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Using Expression Graphs in Optimization Algorithms

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Outline

- The Problem
- Some algorithm ingredients
- Expression graphs
    - various forms
    - derivative computations
    - bound computations
    - convexity detection
- Summary and pointers

The Problem

$$\text{Seek } x^* \text{ to minimize } f(x)$$

$$\text{s.t.} \quad \ell \leq c(x) \leq u$$

$$f : \mathcal{R}^n \rightarrow \mathcal{R}$$

$$c : \mathcal{R}^n \rightarrow \mathcal{R}^m$$

with f, c smooth; $x \in D$ compact.

Settle for $\hat{x}$ with $f(\hat{x}) - f(x^*) < \epsilon$.

For MINLP, $n = p + q$, $D = \mathcal{R}^p \times \mathcal{Z}^q$.

Branch & Bound, Reduce, Cut...

Algorithm ingredients... in parallel,

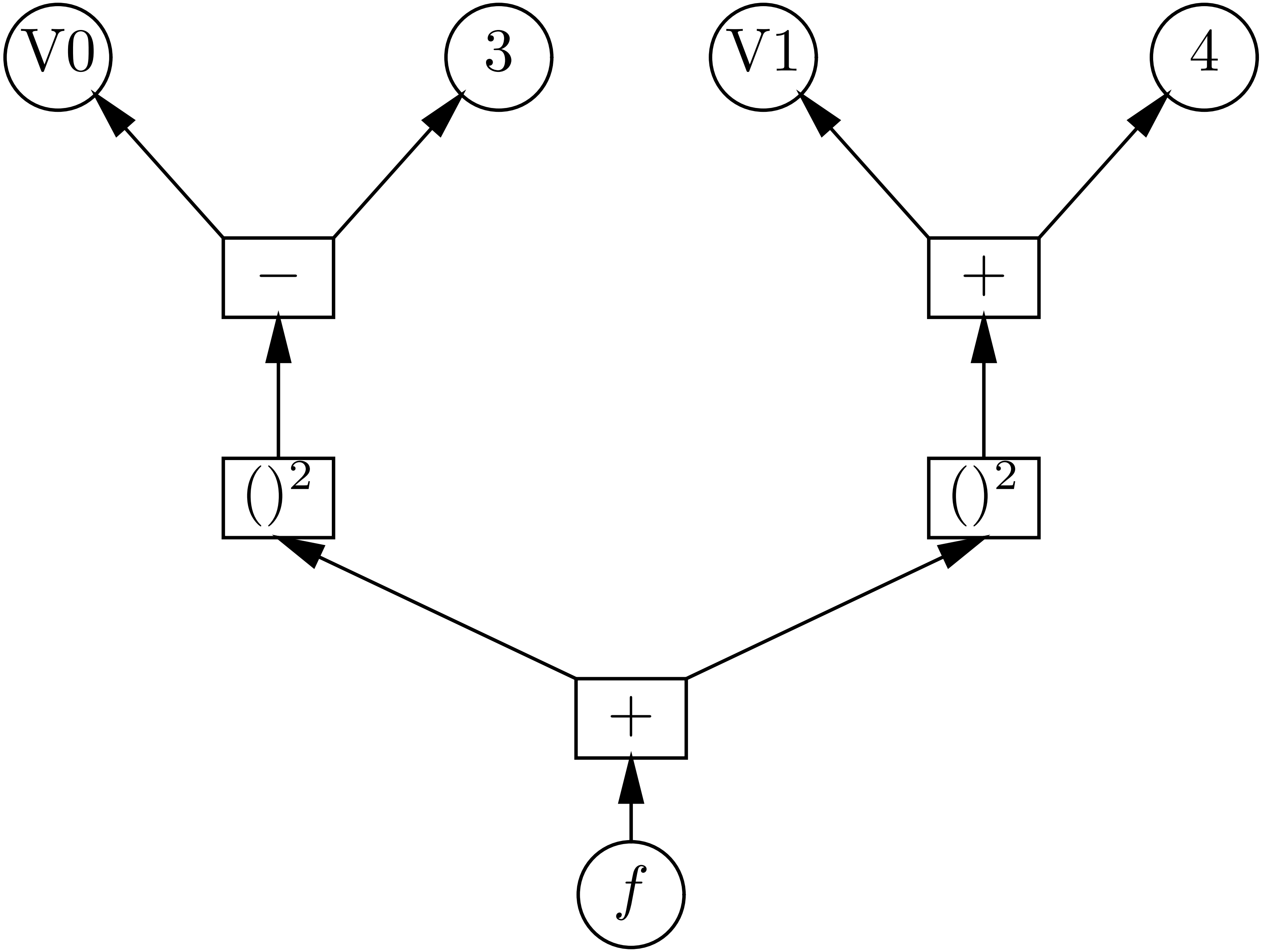
- Local search for good *incumbents*.
- Compute bounds (e.g., relax).
- Compute, refine convex outer approx's.
- Test for sufficiency, exclusion.
- Branch — split domain as needed.
- Reduce domain (using convexity).
- Presolve, updated with new info.

Expression Graphs

Good for

- Function evaluations (doing, simplifying)
- Derivative computations (AD)
- Bound computations, e.g.,
  - interval
  - Taylor series
  - slope
- Convexity detection.

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



Expression Graph Representations

Possible representations include

- graph = list-style data structures
- list of tuples
- Polish prefix or postfix
- XML

Convert from one to another in linear time.

AMPL/solver interface lib. (ASL) uses Polish prefix for external rep., graph for internal.

ASL Graph Walks

Graph walks in ASL currently include...

- conversion to internal form with AD setup
- detection of quadratic forms
- detection of partially-separable structure for efficient Hessian computations
- operator adjustments (for evaluations after some of the above)

Example: ASL Multiplication Operator

Do multiplication and save partials for AD:

```
 double
f_OPMULT(expr *e A_ASL)
{
    expr *e1 = e->L.e;
    expr *e2 = e->R.e;
    return   (e->dR = (*e1->op)(e1))
           * (e->dL = (*e2->op)(e2));
    }
```

Forward AD via Graph Walk

Computing $x_j = o_j(x_k, x_\ell)$ (with $j > n$, $k < j$, $\ell < j$)

$$\Longrightarrow \frac{\partial x_j}{\partial x_i} = \frac{\partial o_j}{x_k}\frac{x_k}{x_i} + \frac{\partial o_j}{x_\ell}\frac{x_\ell}{x_i} \quad \text{for} \quad 1 \le i \le n.$$

Similary recur higher derivatives by graph walk doing forward AD.

Partially Separable Structure

$$f(x) = \sum_i f_i(A_i x))$$

$$\Longrightarrow \nabla^2 f(x) = \sum_i A_i^T \nabla^2 f_i A_i$$

Graph walk finds “group” partial separability:

$$f(x) = \sum_i \theta_i(\sum_j^{r_i} f_{ij}(A_{ij}x))$$

Use of Partially Separable Structure

Good for efficiently computing explicit Hessians and Hessian-vector products.

In ASL, partials are stored during function evaluations (graph walks) for use in Hessian-vector computations by a mix of forward and backward AD.

More Computations by Graph Walks

Walks similar to forward AD can compute

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

“Slopes” are divided differences:

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

Slope Arithmetic

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

$f = \cdots$	$\Rightarrow f[x,z] = \cdots$
$c \in \mathcal{R}$	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 Slopes

Interval X, interval evaluation of $f[X, z]$

$$\Rightarrow f[x, z] \in f[X, z] \; \forall \; x \in X.$$

$$f(x) = f(z) + f[x, z](x - z)$$

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

Quadratic approximation:

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

Extension to n Variables

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

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

Second-Order Slopes

Second-order slopes:

- Not unique.
- $f(x) =$
  $f(z) + f'(z)(x - z) + (x - z)^T f[x, z, z](x - z).$
- $(x - z)^T f[x, z, z] = f[x, z] - f'(z).$
- For $x \in \mathcal{R}^n$,
  $work(f[X, z, z]) = O(n^2 \cdot work(f(x))).$

Convexity

Can specify some problems in a way that guarantees convexity, e.g.,

- CVXMOD [Boyd & Mattingley, 2006]
- Joesph Young thesis (Rice, 2008)

but in general have convexity only in some regions.

Convexity Detection

Can walk expression graphs to detect condition sufficient for convexity in a region.

- [Nenov, Fylstra, Kolev, 2004], in Frontline spreadsheet software
- Dr. AMPL [Fourer, et al., 2008]

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Summary

With walks of expression graphs we can

- Evaluate expressions
- Detect problem structure:
  - convexity, partially separable structure.
- Compute derivatives
- Compute bounds
- Presolve (linear, nonlinear)
- Optimize such computations.

Pointers

- Neumaier global optimization page/pointers: `http://www.mat.univie.ac.at/~neum/glopt.html`
- Coconut (C++ software): `http://www.mat.univie.ac.at/~neum/glopt/coconut`
- AMPL web site (e.g., some papers): `http://www.ampl.com`
- My papers: pointers in `http://www.cs.sandia.gov/~dmgay`