Probabilistic estimation of the accuracy of inner products and application to stochastic validation

Fabienne Jézéquel, Théo Mary
LIP6, Sorbonne Université, CNRS, Paris, France

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Accuracy of inner products

The inner product $s = x^T y$ of $x, y \in \mathbb{R}^n$ is a widely used kernel.

The computed $\widehat{s}$ satisfies

$$\frac{|\widehat{s} - s|}{|s|} \leq nu \frac{|x|^T |y|}{|x^T y|}$$

where u is the unit roundoff (in double precision $u = 2^{-53}$).

But this bound cannot be used as a reliable estimator of the accuracy.

- nu (the backward error) is often **pessimistic**
- $\kappa := \frac{|x|^T |y|}{|x^T y|}$ (the condition number) is in general sharp but **cannot be reliably computed**: it requires the true inner product $x^T y$.

$\Rightarrow$ numerical validation based on **stochastic arithmetic**

Stochastic arithmetic [Vignes'04]

For each arithmetic operation $c = a \operatorname{op} b$ where $\operatorname{op} \in \{+, -, \times, /\}$:

$$c^{(1)} = \operatorname{SR}(a^{(1)} \operatorname{op} b^{(1)})$$
$$\dots$$
$$c^{(d)} = \operatorname{SR}(a^{(d)} \operatorname{op} b^{(d)})$$

where the stochastic rounding operator $\operatorname{SR}(\cdot)$ rounds either up or down at random with equal probability.

computed result: $\bar{c} = \frac{1}{d} \sum_{i=1}^{d} c^{(i)}$

its number of correct digits is estimated as

$$D_c = \log_{10}\left(\frac{\sqrt{d}\,|\bar{c}|}{\sigma \tau_\beta}\right) \text{ where } \sigma^2 = \frac{1}{d-1} \sum_{i=1}^{d} \left(c^{(i)} - \bar{c}\right)^2$$

τ_β is the value of Student's distribution for $d-1$ degrees of freedom and a confidence level β.

Inner product in stochastic arithmetic

The computation of an inner product $s = x^T y$, $x, y \in \mathbb{R}^n$:

$$\begin{aligned} s_0 &= 0, \\ s_k &= s_{k-1} + x_k y_k, \quad \text{for } k = 1\colon n, \\ s &= s_n \end{aligned}$$

becomes with stochastic arithmetic:

$$\begin{aligned} s_0^{(i)} &= 0, \quad \text{for } i = 1\colon d, \\ s_k^{(i)} &= \mathrm{SR}(s_{k-1}^{(i)} + \mathrm{SR}(x_k^{(i)} y_k^{(i)})), \quad \text{for } k = 1\colon n \text{ and } i = 1\colon d, \\ s^{(i)} &= s_n^{(i)}, \quad \text{for } i = 1\colon d. \end{aligned}$$

SR applied after each addition and multiplication
prevents the use of optimized libraries which do not support SR

⇒ **major performance hurdle**

In this talk

We present 2 methods to get a reliable accuracy estimation by **standard deterministic inner products**.

randomness introduced to estimate the accuracy:

- random perturbations to the input x and/or y
- or random perturbations to the output $\widehat{s}$.

⇒ **no intrusive modifications** in the intermediate computations of the inner products

⇒ can rely on **optimized implementations** such as the BLAS.

Overview

1. Principles of the 2 methods
2. Probabilistic analysis of their accuracy estimation
3. Numerical experiments and comparison with CADNA

Method 1

We perturb each representative of x with random perturbations:

$$\Delta x^{(1)}, \dots, \Delta x^{(d)}$$

and compute

$$\begin{aligned} s^{(1)} &= (x^{(1)} + \Delta x^{(1)})^T y, \quad |\Delta x^{(1)}| \le \delta |x^{(1)}|, \\ &\dots \\ s^{(d)} &= (x^{(d)} + \Delta x^{(d)})^T y, \quad |\Delta x^{(d)}| \le \delta |x^{(d)}|. \end{aligned}$$

the perturbed representatives of x differ by a factor of order δ
$\Rightarrow$ the $s^{(i)}$ will differ by a factor of order $\kappa\delta$.

Method 1 **implicitly** estimates the condition number κ.

Method 2

We compute a deterministic inner product $\widehat{s}$.

Then we compute $\widehat{\kappa}$, an explicit estimation of κ.

Randomness introduced in the d representatives of s:

$$s^{(i)} = \widehat{s} + \Delta s^{(i)}, \quad i = 1 : d,$$

where $|\Delta s^{(i)}| \approx \delta \widehat{\kappa} |\widehat{s}|$, δ controlling the size of the perturbations.

Method 2 **explicitly** estimates κ, and randomizes the *output* with a perturbation of size $\kappa\delta$.

Probabilistic analysis of the accuracy estimation

Method 1: input randomization

Given $x, y \in \mathbb{R}^n$, we define perturbed vectors $x^{(1)}, \ldots x^{(d)}$:

$$x^{(1)} = x \circ (1 + \delta \xi^{(1)}),$$
$$\ldots$$
$$x^{(d)} = x \circ (1 + \delta \xi^{(d)}),$$

where $\circ$ denotes the Hadamard (componentwise) product, $\delta > 0$, and $\xi^{(i)} \sim \mathcal{N}(0,1)^n$ (standard normal random vectors).

We compute the d inner products $s^{(i)} = (x^{(i)})^T y$.

We show that:

1. $$\varepsilon = \frac{\sigma_s}{\sqrt{d(d-1)}} \quad \text{where} \quad \bar{s} = \frac{1}{d}\sum_{i=1}^{d} s^{(i)} \quad \text{and} \quad \sigma_s^2 = \sum_{i=1}^{d} (\bar{s} - s^{(i)})^2$$
   is a good estimator of the accuracy $|s - \bar{s}|$ of $\bar{s}$.
2. the rounding errors in the computed $\widehat{\bar{s}}$ do not significantly affect the quality of the estimator as long as $\delta \gg u$.

Method 1: accuracy $|s - \bar{s}|$ of the exact $\bar{s}$

We show that

$$t = \frac{\bar{s} - s}{\varepsilon}$$

follows Student's t-distribution with $d - 1$ degrees of freedom.

Therefore, we can bound the quality of the estimation.

For any probability $\beta > 0$, $\exists \tau_\beta$ s.t.

$$\beta = \mathbb{P}(|t| \leq \tau_\beta) = \mathbb{P}\left(|\bar{s} - s| \leq \tau_\beta \varepsilon\right)$$

For Student's distribution, small values of τ_β suffice to make β close to 1.

$\Rightarrow$ ε is a good estimator of the accuracy of $\bar{s}$.

Method 1: accuracy $|s-\widehat{s}|$ of the computed $\widehat{s}$

We show that

for any probability $\beta > 0$

$$\mathbb{P}(|s-\widehat{s}| \leq 2\tau_\beta \varepsilon) \geq \beta\beta'$$

where

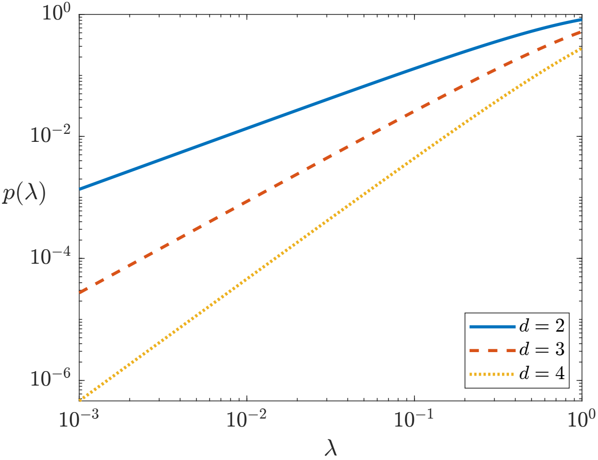
$$\beta' \geq 1 - p\left(\left(\frac{\sqrt{nd(d-1)}}{\tau_\beta}\frac{\gamma_{n+d}}{\delta}\right)^2\right)$$

for any integer k s.t. $ku < 1$, $\gamma_k = \frac{ku}{1-ku} \approx ku$

and for any $\lambda \leq d-1$,

$$p(\lambda) = \left(\frac{\lambda}{d-1}\right)^{(d-1)/2} \exp\Big((d-1-\lambda)/2\Big).$$

Method 1: as closer look at $p(\lambda)$



$p(\lambda)$ quickly vanishes as λ decreases, even for small values of d.

$\Rightarrow$ $\beta' \geq 1 - p(\lambda)$ very close to 1 if λ, and so u/δ, is sufficiently small.

Method 2: output randomization

Given $x, y \in \mathbb{R}^n$, we first compute in deterministic arithmetic the inner products

$$\widehat{s} = x^T y \quad \text{and} \quad \widehat{r} = |x|^T |y|.$$

Then, we compute an estimate of the condition number

$$\widehat{\kappa} = \widehat{r} / |\widehat{s}|.$$

Finally, we randomize the output by defining its d representatives as

$$s^{(i)} = \widehat{s}(1 + \xi^{(i)} \delta \widehat{\kappa}),$$

where $\xi^{(i)} \sim \mathcal{N}(0,1)$ and $\delta > 0$ is an estimation of the numerical noise introduced in the previous computation.

Method 2 estimates the accuracy of the inner product as $\delta \widehat{\kappa}$.

Method 2: output randomization

- if x, y are known exactly, we should set $\delta \approx u$.
  Method 2 only requires the computation of two inner products (s and r) with deterministic arithmetic.

- if x, y are the result of a previous computation, we must estimate the noise δ affecting them.

  With a stochastic validation tool, we have d representatives $x^{(i)}, y^{(i)}$.

  We estimate their noise δ and use Method 2 on an arbitrary choice of representatives, or possibly on

$$\bar{x} = \frac{1}{d}\sum_{i=1}^{d} x^{(i)}, \;\; \bar{y} = \frac{1}{d}\sum_{i=1}^{d} y^{(i)}.$$

Method 2: output randomization

Assuming δ to be a reliable measure of the noise, the loss of accuracy is bounded by $\delta\kappa$ where $\kappa = r/|s|$ is the true condition number.

Is $\delta\widehat{\kappa} = \delta\widehat{r}/|\widehat{s}|$ a reliable estimate?

We show that

$$\kappa \frac{(1-\gamma_n)}{(1+\gamma_n\kappa)} \leq \widehat{\kappa} \leq \kappa \frac{(1+\gamma_n)}{(1-\gamma_n\kappa)}.$$

$\Rightarrow$ $\widehat{\kappa}$ is a reliable estimate of κ as long as $\gamma_n\kappa \ll 1$.

If $\gamma_n\kappa \approx 1$, all digits of the result should be lost to numerical noise.

Numerical experiments and comparison with CADNA

The CADNA library

cadna.lip6.fr

- implements stochastic arithmetic with $\beta = 95\%$ and $d = 3$
  $\Rightarrow$ estimates the number of correct digits within a 95% confidence interval
- can be used in C/C++ or Fortran codes
- provides stochastic types (3 floating-point variables and an integer)
- all operators and mathematical functions overloaded
  $\Rightarrow$ few modifications in user programs
- support for MPI, OpenMP, GPU codes
- in one CADNA execution: accuracy of any result, complete list of numerical instabilities

[Chesneaux'90], [Jézéquel & al'08], [Lamotte & al'10], [Eberhart & al'18], [Jézéquel & al'21],...

Experimental setting

We compute in double precision 200 pairs of vectors x and y of size $n = 100$.

To simulate previous errors, we generate a triplet of perturbed vectors

$$\mathbf{x} = \left(x^{(1)}, x^{(2)}, x^{(3)}\right) = \left(x + \Delta x^{(1)}, x + \Delta x^{(2)}, x + \Delta x^{(3)}\right)$$

where $|\Delta x^{(j)}| \leq \eta |x|$.

η represents the noise affecting the vectors

if $\eta = 0$ the vectors are exact

experiments (not shown here) where y was also perturbed
$\Rightarrow$ similar conclusions

Implementation of Method 1

- if $\eta = 0$ (exact vector), the triplet $\mathbf{x}$ consists of 3 identical copies of x so randomness must be added. We thus define

$$\widetilde{\mathbf{x}} = \left(\widetilde{x}^{(1)}, \widetilde{x}^{(2)}, \widetilde{x}^{(3)}\right) = \left(x + \Delta x^{(1)}, x + \Delta x^{(2)}, x + \Delta x^{(3)}\right)$$

  where $|\Delta x^{(j)}| \leq \delta |x|$.

- if $\eta \neq 0$ ($\mathbf{x}$ affected by noise), we define $\widetilde{\mathbf{x}} = \mathbf{x}$ ($\delta = \eta$).

Method 1 computes $\widetilde{\mathbf{x}}^T y$, producing a stochastic number

$$\mathbf{s}_{M_1} = \left((\widetilde{x}^{(1)})^T y,\ (\widetilde{x}^{(2)})^T y,\ (\widetilde{x}^{(3)})^T y\right)$$

where each inner product $(\widetilde{x}^{(i)})^T y$ is computed with deterministic arithmetic.

Implementation of Method 2

We compute the inner product $s^{(1)} = (x^{(1)})^T y$ with deterministic arithmetic.

We estimate the condition number as

$$\widehat{\kappa} = \frac{|x^{(1)}|^T |y|}{|s^{(1)}|}.$$

We finally compute the stochastic triplet

$$\mathbf{s}_{M_2} = (s^{(1)}, s^{(1)} + \Delta s^{(2)}, s^{(1)} + \Delta s^{(3)})$$

where $|\Delta s^{(j)}| \leq \delta \widehat{\kappa} |s^{(1)}|$ for a given δ.

Similarly to Method 1,

- if $\eta = 0$ (exact vector), we test various values of $\delta \geq u$
- if $\eta \neq 0$ (vector affected by noise), we take $\delta = \eta$

Comparison of CADNA, Method 1, and Method 2

CADNA computes $\mathbf{x}^T y$ with stochastic arithmetic and thus produces a stochastic number

$$\mathbf{s}_C = \left(s_C^{(1)}, s_C^{(2)}, s_C^{(3)}\right).$$

For CADNA, Method 1, and Method 2, we report:

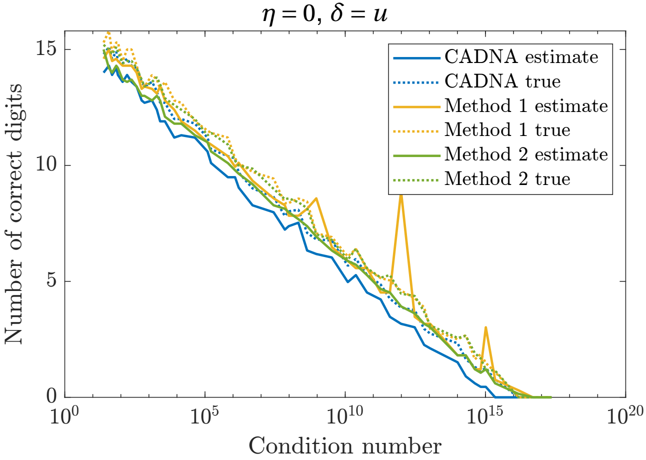
- the *estimated* accuracy provided by the method
- the *true* accuracy obtained by comparing the computed result to the correctly rounded result.

The accuracy is measured as the number of correct decimal digits of the result.

Since the computed result $\mathbf{s} = (s^{(1)}, s^{(2)}, s^{(3)})$ is a stochastic number,

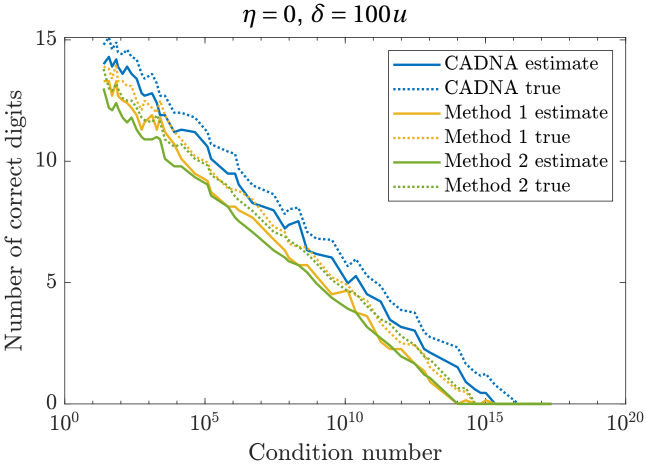
- the estimated accuracy is obtained using a CADNA function
- the true accuracy is measured using the average result $\bar{s} = \sum_{i=1}^{3} s^{(i)}/3$.

Exact input vectors



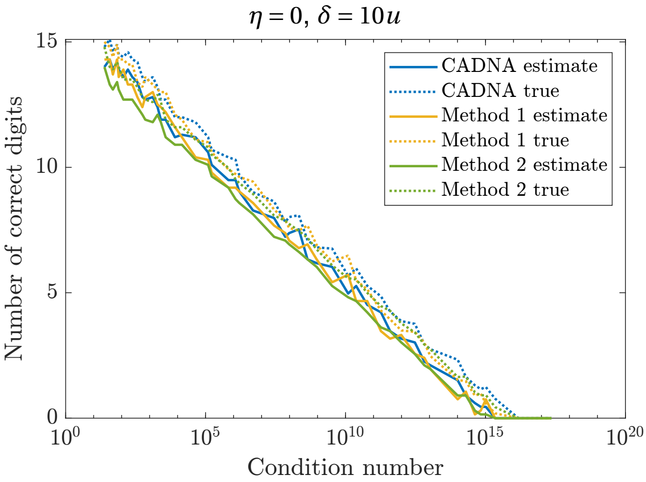
For a too small δ, Method 1 (and Method 2) can overestimate the number of correct digits.

Exact input vectors



For a too large δ, the estimation is reliable but the computed result is noticeably less accurate than with CADNA, due to the introduction of an error $\approx \delta$.

Exact input vectors



$\delta = 10u$ appears to be a suitable choice.

Method 1 and Method 2 compute a result with comparable accuracy to CADNA, while providing a reasonably tight estimate of their accuracy.

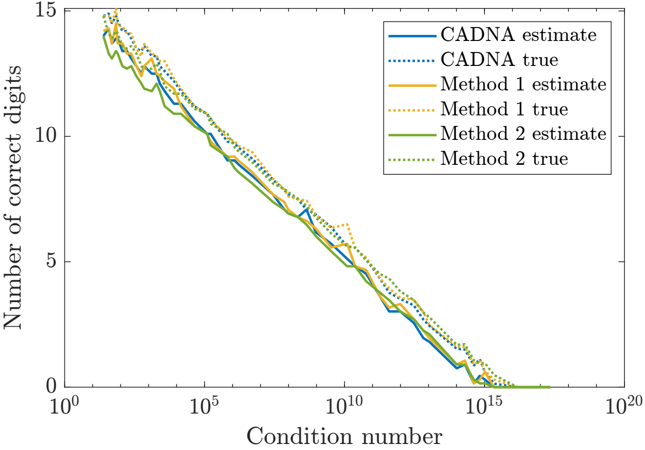
Exact input vectors

- All methods can reliably estimate the accuracy of the inner product.
- A suitable value for δ should be chosen.
- Method 2 underestimates the accuracy more frequently than Method 1
  $\Rightarrow$ slightly more pessimistic, although overall still quite reliable

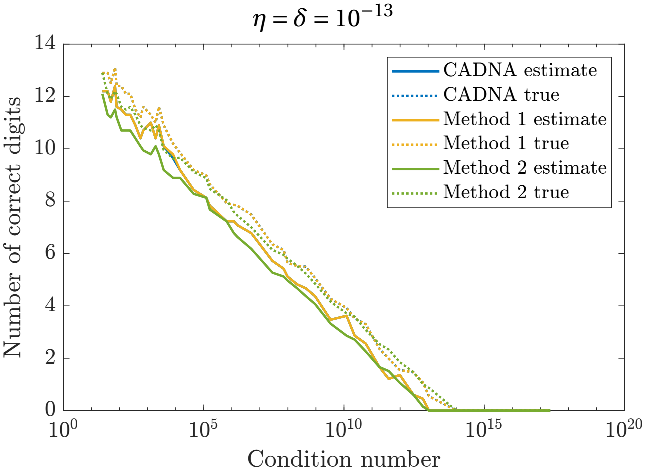
Perturbed input vectors

input vectors affected by a stochastic perturbation of size η ($\delta = \eta$)

$\eta = \delta = 10^{-15}$



Perturbed input vectors



Method 1 equivalent to CADNA

Perturbed input vectors

- When $\eta \gg u$, the initial perturbation dominates the rounding errors.

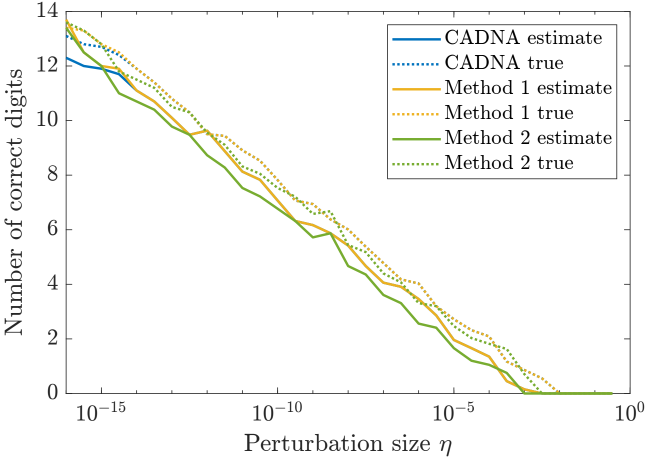
  So deterministic arithmetic in Method 1 does not change the result nor its estimated accuracy compared with CADNA.

  From a certain perturbation η ($\eta \geq 10^{-13}$) Method 1 is as reliable an estimator as CADNA.

- Method 2 is also a reliable estimator, although slightly pessimistic.

Perturbed input vectors

Accuracy of the inner product w.r.t. η, for one pair of input vectors with $\kappa \approx 1.5 \times 10^3$.



As soon as $\eta \gg u$ Method 1 becomes equivalent to CADNA.

Conclusion

- new numerical validation methods to estimate the accuracy of inner products with stochastic arithmetic.
- both methods allow for the use of efficient deterministic inner products
  performance gain for Method 1 already evaluated in [NSV'20]
- probabilistic analysis proves both methods to be reliable estimators
- reliability also confirmed via experiments: both methods compute estimations comparable to the stochastic validation method implemented in CADNA

Which of Method 1 or Method 2 should be preferred?

- Method 2 tends to be slightly more pessimistic than Method 1.
- In terms of cost,
  - Method 1 computes d inner products (in practice $d = 3$), whereas Method 2 only computes 2 of them.
  - when the input vectors are already affected by stochastic perturbations, Method 2 also requires to measure the noise δ.

Recommendation

- Method 2 when the input vectors are exact and performance is paramount
- Method 1 when the input vectors are already perturbed and/or a very tight estimate is desired.

References

This work:

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CADNA: http://cadna.lip6.fr

Thanks for your attention!