Automatic differentiation beyond typedef and operator overloading

Peter Caspers

Quaternion Risk Management

01 December 2015

Agenda

Introduction to AD

Approaches in QuantLib

Source code transformation

Agenda

Introduction to AD

Approaches in QuantLib

Source code transformation

AD in a nutshell 1/3

- for a computer program $f : \mathbb{R}^n \to \mathbb{R}^m$, compute $\partial_x f$
- ... by looking at the program's sequence of basic operations $(+ - */, \exp, \sin, \mathrm{erf} \ldots)$, using basic calculus in each step
- ... and stitching everything together with the chain rule

AD in a nutshell 2/3

- results are exact up to machine precision, also for higher order derivatives
- implementation:
  - operator overloading instrumenting the double type[1]
  - source code transformation tools[2]
  - coding by hand

[1] e.g. CppAD, ADOL-C, Adept, dco, proprietary tools
[2] e.g. ADIC, OpenAD/F

AD in a nutshell 3/3

- local jacobians can be propagated forward ($x \rightsquigarrow y$) (that's intuitive) or backward ($y \rightsquigarrow x$) in a dual or *adjoint* fashion
- one *forward* sweep yields one directional derivative of your choice of the vector of output variables
- one *reverse* sweep yields the gradient w.r.t. all input variables of one linear combination of the output variables
- the complexity for one (forward or reverse) sweep is a constant, low multiple of the complexity for one function evaluation[3]
- in particular: **law of cheap gradient** !

[3] theory: the multiple in adjoint mode is bounded by 4

Adjoint mode example

- program $f : \mathbb{R}^{n+1} \to \mathbb{R}$: $y = \exp\left(\prod_{i=0}^{n} x_i\right) \sin\left(\prod_{i=0}^{n} x_i\right)$
- imagine n to be large, like 1000
- evaluation complexity: $n + 3 = O(n)$ operations $\in \{*, \exp, \sin\}$
- goal: compute $\partial_x f \in \mathbb{R}^{n+1}$
- finite difference approach: $(n + 1)(n + 3) + 2(n + 1) = O(n^2)$ operations in addition to the evaluation

Adjoint mode example - distance 1 nodes

- init $\partial_y y = 1$
- first break down is $y = uv$
- $\partial_u y = \partial_y y \partial_u y = v$, $\partial_v y = \partial_y y \partial_v y = u$
- 2 operations assuming we have
  - evaluated the function and at the same time built the computational graph so that we know ...
  - ... the value of u and v and
  - ... the "analytics" for the local derivatives
- *(disclaimer: we are not overly pedantic on how to count the operations in this example here ...)*

Adjoint mode example - distance 2 nodes

- second break down $u = \exp(x), v = \sin(x)$
- $\partial_x u = \exp(x), \partial_x v = \cos(x)$
- $\partial_x y = \partial_u y \partial_x u + \partial_v y \partial_x v = \sin(x)\exp(x) + \exp(x)\cos(x)$
- again, we know x from the initial function evaluation
- 4 operations (total operations count 6)

Adjoint mode example - distance 3 nodes

- third break down $x = x_0 h_0$
- $\partial_{x_0} x = h_0, \partial_{h_0} x = x_0$
- $\partial_{x_0} y = \partial_x y \partial_{x_0} x = [\sin(x)\exp(x) + \exp(x)\cos(x)]h_0$
- $\partial_{h_0} y = \partial_x y \partial_{x_0} h_0 = [\sin(x)\exp(x) + \exp(x)\cos(x)]x_0$
- ... we know h_0 from the forward sweep ...
- 2 operations (total operations count 8)

Adjoint mode example - nodes with distance n+2

- continue like in the third break down until we arrive at $h_{n-1} = x_n$
- $\partial_{x_i} y = [\sin(\prod x_i) \exp(\prod x_i) + \exp(\prod x_i) \cos(\prod x_i)] \prod_{j \neq i} x_i$
- $2n$ operations from the third break down on
- total operations count $2n + 6$
- one function evaluation was $n + 3$ operations
- naive approach for gradient calculation was $(n+1)(n+3) + 2(n+1)$ operations

Agenda

Introduction to AD

Approaches in QuantLib

Source code transformation

The typedef approach

- just says `typedef CppAD::AD<double> Real`
- it is a bit more complicated than that
- QuantLibAdjoint (CompatibL), with additional logic (tapescript)
- *AD-or-not-AD* decision at compile time and globally, i.e. no selective activation of variables

Matrix multiplication with (sleeping) active doubles

```
Matrix_t<T> A(1024, 1024);
Matrix_t<T> B(1024, 1024);
...
Matrix_t<T> C = A * B;
```

- `T = double`: 764 ms
- `T = CppAD::AD<double>`: 8960 ms
- penalty: 11.7x
- note that we do not get anything for that (AD is disabled)
- this is not an exception, but seems to occur for every "numerically intense" code section (see below for a second example)

Active doubles vs. native doubles 1/2

- for a `MinimalWrapper` consisting of a `double` and a pointer `MinimalWrapper*` (set to `nullptr` always), the penalty is around 2.1x
- for this gcc generates *scalar* double instructions (mulsd, addsd)
- for the native `double` gcc generates *packed* double instructions (mulpd, addpd)[4]
- in addtion the more involved data layout of the `MinimalWrapper` (placing a pointer after each native `double`) leads to more instructions in the innermost loop[5]

[4] with -ftree-vectorize, a similar observation holds for -ffast-math optimizations
[5] we note that cachegrind does not report a higher rate of cache misses though

Active doubles vs. native doubles 2/2

- (current) compilers seem to generate more instructions and possibly less efficient instructions for non-native double wrappers
- memory consumption will go up, too
- it is not clear what the “best possible” OO tool can achieve, but probably it will be something between 2x and 12x
- 2x is already too much, if we do not get anything for that
- we can easily avoid this useless overhead

The template approach

- introduce templated versions of relevant classes (e.g. `Matrix_t`)
- for backward compatibility, `typedef Matrix_t<Real> Matrix`
- it is a bit more complicated than that
- allows mixing of active and native classes, as required, i.e. activation of variables in selected parts of the application only
- work in progress[6], but basic IRD stuff works (like yield and volatility termstructures, swaps, CMS coupons, GSR model)
- `https://github.com/pcaspers/quantlib/tree/adjoint`
- `https://quantlib.wordpress.com/tag/automatic-differentiation/`

[6] conversion rate $\approx$ 2000 LOC / day (manual + an Elisp-little-helper)

Expensive gradients with operator overloading

- the typedef as well as the template approach use operator overloading tools (like CppAD)
- for numerically intense algorithms, we observe dramatic performance loss (because less optimization can be applied to non-native types)
- e.g. a convolution engine for Bermudan swaptions is **80x slower**[7] in adjoint mode compared to one native-double pricing
- if AD is actually not needed, the template approach is the way out, otherwise we need other techniques

[7] see `https://quantlib.wordpress.com/2015/04/14/adjoint-greeks-iv-exotics`

Agenda

Introduction to AD

Approaches in QuantLib

Source code transformation

Source Code Transformation

- generate adjoint code at compile time, which may yield better performance
- however, does not work out of the box like OO tools
- no mature tool for C++ (ADIC 2.0 = “OpenAD/Cpp” under development)
- needs specific preparation of code before it can be applied

OpenAD/F

- OpenAD is a language independent AD backend working with abstract xml representations (XAIF) of the computational model
- OpenAD/F adds a Fortran 90 front end
- Open Source, proven on large scale real-world models
- `http://www.mcs.anl.gov/OpenAD`

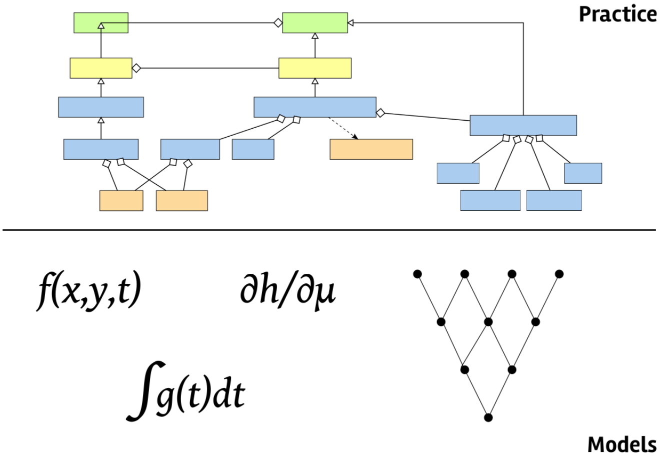
From QuantLib to SCT

- isolate the core computational code and reimplement it in Fortran
- use OpenAD/F to generate adjoint code, build a separate support library from that
- use a wrapper class on the QuantLib side to communicate with the support libary
- minimal library example[8] and LGM swaption engine[9] available
- build via `make` (AD support library) or `make plain` (without OpenAD - transformation, for testing)

[8] `https://github.com/pcaspers/quantlib/tree/master/QuantLibOAD/simplelib`

[9] `https://github.com/pcaspers/quantlib/tree/master/QuantLibOAD/lgm`

By the way ... different motivation, but same idea ?



(taken from Luigi's talk at the 11th FI conference, 2015, Paris)

LGM Bermudan swaption convolution engine

- core computation can be implemented in around 200 lines
- native interface only using (arrays of) doubles and integers
- input: relevant times $\{t_i\}$, model $\{(H(t_i), \zeta(t_i), P(0,t_i))\}$, Termsheet, codified as index lists $\{k_i, l_i, ...\}$
- output: npv, gradient w.r.t. $\{(H(t_i), \zeta(t_i), P(0,t_i))\}$

```
subroutine lgm_swaption_engine(n_times, times, modpar, n_expiries, &
     expiries, callput, n_floats, &
     float_startidxes, float_mults, index_acctimes, float_spreads, &
     float_t1s, float_t2s, float_tps, &
     fix_startidxes, n_fixs, fix_cpn, fix_tps, &
     integration_points, stddevs, res)
```


Building the AD support library

```
emacs@peter-ThinkPad-W520
File Edit Options Buffers Tools Compile Help
-*- mode: compilation; default-directory: "~/OpenAD/" -*-
Compilation started at Sun Nov 22 18:15:21

cd ~/OpenAD/ && source setenv.sh && cd ~/quantlib/QuantLibOAD/lgm && make clean && make -k
rm -f *.o *.so
rm -f ad_template* OAD_* w2f__* iaddr*
rm -f lgm.pre* *.B *.xaif *.o *.mod driver driverE *~
openad -c -m rj lgm.f90
openad log: openad.2015-11-22_18:15:22.log~
preprocessing fortran
parsing preprocessed fortran
analyzing source code and translating to xaif
adjoint transformation
 getting runtime support file OAD_active.f90
 getting runtime support file w2f__types.f90
 getting runtime support file iaddr.c
 getting runtime support file ad_inline.f
 getting runtime support file OAD_cp.f90
 getting runtime support file OAD_rev.f90
 getting runtime support file OAD_tape.f90
 getting template file
translating transformed xaif to whirl
unparsing transformed whirl to fortran
postprocessing transformed fortran
gfortran -g -O3 -o w2f__types.o -c w2f__types.f90 -fpic
gfortran -g -O3 -o OAD_active.o -c OAD_active.f90 -fpic
gfortran -g -O3 -o OAD_cp.o -c OAD_cp.f90 -fpic
gfortran -g -O3 -o OAD_tape.o -c OAD_tape.f90 -fpic
gfortran -g -O3 -o OAD_rev.o -c OAD_rev.f90 -fpic
gfortran -g -O3 -o driver_lgm.o -c driver_lgm.f90 -fpic
gfortran -g -O3 -o lgm.pre.xb.x2w.w2f.post.o -c lgm.pre.xb.x2w.w2f.post.f90 -fpic
gfortran -shared -g -O3 -o liblgmad.so w2f__types.o OAD_active.o OAD_cp.o OAD_tape.o OAD_rev.o driver_lgm.o lgm.pre.xb.x2w.w2f.post.o

Compilation finished at Sun Nov 22 18:15:29

U:@%*-  *compilation*   All L1     (Compilation:exit [0])
Beginning of buffer
```

LGM Bermudan swaption convolution engine

- C++ wrapper is a usual QuantLib pricing engine
- precomputes the values and organizes them in arrays for the Fortran core
- invokes the Fotran routine
- stores the npv and the adjoint gradient as results

```
void LgmSwaptionEngineAD::calculate() const {
    // collect data needed for core computation routine
    ...
    // join all dates and fill index vectors
    ...
    // call core computation routine and set results

    lgm_swaption_engine_ad_(&ntimes, &allTimes[0], &modpar[0], &nexpiries, ...
                    &integration_pts, &std_devs, &res, &dres[0]);
    ...
    results_.value = res;
    results_.additionalResults["sensitivityTimes"] = allTimes;
    results_.additionalResults["sensitivityH"] = H_sensitivity;
    results_.additionalResults["sensitivityZeta"] = zeta_sensitivity;
    results_.additionalResults["sensitivityDiscount"] = discount_sensitivity;
```

Performance

- 10y Bermudan swaption, yearly callable
- 49 grid points per expiry
- single pricing[10] (non-transformed code): 4.2 ms
- pricing + gradient $\in \mathbb{R}^{105}$: **25.6 ms**[11]
- additional stuff[12]: 6.2 ms
- adjoint calculation multiple: **6.1x** (7.6x including add. stuff)
- common, practical target for the adjoint multiple: 5x - 10x

---

[10] Intel(R) Core(TM) i7-2760QM CPU @ 2.40GHz, using one thread
[11] to achieve this, the runtime configuration of OpenAD/F has to be modified
[12] transformation of gradient w.r.t. model parameters to usual vegas, see below

How not to use AD

- avoid to record tapes that go through solvers, optimizers, etc.[13]
  - instead use the implicit function theorem to convert gradients w.r.t. calibrated (model) variables to gradients w.r.t. market variables
  - this is more efficient, less error prone (e.g. `Bisection` produces zero derivatives always, optimizations may produce bogus derivatives depending on the start value)
  - in the case of SCT applied as above this is even necessary from a practical viewpoint
- apply AD only to differentiable programs (e.g. replace a digital payoff by a call spread)
- avoid to record *long* tapes e.g. for *all* paths of a MC simulation, reuse a tape recorded on one path instead (here, ensure *tape-safety*)

[13] not to be confused with feeding AD - derivatives of the target function to optimizers like Levenberg-Marquardt or Newton-style solvers

Calibration of LGM model

To illustrate the usage of the implicit function theorem, consider the calibration to n swaptions[14]

$$\begin{aligned} \text{Black}(\sigma_1) - \text{Npv}_{\text{LGM}}(\zeta_1) &= 0 \\ &\dots \\ \text{Black}(\sigma_n) - \text{Npv}_{\text{LGM}}(\zeta_n) &= 0 \end{aligned}$$

with

$$\frac{\partial \text{Npv}_{\text{LGM}}}{\partial \zeta} = \text{diag}(\nu_1, ..., \nu_n), \text{ all } \nu_i \neq 0 \tag{1}$$

[14] recall that $\zeta(t)$ is the accumulated model variance up to time t

Implicit function theorem

Locally, there exists a unique g

$$g(\sigma_1, ..., \sigma_n) = (\zeta_1, ..., \zeta_n) \tag{2}$$

and

$$\frac{\partial g}{\partial \sigma} = \left(\frac{\partial \mathrm{Npv}_{\mathrm{LGM}}}{\partial \zeta} \right)^{-1} \frac{\partial \mathrm{Black}}{\partial \sigma} \tag{3}$$

Informally, $g = \zeta(\sigma)$ and

$$\frac{\partial \zeta}{\partial \sigma} = \frac{\partial \zeta}{\partial \mathrm{NPV}} \frac{\partial \mathrm{NPV}}{\partial \sigma} = \left(\frac{\partial \mathrm{NPV}}{\partial \zeta} \right)^{-1} \frac{\partial \mathrm{NPV}}{\partial \sigma} \tag{4}$$

Pasting the vega together

$$\frac{\partial \text{Npv}_{\text{Berm}}}{\partial \sigma} = \frac{\partial \text{Npv}_{\text{Berm}}}{\partial \zeta} \frac{\partial \zeta}{\partial \sigma} = \frac{\partial \text{Npv}_{\text{Berm}}}{\partial \zeta} \left(\frac{\partial \text{Npv}_{\text{Calib}}}{\partial \zeta} \right)^{-1} \frac{\partial \text{Black}}{\partial \sigma}$$

- the components can be calculated analytically (calibrating swaptions' market vegas) or using the ad engine[15] (calibrating swaptions' ζ-gradient, but this is much cheaper than for the Bermudan case)
- matrix inversion and multiplication is cheap
- the additional computation time is quite small (see the example above, the addtional costs are the same as for 1.5x original NPV calculations)

[15] in this particular case, bump and revalue would be even cheaper (since we are only sensitive to one ζ per swaption, so only one additional evaluation is needed)

Summary

- global instrumentation (via typedefs) with active variables can lead to performance (and memory) issues
- selective / mixed instrumentation (via templates) solves the issue, but leaves problems when AD is required for numerically intense parts of the code
- source code transformation can solve this issue, we gave an example in terms of a Bermudan swaption engine transformed using OpenAD/F yielding an adjoint multiple of **6.1** compared to **80** with operator overloading (using CppAD)

Quaternion
Risk Management

UK
29th Floor, 1 Canada Square
Canary Wharf, London E145DY
+44 207 712 1645
caroline.tonkin@quaternionrisk.com

Germany
Maurenbrecherstrasse 16
47803 Krefeld
+49 2151 9284 800
heidy.koenings@quaternionrisk.com

Ireland
54 Fitzwilliam Square
Dublin 2
+353 1 678 7922
joelle.higgins@quaternionrisk.com

UK

Germany

Ireland

info@quaternionrisk.com | www.quaternionrisk.com