Regular Singularities
&
Rigorous Numerics

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Periods workgroup, May 19, 2021

Try it online!
http://marc.mezzarobba.net/oaademo-periodswg
Problem

Starting from a linear differential equation

\[ p_r(z) y^{(r)}(z) + \cdots + p_1(z) y'(z) + p_0(z) y(z) = 0 \]

with polynomial coefficients \( p_0, \ldots, p_r \) and initial values, compute “the solution” at a given point.
ODA Solving from a Computer Algebra Perspective

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with polynomial coefficients \( p_0, \ldots, p_r \) and initial values, compute “the solution” at a given point.

Special requirements:

- Complex variables: \( z \in \mathbb{C} \)
- Arbitrary precision
- Rigorous error bounds (\( \Rightarrow \) usable in computer proofs, in “exact” algorithms)
- Singular cases
Applications

- **Special functions**
  via *generating functions* and *singularity analysis*
  random walks on lattices,
  asymptotics of P-recursive sequences...

- **Combinatorics**
  via *generating functions* and *singularity analysis*
  random walks on lattices,
  asymptotics of P-recursive sequences...

- **Numerical (Real) Algebraic Geometry**
  via *Picard-Fuchs equations*
  periods of surfaces [Sertöz 2019, ...],
  volumes of semi-algebraic sets [Lairez, M., Safey 2019]...

- **“Numerical differential Galois theory”**
  via *connection / monodromy / Stokes matrices*
  operator factoring, heuristic diff. Galois groups
  [van der Hoeven 2007, ...]
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  operator factoring, heuristic diff. Galois groups [van der Hoeven 2007, …]
Iterated Integrals

[Ablinger, Blümlein, Raab, Schneider, 2014]

\[
\int_0^1 \frac{x_5}{x_5-1} \, dx_5 \int_{x_5}^1 \frac{dx_4}{x_5 x_4 \sqrt{x_4-\frac{1}{4}}} \int_{x_4}^1 \frac{dx_3}{x_4 x_3 \sqrt{x_3-\frac{1}{4}}} \int_{x_3}^1 \frac{dx_2}{1-x_2} \int_{x_2}^1 \frac{dx_1}{1-x_1} = ?
\]

(with suitable branch choices)
Iterated Integrals

[Ablinger, Blümlein, Raab, Schneider, 2014]

\[ I(x) = \int_0^1 \frac{x_5}{x_5 - 1} \int_0^1 \frac{dx_4}{\sqrt{x_4 - \frac{1}{4}}} \int_0^1 \frac{dx_3}{\sqrt{x_3 - \frac{1}{4}}} \int_0^1 \frac{dx_2}{1 - x_2} \int_0^1 \frac{dx_1}{1 - x_1} \]

(with suitable branch choices)

\[(4 x^9 - 13 x^8 + 15 x^7 - 7 x^6 + x^5) I^{(6)}(x) + (54 x^8 - 140 x^7 + 120 x^6 - 36 x^5 + 2 x^4) I^{(5)}(x) + (202 x^7 - 397 x^6 + 228 x^5 - 34 x^4 + x^3) I^{(4)}(x) + (222 x^6 - 303 x^5 + 90 x^4 + 3 x^3 - 3 x^2) I^{(3)}(x) + (48 x^5 - 37 x^4 + x^3 - 6 x^2 + 6 x) I''(x) + (-x^2 + 6 x - 6) I'(x) = 0\]
Iterated Integrals

[Ablinger, Blümlein, Raab, Schneider, 2014]

\[ I(x) = \int_x^1 \frac{x_5 \ dx_5}{x_5 - 1} \int_{x_5 x_4}^1 \frac{dx_4}{\sqrt{x_4 - \frac{1}{4}}} \int_{x_4 x_3}^1 \frac{dx_3}{\sqrt{x_3 - \frac{1}{4}}} \int_{x_3}^1 \frac{dx_2}{1 - x_2} \int_{x_2}^1 \frac{dx_1}{1 - x_1} = ? \]

(with suitable branch choices)

\[(4 x^9 - 13 x^8 + 15 x^7 - 7 x^6 + x^5) I^{(6)}(x) + (54 x^8 - 140 x^7 + 120 x^6 - 36 x^5 + 2 x^4) I^{(5)}(x) + (202 x^7 - 397 x^6 + 228 x^5 - 34 x^4 + x^3) I^{(4)}(x) + (222 x^6 - 303 x^5 + 90 x^4 + 3 x^3 - 3 x^2) I^{(3)}(x) + (48 x^5 - 37 x^4 + x^3 - 6 x^2 + 6 x) I''(x) + (-x^2 + 6 x - 6) I'(x) = 0\]

\textbf{sage: iint\_value(dop, myini, 1e\(-500\))}
\[0.9708046956249312405 \ldots 59027603834204946 +/- 9.05e\(-501\)]
Pólya Walks

For a random walk on $\mathbb{Z}^d$ ($d \geq 3$) starting at 0:

$$\text{return probability} = 1 - \frac{1}{w(1/2d)}$$

where

$$w(z) = \sum_{n=0}^{\infty} w_n z^n$$

satisfies an LODE with polynomial coefficients

$$d = 3 \quad z^2 (4 z^2 - 1) (36 z^2 - 1) D^3 + (1296 z^5 - 240 z^3 + 3 z) D^2$$
$$+ (2592 z^4 - 288 z^2 + 1) D + 864 z^3 - 48 z$$

$$d = 4 \quad (1024 z^7 - 80 z^5 + z^3) D^4 + (14336 z^6 - 800 z^4 + 6 z^2) D^3$$
$$+ (55296 z^5 - 2048 z^3 + 7 z) D^2 + (61440 z^4 - 1344 z^2 + 1) D$$
$$+ 12288 z^3 - 128 z$$

[thanks to B. Salvy]

$$\text{First return after } n \text{ steps:}$$

$$f(z) = \sum_{n=0}^{\infty} f_n z^n$$

$$f\left(\frac{1}{2d}\right) = \sum_{n=0}^{\infty} \frac{f_n}{(2d)^n}$$

$$w(z) = 1 + f(z) w(z)$$

sage: from ore_algebra.examples import polya
sage: 1 - 1/polya.dop[10].numerical_solution([0]*9+[1], [0, 1/(2*10)], 1e-50).real()
[0.0561975359742678812097369256252412572131681661862 +/- 7.03e-51]
Volumes of Compact Semi-Algebraic Sets

[Lairez, M., Safey El Din, 2019]

- The “slice volume” function satisfies a Picard-Fuchs eqn
- Except at critical values of the projection, it is analytic

→ Compute initial values by recursive calls, integrate the equation

Cost for p digits = $\tilde{O}(p)$

\[ \text{slice #2: } \rho = \frac{10866099}{4849664} \]
\[ \text{slicelength} = [3.95699242690042041342397892533404623584614411033674866606926914003 +/- 5.52e-66] \]
\[ \text{integrating PF equation over } [1.010906176264399, 2.989093823735602] \]
\[ \text{...piece volume} = [8.1084458716614722013317884330079153901325376090443193970231734 +/- 8.50e-62] \]
\[ \text{slice volume} = [24.858639122870438686966646961582254943981378134071631307423220 +/- 5.78e-60] \]
\[ \text{integrating PF equation over } [-1, 1] \]
\[ \text{...piece volume} = [39.478417604357434475337963999504604541254797628963162506 +/- 6.38e-55] \]
\[ [39.478417604357434475337963999504604541254797628963162506 +/- 6.38e-55] \]
$ sage -pip install \\git+https://github.com/mkauers/ore_algebra.git
Try It Yourself

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...Or locally

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Note:

- Code intended both for end users and as a personal playground
- Some experimental/undocumented features
- Talk to me if it does not quite do what you need!
An Implementation of Ore Polynomials

Ore polynomials
≈ skew polynomials that model functional operators

\[ K(z)\langle D \rangle = \{ \text{polynomials in } D \text{ over } K(z) \text{ subject to } Dz = zD + 1 \} \]
\[ \cong \{ \text{differential operators} \} \]

\[ [zf(z)]' = zf'(z) + f(z) \]

```
sage: from ore_algebra import OreAlgebra
sage: Pol.<z> = PolynomialRing(QQ)
```

```
sage: Dop.<Dz> = OreAlgebra(Pol)
sage: Dz*z    # a differential operator
z*Dz + 1
```

Features

- Basic arithmetic (diff, shift, qdiff, qshift, custom)
- Gcrd, lclm, D-finite closure (incl. multivariate)
- Creative telescoping
- Polynomial, rational, asympt. series solutions
- Desingularization
- Guessing
- ...

This talk:
- Numerical connection (differential case)
Analytic Continuation

\[ \mathcal{L} = a_r(z) D_z^r + \cdots + a_1(z) D_z + a_0(z) \]
Analytic Continuation

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Analytic Continuation

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[y(0), y'(0), ...]
Analytic Continuation

\[ \mathcal{L} = a_r(z) D_z^r + \cdots + a_1(z) D_z + a_0(z) \]

\[ [y(0), y'(0), \ldots] \]
Analytic Continuation

\[ \mathcal{L} = a_r(z) D_z^r + \cdots + a_1(z) D_z + a_0(z) \]

\[ [y(0), y'(0), \ldots] \]

\[ f_0(z) = 1 + 0 \cdot z + \cdots + O(z^r) \]
\[ f_1(z) = 0 + 1 \cdot z + \cdots + O(z^r) \]
\[ \vdots \]
\[ y = \alpha_0 f_0 + \cdots + \alpha_r f_r \]
Analytic Continuation

\[ \mathcal{L} = a_r(z) D_z^r + \cdots + a_1(z) D_z + a_0(z) \]

\[ [y(0), y'(0), \ldots] \]

\[ y(\zeta) = ? \]

\[ f_0(z) = 1 + 0 \cdot z + \cdots + O(z^r) \]

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Transition Matrices

\((z^2 + 1) y''(z) + 2 z y'(z) = 0\)
Transition Matrices

\[(z^2 + 1) y''(z) + 2 z y'(z) = 0\]

\[
\begin{vmatrix}
  f_0(z) &= 1 + 0 \cdot z + O(z^2) \\
  f_1(z) &= 0 + 1 \cdot z + O(z^2)
\end{vmatrix}
\]
Transition Matrices

\((z^2 + 1) y''(z) + 2 z y'(z) = 0\)

\[
\begin{align*}
  f_0(z) &= 1 + 0 \cdot z + O(z^2) \\
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\end{align*}
\]
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Transition Matrices

\[(z^2 + 1) y''(z) + 2 z y'(z) = 0\]

\[
y = \beta_0 g_0 + \beta_1 g_1
\]

\[
g_0(z) = 1 + 0 \cdot (z - z_0) + O((z - z_0)^2)
\]

\[
g_1(z) = 0 + 1 \cdot (z - z_0) + O((z - z_0)^2)
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y = \alpha_0 f_0 + \alpha_1 f_1
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\[
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g_1(z) &= 0 + 1 \cdot (z - z_0) + O\left( (z - z_0)^2 \right)
\end{align*}
\]

\[
\begin{bmatrix} y(z_0) \\ y'(z_0) \end{bmatrix} = \begin{bmatrix} \square & \square \\ \square & \square \end{bmatrix} \begin{bmatrix} y(0) \\ y'(0) \end{bmatrix}
\]

\[
\begin{align*}
f_0(z) &= 1 + 0 \cdot z + O(z^2) \\
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\end{align*}
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\[y = \alpha_0 f_0 + \alpha_1 f_1\]
Transition Matrices

\[(z^2 + 1) y''(z) + 2 z y'(z) = 0\]

\[
\begin{bmatrix}
\tilde{y}(z_0) \\
\tilde{y}'(z_0)
\end{bmatrix} = \begin{bmatrix}
\square & \square \\
\square & \square
\end{bmatrix} \begin{bmatrix}
y(0) \\
y'(0)
\end{bmatrix}
\]

\[y = \beta_0 g_0 + \beta_1 g_1\]

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\end{align*}\]

\[y = \alpha_0 f_0 + \alpha_1 f_1\]
Regular Singular Points \[ L = a_r(z) D_z^r + \cdots + a_1(z) D_z + a_0(z) \]

“Definition”. Singular points \( (a_r(\zeta) = 0) \) where all solutions are “tame”:

- \( y(\zeta + z) \sim z^{-3/2} \log z \)
- \( y(\zeta + z) \sim z^{i \sqrt{2}} \)
- \( y(\zeta + z) \sim e^{\pm 1/z} \)

Local solutions at reg. sing. \( \zeta = 0 \) [Fuchs, 1866]

On some slit neighborhood \( D \setminus \mathbb{R}_{\leq 0} \),
\( L \cdot y = 0 \) has a full basis of solutions of the form

\[ z^\lambda (y_0(z) + y_1(z) \log z + \cdots + y_t(z) \log^t z), \quad \lambda \in \tilde{\mathbb{Q}}, \quad y_i \text{ analytic on } D. \]

- **General form:** \( y(z) = \sum_{\nu \in \Lambda} \sum_{k=0}^t y_{\nu,k} z^\nu \log^k z \)
- \( \Lambda \) is the set of \( \lambda_i + \mathbb{N} \) in \( \mathbb{C} \)

- **“Canonical” basis:** dual of \( \{ y \mapsto y_{\nu,k} \quad \nu \text{ root of indicial polynomial,} \quad k < \text{mult}(\nu) \} \)
  - Natural generalization of \( x^i + O(x^r) \) at ordinary points
  - *Not* the usual Frobenius basis!

\[ ✔ \quad y(\zeta + z) \sim z^{-3/2} \log z \quad ✔ \quad y(\zeta + z) \sim z^{i \sqrt{2}} \quad ✗ \quad y(\zeta + z) \sim e^{\pm 1/z} \]
Initial Conditions at Regular Singular Points

\[ \mathcal{L} = z D_z^2 + D_z + z \quad (J_0, Y_0) \]
Initial Conditions at Regular Singular Points

\[ \mathcal{L} = z D_z^2 + D_z + z \quad (J_0, Y_0) \]

\[ f_0(z) = 1 \cdot \log(z) + 0 \cdot 1 + \tilde{O}(z) \]
\[ f_1(z) = 0 \cdot \log(z) + 1 \cdot 1 + \tilde{O}(z) \]
Initial Conditions at Regular Singular Points

\[ \mathcal{L} = z D_z^2 + D_z + z \quad (J_0, Y_0) \]

\[ \begin{align*}
    f_0(z) &= 1 \cdot \log(z) + 0 \cdot 1 + \tilde{O}(z) \\
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    y &= \alpha_0 \log(z) + \alpha_1 + \tilde{O}(z) \Rightarrow y = \alpha_0 f_0 + \alpha_1 f_1
\end{align*} \]
Initial Conditions at Regular Singular Points

\[ \mathcal{L} = z D_z^2 + D_z + z \quad (J_0, Y_0) \]

\[
\begin{align*}
\left. \begin{array}{l}
f_0(z) = 1 \cdot \log(z) + 0 \cdot 1 + \tilde{O}(z) \\
f_1(z) = 0 \cdot \log(z) + 1 \cdot 1 + \tilde{O}(z)
\end{array} \right\} \\
y = \alpha_0 \log(z) + \alpha_1 + \tilde{O}(z) \Rightarrow y = \alpha_0 f_0 + \alpha_1 f_1
\end{align*}
\]
Initial Conditions at Regular Singular Points

\[ \mathcal{L} = z D_z^2 + D_z + z \quad (J_0, Y_0) \]

\[ f_0(z) = 1 \cdot \log(z) + 0 \cdot 1 + \tilde{O}(z) \]
\[ f_1(z) = 0 \cdot \log(z) + 1 \cdot 1 + \tilde{O}(z) \]

\[ y = \alpha_0 \log(z) + \alpha_1 \tilde{O}(z) \Rightarrow y = \alpha_0 f_0 + \alpha_1 f_1 \]

\[ y(\zeta) = ? \]
Regular Singular Transition Matrices
Regular Singular Transition Matrices

\[
\begin{pmatrix}
  f_0(z) \\
  f_1(z) \\
  \vdots
\end{pmatrix}
\]
Regular Singular Transition Matrices

\[ y = \alpha_0 f_0 + \alpha_1 f_1 + \cdots \]
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\[ y = \beta_0 g_0 + \beta_1 g_1 + \cdots \]

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\[ \begin{pmatrix} g_0(z) \\ g_1(z) \\ \vdots \end{pmatrix} \]
Regular Singular Transition Matrices

\[ y = \beta_0 g_0 + \beta_1 g_1 + \cdots \]

\[ y = \alpha_0 f_0 + \alpha_1 f_1 + \cdots \]
\[ \sum_{\nu \in \lambda + \mathbb{Z}} \sum_{k=0}^{K} y_{\nu, k} z^\nu \frac{\log(z)^k}{k!} \]

\[ L(S_n^{-1}, n + S_k) \cdot (y_{n, k}) = 0 \]
Summary

**Numerical solution of linear ODEs with polynomial coefficients**

- full support for regular singular points (incl. algebraic, resonant…)
- arbitrary precision
- rigorous error bounds

**Based on:** Taylor series, an. continuation, recurrences, ball arithmetic, majorants…

**Code available at**

https://github.com/mkauers/ore_algebra/

**Perspectives**

- Irregular singular case
- p-adic points
- Performance improvements

**Bug reports, feature requests, examples welcome!**
A Taylor Series Method

Locally, the solutions are given by convergent power series (Cauchy)

Sum the series numerically to get “initial values” at a new point

Large steps ($\propto$ radius of convergence)

Extends to the regular singular case
Recurrences

The **Taylor coefficients** of a D-finite function \( y(z) = \sum_{n=0}^{\infty} y_n z^n \) obey a linear **recurrence relation** with polynomial coefficients:

\[
 b_s(n) y_{n+s} + \cdots + b_1(n) y_{n+1} + b_0(n) y_n = 0.
\]

(And conversely, for D-finite formal power series.)
Recurrences

The **Taylor coefficients** of a D-finite function \( y(z) = \sum_{n=0}^{\infty} y_n z^n \) obey a linear **recurrence relation** with polynomial coefficients:

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\]

(And conversely, for D-finite formal power series.)

**Proof.**

\[
y = \sum_{n=-\infty}^{\infty} y_n z^n \quad \leftrightarrow \quad Y = (y_n)_{n \in \mathbb{Z}}
\]

\[
D \cdot y = \sum_{n=-\infty}^{\infty} (n+1) y_{n+1} z^n \quad \leftrightarrow \quad (S n) \cdot Y
\]

\[
z \cdot y = \sum_{n=-\infty}^{\infty} y_{n-1} z^n \quad \leftrightarrow \quad S^{-1} \cdot Y
\]
Recurrences

The **Taylor coefficients** of a D-finite function \( y(z) = \sum_{n=0}^{\infty} y_n z^n \) obey a linear **recurrence relation** with polynomial coefficients:

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\]

(And conversely, for D-finite formal power series.)

- Easy to generate
- Leads to **fast algorithms**
  
  Best **boolean** complexity:
  
  time \( O(M(p \log^2 p)) \), space \( O(p) \)
  
  for fixed \( z \) and \( \varepsilon = 2^{-p} \)

The **coefficients** of a D-finite function

\[
\sum_{\nu \in \mathbb{N}} \sum_{k=0}^{K} y_{\nu,k} z^\nu \frac{\log(z)^k}{k!}
\]

obey a linear **recurrence relation** with polynomial coefficients:

\[
[b_s(\nu + S_k) \cdot S^s + \cdots + b_1(\nu + S_k) S^1 + b_0(\nu + S_k)] \cdot (y_{\nu,k}) = 0.
\]

- Easy to generate
- Leads to **fast algorithms**

Best **boolean** complexity:

- time \(O(M(p \log^2 p))\), space \(O(p)\)
- for fixed \(z\) and \(\varepsilon = 2^{-p}\)

Error Bounds

Rounding Errors

Real & complex arithmetic based on Arb
({Real, Complex}BallField in Sage)

- More generally: takes care of error propagation
- Arb supports truncated power series (derivatives, reg. sing. points)
- Manual error analysis still useful when intervals blow up

Truncation Errors

\[ \sum_{n=0}^{\infty} u_n z^n = \sum_{n=0}^{N-1} u_n z^n + \sum_{n=N}^{\infty} u_n z^n \]

- Majorant series
- "Adaptive" bounds using residuals
The Method of Majorants

Instead of directly bounding $|\sum_{n \geq N} u_n \zeta^n|$, compute a **majorant series**:

$$\sum \hat{u}_n z^n \in \mathbb{R}_{\geq 0}[[z]] \quad \text{s.t.} \quad \forall n, \quad |u_n| \leq \hat{u}_n$$

To do that, "replace" L with a simple **model equation**:

$$L(z, \frac{d}{dz}) \cdot u = 0 \quad \ll \quad \hat{u}'(z) - \hat{a}(z) \hat{u}(z) = 0$$

"bounded by" for us: always 1st order

Solve the model equation and study the solutions:

$$\hat{u}(z) = \exp \int_{z}^{\infty} \hat{a}(w) \, dw \quad \left| \sum_{n=N}^{+\infty} u_n z^n \right| \leq \sum_{n=N}^{+\infty} \hat{u}_n |z|^n \leq \ldots$$
Adaptive Bounds

**Problem.** Computing majorants in a (too) naive way leads to catastrophic overestimations

**Idea.** Take into account the last computed / first neglected terms of the series

**Analogy.** Residuals of linear systems

\[ \begin{align*}
A x &= b \\
A \tilde{x} &= \tilde{b}
\end{align*} \]

\[ A \in \text{GL}_n(\mathbb{C}), \quad \|A^{-1}\| \leq M \]

\[ \|x - \tilde{x}\| \leq M \cdot \|b - \tilde{b}\| \]

computed approx. \quad known

residual (≈ 1st negl. term)
Adaptive Majorants

\[ L(z, D_z) \cdot u = 0 \]

**Residual:** \( q(z) := L(z, D_z) \cdot \tilde{u} \)

\[ u(z) = \sum_{n=0}^{\infty} u_n z^n = \sum_{n=0}^{N-1} u_n z^n + \sum_{n=N}^{\infty} u_n z^n \]

\[ \tilde{u}(z) \]

**Model equation**

\[ q(z) \prec \hat{q}(z) \]

\[ L(z, D_z) \cdot (\tilde{u} - u) = q \prec \hat{L}(z, D_z) \cdot v = \hat{q} \]

**Majorant property:**

\[ (\forall n \leq n_0) \quad |u_n| \leq v_n \quad \Rightarrow \quad (\forall n) \quad |u_n| \leq v_n \]

**Solving the model equation**

\[ v(z) = h(z) \left( \text{cst} + \int_{z}^{t} \frac{\hat{q}(t)}{h(t)} \, dt \right) \]

where \( h(z) = \exp \int_{z}^{t} \frac{\hat{a}(t)}{h(t)} \, dt \)

\[ \text{choose cst = 0} \quad \Rightarrow \quad = O(z^N) \]
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