Computing Second Order Derivatives with ADiMat

Facilitating Optimal Experimental Design by Automatic Differentiation

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May 14, 2013 / Colloquium of the Interdisciplinary Center for Scientific Computing (IWR) of Heidelberg University

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Outline

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   - Second Order Derivatives
   - ADiMat
2. Second Order Derivatives with ADiMat
   - Full Second Order Derivatives: Hessians
   - Nested Application of ADiMat
3. Performance Results

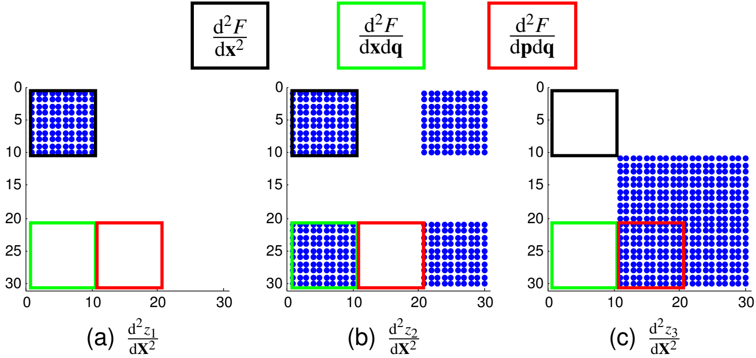
Second Order Derivatives

- Second order derivatives are often required in software for Optimal Experimental Design (OED), for example in VPLAN [Körkel, 2002].
    - We consider functions of the form $\mathbf{z} = F(\mathbf{x}, \mathbf{p}, \mathbf{q}) : (\mathbb{R}^{n_x} \times \mathbb{R}^{n_p} \times \mathbb{R}^{n_q}) \to \mathbb{R}^m$
    - Costs: time T_F and memory M_F
    - Needed derivatives: $\frac{\mathrm{d}^2 F}{\mathrm{d}\mathbf{x}^2}$, $\frac{\mathrm{d}^2 F}{\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{q}}$, and $\frac{\mathrm{d}^2 F}{\mathrm{d}\mathbf{p}\mathrm{d}\mathbf{q}}$
    - Abbreviations: $\mathbf{X} = [\mathbf{x}, \mathbf{p}, \mathbf{q}]$, $n = n_x + n_p + n_q$
- Using Automatic Differentiation (AD) for 2$^{\text{nd}}$ order derivatives is attractive for performance reasons
    - Precise derivatives help in optimization
    - AD is often more efficient than numerical methods
    - AD is more broadly applicable (in the mathematical sense)

Example Function

```
function z = F(x, p, q)
  t1 = 1;
  for i=1:length(x)
    t1 = t1 .* sin(x(i));
  end
  t2 = 1;
  for i=1:length(p)
    t2 = t2 .* sin(x(i) .* q(i));
  end
  t3 = 1;
  for i=1:length(q)
    t3 = t3 .* cos(p(i) .* q(i));
  end
  z = [t1, t2, t3];
```

2^{nd} Order Derivatives of Example Function



(a) $\frac{d^2z_1}{d\mathbf{X}^2}$ (b) $\frac{d^2z_2}{d\mathbf{X}^2}$ (c) $\frac{d^2z_3}{d\mathbf{X}^2}$

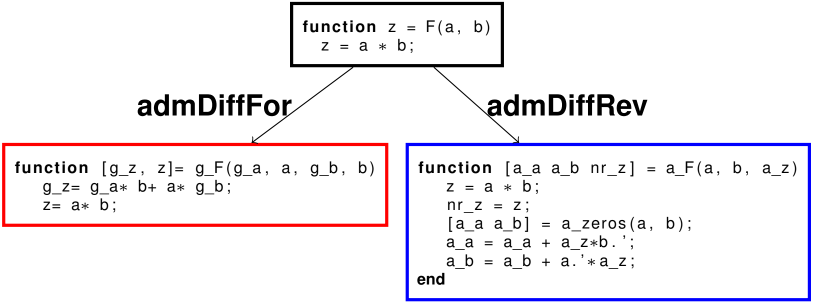
Figure: `spy` plots of the Hessians of the $m = 3$ output components of F for $n_x = n_p = n_q = 10$.

ADiMat

- **A**utomatic **Di**fferentiation for **Mat**lab (**ADiMat**) is an AD tool for MATLAB (http://www.adimat.de)
- Uses source transformation, but combines it with operator overloading [Bischof & Bücker et al., 2002]
- Supports both forward mode (FM) and reverse mode (RM)
- Capitalizes on the high-level mathematical functions and operators in MATLAB, like $*$, \, `eig`, `svd`, `expm`, `cross`, `interp1`, `roots`, ...
- ADiMat features
  - Comfortable user interface [Willkomm & Bischof & Bücker, 2012]
  - Higher order derivatives (univariate and mixed)

ADiMat Internals

- ADiMat transforms function `F` to a new function



```
function z = F(a, b)
  z = a * b;
```

admDiffFor

admDiffRev

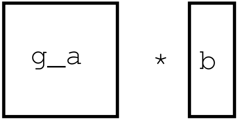
```
function [g_z, z]= g_F(g_a, a, g_b, b)
   g_z= g_a* b+ a* g_b;
   z= a* b;
```

```
function [a_a a_b nr_z] = a_F(a, b, a_z)
   z = a * b;
   nr_z = z;
   [a_a a_b] = a_zeros(a, b);
   a_a = a_a + a_z*b.';
   a_b = a_b + a.'*a_z;
end
```

- Evaluation of derivatives of `F` at certain arguments `a, b` by running the generated functions
- Derivative inputs have to be properly initialized (seeding)

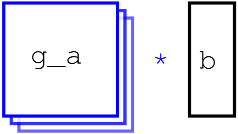
Scalar and Vector Mode

- Derivative variables have the same shape as the originals



This only allows for a single directional derivative in `g_x`: scalar mode

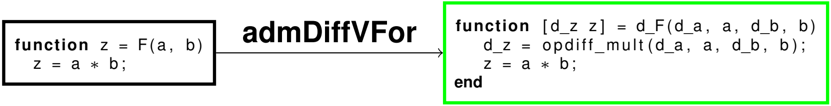
- For vector mode use derivative class objects, with overloaded operators, as containers for $n_{\mathrm{dd}} > 1$ directional derivatives



- Overloaded operator dispatch happens at run time, since MATLAB is weakly typed
- Performance is quite bad

Alternative: Vectorized Code

- Alternative: “vectorize” the code explicitly
  - Replace objects by opaque data type
  - Replace overloaded operators by function calls



```
function z = F(a, b)
  z = a * b;
```

admDiffVFor

```
function [d_z z] = d_F(d_a, a, d_b, b)
   d_z = opdiff_mult(d_a, a, d_b, b);
   z = a * b;
end
```

- Resolution of function calls now at compile time
  - Often very good performance, especially with “scalar” or “F77-style” codes, for small to medium n_{dd}.

Full 2$^{\text{nd}}$ Order Derivatives: Hessians

- Main driver for second order derivatives is **admHessian**
- Computes the full Hessian matrix H
- or (multiple) products $\mathrm{H} \cdot \mathbf{v}$ thereof
  - We can pick out our desired derivatives from H,
  - or compute only the suitable linear combinations $\mathrm{H} \cdot \mathbf{v}$
- Returns the Hessians of all function results H_k, $1 \leq k \leq m$
- Two evaluation strategies:
  - Forward over reverse mode (default)
  - Linear combination of second order univariate Taylor coefficients

Forward over Reverse Mode

- Differentiate function F in RM
- Run RM evaluation with a typical first order FM OO class
  - Obtain first order derivatives of function result by the FM
  - and the derivatives of those w.r.t. all inputs by the RM
- Costs:
  - Time $O(m) \cdot T_F$ for one $\mathrm{H} \cdot \mathbf{v}$ product
  - Time $O(n \cdot m) \cdot T_F$ for full H
  - Space $O(T_F)$ for the stack required by the RM

```
adopts = admOptions('i', [1 2 3]);
adopts.functionResults = {z};
H = admHessian(@F, 1, x, p, q, adopts);
```

- Caveat: FM OO class supports very few builtins as of yet

Forward over Reverse Mode

- We don't need the full Hessian H, in particular not $\frac{\mathrm{d}^2 F}{\mathrm{d}\mathbf{q}^2}$
  - Mask out the columns corresp. to $\mathbf{q}$ with a seed matrix

$$\mathrm{S} = \begin{pmatrix} \mathrm{I}_{n_x} & 0_{n_p} \\ 0_{n_p} & \mathrm{I}_{n_p} \\ 0_{n_q} & 0_{n_q} \end{pmatrix} \in \mathbb{R}^{n \times (n_x + n_p)}$$

  - With the example function F we could even use compression (adding together the $\mathbf{x}$– and $\mathbf{p}$–columns)
- Costs:
  - Time $O((n_x + n_p) \cdot m) \cdot T_F$ for the desired sub blocks of H

```
S = [eye(numel(x))     zeros(numel(x))
     zeros(numel(p))   eye(numel(p))
     zeros(numel(q))   zeros(numel(q))];

H = admHessian(@F, S, x, p, q, adopts);
```

2nd Order Taylor Coefficients

- Propagate 2nd order univariate Taylor coefficients in FM
- Compute the off-diagonal Hessian entries as
  $H_{i,j} = \frac{1}{2}\left(D^2_{\mathbf{e}_i+\mathbf{e}_j}F(\mathbf{X}) - D^2_{\mathbf{e}_i}F(X) - D^2_{\mathbf{e}_j}F(X)\right), \quad i \neq j$
  [Griewank & Walther, 2008]
    - For full H need $n + \frac{n\cdot(n+1)}{2}$ derivative directions
- Costs:
    - Time $O(n^2)\cdot T_F$ for full H
    - Space $O(n^2)\cdot M_F$

```
adopts.hessianStrategy = 't2for';
% Alternatives: use FD, vectorized Taylor mode
% adopts.admDiffFunction = @admDiffFD;
% adopts.admDiffFunction = @admTaylorVFor;
H = admHessian(@F, 1, x, p, q, adopts);
```

Mixed 2nd Order Directional Derivatives

- Generate three functions by twice applying the FM
  - Diff. `F` in FM w.r.t. `x`, then `dx_F` w.r.t. both `x` and `g_x`
  - Also differentiate `dx_F` w.r.t. `q`
  - Differentiate `F` in FM w.r.t. `p`, then `dp_F` w.r.t. `q`

```
alias ac='adimat-client -F'
ac -ix      -d1                  -odx_F.m    F.m
ac -ig_x,x  -d1 -sgradprefix=h_  -odx_dx_F.m dx_F.m
ac -iq      -d1 -sgradprefix=h_  -odq_dx_F.m dx_F.m
ac -ip      -d1                  -odp_F.m    F.m
ac -iq      -d1 -sgradprefix=h_  -odq_dp_F.m dp_F.m
```

- Costs:
  - Time $O(1) \cdot T_F$ and space $O(1) \cdot M_F$ for one entry $H_{i,j}$
  - Time $O(n_x^2/2 + n_x n_q + n_p n_q) \cdot T_F$ for the desired sub blocks
- Caveat: ADiMat may not be able to reprocess its code

Mixed 2^{nd} Order Directional Derivatives

```
h_g_x = zeros(size(x)); h_x = h_g_x; g_x = h_x;
for i=1:numel(x), for j=1:i
    h_x(i) = 1; g_x(j) = 1;
    h_g_f = dx_dx_F(h_g_x, g_x, h_x, x, p, q);
    dF_dxdx(:,i,j) = h_g_f(:);
    dF_dxdx(:,j,i) = h_g_f(:);
    h_x(i) = 0; g_x(j) = 0;
  end end
h_q = zeros(size(q)); g_x = zeros(size(x));
for i=1:numel(x), for j=1:numel(q)
    g_x(i) = 1; h_q(j) = 1;
    h_g_f = dq_dx_F(g_x, x, p, h_q, q);
    dF_dqdx(:,i,j) = h_g_f(:);
    g_x(i) = 0; h_q(j) = 0;
  end end % likewise for dF_dqdp
```

Complex Variable Method over FM

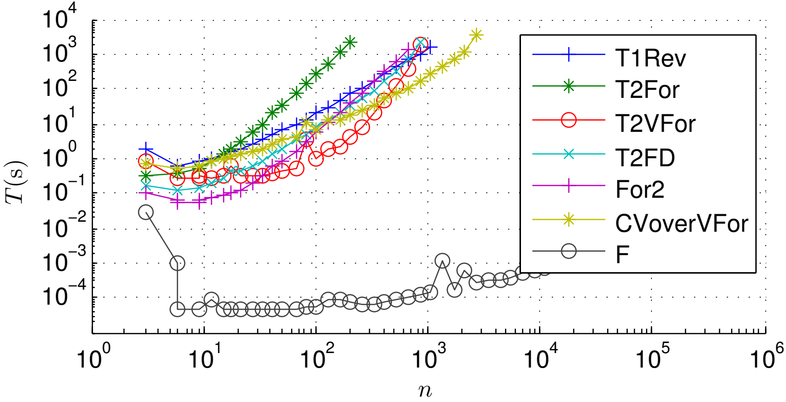
- First order FM to compute Jacobian
- Apply complex variable (CV) method on top of that
  - Only applicable if F is real analytic
  - Very precise and efficient approximation to derivatives

```
adopts2 = admOptions(’i’, [1 2 3] + 2, ’d’, 1);
adopts2.nargout = 1;
H = admDiffComplex(@admDiffVFor, S, ...
      @F, 1, x, p, q, adopts, adopts2);
H = reshape(H, [numel(z) size(S)]);
```

- Costs:
  - Time $O(n) \cdot T_F$ for one $\mathrm{H} \cdot \mathbf{v}$ product
  - Time $O(n \cdot (n_x + n_p)) \cdot T_F$ for the desired sub blocks of H
  - Space $O(n) \cdot M_F$

Performance Test

- Six methods to compute the three Hessian sub blocks:



Summary

- Presented six different methods for evaluation of 2nd order derivatives with ADiMat
  - There are more
  - Certain room to manoeuver w.r.t. performance and language support
- ToDo items
  - Broaden language support of the 2nd higher derivative methods in ADiMat
  - And also enhance performance of them
- Outreach
  - Visit ADiMat on the web at www.adimat.de
  - Subscribe to the ADiMat Users mailing list

References I

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Das Softwarepaket VPLAN
Dissertation, 2002

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Evaluating Derivatives
SIAM, 2008

C. Bischof, M. Bücker, B. Lang, A. Rasch & A. Vehreschild
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Proceedings of the Second IEEE International Workshop on Source Code Analysis and Manipulation (SCAM), 2002

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