

# Probabilistic Error Analysis for Inner Products

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# Why Statistical/Probabilistic Approaches to Roundoff Error Analysis?

Disadvantage of deterministic bounds:

- Too pessimistic, especially for large dimensions  $n$   
(worst-case bounds cannot account for cancellation of errors)
- Valid only for sufficiently small  $n$   
( $n < \frac{1}{u}$ , where  $u$  is unit roundoff, half precision:  $n < 2048$ )
- May specify only first-order error terms

# Existing Work

- Von Neumann & Goldstine (1947): Matrix inversion
- Hull & Swenson (1966): Matrix addition, multiplication, Runge Kutta
- Henrici (1966): ODEs
- Tienari (1970): Matrix inversion
- Barlow & Bareiss (1985): Gaussian elimination
- Chatelin & Brunet (1990): Eigenvalues
- Higham & Mary (2018):  
Backward errors for: Inner products, matvec, matmult, LU, Cholesky

# Overview

- ① Perturbation bounds (perturbed inputs, exact computation)
  - General deterministic worst-case bound
  - Probabilistic bound: **Independent** errors
- ② Roundoff error bounds (exact inputs, roundoff in computation)
  - Probabilistic bound: **Dependent** errors

Assume: All vectors are real

## Perturbation Bounds

Perturbed inputs, exact computation

# Perturbed Inner Product

Exact vectors

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \quad \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \quad \mathbf{x}^T \mathbf{y} = x_1 y_1 + \cdots + x_n y_n$$

Perturbed vectors

$$\hat{\mathbf{x}} = \begin{pmatrix} (1 + \delta_1)x_1 \\ \vdots \\ (1 + \delta_n)x_n \end{pmatrix} \quad \hat{\mathbf{y}} = \begin{pmatrix} (1 + \theta_1)y_1 \\ \vdots \\ (1 + \theta_n)y_n \end{pmatrix} \quad |\delta_j|, |\theta_j| \leq u$$

Relative error

$$\left| \frac{\hat{\mathbf{x}}^T \hat{\mathbf{y}} - \mathbf{x}^T \mathbf{y}}{\mathbf{x}^T \mathbf{y}} \right| \leq ??$$

## General Deterministic Worst-Case Bound

Idea: Express perturbations as Hadamard product

$$\hat{\mathbf{x}} = \begin{pmatrix} x_1 + \delta_1 x_1 \\ \vdots \\ x_n + \delta_n x_n \end{pmatrix} = \mathbf{x} + \boldsymbol{\delta} \circ \mathbf{x}, \quad \hat{\mathbf{y}} = \begin{pmatrix} y_1 + \theta_1 y_1 \\ \vdots \\ y_n + \theta_n y_n \end{pmatrix} = \mathbf{y} + \boldsymbol{\theta} \circ \mathbf{y}$$

Relative error bound

$$\left| \frac{\hat{\mathbf{x}}^T \hat{\mathbf{y}} - \mathbf{x}^T \mathbf{y}}{\mathbf{x}^T \mathbf{y}} \right| \leq \underbrace{\frac{\|\mathbf{x} \circ \mathbf{y}\|_p}{|\mathbf{x}^T \mathbf{y}|}}_{\text{Amplifier}} \underbrace{\|\boldsymbol{\delta} + \boldsymbol{\theta} + \boldsymbol{\delta} \circ \boldsymbol{\theta}\|_q}_{\text{Perturbations}} \quad \frac{1}{p} + \frac{1}{q} = 1$$

- $\boldsymbol{\delta} \circ \boldsymbol{\theta}$  represents second-order errors
- Bound is **exact**

## Deterministic Worst-Case Bound: Special Cases

- $p = 1$ : Traditional amplifier

$$\left| \frac{\hat{\mathbf{x}}^T \hat{\mathbf{y}} - \mathbf{x}^T \mathbf{y}}{\mathbf{x}^T \mathbf{y}} \right| \leq \frac{|\mathbf{x}|^T |\mathbf{y}|}{|\mathbf{x}^T \mathbf{y}|} u(2 + u)$$

- $p = 2$ :

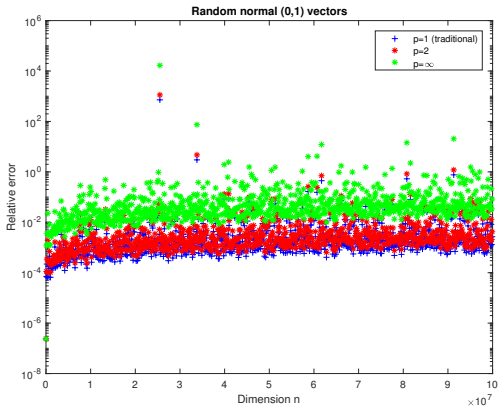
$$\left| \frac{\hat{\mathbf{x}}^T \hat{\mathbf{y}} - \mathbf{x}^T \mathbf{y}}{\mathbf{x}^T \mathbf{y}} \right| \leq \frac{\sqrt{\sum_{j=1}^n |x_j y_j|^2}}{|\mathbf{x}^T \mathbf{y}|} \sqrt{n} u(2 + u)$$

- $p = \infty$ : Smallest amplifier

$$\left| \frac{\hat{\mathbf{x}}^T \hat{\mathbf{y}} - \mathbf{x}^T \mathbf{y}}{\mathbf{x}^T \mathbf{y}} \right| \leq \frac{\max_{1 \leq j \leq n} |x_j y_j|}{|\mathbf{x}^T \mathbf{y}|} n u(2 + u)$$



# Comparison of Deterministic Bounds for $n \leq 10^8$



$p = 1$  (traditional) bound is the best

$p = 2$  bound is almost as good

Single precision perturbations  $u \approx 10^{-8}$ , bounds computed in double

## Probabilistic Bound: Azuma's Inequality

How much does a sum  $Z = Z_1 + \dots + Z_n$  of independent random variables  $Z_1, \dots, Z_n$  differ from its mean  $\mathbb{E}[Z]$ ?

If

$$|Z_j - \mathbb{E}[Z_j]| \leq c_j, \quad 1 \leq j \leq n$$

then for any  $0 < \delta < 1$  with probability at least  $1 - \delta$

$$\Pr[|Z - \mathbb{E}[Z]| \geq \epsilon] \leq 2 \exp\left(-\frac{\epsilon^2}{2 \sum_{j=1}^n c_j^2}\right)$$

- $2 \sum_{j=1}^n c_j^2$  approximates the variance
- All  $Z_j$  close to their means  $\Rightarrow$   
 $Z_1 + \dots + Z_n$  close to its mean, with high probability

# Probabilistic Perturbation Bound

Assume

- All  $\delta_j, \theta_j$  are independent random variables
- Zero mean:  $\mathbb{E}[\delta_j] = 0 = \mathbb{E}[\theta_j]$
- Bounded:  $|\delta_j|, |\theta_j| \leq u$

Then, for any  $0 < \delta < 1$ , with probability at least  $1 - \delta$

$$\left| \frac{\hat{\mathbf{x}}^T \hat{\mathbf{y}} - \mathbf{x}^T \mathbf{y}}{\mathbf{x}^T \mathbf{y}} \right| \leq \underbrace{\frac{\sqrt{\sum_{j=1}^n |x_j y_j|^2}}{|\mathbf{x}^T \mathbf{y}|}}_{\text{Amplifier}} \underbrace{\sqrt{2 \ln(2/\delta)}}_{\text{Probabilistic}} \underbrace{u(2+u)}_{\text{Perturbation}}$$

- Probabilistic factor is small:

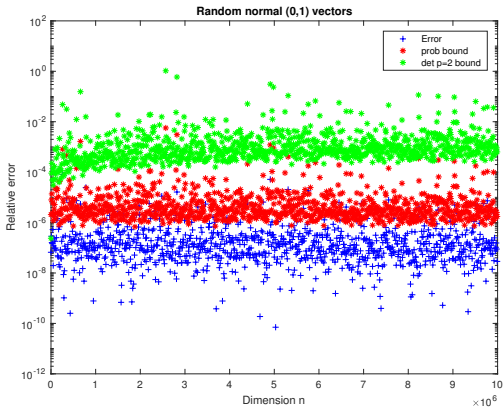
If  $1 - \delta = 1 - 10^{-16}$  then  $\sqrt{2 \ln(2/\delta)} \leq 9$

## Comparison of Perturbation Bounds: Deterministic vs Probabilistic

$$\left| \frac{\hat{\mathbf{x}}^T \hat{\mathbf{y}} - \mathbf{x}^T \mathbf{y}}{\mathbf{x}^T \mathbf{y}} \right| \leq \frac{\sqrt{\sum_{j=1}^n |x_j y_j|^2}}{|\mathbf{x}^T \mathbf{y}|} \Delta u(2+u)$$

- Deterministic ( $p = 2$ ) bound:  $\Delta = \sqrt{n}$   
Increases with dimension  $n$
- Probabilistic bound:  $\Delta = \sqrt{2 \ln(2/\delta)}$   
Independent of dimension  
 $\Delta \leq 9$  for tiny failure probability  $\delta = 10^{-16}$
- Probabilistic bound tighter for  $n \geq 81$

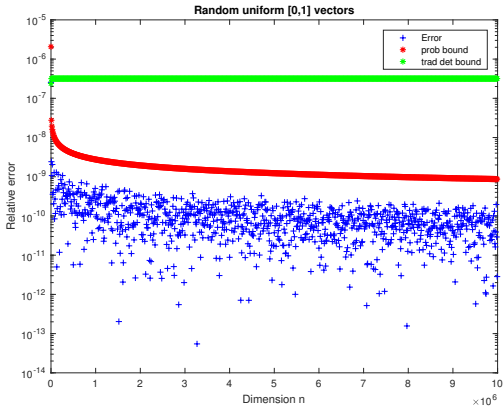
# Comparison: Deterministic vs Probabilistic for $n \leq 10^7$



Probabilistic bound tighter than deterministic bound

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## Perturbation Bounds: Summary

- Component-wise relative perturbation of input vectors, inner product computation is exact
- Bounds for the relative error of  $\mathbf{x}^T \mathbf{y}$
- Deterministic bounds are exact (no big O terms)  
Amplifier in any  $p$ -norm
- Probabilistic bound: Perturbations are random variables
- No assumptions on random variables other than:  
independent, zero-mean, bounded
- Probabilistic bound (with stringent success probability)  
tighter than deterministic bound for dimension  $n \geq 81$

## Roundoff Error Bounds

Exact inputs, computations have round off errors



## Deterministic Roundoff Error Bound

- Exact computation

$$s_1 = x_1 y_1$$

$$s_{k+1} = s_k + x_{k+1} y_{k+1} \quad 2 \leq k < n$$

Output:  $s_n = \mathbf{x}^T \mathbf{y}$

- Floating point arithmetic:  $|\delta_k|, |\theta_k| \leq u$

$$\hat{s}_1 = x_1 y_1 (1 + \theta_1)$$

$$\hat{s}_k = (\hat{s}_{k-1} + x_k y_k (1 + \theta_k)) (1 + \delta_k) \quad 2 \leq k \leq n$$

Output:  $\hat{s}_n$

- If  $nu < 1$  then [Higham 2002]

$$\left| \frac{\hat{s}_n - s_n}{s_n} \right| \leq \underbrace{\frac{|\mathbf{x}|^T |\mathbf{y}|}{|\mathbf{x}^T \mathbf{y}|}}_{\text{Amplifier}} \underbrace{\frac{nu}{1 - nu}}_{\text{Roundoff}}$$

## Probabilistic Roundoff Error Bound

Distinguish **product** roundoffs from **summation** roundoffs

- Exact computation

$$s_1 = s_2 = x_1 y_1$$

$$s_{2k+1} = s_{2(k+1)} = s_{2k} + x_{k+1} y_{k+1} \quad 2 \leq k < n$$

Output:  $s_{2n} = \mathbf{x}^T \mathbf{y}$

- Floating point arithmetic:  $|\delta_k| \leq u$

$$\hat{s}_1 = x_1 y_1 (1 + \delta_1)$$

$$\hat{s}_2 = \hat{s}_1 (1 + \delta_2)$$

$$\hat{s}_{2k+1} = \hat{s}_{2k} + x_{k+1} y_{k+1} (1 + \delta_{2k+1})$$

$$\hat{s}_{2(k+1)} = \hat{s}_{2k+1} (1 + \delta_{2(k+1)}) \quad 2 \leq k < n$$

Output:  $\hat{s}_{2n}$

## Probabilistic Bounds for Forward Error

- Product roundoff

$$\begin{aligned}Z_{2k+1} &= \hat{s}_{2k+1} - s_{2k+1} \\ &= Z_{2k} + x_{k+1}y_{k+1} \delta_{2k+1}\end{aligned}$$

- Summation roundoff

$$\begin{aligned}Z_{2(k+1)} &= \hat{s}_{2(k+1)} - s_{2(k+1)} \\ &= Z_{2k+1} + \hat{s}_{2k+1} \delta_{2(k+1)}\end{aligned}$$

- Assume that roundoffs  $\delta_k$  have zero mean:  $\mathbb{E}[\delta_k] = 0$

## Probabilistic Bounds for Forward Error

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- Assume that roundoffs  $\delta_k$  have zero mean:  $\mathbb{E}[\delta_k] = 0$

Forward error at stage  $j$ , conditioned on previous roundoffs, has mean equal to forward error at stage  $j - 1$

$$\mathbb{E}[Z_j | \delta_1, \dots, \delta_{j-1}] = Z_{j-1} \quad 1 < j \leq 2n$$

Forward errors  $Z_1, Z_2, \dots$ , are Martingale with respect to roundoffs  $\delta_1, \delta_2, \dots$

## Probabilistic Bound: Azuma-Hoeffding Martingale

Sequence of random variables  $Z_0, Z_1, Z_2 \dots$  is Martingale with respect to sequence  $\delta_1, \delta_2 \dots$  if for  $j \geq 1$

- 1  $Z_j$  is function of  $\delta_1, \dots, \delta_j$
- 2  $\mathbb{E}[|Z_j|] < \infty$ ,
- 3  $\mathbb{E}[Z_j | \delta_1, \dots, \delta_{j-1}] = Z_{j-1}$

If also

$$|Z_j - Z_{j-1}| \leq c_j \quad 1 \leq j \leq 2n$$

then, for any  $0 < \delta < 1$ , with probability at least  $1 - \delta$

$$|Z_{2n} - Z_0| \leq \sqrt{\sum_{j=1}^{2n} c_j^2} \sqrt{2 \ln(2/\delta)}$$

## Probabilistic Roundoff Bound

Assume that the roundoffs  $\delta_j$  satisfy:

- Zero mean:  $\mathbb{E}[\delta_j] = 0$
- Bounded:  $|\delta_j| \leq u$

Then, for any  $0 < \delta < 1$ , with probability at least  $1 - \delta$

$$\left| \frac{\hat{S}_{2n} - S_{2n}}{S_{2n}} \right| \leq \frac{|\mathbf{x}|^T |\mathbf{y}|}{|\mathbf{x}^T \mathbf{y}|} \sqrt{n+1} \sqrt{2 \ln(2/\delta)} (1+u)^n u$$

Bound does not depend on the summation order

## Comparison of Roundoff Bounds: Deterministic vs Probabilistic

$$\left| \frac{\hat{s}_{2n} - s_{2n}}{s_{2n}} \right| \leq \frac{|\mathbf{x}|^T |\mathbf{y}|}{|\mathbf{x}^T \mathbf{y}|} \Delta u$$

Assume:  $\delta = 10^{-16}$ ,  $u \approx 6 \cdot 10^{-8}$  (IEEE Single),  $n \leq 10^7$

- Deterministic bound:

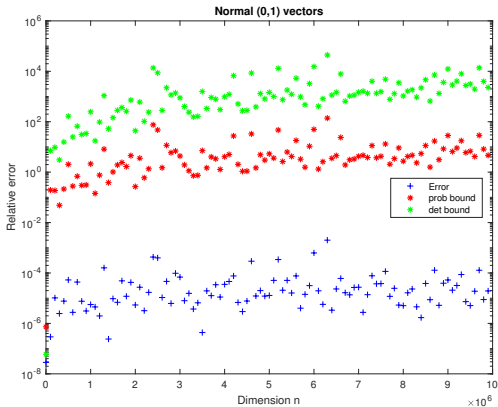
$$\Delta = \frac{n}{1 - nu} \leq 1.5 n$$

- Probabilistic bound:

$$\Delta = \sqrt{n+1} (1+u)^n \sqrt{2 \ln(2/\delta)} \leq 15.7 \sqrt{n+1}$$

- Deterministic bound  $\sim n$   
probabilistic bound  $\sim \sqrt{n}$

# Comparison: Deterministic vs Probabilistic for $n \leq 10^7$

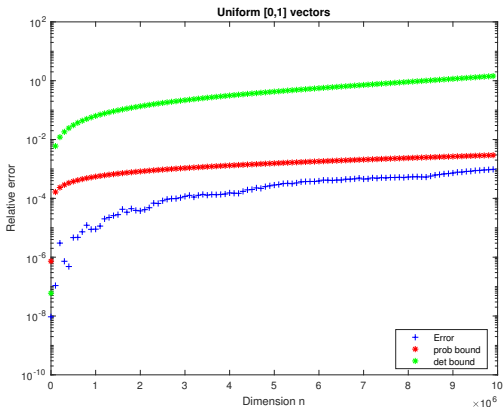


Probabilistic bound tighter than deterministic bound

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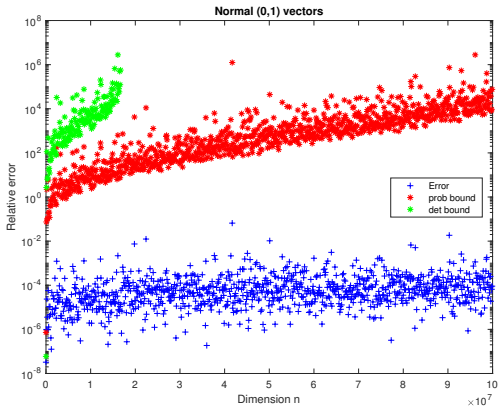
# Comparison: Deterministic vs Probabilistic for $n \leq 10^7$



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# Comparison: Deterministic vs Probabilistic for $n \leq 10^8$



Probabilistic bound tighter than deterministic bound  
But: Need to tighten probabilistic bound

## Tighter Probabilistic Bound

Assume that the roundoffs  $\delta_j$  satisfy:

- Zero mean:  $\mathbb{E}[\delta_j] = 0$
- Bounded:  $|\delta_j| \leq u$

For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$

$$\left| \frac{\hat{s}_{2n} - s_{2n}}{s_{2n}} \right| \leq \kappa \sqrt{2 \ln(2/\delta)} u$$

where

$$\kappa \equiv \frac{\sqrt{\|\mathbf{x} \circ \mathbf{y}\|_2^2 + \sum_{k=1}^n ((\mathbf{x} \circ \mathbf{y})_{1:k}^T \mathbf{u}_k)^2}}{|\mathbf{x}^T \mathbf{y}|}$$

and

$$\mathbf{u}_k \equiv (1 + u \quad (1 + u)^2 \quad \cdots \quad (1 + u)^k)$$

# Summary

Probabilistic **perturbation** bounds:

Independent of  $n$

Probabilistic **roundoff error** bounds:

- Proportional to  $\sim \sqrt{n}$  instead of  $n$
- No limit on dimension  $n$
- No assumption on independence of errors (Martingales)  
Only assumption: zero-mean and bounded
- Exact, non-asymptotic bounds (no big O terms)
- Extremely stringent success probabilities ( $\delta = 10^{-16}$ )

Not covered:

New condition numbers for general forward error bounds  
(from concentration inequalities)