

Computational Economics: Practical Tools and Techniques

Part 1: Overview of scientific computing

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Historical perspectives on computers and economics

- Odhner Arithmometer (1874): 9 digit precision for operands, 13 digits for results
- EDSAC (UK, 1949-1958): 17 bits (one word) or 35 bits (two words) long operands and results, ~220 multiplications per second, 12kW, weight 6t (ENIAC, US, 1946-1955: 10 bits operands and results, ~400 multiplications per second, 160 kW, 27 t) - the first article by Hendrick Houthakker published in econometrics based on results from a digital calculator having a stored memory program. "Some Calculations on Electricity Consumption in Great Britain", Journal of Royal Statistical Society, 1951.
- Orcutt's portable regression analyzer (1945), 2 digit accuracy, 33 items in storage on punch cards, "A Study of the Autoregressive Nature of the Time Series Used for Tinbergen's Model of the Economic System of the United States, 1919-1932", Journal of Royal Statistical Society, 1948.

- "Ninja gap" - performance gap between naively written C/C++ code that is parallelism unaware and best-optimized code on modern multi-/many-core processors
- There is an average Ninja gap of 24X (up to 53X) for a recent 6-core Intel Core i7 X980 Westmere CPU, and that this gap if left unaddressed will inevitably increase (Nadathur Satish et al, Computer Architecture (ISCA), 2012)
- Computational complexity and numerical algorithms complexity: complementary or substitute?
- Massively parallel processors favor **simpler** numerical algorithms: larger block-independent data frames with optimal function calls versus sophisticated (expensive) serial code

Round-off (trivial) errors (logistic functions based models)

MATLAB (standard double data type)

There is no quadruple precision available in standard MATLAB distributions

```
1 1e15*sum([-5, 1e-15, 5])
2 ans = 0.8882
3
4 1e15*sum([-15, 1e-15,15])
5 ans = 1.7764
6
7 eps(-15)+eps(1e-15)+eps(15)
8 ans = 3.5527e-15
```

"Big Data"?

2012: Really Big Objects Coming to R: matrices were limited 46,000 by 46,000 before.

Symbolic computing in MATLAB and Mathematica

ADVANPIX Multiprecision Computing Toolbox for MATLAB - highly optimized for quadruple precision

```
1 tic; [U,S,V] = svd(Y); toc; % MATLAB Symbolic Math Toolbox
2 Elapsed time is 59.357723 seconds.
3 norm(Y-U*S*V',1); 3.061145275981987186191661e-31
4 tic; [U,S,V] = svd(X); toc; % Multiprecision Computing Toolbox
5 Elapsed time is 0.668525 seconds. % ~80 times faster
6 norm(X-U*S*V',1); 5.718086004885703247723198511534649e-31
```

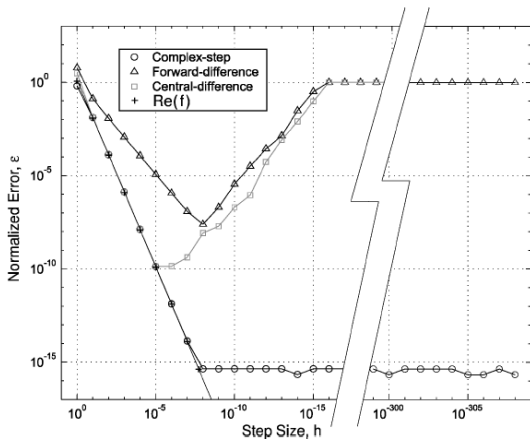
"It is disappointing, certainly, that **no simple finite-difference formula** gives accuracy comparable to the machine accuracy or even the lower accuracy to which f[unction] is evaluated" –William Press, Numerical Recipes in C++

- $f'(x) = \frac{f(x+h)-f(x)}{h} + \mathcal{O}(h)$, truncation error is $\mathcal{O}(h)$
- Truncation error vs. subtractive cancellation (loss of significance)

```
1 %MATLAB
2 x=2; h=10^-1; ((x+h)^3-x^3)/h
3 ans = 12.6100;
4 x=2; h=10^-15; ((x+h)^3-x^3)/h
5 ans = 10.6581;
```

- Taylor series for real function extended into the complex plane
$$f(x + ih) = f(x) + ih \frac{\partial f}{\partial x} - \dots$$
- $\frac{\partial f}{\partial x} \approx \frac{\text{Im}[f(x + ih)]}{h}$
- Error is $O(h^2)$

Complex Step Derivative: Asymptotics



From: J. R. R. A. Martins, P. Sturdza and J. J. Alonso, "The Complex-Step Derivative Approximation". ACM Transactions on Mathematical Software, Vol. 29, No. 3, September 2003, Pages 245-262.

Complex Step Derivative: Implementation in MATLAB using OOP

```
1 % Example
2 %tic;h=@(x) 2*pi*x.^3 + 5*x.^2 + 3*x;d=CSD;nx=100000;x=linspace(-100,100,nx);tt=
   zeros(1,nx);tt=d.gradient(h,x);toc; Elapsed time is 14.981273 seconds.
3 classdef CSD < handle
4     properties
5         def_step = 1e-9;
6     end
7     methods
8         function grad = gradient(this, h, x0, step)
9             num_var= length( x0 );
10            grad = zeros(num_var, 1 );
11            if nargin < 4
12                dx = this.def_step ;
13            else
14                dx = step ;
15            end
16            x_i = x0 + 1i * dx ;
17            for i_x = 1 : num_var
18                x1 = x0;
19                x1( i_x ) = x_i(i_x) ;
20                [ fval ] = h( x1(i_x) ) ;
21                grad(i_x ) = imag( fval / dx ) ;
22            end
23        end
24    end
25end
```

Complex Step Derivative: Implementation in Fortran

```
1  implicit none
2  interface
3  function simple_function(x)
4  implicit none
5  complex(8) :: simple_function
6  complex(8), intent(in) :: x
7  end function simple_function
8  end interface
9  real(8), parameter :: def_step = 1e-9
10 real(8), allocatable :: x_real(:), dfdx(:)
11 real(8) xmin, xmax
12 complex(8), allocatable :: x_complex(:)
13 integer nx, i
14 nx = 100000
15 xmin = -100
16 xmax = 100
17 allocate(x_real(nx), dfdx(nx), x_complex(nx))
18 do i=1,nx
19 x_real(i) = xmin + (i-1)*(xmax-xmin)/(nx-1)
20 x_complex(i) = dcplx(x_real(i), def_step)
21 dfdx(i) = dimag(simple_function(x_complex(i))) / def_step
22 end do
```


Complex Step Derivative: Implementation in Fortran

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20 x_complex(i) = dcplx(x_real(i), def_step)
21 dfdx(i) = dimag(simple_function(x_complex(i))) / def_step
22 end do
```

time ./csd → 0.004s

Speed gain: 3750 times over MATLAB OOP implementation, further gains are possible

pure function-based MATLAB 0.01s

Using Python as glue: Fortran/C to Python

```
1 function simple_function(x)
2
3 implicit none
4 complex(8) :: simple_function
5 complex(8), intent(in) :: x
6
7 ! Declare local constant Pi
8 complex(8), parameter :: Pi = 3.1415927
9
10 simple_function = 2*Pi*x**3 + 5*x**2 + 3*x
11
12 end function simple_function
```

```
1 f2py -c -m ff simple_function.f90
2 python
3 Python 2.7.5 |Anaconda 1.7.0 (x86_64)
4 >>> import ff
5 >>> ff.simple_function(1)
6 (14.283185482025146+0j)
```

Scientific Computing versus Computer Science

- One of the other problems we face, with respect to software, is the fact that we haven't changed our programming model in the last thirty years. FORTRAN and C are the programming paradigms that we used, and we still use, and they have no mechanism for doing parallel processing, so all the processing comes about through functional calls that are made to do the message passing. We really need to think about new languages that can effectively exploit parallel processing.
- The chips in our laptops are capable of high performance; for instance, **if we do the right thing with respect to the memory hierarchy we can see really significant speedup over doing it in a naive way.**

An interview with Jack J. Dongarra, SIAM, 2004.

Benchmarks for serial code performance: naive (inefficient) Python

```
1 #!/usr/bin/env python
2 import time
3
4 def linspace( start , end , count ) :
5
6     delta = (end-start) / float(count)
7     return [start,] + \
8     map( lambda x:delta*x + start , range( 1, count ) ) + [end, ]
9
10 if __name__ == "__main__":
11     t = time.clock()
12     nx = 10000000
13
14     xmin, ymin = float(0), float(0)
15     xmax, ymax = float(1), float(1)
16
17     x = linspace(xmin, xmax, nx)
18     y = linspace(ymin, ymax, nx)
19     vec_mult=linspace(0,0,nx); # initialize vector
20
21     for i in range(1,nx) :
22         vec_mult[i] = x[i]*y[i]
23     print sum(vec_mult)/nx
24     print time.clock() - t
```

0.333333283333 12.832045s

Benchmarks for serial code performance: MATLAB versus Python

(Python Enthought Canopy distribution or Anaconda distribution)

The NumPy array: a structure for efficient numerical computation:

A convenient way of describing blocks of computer memory, so that the numbers represented may be easily manipulated - a view over the memory, **strided** memory model

```
1 #!/usr/bin/env python
2 import numpy
3 import time
4
5 t = time.clock()
6 nx = 10000000
7
8 xmin, ymin = float(0), float(0)
9 xmax, ymax = float(1), float(1)
10 dx = float(xmax-xmin)/(nx-1)
11 dy = float(ymax-ymin)/(nx-1)
12 x = numpy.arange(xmin, xmax, dx)
13 y = numpy.arange(ymin, ymax, dy)
14 print numpy.dot(x,y)/nx
15 print time.clock() - t
```

0.33333325 0.113677s **Speed gain: 100 times over naive implementation, further gains are possible**

```
1 %MATLAB
2 tic; nx = 10000000; x=linspace(0,1,nx); y=linspace(0,1,nx); disp(sum(x.*y)/nx); toc;
```

0.333333349999975 Elapsed time is 0.560156 seconds.

Math libraries

- Basic Linear Algebra Subprograms - BLAS/LAPACK
- Intel MKL: industry-standard, interfaces to C and Fortran; "Intel MKL is indispensable for any high-performance computer user on x86 platforms." Jack Dongarra
- OpenBLAS - multi-threaded high performance implementation for multi-core CPUs
- MacOS X: Accelerate framework
- MATLAB with Intel MKL \Rightarrow 5-6 times faster than open source Fortran/BLAS
- The GNU Scientific Library (GSL) - a C replacement for numerical procedures written in Fortran (Netlib), NO high performance BLAS
- EIGEN templates and Armadillo C++ linear algebra library, the syntax (API) deliberately similar to MATLAB
- IMSL FORTRAN/C Numerical Library

- Gradients and Hessians are critical for Newton-based NL solvers
- Solution update method: Sequential Quadratic Programming (SQP), Interior-Point (IP)
- Global optimum: trust region, line search
- Penalty function, tolerance, feasibility
- SNOPT
 - line-search SQP; null-space CG option
 - l_1 exact penalty function
- IPOPT - open source in COIN-OR
 - line-search filter algorithm
- KNITRO
 - trust-region Newton, interior with CG option or direct
 - l_1 exact penalty function
 - Active Set - for medium size problems with good initial guess

AMPL (GAMS) Modeling and Programming Languages

- use automatic differentiation (AD vs. CSD vs. numeric differentiation)
- natural for optimization problems
- mathematical programming
- access to solvers
- portable code
- NEOS server

(<http://www.neos-server.org/neos/solvers/index.html>) :

input in GAMS or AMPL

dozens of solvers available, including KNITRO, SNOPT,
MOSEK, IPOPT

Non-linear Optimization with derivatives: Example

Structural model estimation with GMM, GMM (initial) = 29

"Constrained optimization approaches to estimation of structural models", C.-L. Su & K. Judd, Econometrica, 2012

```
1 KNITRO 6.0.0
2 Number of variables:                2339
3 Number of constraints:              2300
4   linear equalities:                44   nonlinear equalities:
   2256
5 Number of nonzeros in Jacobian:     133696
6 Number of nonzeros in Hessian:     60879
7 ...
8 25 iterations; 50 function evaluations
9 GMM = 3.72555
10 Total program time (secs)          =      12.79959 (12.774 CPU time)
```

```
1 Ipopt 3.10.3 (NEOS)
2 Number of iterations....: 94 Number of objective function evaluations = 153
3 GMM = 3.72555
4 Total CPU secs in IPOPT (w/o function evaluations) =      61.193
5 Total CPU secs in NLP function evaluations          =     110.733
```

SNOPT 7.2-10 : failed. 26104 iterations, CONOPT 3.15C: failed; objective 1418728.502