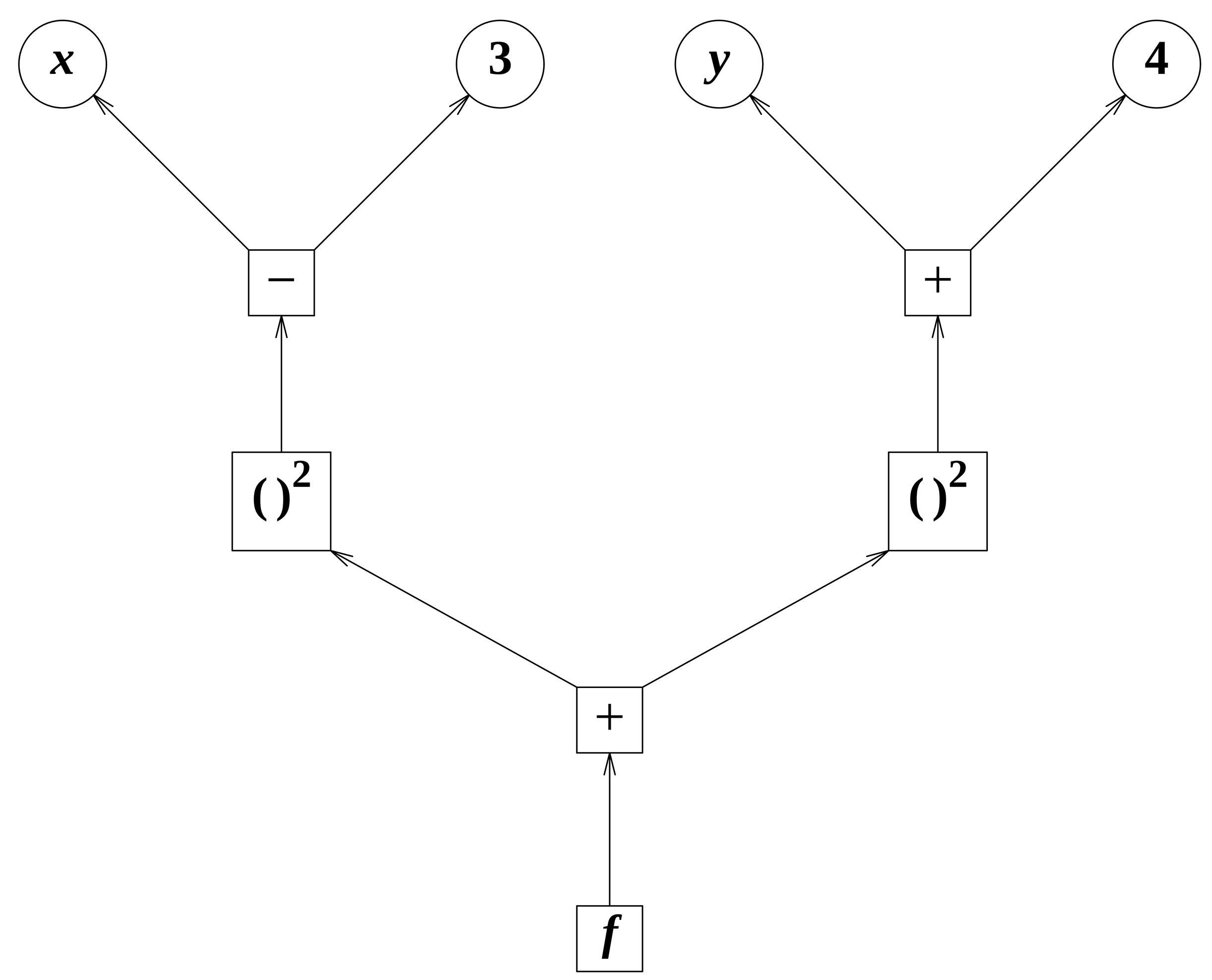
All involve expression graphs.

Expression Graphs

Uses include

- Simplifications before evaluations
- Evaluations
- Derivative computations (AD)
- Bound computations, e.g.,
  - interval
  - Taylor series
  - slope
- Convexity detection.

Expression Graph Example



Expression graph for $f = (x-3)^2 + (y+4)^2$

AD-like Graph Walks

Expression-graph walks similar to forward AD can

- compute interval bounds (by interval arithmetic);
- propagate Taylor series;
- compute interval slopes.

Slopes and Intervals

"Slopes" are divided differences:

$$f[x,z] = \begin{cases} (f(x) - f(z))/(x-z) & \text{if } x \neq z \\ f'(x) & \text{if } x = z \end{cases}$$

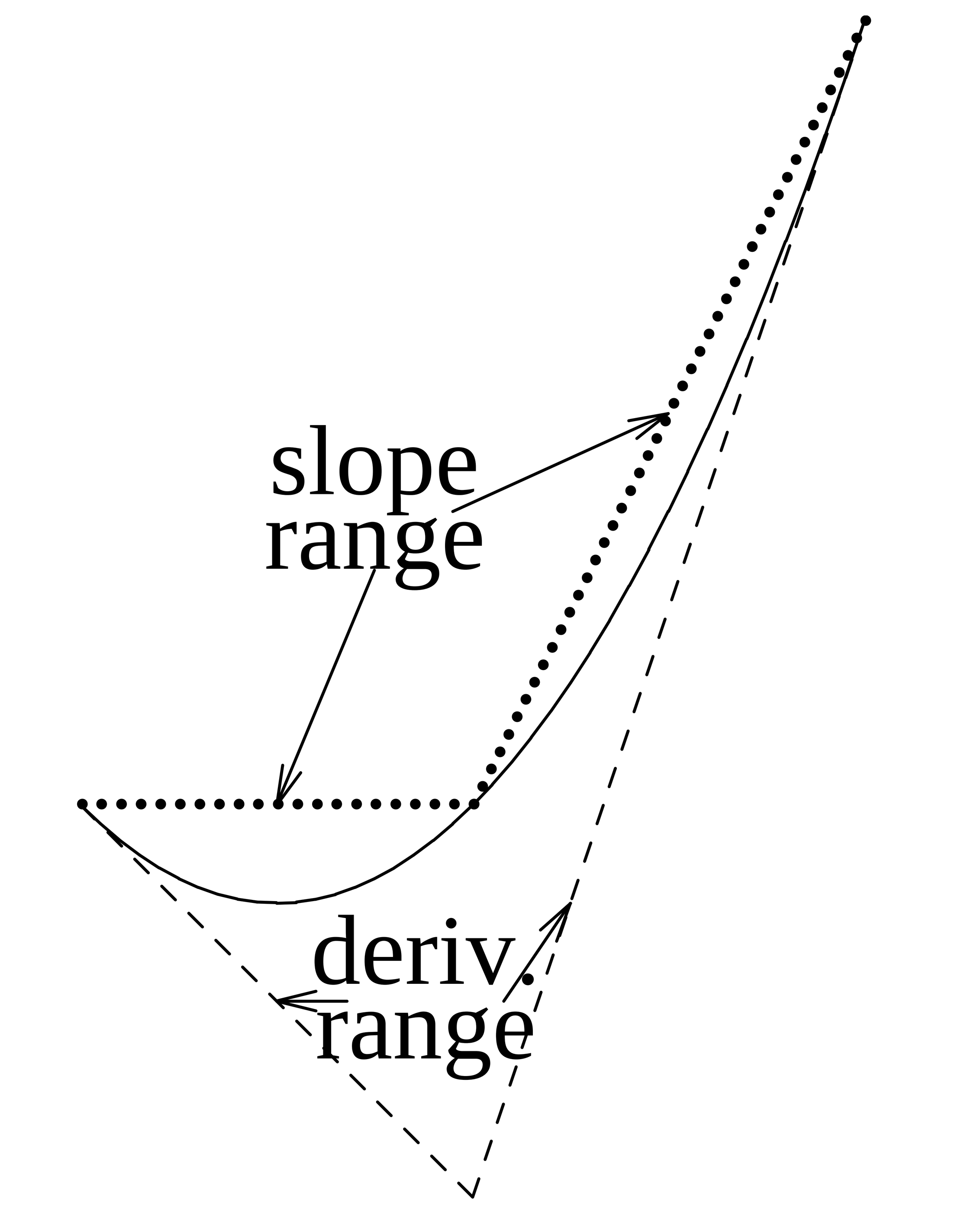
Given interval X, interval evaluation of $f[X,z]$ gives $f[x,z] \in f[X,z]\ \forall\, x \in X$. Since $f(x) = f(z) + f[x,z](x-z)$,

$$f(X) \subseteq F_z(X) \doteq f(z) + f[X,z](X-z).$$

Quadratic approximation:

$$width(F_z(X)) - width(f(X))$$
$$\leq O(width(X)^2).$$

Derivative vs. Slope Ranges



$f(x) = x^2$

Slope Arithmetic

Slope arithmetic, analogous to forward AD [Krawczyk & Neumaier, 1985]:

$f = \cdots$	$\Rightarrow f[X,z] = \cdots$
$c \in \mathbb{R}$	0
X	1
$g \pm h$	$g[X,z] \pm h[X,z]$
$g \cdot h$	$g[X,z] \cdot h(X) + g(z) \cdot h[X,z]$
g/h	$(g[X,z] - h[X,z] \cdot f(z))/h(X)$

Interval slope computations extend readily to n variables and can be done by walk of expression graph.

$$work(f[X,z]) = O(n \cdot work(f(x))).$$

Component-wise computation [Hanson, 1968] can be tighter (but slower).

Second-Order Slopes

Second-order slopes:

- Scalar: $f[x,z,z] = (f[x,z] - f'(z))/(x-z)$.
- $f(x) = f(z) + f'(z)(x-z) + f[x,z,z](x-z)^2$.
- Often get tighter bounds than with slopes.
- Still just quadratic approximation.
- For $x \in \mathbb{R}^n$, component-wise evaluations have

$work(f[X,z,z]) = O(n \cdot work(f(x)))$.

Some Bounding Techniques

interval	$F(X) \supset f(X)$
Taylor 1	$f(z) + F'(X)(X-z)$
slope 1	$f(z) + F[X,z](X-z)$
slope 2	$f(z) + f'(z)(X-z)$ $+F[X,z,z](X-z)^2$
slope 2*	$\{f(z) + f'(z)h + F[X,z,z]h^2 : h \in X - z\}$

Only "slope 2*" and the implementation are new in the present work.

Bound Widths on 2 Examples

Method	Barnes	Sn525
interval	162.417	0.7226
Taylor 1	9.350	0.3609
slope 1	6.453	0.3529
slope 2	3.007	0.1140
slope 2*	2.993	0.1003
true	2.330	0.0903

For problem details, see the paper.
Implementation (not finished) built on facilities in ASL (AMPL/Solver interface library).
Expression graphs from AMPL; use directed roundings (part of IEEE arithmetic standard).
Good for easy development, quick tests.
Contact dmg@acm.org for more details.