Reliable numerical computations

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• H. Ranocha, L. Lóczi, D. I. Ketcheson: *General relaxation methods for initial value problems with application to multistep schemes*, Numerische Mathematik 146, 875–906 (2020), **D1** journal

• L. Lóczi: *Guaranteed- and high-precision evaluation of the Lambert W function*, 30 pages, submitted to a **Q1** journal, positive feedback from the 3 reviewers asking for some revisions

• Y. Hadjimichael, D. I. Ketcheson, L. Lóczi: *Positivity preservation of implicit discretizations of the advection equation*, 25 pages, to be submitted

• L. Hajder, L. Lóczi: *Rapid Estimation of Surface Normals from Affine Transformations*, manuscript

• I. Fekete, L. Lóczi: *Linear multistep methods and global Richardson extrapolation*, under review in a Q1 journal

• L. Lóczi: *On some growth and convexity properties of the solutions of* $x^y = y^x$, under review, submitted to a leading mathematics education journal of Cambridge Univ. Press

Work in progress:
• linear multistep methods and local Richardson extrapolation
• monotonicity preservation of Runge—Kutta—Patankar schemes

Guaranteed- and high-precision evaluation of the Lambert W function

The Lambert function W satisfies $W(x)\, e^{W(x)} = x$ (for $x > -1/e$) — a generalization of the logarithm function

The solutions to many polynomial-exponential-logarithmic equations can be expressed in terms of the W function

```
Solve[x + Exp[x] == y, x] // Quiet
```

$\{\{x \to y - \text{ProductLog}[e^y]\}\}$

```
Solve[x + Log[x] == y, x] // Quiet
```

$\{\{x \to \text{ProductLog}[e^y]\}\}$

```
Solve[x^2 + Log[x] == y, x] // Quiet
```

$$\left\{\left\{x \to -\frac{\sqrt{\text{ProductLog}[2\, e^{2y}]}}{\sqrt{2}}\right\}, \left\{x \to \frac{\sqrt{\text{ProductLog}[2\, e^{2y}]}}{\sqrt{2}}\right\}\right\}$$

```
Solve[x^3 Log[x] == y, x] // Quiet
```

$$\left\{\left\{x \to -\frac{(-3)^{1/3}\, y^{1/3}}{\text{ProductLog}[3y]^{1/3}}\right\}, \left\{x \to \frac{3^{1/3}\, y^{1/3}}{\text{ProductLog}[3y]^{1/3}}\right\}, \left\{x \to \frac{(-1)^{2/3}\, 3^{1/3}\, y^{1/3}}{\text{ProductLog}[3y]^{1/3}}\right\}\right\}$$

```
Solve[Log[x]/x == y, x] // Quiet
```

$$\left\{\left\{x \to -\frac{\text{ProductLog}[-y]}{y}\right\}\right\}$$

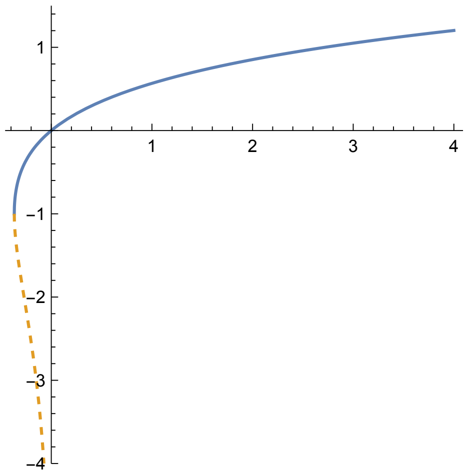
```
Solve[Exp[x]/x^2 == y, x] // Quiet
```

$$\left\{\left\{x \to -2\,\text{ProductLog}\left[-\frac{1}{2\sqrt{y}}\right]\right\}, \left\{x \to -2\,\text{ProductLog}\left[\frac{1}{2\sqrt{y}}\right]\right\}\right\}$$

The W function has two real branches: W_0 (continuous curve) and W_{-1} (dashed curve)

In[ ]:=
```
Plot[{ProductLog[x], ProductLog[-1, x]}, {x, -1 / E, 4},
 PlotRange → {-4, 1.5}, AspectRatio → 1, PlotStyle → {, Dashed}]
```

Out[ ]=



The W function gained popularity in the last few decades, and it is implemented in all major symbolic systems (e.g. *Mathematica*, Maple).

Both branches of the W function are now extensively used in science and engineering:

D.A. Barry et al. / Mathematics and Computers in Simulation 53 (2000) 95–103 97

Table 1
Applications of the real-valued W-function including the branch used

Problem description	Branch of the W-function used	Reference
Water movement in soil	W_{-1} or W_0^- or W_0^+	[5,6]
Enzyme–substrate reactions	W_0^+ or W_0^-	[22,36]
Time of a parachute jump	W_0^+	[29]
Iterated exponentiation	$W_0(x)$, $-\exp(-1) \le x \le \exp(1)$	[13,23]
Jet fuel consumption	W_0^- or W_{-1}	[1,13]
Combustion	W_0^+	[13,30]
Forces in hydrogen ions	W_0^+ or W_0^-	[34,35]
Population growth	W_{-1} and W_0^-	[13]
Roots of trinomials	W_0^+	[21]
Disease spreading	W_0^-	[13]
Recurrences in algorithm analysis	W_0^-	[13,25]
Binary search tree height	W_0^-	[13,15,32]
Hashing with uniform probing	W_0^+	[20]
Hashing methods	W_{-1}	[27]
Optimal wire shapes	W_0^-	[17]
SU(N) gauge theory	W_0^+	[2]
QCD renormalisation	W_0^+ or W_0^- or W_{-1}	[18,19,37]
Star collapse	W_0^+	[14]
Two-body motion	W_0^- and W_{-1}	[28]
Structure learning	W_0^+	[7]
Reaction–diffusion modelling	W_{-1}	[9]
Sample partitioning	W_0^+	[12]
Entropy-constrained scalar quantization	W_0^-	[39]
Redox barrier design	W_0^-	[11]
Photochemical bleaching	W_0^+	[40]
Thin film life time	W_{-1}	[38]
Testing Legendre transform algorithm	W_0^+	[26]
Exponential function approximation	W_{-1} and W_0^-	[33]
Herbivore–plant coexistence	W_0^+	[24]
Photorefractive two-wave mixing	W_0^+	[31]

The W function is not an elementary function, natural question: how to approximate it with elementary functions?
There are several known formulae, including

- Taylor expansions, e.g., about the origin

$$\sum_{k=1}^{\infty} \frac{(-k)^{k-1}}{k!} x^k = x - x^2 + \frac{3x^3}{2} - \frac{8x^4}{3} + \frac{125x^5}{24} + \mathcal{O}\left(x^6\right);$$

- Puiseux expansions, e.g., about the branch point $x = -1/e$;

- asymptotic expansions about $+\infty$, such as

$$\ln(x) - \ln(\ln(x)) + \sum_{k=0}^{\infty} \sum_{m=1}^{\infty} c_{k,m} \frac{(\ln(\ln(x)))^m}{(\ln(x))^{m+k}}$$

  where the coefficients $c_{k,m}$ are defined in terms of the Stirling cycle numbers;

recursive approximations

- the recursion

$$\lambda_{n+1}(x) := \ln(x) - \ln(\lambda_n(x));$$

- the Newton-type iteration

$$\nu_{n+1}(x) := \nu_n(x) - \frac{\nu_n(x) - xe^{-\nu_n(x)}}{1 + \nu_n(x)};$$

- the iteration

$$\beta_{n+1}(x) := \frac{\beta_n(x)}{1 + \beta_n(x)} \left(1 + \ln\left(\frac{x}{\beta_n(x)}\right)\right);$$

- the Halley-type iteration

$$h_{n+1}(x) := h_n(x) - \frac{h_n(x)e^{h_n(x)} - x}{e^{h_n(x)}\left(h_n(x) + 1\right) - \frac{(h_n(x)+2)\left(h_n(x)e^{h_n(x)} - x\right)}{2(h_n(x)+1)}};$$

- the Fritsch–Shafer–Crowley (FSC) scheme;

analytic bounds on different intervals

- the bounds

$$\ln(x) - \ln(\ln(x)) + \frac{\ln(\ln(x))}{2\ln(x)} < \mathrm{W}_0(x) < \ln(x) - \ln(\ln(x)) + \frac{e\ln(\ln(x))}{(e-1)\ln(x)},$$

  valid for $x \in (e, +\infty)$;

Error estimates for the remainder terms in the series expansions?

For the recursive approximations:
What starting value should one pick?
Is the recursion well-defined then?
Will it converge for a particular value of x?
If yes, what is the error committed when n recursive steps are performed?
How many steps to take to approximate $W(x)$ to a given precision?
How to tackle the difficulties when x is close to the branch point at $-1/e$, to the singularity near $x < 0$, or when $x > 0$ is very large?

In our work, we analyzed the following recursion proposed by R. Iacono and J. P. Boyd:

$$\beta_{n+1}(x) := \frac{\beta_n(x)}{1+\beta_n(x)} \left(1 + \ln\left(\frac{x}{\beta_n(x)}\right)\right)$$

• We proposed **simple and suitable starting values** (consisting of the basic operations, logarithms, or square roots) that guarantee monotone convergence on the full domain of definition of both real branches.

• The quadratic rate of convergence of the above recursion is proved via **explicit** and **uniform** error estimates.

• From these estimates, the maximum number of iteration steps needed to achieve a desired precision can easily be determined in advance.

Some results:

$$
\begin{cases}
\beta_0(x) := -1-\sqrt{2}\sqrt{1+ex} & \text{for } -1/e < x \le -1/4,\\
\beta_0(x) := \ln(-x)-\ln(-\ln(-x)) & \text{for } -1/4 < x < 0,\\
\beta_{n+1}(x) := \dfrac{\beta_n(x)}{1+\beta_n(x)}\left(1+\ln\left(\dfrac{x}{\beta_n(x)}\right)\right) & (n\in\mathbb{N}).
\end{cases}
$$

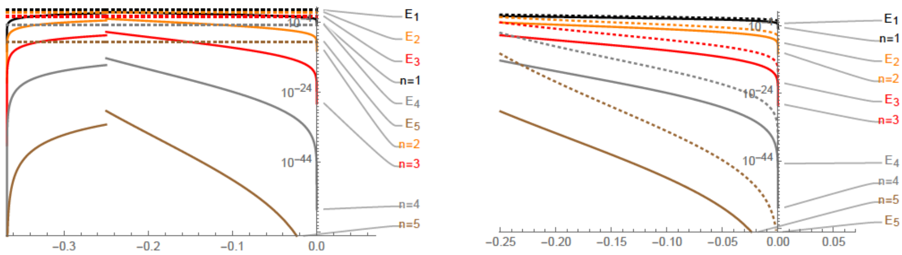
Theorem 2.23. *For any* $-1/e < x < 0$ *and* $n \in \mathbb{N}^+$, *the recursion* (27) *satisfies*

$$0 < \mathrm{W}_{-1}(x) - \beta_n(x) < \left(\frac{1}{2}\right)^{2^n}.$$

In particular, for $-1/4 < x < 0$, *the sharper estimate*

$$\mathrm{W}_{-1}(x) - \beta_n(x) < \left(\frac{1}{2}\right)^{2^n}\left(\frac{1}{|\ln(-x)-\ln(-\ln(-x))|\cdot|1+\ln(-x)-\ln(-\ln(-x))|}\right)^{-1+2^n}$$

also holds.



(a) (b)

The proofs are of symbolic character, e.g.:

$$\frac{ye^{y+1}\left(10+\sqrt{1+ye^{y+1}}\right)\ln\left(1+\sqrt{1+ye^{y+1}}\right)}{10\left(1+ye^{y+1}+\sqrt{1+ye^{y+1}}\right)} < y,$$

$$(w+10)^2z^2+(w+1)(w^3+9w^2-120w-200)z+10(w+1)^3(w^2+10),$$

Some examples (may have relevance in number theory):

• uniform, high-precision approximations (quadratic rate of convergence)

Remark 2.5. *According to* (19), *we have the following uniform estimates for any*

$$0 < \mathrm{W}_0(x) - \beta_5(x) < 8 \cdot 10^{-17},$$

$$0 < \mathrm{W}_0(x) - \beta_{10}(x) < 7 \cdot 10^{-517},$$

$$0 < \mathrm{W}_0(x) - \beta_{15}(x) < 8 \cdot 10^{-16519}.$$

• very large arguments

$$0 < \mathrm{W}_0\left(10^{10^{20}}\right) - \beta_9\left(10^{10^{20}}\right) < 10^{-10000}.$$