

# Small Singular Values *can Increase* in Lower Precision

Petros Drineas (Purdue CS)

Joint work with I. Ipsen (NCSU) & C. Boutsikas, G. Dexter, L. Ma (Purdue)

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[for sufficiently tall-and-thin matrices; using stochastic rounding; with high probability; etc.]

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# Motivation

## Iron Law

All numbers used in a computer shall have a fixed number of digits. Therefore, the output of (almost) all primitive operations executed in a computer are wrong.

- ▶ **Major concern:** These *roundoff* errors accumulate and could be catastrophic<sup>1</sup>.
- ▶ Turing Award (1970) to J. H. Wilkinson for his work in linear algebraic computations and backward error analysis.

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<sup>1</sup>Anecdotally, a very prominent numerical analyst was hesitant to fly after they found out that computers (and, therefore, roundoff errors) were involved in aircraft design and flight planning...

# Motivation, cont'd

## Iron Law

All numbers used in a computer shall have a fixed number of digits. Therefore, the output of (almost) all primitive operations executed in a computer are wrong.

- ▶ We need to *round* numbers in order to be stored/represented/used by a computer.
- ▶ We think of this *rounding* process as a *deficiency*, since it leads to errors.

# Could rounding be a *blessing* for 21st century computing?

## Computing in the 21st century

Data Science, Machine Learning, and Artificial Intelligence *dominate modern computing*.

- ▶ Data are noisy and highly accurate computations could result in overfitting<sup>2</sup>.
- ▶ *Regularization* is fundamental in DS/ML/AI algorithms.
- ▶ **Rounding is a form of implicit regularization!**

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<sup>2</sup>...to irrelevancies, according to Michael W. Mahoney.

## Rounding and the smallest singular value of a matrix

Given a matrix  $\mathbf{A} \in \mathbb{R}^{n \times d}$  (exact representation), what happens to its smallest singular value after rounding  $\mathbf{A}$  to  $\tilde{\mathbf{A}} \in \mathcal{F}^{n \times d}$ ?

- ▶ Here  $\mathcal{F}$  could be, for example, the set of all *double*, *single*, or *half* precision numbers.

## Prior knowledge

Large singular values remain unharmed, but small singular values tend to increase.

See, for example, [Stewart & Sun, 1990, pg. 266]

*“...small singular values tend to increase” [under small perturbations]*

and [Rump, 2009, pg. 261]

*“...even an approximate inverse of an arbitrarily ill-conditioned matrix does, in general, contain useful information. This is due to a kind of regularization by rounding to working precision.”*



# Rounding as a perturbation

## A straight-forward approach

- ▶ Model rounding error as a perturbation  $\mathbf{E}$
- ▶ Formally,  $\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{E}$
- ▶ Use perturbation theory to get bounds

## What does Weyl's inequality reveal about the small singular values?

- ▶ If the **largest** singular value of  $\mathbf{E}$  ("noise" due to rounding) is larger than the **smallest** singular value of  $\mathbf{A}$ , not much...

$$\underbrace{\sigma_{\min}(\mathbf{A}) - \|\mathbf{E}\|_2}_{\text{trivial if } \leq 0} \leq \sigma_{\min}(\underbrace{\mathbf{A} + \mathbf{E}}_{\tilde{\mathbf{A}}})$$

(Building upon [G. W. Stewart LAA '84])

- ▶ Partition the  $n \times d$  matrices  $\mathbf{A}$  and  $\mathbf{E}$
- ▶ ( $\Sigma_1$  is  $(d-1) \times (d-1)$ )

$$\mathbf{A} = \mathbf{U} \begin{pmatrix} \Sigma_1 & \mathbf{0} \\ \mathbf{0} & \sigma_d \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \mathbf{V}^T, \quad \mathbf{E} = \mathbf{U} \begin{pmatrix} \mathbf{E}_{11} & \mathbf{e}_{12} \\ \mathbf{e}_{21}^T & e_{22} \\ \mathbf{E}_{31} & \mathbf{e}_{32} \end{pmatrix} \mathbf{V}^T$$

- ▶ Assume
  - ① Large singular values are large:  $\sigma_{d-1} > 4\|\mathbf{E}\|_2$
  - ② A single small singular value:  $\sigma_d < \|\mathbf{E}\|_2$
- ▶ We prove<sup>3</sup>

$$\sigma_d(\mathbf{A} + \mathbf{E})^2 \geq (\sigma_d + e_{22})^2 + \|\mathbf{e}_{32}\|_2^2 - r_3 - r_4$$

- ▶  $r_3, r_4$  contains terms of  $\mathcal{O}(\|\mathbf{E}\|_2^3)$  or higher

$$r_3 = 2\mathbf{e}_{12}^T (\boldsymbol{\Sigma}_1 + \mathbf{E}_{11})^{-T} \underbrace{\begin{pmatrix} \mathbf{e}_{21} & \mathbf{E}_{31}^T \end{pmatrix} \begin{pmatrix} e_{22} + \sigma_d \\ \mathbf{e}_{32} \end{pmatrix}}_{\mathbf{w}}$$

$$r_4 = \|\mathbf{w}\|_2^2 + 4 \frac{\|\mathbf{E}\|_2^2 \|(\boldsymbol{\Sigma}_1 + \mathbf{E}_{11})^{-1}(\mathbf{e}_{12} + \mathbf{w})\|_2^2}{1 - 4\|\mathbf{E}\|_2^2 \|(\boldsymbol{\Sigma}_1 + \mathbf{E}_{11})^{-1}\|_2^2}$$

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<sup>3</sup>We also prove a generalized version of this result for clusters of small singular values.

# Pros & Cons

## Pros

- ▶ True lower bound (beyond second order)
- ▶ Assumes a small gap between  $\sigma_{d-1}$ ,  $\sigma_d$
- ▶ Numerical experiments confirm our theory

## Cons

- ▶ The higher order terms are challenging to interpret

# Pros & Cons

## Pros

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## Cons

- ▶ The higher order terms are challenging to interpret

Let's use *Randomized Algorithms*, specifically *Stochastic Rounding (SR)*.

# Normalized FP numbers

## FP Model

- ▶ Given a basis  $\beta$  and a precision  $p$

$$x = (-1)^s \cdot m \cdot \beta^{e-p}$$

- ▶  $s$  is the sign bit
- ▶  $e$  is the exponent
- ▶ The significand  $m$  is an integer in

$$\beta^{p-1} \leq m \leq \beta^p$$

## Properties

- ▶ Let  $\mathcal{F}$  be the set of normalized FP numbers and let  $x \in \mathbb{R} - \mathcal{F}$
- ▶ The two FP numbers enclosing  $x$  are denoted by  $\lfloor\!\!\lfloor x \rfloor\!\!\rfloor$ ,  $\lceil\!\!\lceil x \rceil\!\!\rceil$



- ▶ The following inequality holds:

$$\max \{x - \lfloor\!\!\lfloor x \rfloor\!\!\rfloor, \lceil\!\!\lceil x \rceil\!\!\rceil - x\} \leq \beta^{1-p}|x|$$

# Deterministic vs Stochastic Rounding (SR)

## Deterministic

- ▶ Round-to-Nearest (RN)



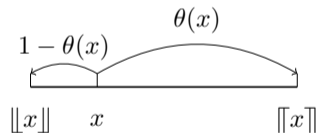
- ▶ For RN

$$\max \{x - \lfloor x \rfloor, \lceil x \rceil - x\} \leq 1/2 \beta^{1-p} |x|$$

## Stochastic

- ▶  $\theta(x) = \frac{x - \lfloor x \rfloor}{\lceil x \rceil - \lfloor x \rfloor}$

- ▶ SR - *nearness*:



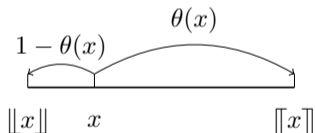
- ▶ Property:  $\mathbb{E}[\text{SR}(x)] = x$

# Stochastic Rounding (SR)

## Stochastic Rounding

- ▶  $\theta(x) = \frac{x - \lfloor x \rfloor}{\lceil x \rceil - \lfloor x \rfloor}$

- ▶ SR - *nearness*:



- ▶ Property:  $\mathbb{E}[\text{SR}(x)] = x$

## History:

- ▶ Can be traced back to [Forsythe 1950](#)
- ▶ Also [von Neumann & Goldstine 1947](#)
- ▶ **Recent resurgence**: increasing interest for low-precision FP arithmetic for ML and DNNs [[Gupta et al. 2015](#)]
- ▶ Many patents held by (GPU) chip designers
- ▶ Review: [Crocì et al. 2022](#)



# SR: A simple example

## Why SR?

- ▶ Let  $\mathcal{F} = \{0, 1\}$  and consider the rank one matrix

$$\begin{pmatrix} 1 & 1 \\ \frac{1}{2} & \frac{1}{2} \\ 1 & 1 \\ \frac{1}{2} & \frac{1}{2} \\ \vdots & \vdots \\ 1 & 1 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \xrightarrow{\text{RN}(\mathbf{A})} \begin{pmatrix} 1 & 1 \\ 1 & 1 \\ \vdots & \vdots \\ 1 & 1 \end{pmatrix}$$

- ▶ Any deterministic rounding will result to a rounded matrix  $\tilde{\mathbf{A}}$  that is also rank one.

This is **not** the case for SR

- ▶ Let  $\mathcal{F} = \{0, 1\}$  and consider the rank one matrix

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \\ \vdots & \vdots \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \xrightarrow{\text{SR}(\mathbf{A})} \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 1 & 1 \end{pmatrix} = \tilde{\mathbf{A}}$$

- ▶ We can prove that for such  $n \times 2$  matrices (with probability at least 0.997)

$$\sigma_{\min}(\tilde{\mathbf{A}}) \gtrsim 1/2\sqrt{n}$$

For simplicity, assume  $\mathbf{A} \in [-1, 1]^{n \times d}$  and let  $\tilde{\mathbf{A}}$  be the stochastically rounded  $\mathbf{A}$ .

$$\sigma_{\min}(\tilde{\mathbf{A}}) \geq$$

## Model

- ▶  $\mathbf{A} \in^{n \times d}$  with  $n \gg d$
- ▶ SR to FP numbers
- ▶  $\mathbf{E} = \tilde{\mathbf{A}} - \mathbf{A}$
- ▶  $\mathbb{E}[\mathbf{E}] = \mathbf{0}$

## Ingredients

- ▶  $\beta$  is the basis of our FP arithmetic
- ▶  $p$  is the working precision

For simplicity, assume  $\mathbf{A} \in [-1, 1]^{n \times d}$  and let  $\tilde{\mathbf{A}}$  be the stochastically rounded  $\mathbf{A}$ .

$$\sigma_{\min}(\tilde{\mathbf{A}}) \geq \beta^{1-p} \sqrt{n} (\sqrt{\nu} - \varepsilon_{n,d})$$

## Model

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## Ingredients

- ▶  $\beta$  is the basis of our FP arithmetic
- ▶  $p$  is the working precision
- ▶  $\nu$  measures the amount of available randomness during the rounding process
- ▶  $\varepsilon_{n,d}$  captures *lower-order* terms

For simplicity, assume  $\mathbf{A} \in [-1, 1]^{n \times d}$  and let  $\tilde{\mathbf{A}}$  be the stochastically rounded  $\mathbf{A}$ .

$$\sigma_{\min}(\tilde{\mathbf{A}}) \geq \beta^{1-p} \sqrt{n} (\sqrt{\nu} - \varepsilon_{n,d})$$

## Model

- ▶  $\mathbf{A} \in^{n \times d}$  with  $n \gg d$
- ▶ SR to FP numbers
- ▶  $\mathbf{E} = \tilde{\mathbf{A}} - \mathbf{A}$
- ▶  $\mathbb{E}[\mathbf{E}] = \mathbf{0}$

## Understanding $\nu$

- ▶ Consider a matrix with, say, two identical columns whose entries are FPs:  $\sigma_{\min}(\mathbf{A}) = 0$ .
- ▶ SR will **not** modify those columns:  $\sigma_{\min}(\tilde{\mathbf{A}}) = 0$ .
- ▶ Intuitively: **no randomness** for SR to exploit.
- ▶ This **lack of randomness** is captured by  $\nu$ , which, in this case, is equal to zero.

For simplicity, assume  $\mathbf{A} \in [-1, 1]^{n \times d}$  and let  $\tilde{\mathbf{A}}$  be the stochastically rounded  $\mathbf{A}$ .

$$\sigma_{\min}(\tilde{\mathbf{A}}) \geq \beta^{1-p} \sqrt{n} (\sqrt{\nu} - \varepsilon_{n,d})$$

### Model

- ▶  $\mathbf{A} \in^{n \times d}$  with  $n \gg d$
- ▶ SR to FP numbers
- ▶  $\mathbf{E} = \tilde{\mathbf{A}} - \mathbf{A}$
- ▶  $\mathbb{E}[\mathbf{E}] = \mathbf{0}$

### Understanding $\nu$

- ▶ Formally<sup>a</sup>:  $\nu \propto \min_{\text{all columns } j} \sum_{i=1}^n \text{Var}(\mathbf{E}_{ij})$
- ▶  $0 \leq \nu \leq 1$

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<sup>a</sup>Skipping a normalization factor

# Interpreting our bound

For simplicity, assume  $\mathbf{A} \in [-1, 1]^{n \times d}$  and let  $\tilde{\mathbf{A}}$  be the stochastically rounded  $\mathbf{A}$ .

$$\sigma_{\min}(\tilde{\mathbf{A}}) \geq \beta^{1-p} \sqrt{n} (\sqrt{\nu} - \varepsilon_{n,d})$$

- ▶ As  $n$  grows,  $\sigma_{\min}(\tilde{\mathbf{A}})$  increases
- ▶  $\beta^{1-p}$  captures the parameters of FP arithmetic
- ▶  $\nu$  captures the amount of available *stochasticity* in  $\text{SR}(\mathbf{A})$
- ▶  $\varepsilon_{n,d}$  depends only on  $n, d$ :
  - If  $n$  is  $\omega(d^4)$ , then  $\lim_{n \rightarrow \infty} \varepsilon_{n,d} = 0$ .
  - (hiding log factors)

# Our main result: A perturbation theory bound

## Main Theorem

Let  $\mathbf{A}$  and  $\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{E}$  be real  $n \times d$  matrices. Here  $\mathbf{E}$  models a zero-mean random perturbation matrix with minimal (normalized) column variance  $\nu$  and  $\max_{i,j} |\mathbf{E}_{ij}| \leq \mathbf{R}$ .

If  $n \geq 836$ , then with probability at least  $1 - 1/n^c - 2d^2/n^2$ ,

$$\sigma_{\min}(\tilde{\mathbf{A}}) \geq \mathbf{R}\sqrt{n}(\sqrt{\nu} - \varepsilon_{n,d}),$$

where

$$\varepsilon_{n,d} \equiv \sqrt{\frac{d}{n}} + 2d^2\sqrt{\frac{\log n}{n}} + \frac{C(\log n)^{2/3}}{n^{1/30}} \cdot \left(\frac{d}{n}\right)^{\frac{1}{54}},$$

and  $c$  and  $C$  are absolute constants.



## Tightness of our bound

Let  $\mathbf{A}$  and  $\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{E}$  be real  $n \times d$  matrices. Here  $\mathbf{E}$  models a zero-mean random perturbation matrix with minimal (normalized) column variance  $\nu$  and  $\max_{i,j} |\mathbf{E}_{ij}| \leq \mathbf{R}$ . Our main bound is that, with high probability,

$$\sigma_{\min}(\tilde{\mathbf{A}}) \gtrsim \mathbf{R}\sqrt{n\nu}.$$

We exhibit  $n \times d$  matrices  $\mathbf{A}$  for which SR returns the matrix  $\tilde{\mathbf{A}}$  such that

$$\sigma_{\min}(\tilde{\mathbf{A}}) \leq \left(1 + \sqrt{1/(d-1)}\right) \cdot \mathbf{R}\sqrt{n\nu}.$$

# Proof outline

## Steps:

- 1 We introduce the orthogonal projector  $\mathbf{P}_A$  onto the left column space of  $\mathbf{A}$ . This allows us to focus on  $\mathbf{P}_A \mathbf{E}$ .
- 2 Weyl's inequality yields a lower bound on the smallest singular value of  $(\mathbf{I} - \mathbf{P}_A) \mathbf{E}$  by lower bounding the smallest singular value of  $\mathbf{E}$  and upper bounding the largest singular value of  $\mathbf{P}_A \mathbf{E}$ .
- 3 Application of a Random Matrix Theory bound from [Dumitriu & Zhu '23] shows that the smallest singular value of  $\mathbf{E}$  is sufficiently large.
- 4 The largest singular value of the projection  $\mathbf{P}_A \mathbf{E}$  is small, because  $\mathbf{P}_A$  projects  $\mathbf{E}$  on the low-dimensional subspace of dimension  $d$ .
- 5 Standard measure concentration bounds show that  $\mathbf{E}$  *does not concentrate* in any low-dimensional subspace.
- 6 Finally, we combine the bounds for the smallest singular value of  $\mathbf{E}$  and the largest singular value of  $\mathbf{P}_A \mathbf{E}$ .

# Experiments (1)

## Our universe

- ▶  $\mathbf{A} \in [-1, 1]^{n \times d}$

- ▶ All elements of  $\text{SR}(\mathbf{A}) \in \mathcal{F}^{\{p\}}$ ,  $1 \leq p \leq 5$

$$\mathcal{F}^{\{p\}} = \{\pm m/10^p, \text{ for all integers } m = \underbrace{0, 1, 2, \dots, 10^p - 1}_{\leq p \text{ digits}}\} \cup \{\pm 1\}$$

## Setting (1)

- ▶  $\sigma_{\min}(\mathbf{A}) = 0$

- ▶  $n = 10^4; 10^5; 10^6$  and  $d = 10; 100; 1000$

- ▶ For a fixed  $d$ , all  $\mathbf{A}$  have the same singular values

# Experiments (1) [recall: $n \times d$ matrix $A$ and $\sigma_{\min}(A) = 0$ ]

Each entry in the tables shows the pair of values  $(\sigma_{\min}(\tilde{A}), \mathbf{R}\sqrt{n\nu})$

Precision $p = 1$		
$d ; n$	$10^4$	$10^6$
$10$	(4.11, 4.08)	(34.11, 32.96)
$10^2$	(4.08, 4.07)	(32.76, 32.46)
$10^3$	(3.84, 4.05) <sup>a</sup>	(33.26, 33.03)

<sup>a</sup>Square-ish matrix

Precision $p = 3$		
$d ; n$	$10^4$	$10^6$
$10$	(0.04, 0.04)	(0.41, 0.41)
$10^2$	(0.04, 0.04)	(0.41, 0.41)
$10^3$	(0.039, 0.04) <sup>a</sup>	(0.41, 0.41)

<sup>a</sup>Square-ish matrix

# Experiments (2)

## Our universe

- ▶  $\mathbf{A} \in [-1, 1]^{n \times d}$

- ▶ All elements of  $\text{SR}(\mathbf{A}) \in \mathcal{F}^{\{p\}}$ ,  $1 \leq p \leq 5$

$$\mathcal{F}^{\{p\}} = \{\pm m/10^p, \text{ for all integers } m = \underbrace{0, 1, 2, \dots, 10^p - 1}_{\leq p \text{ digits}}\} \cup \{\pm 1\}$$

## Setting (2)

- ▶  $\mathbf{A}^h$  with  $\nu \approx 1$  (*high value*)

- ▶  $\mathbf{A}^l$  with  $\nu \approx 5 \cdot 10^{-4}$  (*low value*)

- ▶  $\sigma_{\min}(\mathbf{A}^h) = \sigma_{\min}(\mathbf{A}^l) = 0$

- ▶ Fixed  $n = 10^4$  and  $d = 10; 100; 1000$

## Experiments (2) [recall: $10^4 \times d$ matrix $\mathbf{A}$ and $\sigma_{\min}(\mathbf{A}) = 0$ ]

Each entry in the tables shows the pair of values  $(\sigma_{\min}(\tilde{\mathbf{A}}), \mathbf{R}\sqrt{n\nu})$ ;  $n = 10^4$  **fixed**

Precision  $p = 1$

$\mathbf{d} ; \nu$	(high)	(low)
$10$	(5.01, 5)	(2.34, 2.31)
$10^2$	(4.95, 5)	(2.27, 2.30)
<sup>a</sup> $10^3$	(4.79, 5)	(2.20, 2.29)

<sup>a</sup>Square-ish matrix

Precision  $p = 3$

$\mathbf{d} ; \nu$	(high)	(low)
$10$	(0.05, 0.05)	(0.023, 0.023)
$10^2$	(0.05, 0.05)	(0.023, 0.023)
<sup>a</sup> $10^3$	(0.047, 0.05)	(0.022, 0.023)

<sup>a</sup>Square-ish matrix

## Experiments (3)

### Our universe

- ▶  $\mathbf{A} \in [-1, 1]^{n \times d}$

- ▶ All elements of  $\text{SR}(\mathbf{A}) \in \mathcal{F}^{\{p\}}$ ,  $1 \leq p \leq 5$

$$\mathcal{F}^{\{p\}} = \{\pm m/10^p, \text{ for all integers } m = \underbrace{0, 1, 2, \dots, 10^p - 1}_{\leq p \text{ digits}}\} \cup \{\pm 1\}$$

### Setting (3)

- ▶  $\sigma_{\min}(\mathbf{A}) = 10^{-2}$

- ▶  $n = 10^4; 10^5; 10^6$  and  $d = 10; 100; 1000$

- ▶ For a fixed  $d$ , all  $\mathbf{A}$  have the same singular values

## Experiments (3) [recall: $n \times d$ matrix $A$ and $\sigma_{\min}(A) = 10^{-2}$ ]

Each entry in the tables shows the pair of values  $(\sigma_{\min}(\tilde{A}), \mathbf{R}\sqrt{n\nu})$

Precision $p = 1$		
$d ; n$	$10^4$	$10^6$
$10$	(4.11, 4.07)	(31.87, 30.85)
$10^2$	(4.07, 4.06)	(34.59, 34.09)
$10^3$	(3.86, 4.05) <sup>a</sup>	(33.24, 33.01)

<sup>a</sup>Square-ish matrix

Precision $p = 4$		
$d ; n$	<sup>a</sup> $10^4$	<sup>b</sup> $10^6$
$10$	(0.01, 0.004)	(0.04, 0.04)
$10^2$	(0.01, 0.004)	(0.04, 0.04)
$10^3$	(0.01, 0.004)	(0.04, 0.04)

<sup>a</sup> $n$  is “small”  $\rightarrow$  smaller singular value does not increase much; bounds are tight

<sup>b</sup> $n$  is “large”  $\rightarrow$  smaller singular increases more; bounds are tight



# Future work

## Theory

- ▶ New Random Matrix Theory bounds for matrices whose entries are independent, but not identically distributed random variables.
  - ① Can be used to prove similar bounds for square-ish matrices.
  - ② Can be used to remove or reduce the  $\epsilon_{n,d}$  factor.
- ▶ Effect of stochastic rounding in downstream applications<sup>a</sup>.

## Experiments

- ▶ Experimental evaluation in GPUs/IPUs that support stochastic rounding, e.g., GraphCore IPU.
- ▶ Effect of stochastic rounding in downstream applications<sup>a</sup>.

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<sup>a</sup>From simple regression problems to DNN training.

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