# Efficient computation of Hankel transforms based on Levin's method 

Oskar Grocholski<br>in collaboration with Markus Diehl

DESY Hamburg

HELMHOLTZ


February 17, 2023

## Motivation

TMD factorization: unpolarized structure functions expressed as

$$
\begin{equation*}
\tilde{W}\left(q_{\perp}\right)=\int \frac{d^{2} \mathbf{z}_{\perp}}{(2 \pi)^{2}} e^{-i \mathbf{z}_{\perp} \cdot \mathbf{q}_{\perp}} W\left(z_{\perp}\right)=\int_{0}^{\infty} \frac{d z_{\perp}}{2 \pi} J_{0}\left(q_{\perp} z_{\perp}\right) z_{\perp} W\left(z_{\perp}\right) \tag{1}
\end{equation*}
$$

$W\left(z_{\perp}\right)$ - product of TMDs and FFs.
Polarized structure functions $\rightarrow$ also integrals involving $J_{1}, J_{2}$.

## Motivation

TMD factorization: unpolarized structure functions expressed as

$$
\begin{equation*}
\tilde{W}\left(q_{\perp}\right)=\int \frac{d^{2} \mathbf{z}_{\perp}}{(2 \pi)^{2}} e^{-i \mathbf{z}_{\perp} \cdot \mathbf{q}_{\perp}} W\left(z_{\perp}\right)=\int_{0}^{\infty} \frac{d z_{\perp}}{2 \pi} J_{0}\left(q_{\perp} z_{\perp}\right) z_{\perp} W\left(z_{\perp}\right) \tag{1}
\end{equation*}
$$

$W\left(z_{\perp}\right)$ - product of TMDs and FFs.
Polarized structure functions $\rightarrow$ also integrals involving $J_{1}, J_{2}$.
Adaptative quadrature methods use different grid points in $z_{\perp}$, depending on $q_{\perp} \Longrightarrow$ if computation of $W(z)$ becomes costly, then computation of every point $\tilde{W}\left(q_{\perp}\right)$ becomes proportionally longer.
$\Longrightarrow$ Find a method that can use a fixed grid in a wide range of $q_{\perp}$ !

## Levin's method: the general idea

D. Levin Fast integration of rapidly oscillatory functions, J. of Computational and Applied Mathematics 67 (1996) 95-101

Rewrite the integral as

$$
\begin{equation*}
\int_{z_{0}}^{z_{1}} \vec{\omega} \cdot \vec{g} d z \tag{2}
\end{equation*}
$$

with the quickly oscillating part $\vec{\omega}$ such that

$$
\begin{equation*}
\frac{d}{d z} \vec{\omega}=A^{T} \vec{\omega}, \tag{3}
\end{equation*}
$$

e.g.

$$
\vec{\omega}(z)=\left[J_{\nu}(q z), J_{\nu+1}(q z)\right]^{T}, \quad \vec{g}(z)=[f(z), 0]^{T} .
$$

## Levin's method: the general idea

Find a function $\vec{h}(z)$ such that

$$
\begin{equation*}
\left(\frac{d}{d z}+A\right) \vec{h}=\vec{g} \tag{4}
\end{equation*}
$$

then

$$
\begin{equation*}
\frac{d}{d z}(\vec{h} \cdot \vec{\omega})=\left(\frac{d}{d z} \vec{h}\right) \cdot \vec{\omega}+\vec{h} \cdot\left(A^{T} \vec{\omega}\right)=\vec{g} \cdot \vec{\omega} . \tag{5}
\end{equation*}
$$

## Levin's method: the general idea

Find a function $\vec{h}(z)$ such that

$$
\begin{equation*}
\left(\frac{d}{d z}+A\right) \vec{h}=\vec{g} \tag{4}
\end{equation*}
$$

then

$$
\begin{equation*}
\frac{d}{d z}(\vec{h} \cdot \vec{\omega})=\left(\frac{d}{d z} \vec{h}\right) \cdot \vec{\omega}+\vec{h} \cdot\left(A^{T} \vec{\omega}\right)=\vec{g} \cdot \vec{\omega} . \tag{5}
\end{equation*}
$$

The integral can be easily computed:

$$
\begin{equation*}
\int_{z_{0}}^{z_{1}} \vec{\omega} \cdot \vec{g} d z=\vec{h}\left(z_{1}\right) \cdot \vec{\omega}\left(z_{1}\right)-\vec{h}\left(z_{0}\right) \cdot \vec{\omega}\left(z_{0}\right) \tag{6}
\end{equation*}
$$

## Levin's method: the general idea

One can choose

$$
\vec{\omega}(z)=\left[\begin{array}{c}
J_{\nu}(q z)  \tag{7}\\
J_{\nu+1}(q z)
\end{array}\right], \quad \vec{g}(z)=\left[\begin{array}{c}
f(z) \\
0
\end{array}\right] .
$$

In that case:

$$
A=\left[\begin{array}{cc}
\nu / z & -q  \tag{8}\\
q & -(\nu+1) / z
\end{array}\right]
$$

Side remark: integral with $J_{\nu+1} \rightarrow$ just use $\vec{g}=[0, f(z)]^{T}$.

## Levin's method: application to Hankel transform

Obtained system of differential equations:

$$
\left(\frac{d}{d z}+\left[\begin{array}{cc}
\nu / z & -q  \tag{9}\\
q & -(\nu+1) / z
\end{array}\right]\right)\left[\begin{array}{l}
h_{1}(z) \\
h_{2}(z)
\end{array}\right]=\left[\begin{array}{c}
f(z) \\
0
\end{array}\right] .
$$

$x$ Singularity at $z=0$ !

## Levin's method: singularity at $z=0$

Make a different splitting of the oscillatory and non-oscillatory part of the integral:

$$
\begin{equation*}
\int_{0}^{\infty} J_{\nu}(q z) f(z) d z=\int_{0}^{\infty}\left(z^{-\nu} J_{\nu}(q z)\right) z^{\nu} f(z) d z \tag{10}
\end{equation*}
$$

## Levin's method: singularity at $z=0$

Make a different splitting of the oscillatory and non-oscillatory part of the integral:

$$
\begin{equation*}
\int_{0}^{\infty} J_{\nu}(q z) f(z) d z=\int_{0}^{\infty}\left(z^{-\nu} J_{\nu}(q z)\right) z^{\nu} f(z) d z \tag{10}
\end{equation*}
$$

Use the rescaled vector of oscillatory functions:

$$
\vec{\omega}_{2}=\left[\begin{array}{c}
z^{-\nu} J_{\nu}(q z)  \tag{11}\\
z^{-\nu} J_{\nu+1}(q z)
\end{array}\right], \quad \lim _{z \rightarrow 0} \vec{\omega}_{2}(z) \text { is finite. }
$$

## Levin's method: singularity at $z=0$

Make a different splitting of the oscillatory and non-oscillatory part of the integral:

$$
\begin{equation*}
\int_{0}^{\infty} J_{\nu}(q z) f(z) d z=\int_{0}^{\infty}\left(z^{-\nu} J_{\nu}(q z)\right) z^{\nu} f(z) d z \tag{10}
\end{equation*}
$$

Use the rescaled vector of oscillatory functions:

$$
\vec{\omega}_{2}=\left[\begin{array}{c}
z^{-\nu} J_{\nu}(q z)  \tag{11}\\
z^{-\nu} J_{\nu+1}(q z)
\end{array}\right], \quad \lim _{z \rightarrow 0} \vec{\omega}_{2}(z) \text { is finite } .
$$

The resulting matrix $A_{2}$ is

$$
A_{2}=\left[\begin{array}{cc}
0 & -q  \tag{12}\\
q & -(2 \nu+1) / z
\end{array}\right] .
$$

## Levin's method: singularity at $z=0$

Introduce $z \tilde{h}_{3}=\tilde{h}_{2}$, to remove the $1 / z$ factor.
$\nu \geq 1 \Longrightarrow \tilde{h}_{3}$ is well-behaved at $z=0$.

## Levin's method: singularity at $z=0$

Introduce $z \tilde{h}_{3}=\tilde{h}_{2}$, to remove the $1 / z$ factor.
$\nu \geq 1 \Longrightarrow \tilde{h}_{3}$ is well-behaved at $z=0$.
Differential equations for the rescaled functions:

$$
\begin{cases}z^{\nu} f(z) & =\frac{d}{d z} \tilde{h}_{1}(z)-q z \tilde{h}_{3}  \tag{13}\\ 0 & =z \frac{d}{d z} \tilde{h}_{3}-2 \nu \tilde{h}_{3}+q \tilde{h}_{1}\end{cases}
$$

Remark: for larger $z$, it is better to use $\frac{z}{z+1} \tilde{h}_{3}=\tilde{h}_{2}$ $\Longrightarrow$ longer formulas, but the method is the same.

In fact, one takes also $z /(1+z)$ instead of $z$ in $\omega_{2}$.

## The case $0 \leq \nu<1$

Can integrate by parts:

$$
\begin{align*}
& \int_{z_{0}}^{z_{1}} J_{\nu}(q z) f(z) d z= \\
& \left.\quad \frac{1}{q} J_{\nu+1}(q z) f(z)\right|_{z_{0}} ^{z_{1}} \\
& \quad-\frac{1}{q} \int_{z_{0}}^{z_{1}} z^{\nu}\left(\frac{d}{d z}(z f(z))-(\nu+2) f(z)\right) z^{-(\nu+1)} J_{\nu+1}(q z) . \tag{14}
\end{align*}
$$

## Infinite interval

In general, one can make a variable transformation:

$$
\begin{equation*}
\int_{0}^{\infty} f(z) J_{\nu}(q z) d z=\int_{-1}^{1}\left(\frac{d z}{d u}\right) f(z(u)) J_{\nu}(z(u)) d u \tag{15}
\end{equation*}
$$

The resulting equation for $\tilde{h}(u)$ reads:

$$
\left[\begin{array}{c}
f(z(u))  \tag{16}\\
0
\end{array}\right]=\left(\left(\frac{d u}{d z}\right) \frac{d}{d u}+A\right)\left[\begin{array}{c}
\tilde{h}_{1}(u) \\
\tilde{h}_{2}(u)
\end{array}\right]
$$

## Chebyshev pseudospectral method

$p_{1}, p_{3}$ - Chebyshev polynomials of order $N-1$ approximating $\tilde{h}_{1,3}$.

$$
\begin{align*}
& u_{j}=\cos \left(\frac{j \pi}{N}\right), \quad j \in\{0, \ldots, N-1\} \quad \text { interpolation points, }  \tag{17}\\
& p_{1,3}\left(u_{j}\right)=\tilde{h}_{1,3}\left(u_{j}\right), \quad f\left(z_{j}\right)=f\left(z\left(u_{j}\right)\right),  \tag{18}\\
& \frac{d}{d u} p\left(u_{j}\right)=\sum_{k=0}^{N-1} D_{j k} p\left(u_{k}\right) \approx \frac{d}{d u} \tilde{h}\left(u_{j}\right) . \tag{19}
\end{align*}
$$

$D$ - Chebyshev differentiation matrix.

## Chebyshev pseudospectral method

Find the approximate solution by discretizing the system:

$$
\text { Let } z_{j}=z\left(u_{j}\right)
$$

$$
\begin{cases}z_{j}^{\nu} f\left(z_{j}\right) & =\left(\frac{d u}{d z}\right) \sum_{j k} p_{1}\left(u_{k}\right)-q z_{j} p_{3}\left(u_{j}\right),  \tag{20}\\ 0 & =z_{j}\left(\frac{d u}{d z}\right) \sum_{j k} p_{3}\left(u_{k}\right)-2 \nu p_{3}\left(u_{j}\right)+q p_{1}\left(u_{j}\right)\end{cases}
$$

## Chebyshev pseudospectral method

Find the approximate solution by discretizing the system:
Let $z_{j}=z\left(u_{j}\right)$,

$$
\begin{cases}z_{j}^{\nu} f\left(z_{j}\right) & =\left(\frac{d u}{d z}\right) \sum_{j k} p_{1}\left(u_{k}\right)-q z_{j} p_{3}\left(u_{j}\right),  \tag{20}\\ 0 & =z_{j}\left(\frac{d u}{d z}\right) \sum_{j k} p_{3}\left(u_{k}\right)-2 \nu p_{3}\left(u_{j}\right)+q p_{1}\left(u_{j}\right)\end{cases}
$$

Let:

$$
\begin{align*}
\vec{F} & =\left[z_{0}^{\nu} f\left(z_{0}\right), \ldots, z_{N-1}^{\nu} f\left(z_{N-1}\right), 0, \ldots, 0\right]^{T}  \tag{21}\\
\vec{P} & =\left[p_{1}\left(u_{0}\right), \ldots, p_{1}\left(u_{N-1}\right), p_{3}\left(u_{0}\right), \ldots, p_{3}\left(u_{N-1}\right)\right]^{T}  \tag{22}\\
B \vec{P} & =\vec{F} \tag{23}
\end{align*}
$$

## Chebyshev pseudospectral method

$\longrightarrow 2 N$ equations.
$\longrightarrow$ Need to find appropriate variable transformation (so that one can interpolate the integrand and the solution well on the resulting grid).
M. Diehl, R. Nagar, F. J. Tackmann, ChiliPDF: Chebyshev Interpolation for Parton Distributions, [arXiv:2112.09703] - efficient use of Chebyshev grids, many kinds of variable transformation implemented.

## Technical remarks

For $\sim 50$ nodes the best accuracy is obtained when splitting the integral into 2 parts:

$$
\begin{equation*}
\int_{0}^{\infty} J_{\nu}(q z) f(z) d z=\int_{0}^{z_{1}} J_{\nu}(q z) f(z) d z+\int_{z_{1}}^{\infty} J_{\nu}(q z) f(z) d z . \tag{24}
\end{equation*}
$$

## Technical remarks

For $\sim 50$ nodes the best accuracy is obtained when splitting the integral into 2 parts:

$$
\begin{equation*}
\int_{0}^{\infty} J_{\nu}(q z) f(z) d z=\int_{0}^{z_{1}} J_{\nu}(q z) f(z) d z+\int_{z_{1}}^{\infty} J_{\nu}(q z) f(z) d z \tag{24}
\end{equation*}
$$

- $q z_{1}$ smaller then the first zero of $J_{\nu} \Longrightarrow$ can integrate on the first subinterval using the Clenshaw-Curtis quadrature.


## Technical remarks

For $\sim 50$ nodes the best accuracy is obtained when splitting the integral into 2 parts:

$$
\begin{equation*}
\int_{0}^{\infty} J_{\nu}(q z) f(z) d z=\int_{0}^{z_{1}} J_{\nu}(q z) f(z) d z+\int_{z_{1}}^{\infty} J_{\nu}(q z) f(z) d z . \tag{24}
\end{equation*}
$$

- $q z_{1}$ smaller then the first zero of $J_{\nu} \Longrightarrow$ can integrate on the first subinterval using the Clenshaw-Curtis quadrature.
- larger $q z_{1} \Longrightarrow$ construct the matrix $B$ needed to solve (20).


## Technical remarks

For $\sim 50$ nodes the best accuracy is obtained when splitting the integral into 2 parts:

$$
\begin{equation*}
\int_{0}^{\infty} J_{\nu}(q z) f(z) d z=\int_{0}^{z_{1}} J_{\nu}(q z) f(z) d z+\int_{z_{1}}^{\infty} J_{\nu}(q z) f(z) d z \tag{24}
\end{equation*}
$$

- $q z_{1}$ smaller then the first zero of $J_{\nu} \Longrightarrow$ can integrate on the first subinterval using the Clenshaw-Curtis quadrature.
- larger $q z_{1} \Longrightarrow$ construct the matrix $B$ needed to solve (20).
- First, compute the LU decomposition of $B$.


## Technical remarks

For $\sim 50$ nodes the best accuracy is obtained when splitting the integral into 2 parts:

$$
\begin{equation*}
\int_{0}^{\infty} J_{\nu}(q z) f(z) d z=\int_{0}^{z_{1}} J_{\nu}(q z) f(z) d z+\int_{z_{1}}^{\infty} J_{\nu}(q z) f(z) d z . \tag{24}
\end{equation*}
$$

- $q z_{1}$ smaller then the first zero of $J_{\nu} \Longrightarrow$ can integrate on the first subinterval using the Clenshaw-Curtis quadrature.
- larger $q z_{1} \Longrightarrow$ construct the matrix $B$ needed to solve (20).
- First, compute the LU decomposition of $B$.
- If $B$ is ill-conditioned (zero or small elements on diagonal), use the singular value decomposition (SVD) of $B$.


## Benchmarking the precision

Compare with precision obtained using optimised Ogata quadrature: Kang:2019ctl [arXiv:1906.05949v2].

## Benchmarking the precision

Compare with precision obtained using optimised Ogata quadrature: Kang:2019ctl [arXiv:1906.05949v2].
"Toy function" used in the cited work:

$$
\begin{equation*}
W(z)=\frac{1}{z}\left(\frac{\beta z}{\sigma^{2}}\right)^{\beta^{2} / \sigma^{2}} \exp \left(-\frac{z \beta}{\sigma^{2}}\right) \tag{25}
\end{equation*}
$$

$Q^{-1}=\frac{\beta}{\beta^{2}-\sigma^{2}}$ - maximum of $W \rightarrow$ mimicks the inverse of the hard scale.

## Benchmarking the precision

$W(z)$ including LO evolution effects at low $z$ and various Ansaetze for large $z$ behavior:

$$
\begin{equation*}
W(z)=\exp \left(S\left(\mu_{z}, Q\right)\right) \times[F(z)]^{2} \tag{26}
\end{equation*}
$$

$\exp \left(S\left(\mu_{z}, Q\right)\right)$ - Sudakov factor with $z$-dependent renormalization scale $\mu_{z} \propto 1 / z$.
$F(z)$ - Ansatz for large-z behavior of TMD:

- Gaussian behavior from Bacchetta et al., [arXiv:1703.10157],
- Exponential form from Scimemi and Vladimirov, [arXiv:1706.01473].


## Benchmarking the precision



## Benchmarking the precision



## Benchmarking the precision



## Benchmarking the precision



## Benchmarking the precision



## Benchmarking the precision



## Benchmarking the precision



## Benchmarking the precision



## Error estimation

Estimate the error by comparing with results for grid with twice as many points.


## Error estimation

Gauss_Q20, error estimation


## Summary

- Need to find good grid settings (subgrid splitting, variable transformation).
- Can use the Levin's method on a fixed grid in $z$-space (independently on $q$ !)
- Much better precision for higher $q$.
- Can handle integration on intervals different than $(0, \infty)$, e.g. when integrating with a lower cut-off $z_{\text {min. }}$.
- Computation of the relevant matrix decomposition allows to quickly compute integrals involving $J_{\nu}, J_{\nu-1}$ and $J_{\nu+1}$.


## Backup: speeding up the computation

- n-point grid $\Longrightarrow$ a system of $2 n$ linear equations.


## Backup: speeding up the computation

- n-point grid $\Longrightarrow$ a system of $2 n$ linear equations.
- The most costly part: computation of the LU (possibly also SV) decomposition $\propto n^{3}$ operations.


## Backup: speeding up the computation

- n-point grid $\Longrightarrow$ a system of $2 n$ linear equations.
- The most costly part: computation of the LU (possibly also SV) decomposition $\propto n^{3}$ operations.
- Can use 3 subgrid with $\{16,16,16\}$ points instead of $\{16,32\}$.


## Backup: speeding up the computation

- n-point grid $\Longrightarrow$ a system of $2 n$ linear equations.
- The most costly part: computation of the LU (possibly also SV) decomposition $\propto n^{3}$ operations.
- Can use 3 subgrid with $\{16,16,16\}$ points instead of $\{16,32\}$.
$\longrightarrow \sim 40 \%$ faster computation, but slightly worse accuracy.


## Backup: 2 vs 3 subgrids



3 subgrids, $\{16,16,16\}$ points
toy_TMD_Q100

2 subgrids, $\{16,32\}$ points

## Backup: 2 vs 3 subgrids

Yukawa_Q2
3 subgrids, $\{16,16,16\}$ points



Yukawa_Q100


## Backup: 2 vs 3 subgrids



## Backup: LU decomposition of the matrix B

$$
\begin{gather*}
P=\left(\begin{array}{ccccc}
1 & 0 & 0 & \ldots & 0 \\
I_{1,2} & 1 & 0 & \ldots & 0 \\
& & \ldots & & \\
I_{1, n-1} & l_{2, n-1} & \ldots & \ddots & 0 \\
I_{1, n} & l_{2, n} & \ldots & I_{n-1, n} & 1
\end{array}\right) \quad U=\left(\begin{array}{ccccc}
u_{1,1} & u_{2,1} & u_{3,1} & \ldots & u_{n, 1} \\
0 & u_{2,2} & u_{3,2} & \ldots & u_{n, 2} \\
& & \ldots & & \\
0 & 0 & \ldots & \ddots & u_{n, n-1} \\
0 & 0 & \ldots & 0 & u_{n, n}
\end{array}\right)
\end{gather*}
$$

$P$ - permutation matrix.

Can solve $B \vec{h}=\vec{g}$ using the backward substitution method.

## Backup: SV decomposition of the matrix B

$$
\begin{equation*}
B=U\left[\operatorname{diag}\left(w_{j}\right)\right] V^{T} \tag{29}
\end{equation*}
$$

$U, V$ - orthogonal matrices, $w_{j}$ - singular values.

$$
\begin{equation*}
B^{-1}=V\left[\operatorname{diag}\left(1 / w_{j}\right)\right] U^{T} . \tag{30}
\end{equation*}
$$

$w_{j}=0\left(\right.$ or $\left|w_{j}\right|<\varepsilon-$ arbitrarily chosen small value) $\rightarrow$ replace $1 / w_{j}$ by 0 . Solution $h^{\prime}$ obtained this way minimizes the error

$$
\begin{equation*}
\sum_{j}\left|\left(B \vec{h}^{\prime}-\vec{g}\right)_{j}\right| \tag{31}
\end{equation*}
$$

## Backup: $z W(z)$ in position space



