Algorithmic Differentiation

C++ & Extremum Estimation

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Outline

Slides

- Latest version: https://speakerdeck.com/mattpd

Why?

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- Nowadays one of the most widely applied approaches — estimation (econometrics, statistics), calibration (finance), training ((supervised) machine learning)
- In practice: Generally no are closed-form expressions — estimation relies on numerical optimization

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  - class includes OLS (Ordinary Least Squares), NLS (Nonlinear Least Squares), GMM (Generalized Method of Moments), and QMLE (Quasi Maximum Likelihood Estimation)

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    - H_k:
      $H_k = I$ (Steepest Ascent) — many variants, including SGD (Stochastic Gradient Descent)
      $H_k = \nabla^2 Q(\theta_k)$ (Newton)
      H_k = Hessian approximation satisfying the secant equation:
      $H_{k+1} s_k = \nabla Q_{k+1} - \nabla Q_k$ (Quasi-Newton)

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  - Inference: Covariance matrix estimators also involve the use of derivative information.

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- How does it compare to other computational differentiation methods?

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  - Symbolic Differentiation

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- "Many a serious mathematician has attempted to give rigorous analyses of a sequence of floating point operations, but has found the task to be so formidable that he has tried to content himself with plausibility arguments instead." — Donald E. Knuth, TAOCP2

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    - a measure of precision in numeric calculations. In base b, if x has exponent E, then ULP(x) = $\epsilon_M \cdot b^E$.

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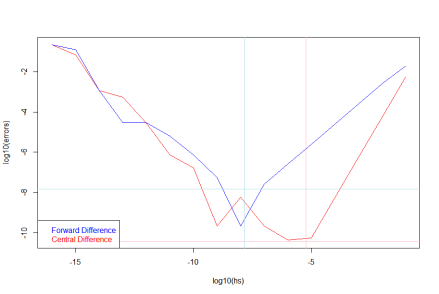

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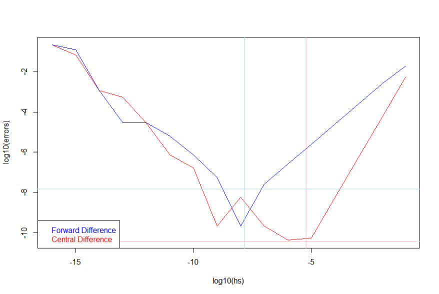

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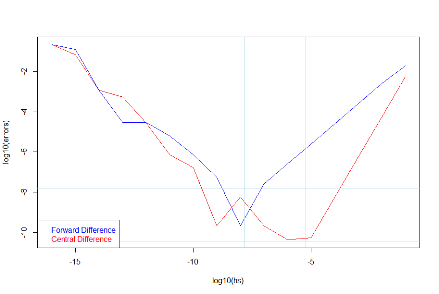

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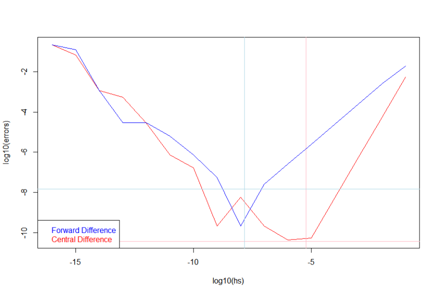

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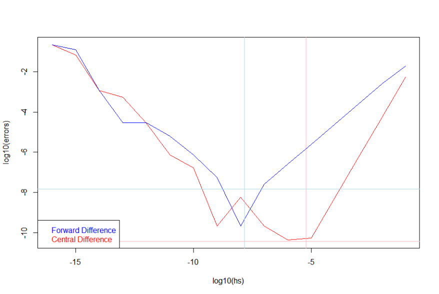

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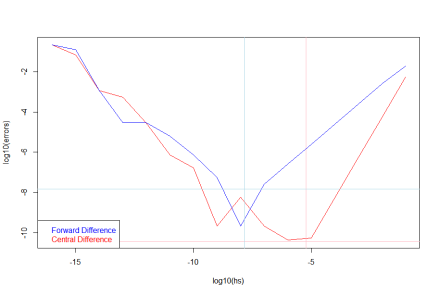

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Algorithmic Differentiation — Idea II

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Algorithmic Differentiation — Idea II

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- round-off error: equivalent to using a source code analogously implementing the analytical derivatives.

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- our parameter vector is $\theta = (\mu,\, \sigma^2)$
- the likelihood function is $\mathcal{L}(\theta; x) = f(x; \theta) = (\sigma\sqrt{2\pi})^{-T} \exp[-\frac{1}{2} \sum_{t=1}^{T} (x_t - \mu)^2 / \sigma^2]$

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- goal: compute the value of ℓ_t corresponding to the arguments $x_t = 6$, $\mu = 6$, and $\sigma^2 = 4$.
- A computer program may execute the sequence of operations represented by an *evaluation trace*, Griewank and Walther (2008)

Variable		Operation		Expression		Value
v_{-1}			$=$	μ	$=$	6
v_0			$=$	σ^2	$=$	4
v_1	$=$	$\phi_1(v_0)$	$=$	$log(v_0)$	$=$	1.386294
v_2	$=$	$\phi_2(v_1)$	$=$	$-\frac{1}{2}log(2\pi) - \frac{1}{2}v_1$	$=$	-1.612086
v_3	$=$	$\phi_3(v_{-1})$	$=$	$x_t - v_{-1}$	$=$	0
v_4	$=$	$\phi_4(v_3)$	$=$	v_3^2	$=$	0
v_5	$=$	$\phi_5(v_0, v_4)$	$=$	v_4/v_0	$=$	0
v_6	$=$	$\phi_6(v_5)$	$=$	$-\frac{1}{2}v_5$	$=$	0
v_7	$=$	$\phi_7(v_2, v_6)$	$=$	$v_2 + v_6$	$=$	-1.612086
ℓ_t	$=$	v_7	$=$	-1.612086		

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- Recall: Two *modes* of propagating the intermediate information: the *forward mode* and the *reverse mode*
  - forward mode: Eigen's Auto Diff module used here

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- by continuing this procedure we ultimately obtain an augmented, forward-derived, evaluation trace

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$\dot{v}_7$	$=$	$(\partial\phi_7/\partial v_2)\dot{v}_2 + (\partial\phi_7/\partial v_6)\dot{v}_6$	$=$	$\dot{v}_2 + \dot{v}_6$	$=$	0
ℓ_t	$=$	v_7	$=$	-1.612086		
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- The problem addressed by the implementations:
  - ”transform a program with a particular evaluation trace into an augmented program whose evaluation trace also contains exactly the same extra variables and additional lines as in the derived evaluation trace,” Griewank and Walther (2008).

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AD — Reverse Mode

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- Griewank and Walther (2008): ”Rather than choosing an input variable and calculating the sensitivity of every intermediate variable with respect to that input, we choose instead an output variable and calculate the sensitivity of that output with respect to each of the intermediate variables. As it turns out adjoint sensitivities must naturally be computed backward, i.e., starting from the output variables.”

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- Worth noting: the choice between the modes depends on the computational cost.

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- Which is better? Depends: e.g., gradient vs. Jacobian
  - Foward mode performance: can establish a worst-case performance bound for AD when used for gradient computation

The Model: GARCH(1, 1)

The spot asset price S follows the following process under the physical probability measure P:

$$\log \frac{S_{t+1}}{S_t} \equiv r_{t+1} = \mu + \epsilon_{t+1} \tag{1}$$

$$\epsilon_{t+1} = \sqrt{v_{t+1}} w_{t+1} \tag{2}$$

$$v_{t+1} = \omega + a\epsilon_t^2 + b v_t \tag{3}$$

$$w \overset{P}{\sim} GWN(0, 1) \tag{4}$$

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  - common finding: p_v close to 1 in financial data, ”near-integrated” process, Bollerslev and Engle (1993).

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    - S&P 500 from January 3rd, 1950 — over 16,000 observations

Illustration: Reliability — AD, L-BFGS

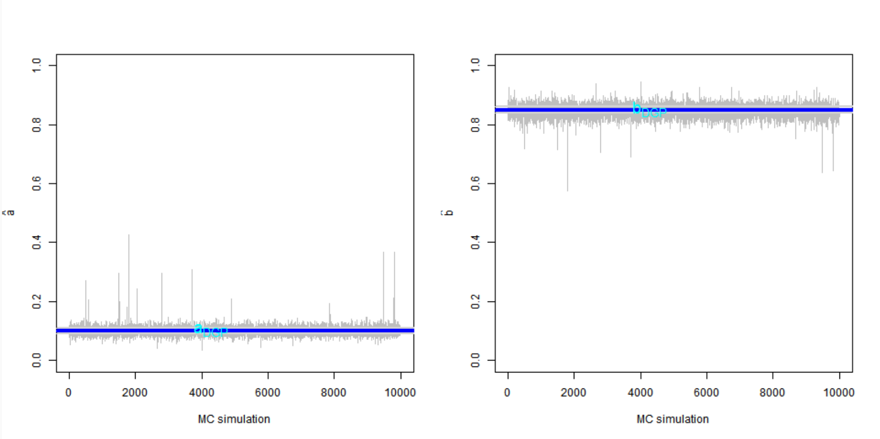

Illustration: Reliability — FD, TNR

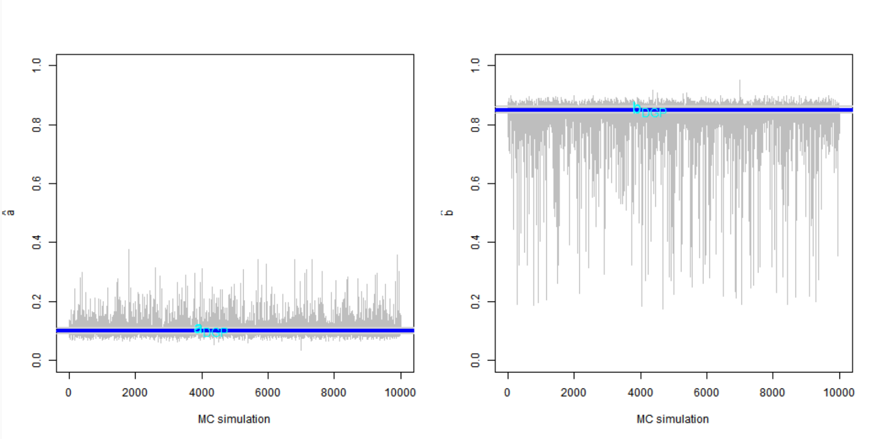

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Illustration: Findings — Reliability

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  - using AD: successful convergence in the vast majority of Monte Carlo experiments
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  - L-BFGS(AD): average = 0.811, median: 0.99999903,
  - L-BFGS(FD): average = 0.446, median: 0.02893254 (*sic*),
  - Truncated Newton with restarting (TNR) (FD): average = 0.708, median: 0.99856261.

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Illustration: Findings

- Overall: When using the fastest successful algorithm-gradient pair for both AD and FD:
    - AD achieves 12.5 times higher accuracy (in terms of the error norm) with a 3 slowdown compared to L-BFGS(FD)
    - while achieving 4 times higher accuracy and 1.1 speedup compared to TNR(FD).

Example Source Code

```r
Rcpp::sourceCpp('ExampleGaussianRcpp.cpp')
```

- Note: Rcpp not necessary for any of this:

Example using Rcpp

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```

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Example using Rcpp

```
Rcpp::sourceCpp('ExampleGaussianRcpp.cpp')
```

- Note: Rcpp not necessary for any of this:
  - Feel free to skip over any line with `Rcpp::`
  - Add `#include <Eigen/Dense>` and `#include <unsupported/Eigen/AutoDiff>` for plain vanilla Eigen

ExampleGaussianRcpp.cpp I

```
// [[Rcpp::plugins("cpp11")]]
#include <cstddef>

// [[Rcpp::depends(BH)]]
#include <boost/math/constants/constants.hpp>

// [[Rcpp::depends(RcppEigen)]]
#include <RcppEigen.h>

#include <cmath>
```

```cpp
namespace model
{
    // 2 parameters: mu, sigma^2
    enum parameter : std::size_t { mu, s2 };
    constexpr std::size_t parameters_count = 2;
}
```

```cpp
// [[Rcpp::export]]
double l_t_cpp(double xt,
               const Eigen::Map<Eigen::VectorXd> parameters)
{
    const auto mu = parameters[model::parameter::mu];
    const auto s2 = parameters[model::parameter::s2];
    constexpr auto two_pi =
      boost::math::constants::two_pi<double>();
    using std::log;
    using std::pow;
    return -.5 * log(two_pi) - .5 * log(s2) -
            .5 * pow(xt - mu, 2) / s2;
}
```

```r
Rcpp::sourceCpp('ExampleGaussianRcppEigen.cpp')
```

ExampleGaussianRcppEigen.cpp I

```
// [[Rcpp::plugins("cpp11")]]
#include <cstddef>

// [[Rcpp::depends(BH)]]
#include <boost/math/constants/constants.hpp>

// [[Rcpp::depends(RcppEigen)]]
#include <RcppEigen.h>
#include <unsupported/Eigen/AutoDiff>

#include <cmath>
```

ExampleGaussianRcppEigen.cpp II

```cpp
namespace model
{
  // 2 parameters: mu, sigma^2
  enum parameter : std::size_t { mu, s2 };
  constexpr std::size_t parameters_count = 2;

  template <typename ScalarType>
  using parameter_vector =
    Eigen::Matrix<ScalarType, parameters_count, 1>;
}
```

```
// note: data `xt` -- double-precision number(s), just as before
// only the parameters adjusted to `ScalarType`
template <typename VectorType>
typename VectorType::Scalar
l_t_cpp_AD(double xt,
           const VectorType & parameters)
{
  using Scalar = typename VectorType::Scalar;
  const Scalar & mu = parameters[model::parameter::mu];
  const Scalar & s2 = parameters[model::parameter::s2];
  // note: `two_pi` is, as always, a double-precision constant
  constexpr auto two_pi =
    boost::math::constants::two_pi<double>();
  using std::log; using std::pow;
  return -.5 * log(two_pi) - .5 * log(s2) -
          .5 * pow(xt - mu, 2) / s2;
}
```

```
// wrapper over `l_t_cpp_AD`
// (simply dispatching to the existing implementation)
//
// (Rcpp-exportable explicit template instantiations
//  would render this unnecessary)

// [[Rcpp::export]]
double l_t_value_cpp(double xt,
                     const Eigen::Map<Eigen::VectorXd> parameters)
{
  return l_t_cpp_AD(xt, parameters);
}
```

```
// objective function together with its gradient
// `xt`: input (data)
// `parameters_input`: input (model parameters)
// `gradient_output`: output (computed gradient)
// returns: computed objective function value
// [[Rcpp::export]]
double l_t_value_gradient_cpp
(
  double xt,
  const Eigen::Map<Eigen::VectorXd> parameters_input,
  Eigen::Map<Eigen::VectorXd> gradient_output
)
{
  using parameter_vector = model::parameter_vector<double>;
  using AD = Eigen::AutoDiffScalar<parameter_vector>;
  using VectorAD = model::parameter_vector<AD>;
```

```
  parameter_vector parameters = parameters_input;
  VectorAD parameters_AD = parameters.cast<AD>();

  constexpr auto P = model::parameters_count;
  for (std::size_t p = 0; p != P; ++p)
  {
    // forward mode:
    // active differentiation variable `p`
    // (one parameter at a time)
    parameters_AD(p).derivatives() = parameter_vector::Unit(p);
  }

  const AD & loglikelihood_result = l_t_cpp_AD(xt, parameters_AD);
  gradient_output = loglikelihood_result.derivatives();
  return loglikelihood_result.value();
}
```

Data Parallel Objective Function I

```
// First: make the data parallelism (DP) explicit
// [[Rcpp::export]]
Eigen::VectorXd l_t_value_cppDP
(
  const Eigen::Map<Eigen::VectorXd> xs,
  const Eigen::Map<Eigen::VectorXd> parameters
)
{
  const std::size_t sample_size = xs.size();
  Eigen::VectorXd result(sample_size);
  for (std::size_t t = 0; t != sample_size; ++t)
  {
    result[t] = l_t_cpp_AD(xs[t], parameters);
  }
  return result;
}
```

Data Parallel Objective Function II

```cpp
// Second: Parallelize using OpenMP
// [[Rcpp::export]]
Eigen::VectorXd l_t_value_cppDP_OMP
(
  const Eigen::Map<Eigen::VectorXd> xs,
  const Eigen::Map<Eigen::VectorXd> parameters
)
{
  const std::size_t sample_size = xs.size();
  Eigen::VectorXd result(sample_size);
  #pragma omp parallel for default(none) shared(result)
  for (std::size_t t = 0; t < sample_size; ++t)
  {
    result[t] = l_t_cpp_AD(xs[t], parameters);
  }
  return result;
}
```

Data Parallel Objective Function Performance I

```
> require("microbenchmark")

> microbenchmark(
+   l_t(xs, fixed_parameters),
+   l_t_value_cppDP(xs, fixed_parameters),
+   l_t_value_cppDP_OMP(xs, fixed_parameters)
+ )
Unit: microseconds
                                      expr  median neval
     l_t_value_cppDP(xs, fixed_parameters) 458.618   100
 l_t_value_cppDP_OMP(xs, fixed_parameters) 213.526   100
```

Note: changing `l_t_cpp_AD` to `l_t_cpp_AD_DP` (analogously) can also help, but we're not done, yet...

```
// [[Rcpp::export]]
Eigen::VectorXd l_t_value_gradient_cppDP
(
  const Eigen::Map<Eigen::VectorXd> xs,
  const Eigen::Map<Eigen::VectorXd> parameters_input,
  Eigen::Map<Eigen::MatrixXd> gradient_output
)
{
  const std::size_t sample_size = xs.size();
  Eigen::VectorXd result(sample_size);
  for (std::size_t t = 0; t != sample_size; ++t)
  {
    using parameter_vector = model::parameter_vector<double>;
    using AD = Eigen::AutoDiffScalar<parameter_vector>;
    using VectorAD = model::parameter_vector<AD>;
```

```
    parameter_vector parameters = parameters_input;
    VectorAD parameters_AD = parameters.cast<AD>();

    constexpr auto P = model::parameters_count;
    for (std::size_t p = 0; p != P; ++p)
    {
      parameters_AD(p).derivatives() = parameter_vector::Unit(p);
    }
    const AD & loglikelihood_result = l_t_cpp_AD(xs[t],
                                                 parameters_AD);
    gradient_output.row(t) = loglikelihood_result.derivatives();
    result[t] = loglikelihood_result.value();
  }
  return result;
}
```

Data Parallel Gradient III

```
// [[Rcpp::export]]
Eigen::VectorXd l_t_value_gradient_cppDP_OMP
(
  const Eigen::Map<Eigen::VectorXd> xs,
  const Eigen::Map<Eigen::VectorXd> parameters_input,
  Eigen::Map<Eigen::MatrixXd> gradient_output
)
{
  const std::size_t sample_size = xs.size();
  Eigen::VectorXd result(sample_size);
  #pragma omp parallel for default(none) \
          shared(result, gradient_output)
  for (std::size_t t = 0; t < sample_size; ++t)
  {
    using parameter_vector = model::parameter_vector<double>;
    using AD = Eigen::AutoDiffScalar<parameter_vector>;
    using VectorAD = model::parameter_vector<AD>;
```

```
    parameter_vector parameters = parameters_input;
    VectorAD parameters_AD = parameters.cast<AD>();

    constexpr auto P = model::parameters_count;
    for (std::size_t p = 0; p != P; ++p)
    {
      parameters_AD(p).derivatives() = parameter_vector::Unit(p);
    }
    const AD & loglikelihood_result = l_t_cpp_AD(xs[t],
                                                 parameters_AD);
    gradient_output.row(t) = loglikelihood_result.derivatives();
    result[t] = loglikelihood_result.value();
  }
  return result;
}
```

Data Parallel Gradient Performance I

```
microbenchmark(
  l_t_value_gradient_cppDP(xs, fixed_parameters, gradient),
  l_t_value_gradient_cppDP_OMP(xs, fixed_parameters, gradient)
)
Unit: microseconds
                        expr   median neval
    l_t_value_gradient_cppDP 631.3375   100
l_t_value_gradient_cppDP_OMP 258.6945   100
```

Worth noting:

- speed-up over naive serial version thanks to OpenMP

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- we can do better: truly data-parallel (non-naive) objective function implementation `l_t_cpp_AD_DP`, reverse mode AD

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- we can do better: truly data-parallel (non-naive) objective function implementation `l_t_cpp_AD_DP`, reverse mode AD
- left as an exercise for the audience! :-)

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- Perverse (but valid) code:

```
if (x == 1.0) then y = 0.0 else y = x - 1.0
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- Reverse mode — memory requirements
- Perverse (but valid) code:

```
if (x == 1.0) then y = 0.0 else y = x - 1.0
```

  - derivative at $x = 1$?

Resources

http://www.autodiff.org/

http://en.wikipedia.org/wiki/Automatic_differentiation

Resources I

A Gentle Introduction to Backpropagation
http://numericinsight.blogspot.com/2014/07/a-gentle-introduction-to-backpropagation.html
http://www.numericinsight.com/uploads/A_Gentle_Introduction_to_B

A Multi-Core Benchmark Used to Improve Algorithmic Differentiation
http://www.seanet.com/~bradbell/cppad_thread.htm

A Multi-Core Algorithmic Differentiation Benchmarking System — Brad Bell
https://vimeo.com/39008544

Resources II

A Step by Step Backpropagation Example
http://mattmazur.com/2015/03/17/a-step-by-step-backpropagation-example/

Adjoint Methods in Computational Finance
http://www.hpcfinance.eu/sites/www.hpcfinance.eu/files/Uwe%20Nau
http://www.nag.com/Market/seminars/Uwe_AD_Slides_July13.pdf

Adjoints and Automatic (Algorithmic) Differentiation in Computational Finance
http://arxiv.org/abs/1107.1831v1

Algorithmic Differentiation in More Depth
http://www.nag.com/pss/ad-in-more-depth

Algorithmic Differentiation of a GPU Accelerated Application
http://www.nag.co.uk/Market/events/jdt-hpc-new-thinking-in-finance-presentation.pdf

Automatic Differentiation and QuantLib
https://quantlib.wordpress.com/tag/automatic-differentiation/

Automatic differentiation in deep learning by Shawn Tan
https://cdn.rawgit.com/shawntan/presentations/master/Deep Learning-Copy1.slides.html

Calculus on Computational Graphs: Backpropagation
https://colah.github.io/posts/2015-08-Backprop/

Resources IV

Computing derivatives for nonlinear optimization: Forward mode automatic differentiation
http://nbviewer.ipython.org/github/joehuchette/OR-software-tools-2015/blob/master/6-nonlinear-opt/Nonlinear-DualNumbers.ipynb

Introduction to Automatic Differentiation
http://alexey.radul.name/ideas/2013/introduction-to-automatic-differentiation/

Jarrett Revels: Automatic differentiation
https://www.youtube.com/watch?v=PrXUl0sanro

Neural Networks (Part I) – Understanding the Mathematics behind backpropagation https://biasvariance.wordpress.com/2015/08/18/neural-networks-understanding-the-math-behind-backpropagation-part-i/

- http://www.johndcook.com/blog/2009/04/06/anatomy-of-a-floating-point-number/

Everything by Bruce Dawson:

- https://randomascii.wordpress.com/category/floating-point/

In particular:

- `https://randomascii.wordpress.com/2012/02/25/comparing-floating-point-numbers-2012-edition/`
- `https://randomascii.wordpress.com/2012/04/05/floating-point-complexities/`
- `https://randomascii.wordpress.com/2013/01/03/top-eight-entertaining-blog-facts-for-2012/`

https://en.wikipedia.org/wiki/Automatic_differentiation#Software

ADNumber, Adept, ADOL-C, CppAD, Eigen (Auto Diff module)

CasADi
https://github.com/casadi/casadi/wiki
CasADi is a symbolic framework for algorithmic (a.k.a. automatic) differentiation and numeric optimization.

CppAD
https://github.com/coin-or/CppAD/

Dali
https://github.com/JonathanRaiman/Dali
An automatic differentiation library that uses reverse-mode differentation (backpropagation) to differentiate recurrent neural networks, or most mathematical expressions through control flow, while loops, recursion.

Open Porous Media Automatic Differentiation Library
https://github.com/OPM/opm-autodiff
Utilities for automatic differentiation and simulators based on AD.

The Stan Math Library (`stan::math`: includes a C++ reverse-mode automatic differentiation library)
https://github.com/stan-dev/math

References

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Giles, Michael, and Paul Glasserman. 2006. "Smoking Adjoints: Fast Monte Carlo Greeks." *Risk* 19: 88–92.

Griewank, Andreas. 2012. "Who Invented the Reverse Mode of Differentiation?" *Optimization Stories* Documenta Matematica, Extra Volume ISMP (2012): 389–400.

Griewank, Andreas, and Andrea Walther. 2008. *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*. 2nd ed. Other Titles in Applied Mathematics 105.

Philadelphia, PA: SIAM.
`http://www.ec-securehost.com/SIAM/OT105.html`.

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Naumann, Uwe. 2012. *The Art of Differentiating Computer Programs: An Introduction to Algorithmic Differentiation*. Computer software, Environments, and Tools 24. Philadelphia, PA: SIAM. `http://www.ec-securehost.com/SIAM/SE24.html`.

Nocedal, Jorge, and Stephen J. Wright. 2006. *Numerical Optimization*. 2. ed. Springer: New York, NY.

Thank You!
Questions?