

AD in FORTRAN

Implementation *via* Preprocessor

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Outline of Talk

- ▶ motivation
- ▶ description by example
- ▶ implementation sketch
- ▶ take-home lessons

motivation

desiderata

AD which is:

- ▶ first class
 - ▶ integrated into language
 - ▶ can be used anywhere
 - ▶ can apply to anything
- ▶ convenient & natural
- ▶ modular
- ▶ expressive
- ▶ fast



what we did:

add AD to FORTRAN

(implementation: leverage existing AD tools)

THE THRILLS - THE CHILLS OF WITCHCRAFT TODAY

THE City OF THE dead

CHRISTOPHER LEE · DENNIS LOTIS
BETTA ST JOHN · PATRICIA JESSEL

WITH
VALENTINE DYALL

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VENETIA STEVENSON

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Executive Producers: SEYMOUR DORNER & MILTON SUBOTSKY
Screenplay by GEORGE BAXT Story by MILTON SUBOTSKY
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X ADULTS ONLY

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Starring

JONATHAN HAZE

JACKIE JOSEPH

MEL WELLES

the flowers that kill in the Spring

TRA-LA

THE FUNNIEST
PICTURE
THIS YEAR!

Produced and Directed by ROGER CORMAN

A FILMGROUP PRESENTATION



Traditional API for AD

```
FUNCTION RAPHSN(F, FPRIME, X0, N)
EXTERNAL F, FPRIME
X = X0
DO 1690 I=1,N
1690 X = X-F(X)/FPRIME(X)
RAPHSN = X
END
```

Note: *caller* provides both F and FPRIME.

Manually coding FPRIME from F is often mechanical, tedious, and error prone.

Automatic differentiation (Speelpenning, 1980; Wengert, 1964) eliminates that, but the *caller* of RAPHSN still needs to provide FPRIME, perhaps also arranging for it to be generated automatically from F.

allow *callee derives*

FARFEL: add AD block constructs to FORTRAN

Compute derivative PHI_{PRM} of PHI wrt SIGMA by forward AD:

```
ADF( TANGENT( SIGMA ) = 1.0 )
PHI = 1 / SQRT( 2 * PI * SIGMA ** 2 ) * EXP( - 0.5 *
END ADF( PHIPRM=TANGENT( PHI ) )
```

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END ADF( PHIPRM=TANGENT( PHI ) )
```

Same, by reverse AD:

```
ADR( COTANGENT( PHI ) ) = 1.0  
PHI = 1/SQRT( 2*PI*SIGMA**2 ) * EXP( -0.5 *  
END ADR( PHIPRM=COTANGENT( SIGMA ) )
```

FARFEL: add AD block constructs to FORTRAN

Compute derivative PHI_{PRM} of PHI wrt SIGMA by forward AD:

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Same, by reverse AD:

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PHI = 1 / SQRT( 2 * PI * SIGMA ** 2 ) * EXP( - 0.5 *  
END ADR( PHIPRM=COTANGENT( SIGMA ) )
```

Syntactically similar to the Naumann and Riehme (2005) NAGWARE 95 extensions, but more (a) general, (b) expressive, (c) available, (d) performant, (e) examples to follow.

```
SUBROUTINE GRAD(F, X, N, DX)
EXTERNAL F
DIMENSION X(N), DX(N)
DO 1492 I=1,N
    ADF((TANGENT(X(J))=0.0, J=1,N), TANGENT(X(I))=1.0)
    Y = F(X, N)
1492 END ADF(DX(I)=TANGENT(Y))
END
```

```
SUBROUTINE GRAD(F, X, N, DX)
EXTERNAL F
DIMENSION X(N), DX(N)
ADR(COTANGENT(Y)=1.0)
Y = F(X, N)
END ADR((DX(I)=COTANGENT(X(I)), I=1,N))
END
```

- ▶ callee derives
- ▶ same API for both versions
- ▶ implied **DO** syntax for arrays
- ▶ no restrictions, **EXTERNAL** parameters allowed

XSTAR = ARGMAX(F , X0)

C CHECKPOINT REVERSE F->G.

C BOTH F AND G ARE 1ST ARG IN, 2ND ARG OUT

CALL F(X, Y)

ADR((COTANGENT(Z(I))=DZ(I), I=1,NZ))

CALL G(Y, Z)

END ADR((DY(I)=COTANGENT(Y(I)), I=1,NY))

ADR((COTANGENT(Y(I))=DY(I), I=1,NY))

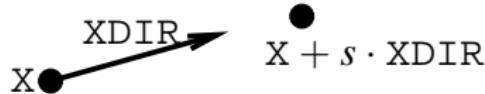
CALL F(X, Y)

END ADR((DX(I)=COTANGENT(X(I)), I=1,NX))

FARFEL allows nested subprograms

Allowing nested definitions is synergistic with first-class AD.

```
C      MAXIMIZE F ALONG THE LINE PARALLEL TO XDIR THROUGH X
      SUBROUTINE LINMAX(F, X, XDIR, LENX, N, XOUT)
      EXTERNAL F
      DIMENSION X(LENX), XDIR(LENX), XOUT(LENX)
      FUNCTION ALINE(DIST)
      DIMENSION Y(50)
      DO 2012 I=1,LENX
2012    Y(I) = X(I)+DIST*XDIR(I)
      ALINE = F(Y, LENX)
      END
      BESTD = ARGMAX(ALINE, 0.0, N)
      DO 2013 I=1,LENX
2013    XOUT(I) = X(I)+BESTD*XDIR(I)
      END
```



optimise scalar $a(s) = f(\vec{x} + s \cdot \vec{dir})$

encapsulation

modularity

nesting for modularity?

nesting for expressivity!

Two player non-zero-sum continuous-strategy game

Player A 's strategy is a .

Player A 's return is $A(a, b)$.

Player B 's strategy is b .

Player B 's return is $B(a, b)$.

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Equilibria must satisfy:

$$a^* = \underset{a}{\operatorname{argmax}} A(a, b^*)$$

$$b^* = \underset{b}{\operatorname{argmax}} B(a^*, b)$$

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Find by solving:

$$a^* = \underset{a}{\operatorname{argmax}} A(a, \underset{b}{\operatorname{argmax}} B(a^*, b))$$

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nesting

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Find by solving:

$$a^* = \underset{a}{\operatorname{argmax}} A(a, \underset{b}{\operatorname{argmax}} B(a^*, b))$$

↖ ↖ ↗ ↗
nesting

aka

$$\text{root } \underset{a^*}{\operatorname{argmax}} \underset{a}{\operatorname{argmax}} A(a, \underset{b}{\operatorname{argmax}} B(a^*, b)) - a^*$$

↗
more nesting

$$\underset{a^*}{\text{root}} \underset{a}{\arg\max} A(a, \underset{b}{\arg\max} B(a^*, b)) - a^*$$

Five levels of nesting. (One from ROOT, two from each ARGMAX.)

C ASTAR & BSTAR: GUESSES IN, OPTIMIZED VALUES OUT

SUBROUTINE EQLBRM(BIGA, BIGB, ASTAR, BSTAR, N)

EXTERNAL BIGA, BIGB

FUNCTION F(ASTAR)

FUNCTION G(A)

FUNCTION H(B)

 H = BIGB(ASTAR, B)

END

 BSTAR = ARGMAX(H, BSTAR, N)

 G = BIGA(A, BSTAR)

END

 F = ARGMAX(G, ASTAR, N)-ASTAR

END

ASTAR = ROOT(F, ASTAR, N)

END

```
FUNCTION ARGMAX(F, X0, N)
    FUNCTION FPRIME(X)
        FPRIME = DERIV1(F, X)
    END
    ARGMAX = ROOT(FPRIME, X0, N)
END
```

```
FUNCTION ROOT(F, X0, N)
X = X0
DO 1669 I=1,N
CALL DERIV2(F, X, Y, YPRIME)
1669 X = X-Y/YPRIME
ROOT = X
END
```

```
FUNCTION DERIV1(F, X)
EXTERNAL F
ADDF(X)
Y = F(X)
END ADDF(DERIV1 = TANGENT(Y))
END
```

```
SUBROUTINE DERIV2(F, X, Y, YPRIME)
EXTERNAL F
ADDF(X)
Y = F(X)
END ADDF(YPRIME = TANGENT(Y))
END
```

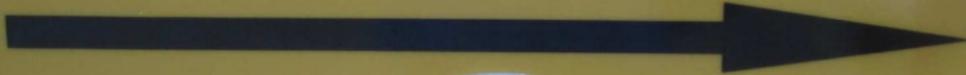
implementation

al Estates
t Nuclear Bunker

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REMOVED
WHEN FINISHED

CLOTHES MAY BE
REMOVED BY
WAITING CUSTOMERS
OR MANAGEMENT

Curry Prevention Services



Possible Implementation Strategies:

- ▶ native (integrated into compiler)
- ▶ preprocessor (generate FORTRAN)
- ▶ preprocessor (generate input to AD tools)

Possible Implementation Strategies:

- ▶ native (integrated into compiler)
- ▶ preprocessor (generate FORTRAN)
- ▶ preprocessors (generate input to AD tools)

FARFALLEN implementation of FARFEL:

- ▶ move contents of AD blocks into (nested) subroutines
- ▶ closure-convert nested subprograms to top level
- ▶ specialize away **EXTERNAL** constructs
- ▶ target TAPENADE or ADIFOR

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등산길 경고문

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분들은 이 표지판 뒤로 넘어가지 말아주시길
바랍니다.

ブッシュ・ウォーキング(山歩き) コース

ブッシュ・ウォーキング(山歩き)の熟練者
以外は、これより先には行かないで
下さい。

THIS SIGN IS TO PREVENT FOREIGN
TOURISTS FROM GETTING LOST



AD block contents to nested subroutines

```
PROGRAM MAIN
SIGMA = 1.0
PI = 3.14159
X = 1.0
XBAR = 1.0
ADF(TANGENT(SIGMA) = 1.0)
PHI = 1/SQRT(2*PI*SIGMA**2)*EXP(-0.5*((X-XBAR)/SIGMA)**2)
END ADF(PHIPRM = TANGENT(PHI))
PRINT *, PHIPRM
END
```



```
PROGRAM MAIN
SIGMA = 1.0
PI = 3.14159
X = 1.0
XBAR = 1.0
SUBROUTINE ADF1(PHI, SIGMA)
PHI = 1/SQRT(2*PI*SIGMA**2)*EXP(-0.5*((X-XBAR)/SIGMA)**2)
END
SIGMA_G1 = 1.0
ADF CALL ADF1(PHI, PHI_G1, SIGMA, SIGMA_G1)
PHIPRM = PHI_G1
PRINT *, PHIPRM
END
```

Closure Conversion

```
PROGRAM MAIN
SIGMA = 1.0
PI = 3.14159
X = 1.0
XBAR = 1.0
SUBROUTINE ADF1(PHI, SIGMA)
    PHI = 1/SQRT(2*PI*SIGMA**2)*EXP(-0.5*((X-XBAR)/SIGMA)**2)
END
SIGMA_G1 = 1.0
ADF CALL ADF1(PHI, PHI_G1, SIGMA, SIGMA_G1)
PHIPRM = PHI_G1
PRINT *, PHIPRM
END
```



```
SUBROUTINE MAIN_ADF1(PHI, SIGMA, PI, X, XBAR)
    PHI = 1/SQRT(2*PI*SIGMA**2)*EXP(-0.5*((X-XBAR)/SIGMA)**2)
END

PROGRAM MAIN
SIGMA = 1.0
PI = 3.14159
X = 1.0
XBAR = 1.0
SIGMA_G1 = 1.0
ADF CALL MAIN_ADF1(PHI, PHI_G1, SIGMA, SIGMA_G1, PI, X,
+ XBAR)
PHIPRM = PHI_G1
PRINT *, PHIPRM
END
```

Specialization

```
SUBROUTINE QUAD(F, A, B, STEP, OUT)
EXTERNAL F
OUT = 0.0
DO 5 X = A,B,STEP
5    OUT = OUT+F(X)
END

...
CALL QUAD(EXP, 0.0, 5.0, 0.1, Z)
CALL QUAD(SQRT, 1.0, 6.0, 0.1, X)
```



```
SUBROUTINE QUAD_SQRT(A, B, STEP, OUT)
OUT = 0.0
DO 5 X = A,B,STEP
5    OUT = OUT+SQRT(X)
END

SUBROUTINE QUAD_EXP(A, B, STEP, OUT)
OUT = 0.0
DO 5 X = A,B,STEP
5    OUT = OUT+EXP(X)
END

...
CALL QUAD_EXP(0.0, 5.0, 0.1, Z)
CALL QUAD_SQRT(1.0, 6.0, 0.1, X)
```

Calling Conventions

```
SUBROUTINE MAIN_ADF1(PHI, SIGMA, PI, X, XBAR)
PHI = 1/SQRT(2*PI*SIGMA**2)*EXP(-0.5*((X-XBAR)/SIGMA)**2)
END

PROGRAM MAIN
SIGMA = 1.0
PI = 3.14159
X = 1.0
XBAR = 1.0
SIGMA_G1 = 1.0
ADF CALL MAIN_ADF1(PHI, PHI_G1, SIGMA, SIGMA_G1, PI, X,
+ XBAR)
PHIPRM = PHI_G1
PRINT *, PHIPRM
END
```



```
SUBROUTINE MAIN_ADF1(PHI, SIGMA, PI, X, XBAR)
PHI = 1/SQRT(2*PI*SIGMA**2)*EXP(-0.5*((X-XBAR)/SIGMA)**2)
END

PROGRAM MAIN
SIGMA = 1.0
PI = 3.14159
X = 1.0
XBAR = 1.0
SIGMA_G1 = 1.0
CALL MAIN_ADF1_G1(PHI, PHI_G1, SIGMA, SIGMA_G1, PI, X,
+ XBAR)
PHIPRM = PHI_G1
PRINT *, PHIPRM
END
```

The full EQLBRM example

```
FUNCTION GMBIGB(A, B)
PRICE = 20.0-1.0*B
COSTS = B*(10.05-0.05*B)
GMBIGB = B*PRICE-COSTS
END

FUNCTION EQLBRM_GMBIGA_GMBIGB_F_G_H(ASTAR, B)
EQLBRM_GMBIGA_GMBIGB_F_G_H = GMBIGB(ASTAR, B)
END

SUBROUTINE DERIV1_EQLBRM_GMBIGA_GMBIGB_F_G_H(ADP, ASTAR, X, Y)
Y = EQLBRM_GMBIGA_GMBIGB_F_G_H(ASTAR, X)
END

FUNCTION DERIV1_EQLBRM_GMBIGA_GMBIGB_F_G_H(ADP, ASTAR, X)
X_G1 = 1.0
ASTAR_G1 = 0.0
Y_G1 = 0.0
CALL DERIV1_EQLBRM_GMBIGA_GMBIGB_F_G_H_DGP1(ADP, ASTAR, ASTAR_G1, X, X_G1, Y, Y_G1)
DERIV1_EQLBRM_GMBIGA_GMBIGB_F_G_H = Y_G1
END

FUNCTION ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H_FPRIME(ADP, ASTAR, X)
ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H_FPRIME = DERIV1_EQLBRM_GMBIGA_GMBIGB_F_G_H(ADP, ASTAR, X)
END

SUBROUTINE DERIV2_ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H_FPRIME(ADP, ASTAR, X, Y)
Y = ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H_FPRIME(ADP, ASTAR, X)
END

SUBROUTINE DERIV2_ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H_FPRIME(ADP, ASTAR, X, Y, YPRIME)
X_G2 = 1.0
ASTAR_G2 = 0.0
Y_G2 = 0.0
CALL DERIV2_ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H_FPRIME(ADP, ASTAR, ASTAR_G2, X, X_G2, Y, Y_G2)
YPRIME = Y_G2
END

FUNCTION ROOT_ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H_FPRIME(ADP, ASTAR, X0, N)
X = X0
DO 1669 I = 1, N
CALL DERIV2_ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H_FPRIME(ADP, ASTAR, X, Y, YPRIME)
X = X - Y*YPRIME
ROOT_ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H_FPRIME = X
END

FUNCTION GMBIGA(A, B)
PRICE = 20.0-1.0*A+1.0*B
COSTS = A*(10.0-0.05*A)
GMBIGA = A*PRICE-COSTS
END

FUNCTION ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H(ADP, ASTAR, X0, N)
ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H = ROOT_ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H(ADP, ASTAR, X0, N)
END

FUNCTION EQLBRM_GMBIGA_GMBIGB_F_G_H(ADP, ASTAR, BSTAR, N)
BSTAR = ARGMAX_EQLBRM_GMBIGA_GMBIGB_F_G_H(ADP, ASTAR, BSTAR, N)
EQLBRM_GMBIGA_GMBIGB_F_G_H = GMBIGA(A, BSTAR)
END

SUBROUTINE DERIV1_EQLBRM_GMBIGA_GMBIGB_F_G_H(ADP, ASTAR, BSTAR, N, X, Y)
Y = EQLBRM_GMBIGA_GMBIGB_F_G_H(ADP, ASTAR, BSTAR, N, X)
END

FUNCTION DERIV1_EQLBRM_GMBIGA_GMBIGB_F_G(ADP, ASTAR, BSTAR, N, X)
X_G3 = 1.0
ASTAR_G3 = 0.0
BSTAR_G3 = 0.0
N_G3 = 0.0
Y_G3 = 0.0
CALL DERIV1_EQLBRM_GMBIGA_GMBIGB_F_G(ADP, ASTAR, BSTAR, N, X, X_G3, BSTAR_G3, ASTAR_G3, BSTAR)
```

```
#!/bin/bash

tapenade -root deriv1_2_adf2 -d -o eqlbrm42 \
    -diffvarname "_g2" -difffuncname "_g2" \
    eqlbrm42.f

tapenade -root deriv2_1_2_adf4 -d -o eqlbrm42 \
    -diffvarname "_g4" -difffuncname "_g4" \
    eqlbrm42{,_g2}.f

tapenade -root deriv1_1_adf1 -d -o eqlbrm42 \
    -diffvarname "_g1" -difffuncname "_g1" \
    eqlbrm42{,_g2,_g4}.f

tapenade -root deriv2_1_1_adf3 -d -o eqlbrm42 \
    -diffvarname "_g3" -difffuncname "_g3" \
    eqlbrm42{,_g2,_g4,_g1}.f

tapenade -root deriv2_2_adf5 -d -o eqlbrm42 \
    -diffvarname "_g5" -difffuncname "_g5" \
    eqlbrm42{,_g2,_g4,_g1,_g3}.f
```

bugs

“issues”



BUGS BUGS BUGS! (Just a taste of the yummy bug juice.)

- (a) Deliberate errors on corner cases complicates automated use.
(E.g., refusal to process routine with no active inputs or no body.)
- (b) Inconsistent or incomplete or unpredictable name transformation.
 - ▶ `DIFFSIZES.INC`, `ND`, `NBDIRS`, `NBDIRSMAX`, etc.
 - ▶ ADIFOR prefixing interacts poorly with **IMPLICIT** declarations.
 - ▶ One-character ADIFOR prefix limit constitutes a limited resource.
- (c) Activity declarations are not respected.
 - ▶ Only sometimes.
 - ▶ By both ADIFOR and TAPENADE.
 - ▶ In different ways.
 - ▶ That vary by release.
 - ▶ (sometimes they determine an input inactive but if you *ask* for it to be inactive it will be made active.)
 - ▶ Need to know in order to call.
 - ▶ Must parse tool output to determine.
- (d) Reverse mode sometimes does not generate primal result.
 - ▶ Must parse tool output to determine.
 - ▶ Workarounds can interact catastrophically with impure primal.
- (e) No way to make cotangent inputs dependent upon primal result.
- (f) Many nesting issues, e.g., ADIFOR by default generates singularity check code which cannot itself be transformed, must set `AD_EXCEPTION_ELAVOB=performance`.

EQLBRM example in VLAD





Same “EQLBRM” example in VLAD

```
EQLBRM( $A, B, a_0, b_0, n$ )  $\triangleq$ 
  let  $a^* = \text{ROOT}_{a^*}(\text{ARGMAX}_a(A(a, (\text{ARGMAX}_b(B(a^*, b), b_0, n))), a_0, n) - a^*, a_0, n)$ 
       $b^* = \text{ARGMAX}_b(B(a^*, b), b_0, n)$ 
  in  $\langle a^*, b^* \rangle$ 
ARGMAX( $f, x_0, n$ )  $\triangleq$  let  $f'(x) \triangleq \text{DERIV1}(f, x)$  in  $\text{ROOT}(f', x_0, n)$ 
ROOT( $f, x, n$ )  $\triangleq$ 
  if  $n = 0$  then  $x$  else let  $\langle y, y' \rangle = \text{DERIV2}(f, x)$  in  $\text{ROOT}(f, x - \frac{y}{y'}, n - 1)$ 
DERIV1( $f, x$ )  $\triangleq$  let  $\langle x, \dot{y} \rangle = \vec{\mathcal{J}}(f, x, 1)$  in  $\dot{y}$ 
DERIV2( $f, x$ )  $\triangleq$   $\vec{\mathcal{J}}(f, x, 1)$ 
```

The $\vec{\mathcal{J}}$ symbol is a differential-geometric pushforward operator, analogous to the FARFEL **ADF** block construct.

There is an analogous $\overleftarrow{\mathcal{J}}$ pullback operator that corresponds to the **ADR** block construct.

For details on the language and its implementation see Pearlmutter and Siskind (2008a,b); Siskind and Pearlmutter (2008).

performance

THEIR FIRST **BIG** SCREEN ADVENTURE IN **COLOUR!**

GERRY ANDERSON'S

THUNDERBIRDS ARE GO

IN
SUPERMARIONATION

AND
TECHNICOLOR

*ADULTS OVER 16
SHOULD BE
ACCOMPANIED
BY CHILDREN

PRODUCED BY SYLVIA ANDERSON • DIRECTED BY DAVID LANE • RELEASED THROUGH UNITED ARTISTS



JOHN TRACY



BRISCOE



ALAN TRACY



JOHNNY TRACY



GORDON TRACY



SCOTT TRACY



BARBARA



LADY PENELAPE



PROFESSOR

FARFALLEN

TAPENADE

6.97

ADIFOR

8.92

STALINGRAD

5.83

AVAILABLE NOW!

lessons

seeking PhD students / postdocs

Support

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FAQs

FORTRAN 77

We would *love* to extend FARFALLEN from FORTRAN 77 to
FORTRAN 95 or FORTRAN 2008 *aka* ISO/IEC 1539-1:2010.

no

yes

GAME EXAMPLE DISCLAIMER

The EXISTENCE OR UNIQUENESS OF AN EQUILIBRIUM IS NOT IN GENERAL GUARANTEED, but our particular A and B have a unique equilibrium.

COORDINATE DESCENT (alternating optimization of a^* and b^*) would require less nesting, but HAS INFERIOR CONVERGENCE PROPERTIES.

Although this example involves AD THROUGH ITERATIVE PROCESSES, we do not address that issue in this work: it IS BEYOND THE SCOPE OF THIS PAPER, and used here only in a benign fashion, for vividness.

On our concrete objective functions THESE CONVERGE RAPIDLY, so for clarity we SKIP the clutter of CONVERGENCE DETECTION.

A stylized illustration of a woman's face in profile, facing right. Her head is split open at the top, revealing a bright, glowing yellow brain with white radial lines emanating from it. She has dark, wavy hair, heavy black eyeliner, and red lips. Her eyes are yellow and have black pupils. The background is a dark blue.

CRAWLING, SLIMY THINGS
TERROR-BENT ON
DESTROYING THE WORLD!

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FARFEL vs Naumann and Riehme (2005)

FARFEL constructs and features that the NAGWARE 95 AD extensions could not, to our knowledge, handle:

- ▶ **EXTERNAL** arguments
- ▶ nested internal definitions (lexically scoped)
- ▶ derivatives of derivatives (nesting)

This would impact all of the examples in this talk.