Elementary Integral Series for Heun Functions
Numerical implementation

Pierre-Louis Giscard   Aditya Tamar

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We give below the pseudo code for the numerical evaluation of general Heun functions using their integral formulation. The code takes Heun parameters and boundary conditions as inputs and returns the value of the Heun function over a chosen interval $]a, b[$. The code is optimized mathematically and requires only one single integral.

The code must be written in a language with the following capabilities: creating real and complex valued matrices; inverting triangular matrices; calculate the exponential of a real number. Not required but could be a bonus : numerical integration subroutine. This can be replaced with a linear approximation as the interval integrated over is always infitesimal in size. This latter option might prove much faster.

We advise starting to run the code with the initial condition located at z_0 on the left hand side of the interval, i.e. $z_0 = a$. Once validated in this situation, the code can be run for $z_0 \neq a$. This is because when $z_0 > a$, the integral might pick a minus sign which may or may not be automatically added depending on the language used.

Procedure 1 Numerical evaluation of the general Heun function $H_G(z)$ for z in a chosen interval $I =]a, b[$ with boundary conditions $H_0 = H_G(z_0)$ and $H_0' = H_G(z_0')$ at $z_0 \in I$. Numerical accuracy parameter: step size Δ. The algorithm supposes that the divergences of H_G, at t, 1 and 0 are not in I.

Inputs:
Real numbers: a, b, z_0, Δ; `% Step size must not be 1`
Mathematical parameters, possibly complex: H_0, H_0'; α, β, q, t, γ, δ, ϵ.
Output: list Z of discrete real values of z; complex list $H = H_G(Z)$.

Initialization: Param $\leftarrow (a, b, \Delta, H_0, H_0', \alpha, \beta, q, t, \gamma, \delta, \epsilon)$

if $H_0 = 0$ **and** $H_0' = 0$ **then**
  $Z \leftarrow Z_i = a + (i-1)\Delta$ `% List of size` $d = (b-a)/\Delta$
  $H \leftarrow 0$ `% List of size` d `full of 0`
else if $H_0 = 0$ **then**
  $(Z, H) \leftarrow$ Procedure3(Param) `% Launch subfunction computing only the required piece of the integral formulation`
else if $H_0 = H_0'$ **then**
  $(Z, H) \leftarrow$ Procedure2(Param) `% Launch subfunction computing only the required piece of the integral formulation`
else
  $(Z, H_1) \leftarrow$ Procedure2(Param)
  $(., H_2) \leftarrow$ Procedure3(Param)
  $H \leftarrow H_1 + H_2$
end if
return Z, H

Procedure 2 Numerical evaluation of the general Heun function $H_G(z)$ for z in a chosen interval $I\ =]a,b[$ with **boundary conditions** $\mathbf{H_0 := H_G(z_0) = H_G(z_0') \neq 0}$ at $z_0 \in I$. Numerical accuracy parameter: step size Δ. The algorithm supposes that the divergences of H_G, at t, 1 and 0 are not in I.

Inputs:

Real numbers: a, b, z_0, Δ; `% Step size must not be 1`

Mathematical parameters, possibly complex: H_0, $H_0' = 0$; α, β, q, t, γ, δ, ϵ.

Output: list Z of discrete real values of z; complex list $H = H_G(Z)$.

Initialization:

$d \leftarrow (b-a)/\Delta + 1$ `% Real number`

$Z \leftarrow Z_i = a + (i-1)\Delta$ `% Real list, size` $d \times 1$

$T \leftarrow T_{ij} = 0$ if $i > j$ and $T_{ij} = 1$ otherwise `% Real` $d \times d$ `matrix`

$\mathrm{Id} \leftarrow \mathrm{Id}_{ij} = 1$ if $i = j$ and 0 otherwise `% Real` $d \times d$ `matrix`

Computations:

$K_1 \leftarrow (K_1)_{ij} = 0$ if $i > j$ and otherwise $(K_1)_{ij} = 1 + I_{ij}$ with

$$I_{ij} = e^{-Z_j} \int_{Z_i}^{Z_j} \left\{ \frac{\zeta^\gamma (\zeta-1)^\delta (t-\zeta)^\epsilon e^\zeta}{Z_j^\gamma (Z_j-1)^\delta (t-Z_j)^\epsilon} \left(\frac{q - \alpha\beta\zeta}{(\zeta-1)\,\zeta\,(\zeta-t)} - \frac{\epsilon}{\zeta-t} - \frac{\gamma}{\zeta} - \frac{\delta}{\zeta-1} - 1 \right) \right\} d\zeta$$

`% This requires coputing` d `local integrals. To reach this linear computational cost, create a subroutine computing the` d `integrals running over 'local' intervals` $Z_i \to Z_{i+1}$ `for` $i = 1$ `up to` $d - 1$`. Then add these as required to form the interval` $Z_i \to Z_j$`. Each of the` d `local integrals over` $Z_i \to Z_{i+1}$ `can be performed either by a standard numerical integration subroutine or, for` Δ `small enough, via the linear approximation: integral =` $\Delta\times$ `integrand evaluated at mid interval point.`

`%` K_1 `is a` $d \times d$ `complex matrix, indices` i `and` j `run from 1 to` d.

$R \leftarrow (\mathrm{Id} - K_1\Delta)^{-1} - \mathrm{Id}$.

`%` R `is a` $d \times d$ `matrix, requiring one matrix inverse computation. All matrices are triangular making this easy. Multiplication by a scalar here means all entries of the matrix are multiplied by the scalar. For example` $(K_1\Delta)_{ij} = (K_1)_{ij} \times \Delta$.

$R \leftarrow R.T$ `% Matrix` R `now contains the Heun function`

$H_0 \leftarrow H_G(z_0)$ `% Boundary condition`

$H \leftarrow H_0(1 + R_{\{1,:\}})$ `%` $R_{\{1,:\}}$ `denotes the first line of matrix` R.

return Z, H

Procedure 3 Numerical evaluation of the general Heun function $H_G(z)$ for z in a chosen interval $I =]a, b[$ **with boundary conditions** $\mathbf{H_0} = \mathbf{H_G}(\mathbf{z_0}) = \mathbf{0}$ **and** $\mathbf{H'_0} = \mathbf{H_G}(\mathbf{z'_0})$ at $z_0 \in I$. Numerical accuracy parameter: step size Δ. The algorithm supposes that the divergences of H_G, at t, 1 and 0 are not in I.

Inputs:
Real numbers: a, b, z_0, Δ; `% Step size must not be 1`
Mathematical parameters, possibly complex: $H_0 = 0$, H'_0; α, β, q, t, γ, δ, ϵ.
Output: list Z of discrete real values of z; complex list $H = H_G(Z)$.

Initialization:
$d \leftarrow (b-a)/\Delta + 1$ `% Real number`
$Z \leftarrow Z_i := a + (i-1)\Delta$ `% Real list of size` $d \times 1$
$\mathrm{Id} \leftarrow \mathrm{Id}_{ij} = 1$ if $i = j$ and 0 otherwise `% Real` $d \times d$ `matrix`
$T \leftarrow T_{ij} = 0$ if $i > j$ and $T_{ij} = e^{(j-i)\Delta} - 1$ otherwise `% Real` $d \times d$ `matrix`
$K_2 \leftarrow (K_2)_{ij} = 0$ if $i > j$ and otherwise

$$(K_2)_{ij} = \left(\frac{q - \alpha\beta Z_j}{(Z_j - 1)Z_j(Z_j - t)} - \frac{\epsilon}{t - Z_j} - \frac{\gamma}{Z_j} - \frac{\delta}{Z_j - 1} - 1 \right) e^{Z_j - Z_i} - \frac{q - \alpha\beta Z_j}{(Z_j - 1)Z_j(Z_j - t)}$$

`%` K_2 `is a` $d \times d$ `complex matrix`

Computations:
$R \leftarrow (\mathrm{Id} - K_2\Delta)^{-1}.T$
`%` R `is a` $d \times d$ `matrix`

$H \leftarrow (H'_0 - H_0) \times R_{\{1,:\}}$ `%` $R_{\{1,:\}}$ `denotes the first line of matrix` R.

return Z, H