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Accurate dot products with FMA

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Motivation: what is the best way to use FMA for accurate dot products?

- IEEE-754 floating point arithmetic + FMA:
  - $\mathbf{F}$ denotes the set of the floating point numbers,
  - $\mathbf{u}$ is the working precision:
    $e.g.,\ \mathbf{u} = 2^{-53} \approx 10^{-16}$ in IEEE-754 double precision.
- $x = (x_1, \ldots, x_n)^T$ and $y = (y_1, \ldots, y_n)^T$ belong to $\mathbf{F}^{n\times 1}$.

- Floating point Fused Multiply and Add (FMA):
  - given a, b and c in $\mathbf{F}$, FMA(a, b, c) equals $a \times b + c$ rounded to the nearest floating point value.
  - only one rounding error for two arithmetic operations!
- Available on Intel IA-64, IBM RS/6000 and PowerPC.

Accuracy of Classic Dot Product

- We consider dot products without/with FMA:

Classic dot product

function $\widehat{s} = \mathbf{Dot}(x, y)$
  $\widehat{s} = x_1 \otimes y_1$
  for $i = 2 : n$
    $\widehat{s} = \widehat{s} \oplus x_i \otimes y_i$

Dot product with FMA

function $\widehat{s} = \mathbf{DotFMA}(x, y)$
  $\widehat{s} = x_1 \otimes y_1$
  for $i = 2 : n$
    $\widehat{s} = \mathrm{FMA}(x_i, y_i, \widehat{s})$

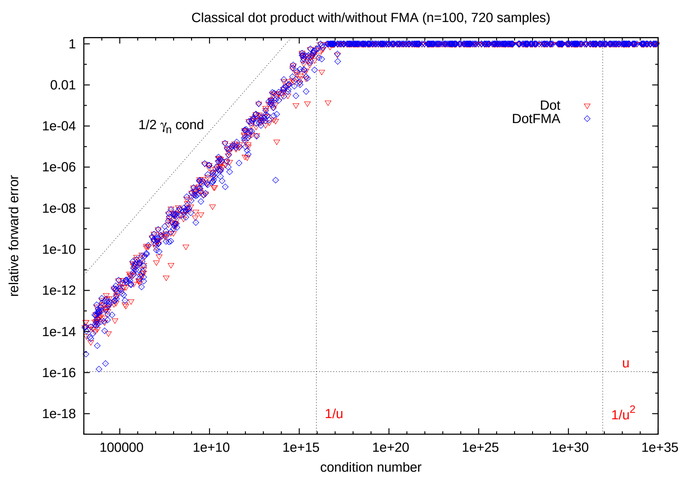
- The condition number for dot product computation is

$$\mathrm{cond}(x^T y) = 2\frac{|x|^T|y|}{|x^T y|}, \quad \text{with} \quad x^T y \neq 0.$$

- **Worst case accuracy:** FMA does not improve the accuracy of computed dot product since **Dot** and **DotFMA** both verifies

$$\frac{|\widehat{s} - x^T y|}{|x^T y|} \leq \frac{1}{2} \underbrace{\gamma_n}_{\approx n\,\mathbf{u}} \mathrm{cond}(x^T y).$$

- **Practical accuracy:** FMA only slightly improves the actual accuracy.



- Classic dot product is not accurate enough when applied to ill-conditioned dot products $e.g.,$ when computing residuals for ill-conditioned linear systems.
- **Question:** How can we obtain more accurate dot products?

Compensated Dot Products

- More accuracy can be achieved thanks to
  - double-double computations (see algorithm **DotXBLAS** below),
  - or with **compensated algorithms**: the forward error in the floating point evaluation of $x^T y$ is

$$c = x^T y - \mathrm{computed}(x^T y).$$

The main idea is to compute an approximate $\widehat{c}$ of the global error c thanks to **Error Free Transformations** (EFT). Then a **compensated result** $\overline{r}$ is provided correcting the computed $x^T y$ as follows,

$$\overline{r} = \mathrm{computed}(x^T y) \oplus \widehat{c}.$$

- From **Dot** and **DotFMA**, we derive two compensated algorithms using EFT (**2Sum**, **2ProdFMA** and **3FMA** are presented in the EFT frame below),
  - **CompDot**: correcting $+$ and $\times$ in **Dot** with **2Sum** and **2ProdFMA** (see [2]).
  - **CompDotFMA**: correcting FMA in **DotFMA** with **3FMA**.

Compensated Dot

function $\overline{r} = \mathbf{CompDot}(x, y)$
  $[\widehat{s}, \widehat{c}] = \mathbf{2ProdFMA}(x_1, y_1)$
  for $i = 2 : n$
    $[\widehat{p}, \pi] = \mathbf{2ProdFMA}(x_i, y_i)$
    $[\widehat{s}, \sigma] = \mathbf{2Sum}(\widehat{s}, \widehat{p})$
    $\widehat{c} = \widehat{c} \oplus (\pi \oplus \sigma)$
  end
  $\overline{r} = \widehat{s} \oplus \widehat{c}$

Compensated DotFMA

function $\overline{r} = \mathbf{CompDotFMA}(x, y)$
  $[\widehat{s}, \widehat{c}] = \mathbf{2ProdFMA}(x_1, y_1)$
  for $i = 2 : n$
    $[\widehat{s}, \alpha, \beta] = \mathbf{3FMA}(x_i, y_i, \widehat{s})$
    $\widehat{c} = \widehat{c} \oplus (\alpha \oplus \beta)$
  end
  $\overline{r} = \widehat{s} \oplus \widehat{c}$

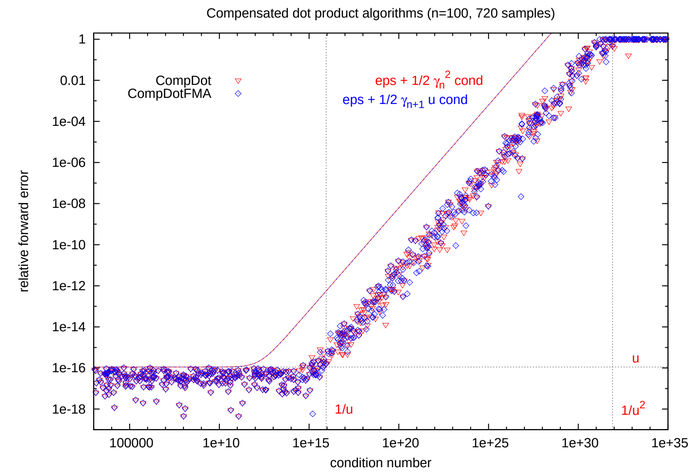
- The relative accuracy of the compensated result now verifies:

$$\frac{|\overline{r} - x^T y|}{|x^T y|} \leq \begin{cases} \mathbf{u} + \frac{1}{2} \underbrace{\gamma_n^2}_{\approx n^2\,\mathbf{u}^2} \mathrm{cond}(x^T y), & \text{with} \quad \mathbf{CompDot}, \\ \mathbf{u} + \frac{1}{2} \underbrace{\gamma_{n+1}\,\mathbf{u}}_{\approx (n+1)\,\mathbf{u}^2} \mathrm{cond}(x^T y), & \text{with} \quad \mathbf{CompDotFMA}. \end{cases}$$

- **CompDot** and **CompDotFMA** are as accurate as classic dot product computed in doubled working precision $\mathbf{u}^2$.

Experimental results

- Algorithms **CompDot** and **CompDotFMA** as accurate as the classic dot product performed in doubled working precision means:
  - while $\mathrm{cond}(x^T y) \lesssim \mathbf{u}^{-1}$, the accuracy is about the working precision $\mathbf{u}$,
  - when $\mathbf{u}^{-1} \lesssim \mathrm{cond}(x^T y) \lesssim \mathbf{u}^{-2}$, the accuracy decreases from 16 digits to 0,
  - for $\mathrm{cond}(x^T y) \gtrsim \mathbf{u}^{-2}$, no correct digit is returned.



- What is the running time over-cost compared to **DotFMA**?

n	DotFMA	CompDot	CompDotFMA	DotXBLAS
50	1.0	1.63	2.61	9.87
100	1.0	1.35	2.43	9.65
1000	1.0	1.26	2.6	10.86
10000	1.0	1.25	2.62	10.97
100000	1.0	1.25	2.35	9.8

Measured computing times on Intel Itanium 2
(1.6 GHz, ICC v9.0, IEEE-754 double precision)

- **Observations:**
  1. **CompDot** and **CompDotFMA** run both faster than **DotXBLAS**,
  2. **CompDot** is the most efficient alternative to **DotXBLAS**.

Error Free Transformations (EFT)

- Error Free Transformations are properties and algorithms to compute the generated rounding errors at the working precision $\mathbf{u}$. The following table sums up the EFT for $+$, $\times$ and FMA.

$+$	$(x, y) = \mathbf{2Sum}(a, b)$ such that $a + b = x + y$ and $x = a \oplus b$	6 flops	Knuth (74)
$\times$	$(x, y) = \mathbf{2ProdFMA}(a, b)$ such that $a \times b = x + y$ and $x = a \otimes b$ Indeed $y = a \times b - x = \mathrm{FMA}(a, b, -x)$	2 flops	
FMA	$(x, y, z) = \mathbf{3FMA}(a, b, c)$ such that $x = \mathrm{FMA}(a, b, c)$ and $a \times b + c = x + y + z$	17 flops	Boldo Muller (05)

- Remark: x, y and z belongs to $\mathbf{F}$ when a, b and c are in $\mathbf{F}$.
- Algorithm **2ProdFMA** is used instead of the classic **2Prod** (by Dekker and Veltkamp, 17 flops) to benefit from FMA.

XBLAS Dot Product

- **XBLAS** = BLAS + Bailey's double-doubles = eXtended and mixed precision BLAS [1].
- A double-double number = unevaluated sum of two IEEE-754 double precision numbers = at least 106 significand bits.
- **DotXBLAS** = Classic dot product (**Dot**) + double-doubles.
- **DotXBLAS** also benefits from the availability of FMA.

Conclusions

- FMA only slightly improves the accuracy of the classic dot product.
- Nevertheless FMA is useful for designing accurate algorithms: **CompDot** and **CompDotFMA** are very efficient for doubling the working precision.
- In particular **CompDot** is about 6 times faster than XBLAS algorithm **DotXBLAS** in our experiments.

[1] X. S. Li, J. W. Demmel, D. H. Bailey, G. Henry, Y. Hida, J. Iskandar, W. Kahan, S. Y. Kang, A. Kapur, M. C. Martin, B. J. Thompson, T. Tung and D. J. Yoo. Design, implementation and testing of extended and mixed precision BLAS. *ACM Transactions on Mathematical Software*, 28(2), 2002.

[2] T. Ogita, S. M. Rump, and S. Oishi. Accurate sum and dot product. *SIAM Journal on Scientific Computing*, 26(6), 2005.