Accuracy and Stability of Numerical Algorithms

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January 21, 2013
SIAM

- ~ 13,500 members: ~ 9000 USA, ~ 500 UK.
- 59% in maths depts
  16% in eng depts
  11% in CS depts
- 108 student chapters:

<table>
<thead>
<tr>
<th>University</th>
<th>Chapter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxford (2007)</td>
<td>#53</td>
</tr>
<tr>
<td>Heriot Watt &amp; Edinburgh</td>
<td>#71</td>
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<tr>
<td>Manchester</td>
<td>#76</td>
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<td>Strathclyde</td>
<td>#93</td>
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<td>Warwick</td>
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<td>Reading</td>
<td>#100</td>
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<td>Cardiff</td>
<td>#104</td>
</tr>
<tr>
<td>Bath</td>
<td>#105</td>
</tr>
</tbody>
</table>
Floating Point Number System

Floating point number system $F \subset \mathbb{R}$:

$$y = \pm m \times \beta^{e-t}, \quad 0 \leq m \leq \beta^t - 1.$$  

- **Base** $\beta$,  
- **precision** $t$,  
- **exponent range** $e_{\text{min}} \leq e \leq e_{\text{max}}$.  

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Floating point numbers are **not equally spaced**.

If $\beta = 2$, $t = 3$, $e_{\text{min}} = -1$, and $e_{\text{max}} = 3$:

```
0  0.5  1.0  2.0  3.0  4.0  5.0  6.0  7.0
```
For \( x \in \mathbb{R} \), \( fl(x) \) is an element of \( F \) nearest to \( x \), and the transformation \( x \rightarrow fl(x) \) is called **rounding** (to nearest).

**Theorem**

If \( x \in \mathbb{R} \) lies in the range of \( F \) then

\[
fl(x) = x(1 + \delta), \quad |\delta| \leq u := \frac{1}{2}\beta^{1-t}.
\]

\( u \) is the **unit roundoff**, or machine precision.
Types of Rounding

- **Round to nearest**—with rule for breaking ties.
  
  \[
  8.12 \rightarrow 8.1, \quad 8.17 \rightarrow 8.2, \quad 8.15 \rightarrow 8.1 \text{ or } 8.2.
  \]
Types of Rounding

- **Round to nearest**—with rule for breaking ties.
  
  \[
  \begin{align*}
  8.12 \rightarrow 8.1, & \quad 8.17 \rightarrow 8.2, \\
  8.15 \rightarrow 8.1 \text{ or } 8.2.
  \end{align*}
  \]

- **Round up**: to \( +\infty \).
  
  \[
  \begin{align*}
  8.11 \rightarrow 8.2.
  \end{align*}
  \]
Types of Rounding

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■ **Round down**: to $-\infty$.
  - 8.68 $\rightarrow$ 8.6.
Types of Rounding

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  8.15 → 8.1 or 8.2.
- **Round up**: to $+\infty$.
  8.11 → 8.2.
- **Round down**: to $-\infty$.
  8.68 → 8.6.

Thomas (9) homework

- **Round 17.37 to the nearest tenth.**  “17.4”
- **Round 13.75 to the nearest tenth.**  “13.8”
“The American was given a time of 9.76sec at the Qatar Super grand prix but his official time was 9.766, which was rounded down instead of being rounded up to Powell’s time of 9.77 set in Athens last year according to rules set out by track and field’s governing body, the timekeeper Tissot admitted.”

King faces a point of embarrassment

A TINY price movement equivalent to one hundred thousandth of one per cent on the inflation rate could make all the difference to the Bank of England this week. With Government statisticians crunching cost of living numbers to six decimal places, the slightest rise could force Bank governor Mervyn King to explain what went wrong.

The Office for National Statistics publishes inflation numbers to one decimal place, meaning that a 3.049 rate would appear as three per cent, letting the MPC off the hook.
Vancouver Stock Exchange Index

- January 1982: Index established at 1000.
- November 1983: Index was 520.

But exchange seemed to be doing well.
Vancouver Stock Exchange Index

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- November 1983: Index was 520.

But exchange seemed to be doing well.

**Explanation:**

- Index *rounded down* to three digits at each recomputation.
- Errors always in same direction $\Rightarrow$ thousands of small errors add up to a large error.

Upon correct recalculation, the index doubled!
Important information on your Virgin Media services

Dear Mr Higham

We’re writing to tell you about changes to your phone charges that will be coming into effect from 1st May 2007.

The price of our monthly phone packages is coming down, so Size: XL (Talk Unlimited) will go from £14 a month to £9.95 and Size: L (Talk Evenings and Weekends) will go from £5.50 to £3.95. Your phone line will stay the same at £11 a month.

The way your call charges are calculated is also changing. Instead of charging to the nearest second, calls will be rounded up to the next minute. So, for example, a call that lasts 4 minutes 50 seconds will be rounded up to 5 minutes. If you have a phone package, any calls made outside your call plan will be rounded up to the next minute.
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Remember

Rounding doesn’t always mean round to nearest!
Next time, no rounding off!
Precision versus Accuracy

Unit roundoff \( u = \frac{1}{2} \beta^{1-t} \).

\[
fl(abc) = ab(1 + \delta_1) \cdot c(1 + \delta_2) \quad |\delta_i| \leq u,
\]
\[
= abc(1 + \delta_1)(1 + \delta_2)
\]
\[
\approx abc(1 + \delta_1 + \delta_2).
\]

- Precision = \( u \).
- Accuracy \( \approx 2u \).
Precision versus Accuracy

Unit roundoff $u = \frac{1}{2} \beta^{1-t}$.

$$fl(abc) = ab(1 + \delta_1) \cdot c(1 + \delta_2) \quad |\delta_i| \leq u,$$

$$= abc(1 + \delta_1)(1 + \delta_2)$$

$$\approx abc(1 + \delta_1 + \delta_2).$$

- **Precision** $= u$.
- **Accuracy** $\approx 2u$.

Accuracy is not limited by precision.
Walkers’ Trouser Review

THE LOWDOWN

Fabric Nikwax Analogy Insulator (polyester microfibre outer, 100g polyester fill)
Sizes XS-XL (unisex)
Inside leg 79cm only
Waist integral belt, front flap with Velcro tabs
Pockets none

RATINGS

Comfort 80%
Fabric performance 100%
Versatility 50%
Quality/value 85%
Overall 78.75%
RGB to XYZ

From CIE Standard (1931):

\[
\begin{bmatrix}
X \\
Y \\
Z
\end{bmatrix} =
\begin{bmatrix}
0.49 & 0.31 & 0.20 \\
0.17697 & 0.81240 & 0.01063 \\
0 & 0.01 & 0.99
\end{bmatrix}
\begin{bmatrix}
R \\
G \\
B
\end{bmatrix}.
\]
RGB to XYZ

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\begin{bmatrix}
    X \\
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= 
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    0 & 0.01 & 0.99 \\
\end{bmatrix}
\begin{bmatrix}
    R \\
    G \\
    B \\
\end{bmatrix}
\]

But in many books:

\[
\begin{bmatrix}
    X \\
    Y \\
    Z \\
\end{bmatrix}
= 
\begin{bmatrix}
    0.49000 & 0.31000 & 0.20000 \\
    0.17697 & 0.81240 & 0.01063 \\
    0 & 0.01000 & 0.99000 \\
\end{bmatrix}
\begin{bmatrix}
    R \\
    G \\
    B \\
\end{bmatrix}
\]
Rational Function

\[ r(x) = \frac{(((7x - 101)x + 540)x - 1204)x + 958}{(((x - 14)x + 72)x - 151)x + 112} \]
Continued Fraction

\[ r(x) = 7 - \frac{3}{x - 2 - \frac{1}{x - 7 + \frac{10}{x - 2 - \frac{2}{x - 3}}}} \]

Division by zero at \( x = 1, 2, 3, 4 \), but \( r \) evaluates correctly in IEEE arithmetic!
Cancellation Example

\[ 0 \leq \frac{1 - \cos x}{x^2} < \frac{1}{2}, \quad x \neq 0. \]

With \( x = 1.2 \times 10^{-5} \), \( \cos x \) rounded to 10 sig figs is

\[ c = 0.9999\,999\,99 \ \Rightarrow \ 1 - c = 0.0000\,0000\,01. \]

Then \( (1 - c)/x^2 = 10^{-10}/1.44 \times 10^{-10} = 0.6944\ldots! \)

To avoid cancellation, rewrite as

\[ \frac{1}{2} \left( \frac{\sin(x/2)}{x/2} \right)^2. \]
Cancellation Example

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With \( x = 1.2 \times 10^{-5} \), \( \cos x \) rounded to 10 sig figs is

\[ c = 0.9999999999 \Rightarrow 1 - c = 0.000000001. \]

Then \( (1 - c)/x^2 = 10^{-10}/1.44 \times 10^{-10} = 0.6944 \ldots! \)

To avoid cancellation, rewrite as

\[ \frac{1}{2} \left( \frac{\sin(x/2)}{x/2} \right)^2. \]

\[ \text{The subtraction } 1 - c \text{ is exact.} \]
Cancellation

**Theorem (Sterbenz)**

Let $x$ and $y$ be floating point numbers with $y/2 \leq x \leq 2y$. Then $x - y$ is computed exactly (assuming $x - y$ does not underflow).
Cancellation

Theorem (Sterbenz)

Let $x$ and $y$ be floating point numbers with $y/2 \leq x \leq 2y$. Then $x - y$ is computed exactly (assuming $x - y$ does not underflow).

Cancellation brings earlier errors into prominence but is not always a bad thing.

- Numbers being subtracted may be error free.
- Cancellation may be a symptom of intrinsic ill conditioning of problem.
Guo, H & Tisseur (2009):

- **Problem**: Find midpoint $c$ of an arc $(a, b)$.

- Obvious formula $c = (a + b)/|a + b|$ is unstable when $a \approx -b$.

- **Solution**: If $a = e^{i\theta_1}$, $b = e^{i\theta_2}$ then $c = e^{i(\theta_1 + \theta_2)/2}$. 
How to Compute $\log \lambda_2 - \log \lambda_1$

Define the **unwinding number**

$$\mathcal{U}(z) := \frac{z - \log e^z}{2\pi i} = \left\lfloor \frac{\text{Im } z - \pi}{2\pi} \right\rfloor \in \mathbb{Z}.$$ 

Let $z = (\lambda_2 - \lambda_1)/(\lambda_2 + \lambda_1)$. 
How to Compute $\log \lambda_2 - \log \lambda_1$

Define the **unwinding number**

$$U(z) := \frac{z - \log e^z}{2\pi i} = \left\lfloor \frac{\text{Im } z - \pi}{2\pi} \right\rfloor \in \mathbb{Z}.$$ 

Let $z = (\lambda_2 - \lambda_1)/(\lambda_2 + \lambda_1)$. Then

$$\log \lambda_2 - \log \lambda_1 = \log \left(\frac{\lambda_2}{\lambda_1}\right) + 2\pi i U(\log \lambda_2 - \log \lambda_1)$$

$$= \log \left(\frac{1 + z}{1 - z}\right) + 2\pi i U(\log \lambda_2 - \log \lambda_1)$$

$$= \text{atanh}(z) + 2\pi i U(\log \lambda_2 - \log \lambda_1).$$

Outline

1. Rounding
2. Precision
3. Accuracy
4. Higher Precision
5. Tiny Relative Errors
IEEE Standard 754-2008 and 1985

<table>
<thead>
<tr>
<th>Type</th>
<th>Size</th>
<th>Range</th>
<th>$u = 2^{-t}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>single</td>
<td>32 bits</td>
<td>$10^{\pm38}$</td>
<td>$2^{-24} \approx 6.0 \times 10^{-8}$</td>
</tr>
<tr>
<td>double</td>
<td>64 bits</td>
<td>$10^{\pm308}$</td>
<td>$2^{-53} \approx 1.1 \times 10^{-16}$</td>
</tr>
<tr>
<td>quadruple</td>
<td>128 bits</td>
<td>$10^{\pm4932}$</td>
<td>$2^{-113} \approx 9.6 \times 10^{-35}$</td>
</tr>
</tbody>
</table>

- Arithmetic ops ($+,-,\times,/,\sqrt{}$) performed as if first calculated to infinite precision, then rounded.
- Default: round to nearest, round to even in case of tie.
Need for Higher Precision


- Long-time simulations.
- Large-scale simulations.
- Resolving small-scale phenomena.
Increasing the Precision

\[ y = e^{\pi \sqrt{163}} \] evaluated at \( t \) digit precision:

<table>
<thead>
<tr>
<th>( t )</th>
<th>( y )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>262537412640768744.00</td>
</tr>
<tr>
<td>25</td>
<td>262537412640768744.0000000</td>
</tr>
<tr>
<td>30</td>
<td>262537412640768743.9999999999999</td>
</tr>
</tbody>
</table>

Is the last digit before the decimal point 4?
Increasing the Precision

\[ y = e^{\pi \sqrt{163}} \] evaluated at \( t \) digit precision:

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<tbody>
<tr>
<td>35</td>
<td>262537412640768743.99999999999999999925007</td>
</tr>
<tr>
<td>40</td>
<td>262537412640768743.9999999999999999992500725972</td>
</tr>
</tbody>
</table>

So no, it’s 3!
Zimbabwe resorts to the $100 trillion note

By Our Foreign Staff

ZIMBABWE’S central bank will introduce a $100 trillion Zimbabwean dollar banknote, worth about £22, on the black market, to try to ease desperate cash shortages, state-run media said yesterday. Prices are doubling every day and food and fuel are in short supply. A cholera epidemic has killed more than 2,000 people and a deadlock between Mr Mugabe and the opposition has put hopes of ending the crisis on hold. Hyper-inflation has forced the central bank to continue to release new banknotes which quickly become almost worthless. There is an official exchange rate, but most Zimbabweans use the informal market for currency deals.

As well as the Z$100 trillion dollar note, the Reserve Bank of Zimbabwe plans to introduce Z$10 trillion, Z$20 trillion and Z$50 trillion notes, the Herald newspaper reported.

Zimbabweans often line up for hours outside banks to withdraw barely enough to buy a loaf of bread.

Old Mutual’s new chief weighs rescue options

JUDGING by the empty state of his spacious South African office, it is quite clear that Julian Roberts has yet to settle into his role as the new chief executive of Old Mutual.

While his secretary bustles around, tidying away his few possessions – a 5p piece and a penny coin left lying on his desk – the four books on his vacant shelves stand out. The titles Blown to Bits and On the Brink of Failure could almost sum up the state of the blue-chip company Mr Roberts has just taken over. Old Mutual was the worst-performing European going to be immune. South Africa lags the rest of the world by six months to a year.

Political tensions are also playing on his mind. Old Mutual is listed not only in the UK and Johannesburg but also on the Zimbabwe Stock Exchange. Due to technical difficulties of transferring a figure with so many noughts on the end of it, Old Mutual struggled to pay shareholders an interim dividend of Z$453 trillion per share – which in November equated to just 2.45p.

“IT is absolutely tragic. We have a significant business with a large

PROFILE

Julian Roberts

Chief executive, Old Mutual

The economic turmoil revealed cracks in Old Mutual’s model when it emerged that its $2.8bn (£1.9bn) variable annuity business in the US could not meet guarantees due to adverse movements in the Asian markets. It has been forced to inject...
If we have quadruple or higher precision, what do we need to do to modify existing algorithms?

To what extent are existing algs precision-independent?
Matrix Functions

(Inverse) scaling and squaring-type algorithms for $e^A$, \log(A), \cos(A), A^t$ use Padé approximants.

- Padé degree chosen to achieve accuracy $u$.
- Padé coeffs and algorithm parameters need rederiving for a different $u$. Logic may change!
- MATLAB’s `expm, logm` need changing for smaller $u$.

Methods based on best $L_\infty$ approximations to $e^A$ for Hermitian $A$ also need higher order approximations deriving.

- Scalar elementary functions!
Outline

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5. Tiny Relative Errors
Tiny Relative Errors

Normwise relative errors

\[ \frac{\| x - y \|_\infty}{\| x \|_\infty} = \frac{\max_i |x_i - y_i|}{\max_i |x_i|} \]

from a numerical experiment:

\[
\begin{array}{cccc}
1.32e-22 & 3.39e-22 & 3.39e-21 & 8.67e-20 \\
1.39e-18 & 4.36e-18 & 5.30e-18 & 5.83e-18 \\
1.45e-17 & 3.76e-17 & 3.76e-17 & 4.27e-17 \\
\ldots
\end{array}
\]

How can errors be \( \ll u \approx 10^{-16} \)?
Base $\beta = 2$, $u = 2^{-t}$. Dingle & H (2011):

**Theorem**

If $x \neq 0$ and $y$ are distinct normalized flpt numbers then $|x - y|/|x| \geq u$ and this lower bound is attainable.
Base $\beta = 2$, $u = 2^{-t}$. Dingle & H (2011):

**Theorem**

*If* $x \neq 0$ *and* $y$ *are distinct normalized flpt numbers then* $|x - y|/|x| \geq u$ *and this lower bound is attainable.*

But $\frac{\|x - y\|_\infty}{\|x\|_\infty} \ll u$ *is possible.*

\[
\begin{align*}
x &= \begin{bmatrix} 1 \\ 10^{-22} \end{bmatrix}, \quad y = \begin{bmatrix} 1 \\ 2 \times 10^{-22} \end{bmatrix}, \quad \frac{\|x - y\|_\infty}{\|x\|_\infty} = 10^{-22}.
\end{align*}
\]
Relative Errors

- Schur–Pade
- SP–Pade
- powerm
- SP–ss–iss
Performance Profiles


For the given set of solvers and test problems, plot

\begin{align*}
x\text{-axis:} & \quad \alpha \\
y\text{-axis:} & \quad \text{probability that solver has error within factor } \alpha \text{ of smallest error over all solvers on the test set.}
\end{align*}
Performance Profile

Graph showing the performance profile with different methods:
- Schur–Pade
- SP–Pade
- powerm
- SP–ss–iss

The x-axis represents \( \alpha \) ranging from 1 to 10, and the y-axis represents \( \pi \) from 0 to 1.

Legend:
- Black solid line: Schur–Pade
- Blue dashed line: SP–Pade
- Green dotted line: powerm
- Red dashed line: SP–ss–iss

The graph illustrates the accuracy and stability of these methods under varying conditions.
The Effect of Tiny Errors

<table>
<thead>
<tr>
<th>Problem</th>
<th>Algorithm 1</th>
<th>Algorithm 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4e-14</td>
<td>1e-16</td>
</tr>
<tr>
<td>2</td>
<td>6e-16</td>
<td>4e-16</td>
</tr>
<tr>
<td>3</td>
<td>1e-16</td>
<td>3e-16</td>
</tr>
<tr>
<td>4</td>
<td>9e-23</td>
<td>1e-17</td>
</tr>
<tr>
<td>5</td>
<td>6e-20</td>
<td>5e-17</td>
</tr>
</tbody>
</table>

Which algorithm is better?
Profile

Algorithm 1

Algorithm 2

<table>
<thead>
<tr>
<th></th>
<th>Alg 1</th>
<th>Alg 2</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1e-16</td>
<td></td>
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<tr>
<td>6e-16</td>
<td>4e-16</td>
<td></td>
</tr>
<tr>
<td>1e-16</td>
<td>3e-16</td>
<td></td>
</tr>
<tr>
<td>9e-23</td>
<td>1e-17</td>
<td></td>
</tr>
<tr>
<td>6e-20</td>
<td>5e-17</td>
<td></td>
</tr>
</tbody>
</table>
Transform the Data

- Map 0 to \( a \) (parameter). Typically, \( a = u/20 \).
- Map \([0, u]\) to \([a, u]\) linearly.
- Leave values \( \geq u \) alone.

- Imposes positive minimum.
- Preserves ordering of errors.
Before

Algorithm 1
Algorithm 2

<table>
<thead>
<tr>
<th>α</th>
<th>4e-14</th>
<th>1e-16</th>
</tr>
</thead>
<tbody>
<tr>
<td>10^1</td>
<td>6e-16</td>
<td>4e-16</td>
</tr>
<tr>
<td>10^2</td>
<td>1e-16</td>
<td>3e-16</td>
</tr>
<tr>
<td>10^3</td>
<td>9e-23</td>
<td>1e-17</td>
</tr>
<tr>
<td>10^5</td>
<td>6e-20</td>
<td>5e-17</td>
</tr>
</tbody>
</table>
Algorithm 1          Algorithm 2
<table>
<thead>
<tr>
<th>f</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.6</td>
<td>4.0e-14</td>
<td>1.0e-16</td>
</tr>
<tr>
<td>0.8</td>
<td>6.0e-16</td>
<td>4.0e-16</td>
</tr>
<tr>
<td>0.8</td>
<td>1.0e-16</td>
<td>3.0e-16</td>
</tr>
<tr>
<td>1.0</td>
<td>5.6e-18</td>
<td>1.1e-17</td>
</tr>
<tr>
<td>1.0</td>
<td>5.6e-18</td>
<td>5.0e-17</td>
</tr>
</tbody>
</table>

After
Matrix Exponential (Al-Mohy & H, 2011)

Algorithm 1
Algorithm 2

$\alpha$

$\rho$

$0.4$ $0.5$ $0.6$ $0.7$ $0.8$ $0.9$ $1$

$20$ $40$ $60$ $80$ $100$
Matrix Exponential Transformed

Algorithm 1
Algorithm 2

University of Manchester
Nick Higham
Accuracy and Stability
Accuracy and Stability of Numerical Algorithms gives a thorough, up-to-date treatment of the behavior of numerical algorithms in finite-precision arithmetic. It combines algorithmic derivations, perturbation theory, and rounding error analysis, all enlivened by historical perspective and informative quotations.

This second edition expands and updates the coverage of the first edition (1996) and includes numerous improvements to the original material. Two new chapters (one on symmetric indefinite systems and one on skew-symmetric systems) and new sections on Hannan’s method, an improved treatment of Gaussian elimination incorporating rook pivoting, and additional error bounds. Other changes include a more intuitive approach to the two-norm condition number for linear systems, and the added multidigit arithmetic based on some recent computer architectures.

Although not designed specifically as a textbook, this new edition is a suitable reference for an advanced course. It can also be used by instructors at all levels as a supplementary text from which to draw examples, historical perspective, statements of results, and exercises.

From reviews of the first edition:

"This definitive source on the accuracy and stability of numerical algorithms is quite a bargain and a worthwhile addition to any library..." —Robert L. Strawderman, 1999

"This text may become the new ‘Bible’ about accuracy and stability for the solution of systems of linear equations. It covers more than 600 pages carefully collected, investigated, and written..." —N. Köckler, 1996

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