Nonnegative tensor train for the multicomponent Smoluchowski equation

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Multicomponent Smoluchowsi equation

$$\frac{\partial n(\bar{v},t)}{\partial t} = \frac{1}{2}\int_0^{v_1}\dots\int_0^{v_d} K(\bar{v}-\bar{u};\bar{u})n(\bar{v}-\bar{u},t)n(\bar{u},t)du_1\dots du_d - \\ -n(\bar{v},t)\int_0^{\infty}\dots\int_0^{\infty} K(\bar{u};\bar{v})n(\bar{u},t)du_1\dots du_d + q(\bar{v},t), \tag{1}$$

- $n(v,t)$ is particle number density function
- $\bar{v} = [v_1,\dots,v_d]^T$ is complex particles with size of v_i for ith component
- $K(\bar{u},\bar{v}) = K(\bar{v},\bar{u}) \geq 0$ the coagulation kernel, $q(\bar{v},t)$ is particles source function

Key aspects of solver

1. Representation of solution at any time moment in the tensor-train format ($O(N^d) \to O(dNR^2)$ memory cells) [1, 2]
2. Right-hand-side of the equation approximate in this format (lower-triangular TT-convolution $O(d^2R^4N\log N)$ + integration $O(d^2NR^4)$)
3. Time scheme for integrate of this equation translate on tensor-train format using standard TT-operations

$$n^{k+\frac{1}{2}}(\bar{i}) = \frac{\tau}{2}\left(L_1^k(\bar{i}) - n^k(\bar{i})\,L_2^k(\bar{i})\right) + n^k(\bar{i}), \\ n^{k+1}(\bar{i}) = \tau\left(L_1^{k+\frac{1}{2}}(\bar{i}) - n^{k+\frac{1}{2}}(\bar{i})\,L_2^{k+\frac{1}{2}}(\bar{i})\right) + n^k(\bar{i}), \tag{2}$$

4. *Main feature*: nonnegative correction of the solution (**Algorithm 2** in [3])

The two-component problem with the constant kernel

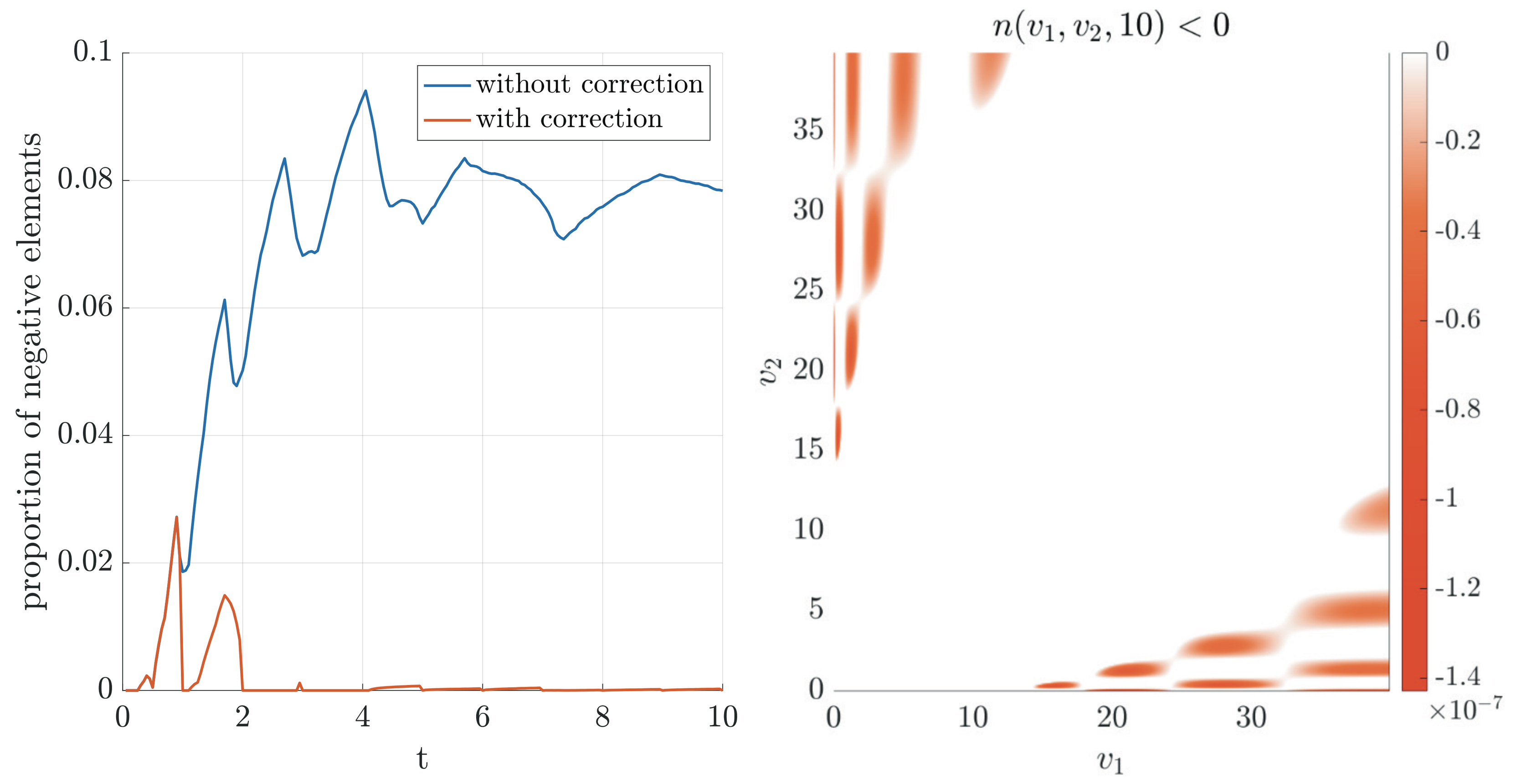

Figure 1. $h = 0.1, \tau = 0.05$. Left panel: Dynamics of the relative number of negative elements with correction at the each integer time moment $t = 1,2,3,\dots,10$ (red line) and without (blue line); Right panel: negative elements in the numerical solution at $t = 10$ arising after its approximation with $R = 10$.

Nonnegative tensor-train based solver

1. Get TT-representations of initial condition $n^0(\bar{i})$ and coagulation kernel K, τ - time step, N_t - number of time steps, s - nonegative correction step.
2. **while** ($k \leq N_t$) **do**

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    n^k ← do_predictor_corrector_step(n^{k-1}, K, τ)
    if (k == s) then
        M ← TT_max(n^k)
        m ← TT_max(|n^k − M · I|)
        if (m − M) > 0 then
            n^k = n^k + (m − M)TT_ones(n^k)
        end if
    end if
k = k + 1
end while
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For find minimal element we use optimal property of $\mathrm{TT-CROSS}$ method and base of this idea $\mathrm{TT\_max}$ procedure [4].

Plots of the total density for the two-component problem

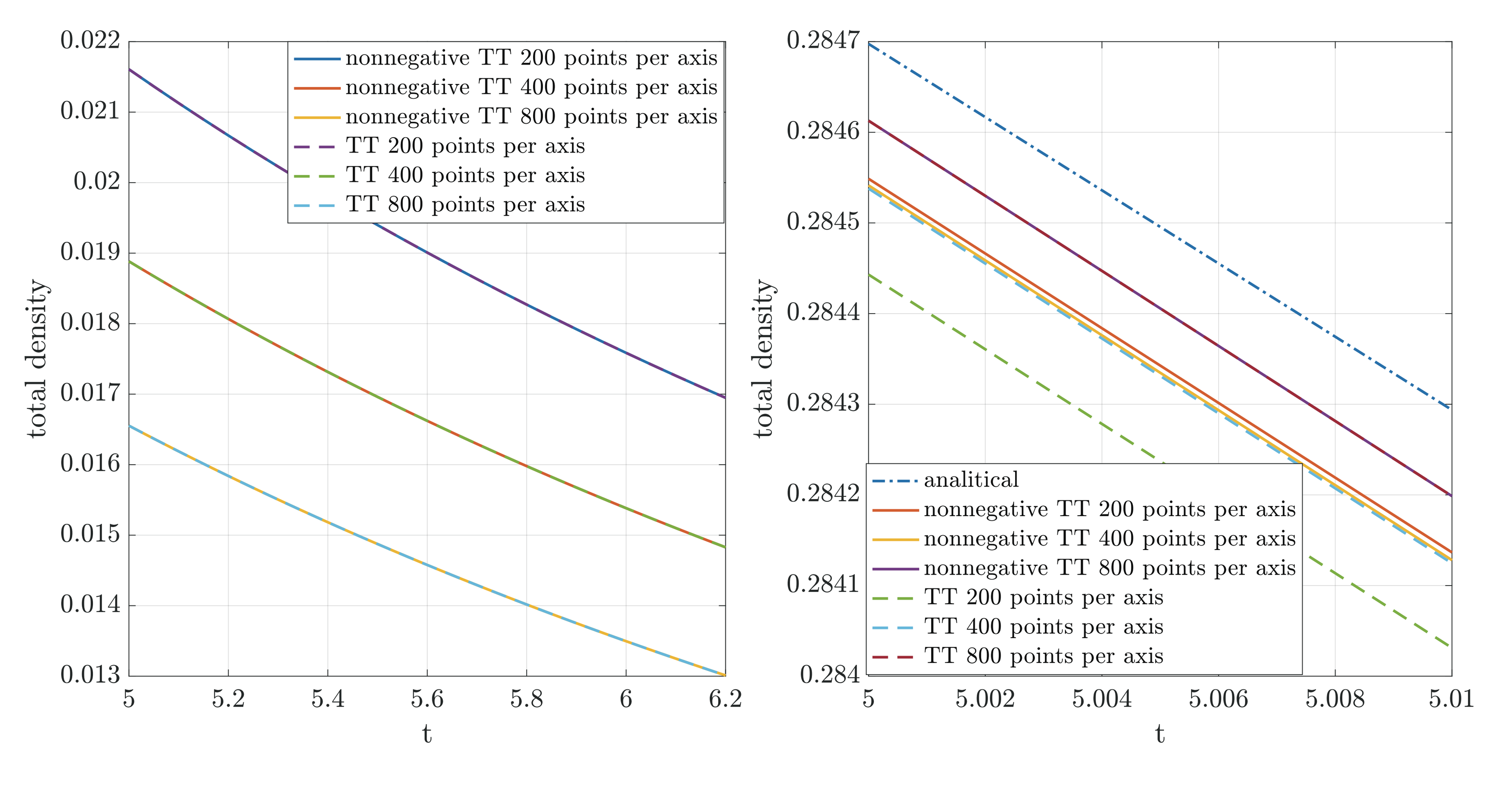

Figure 2. Ballistic kernel (left) and constant kernel (right) for $t \in [5, 6.2]$ and $t \in [5, 5.01]$ simulations time respectively.

Evolution of total mass and density for experiments with source

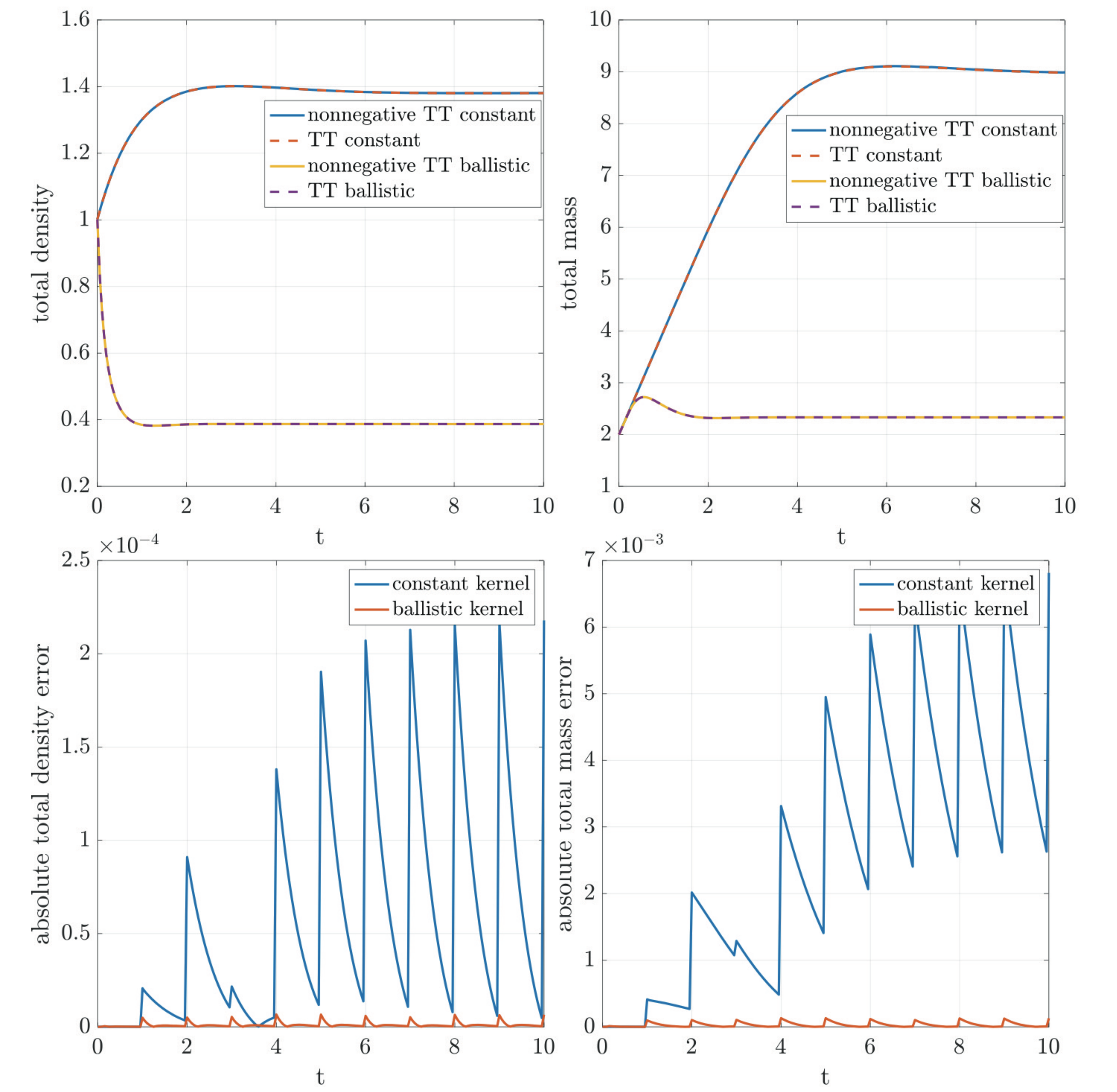

Figure 3. Experiments with source for constant and ballistic kernels: total density (left column) and mass (right column) for nonnegative and standard solution (top row) and absolute difference between the two approaches in terms of the total density and total mass characteristics (bottom row), $V_{max} = 20$ and $t \in [0, 10]$.

Performance of the nonnegative solver

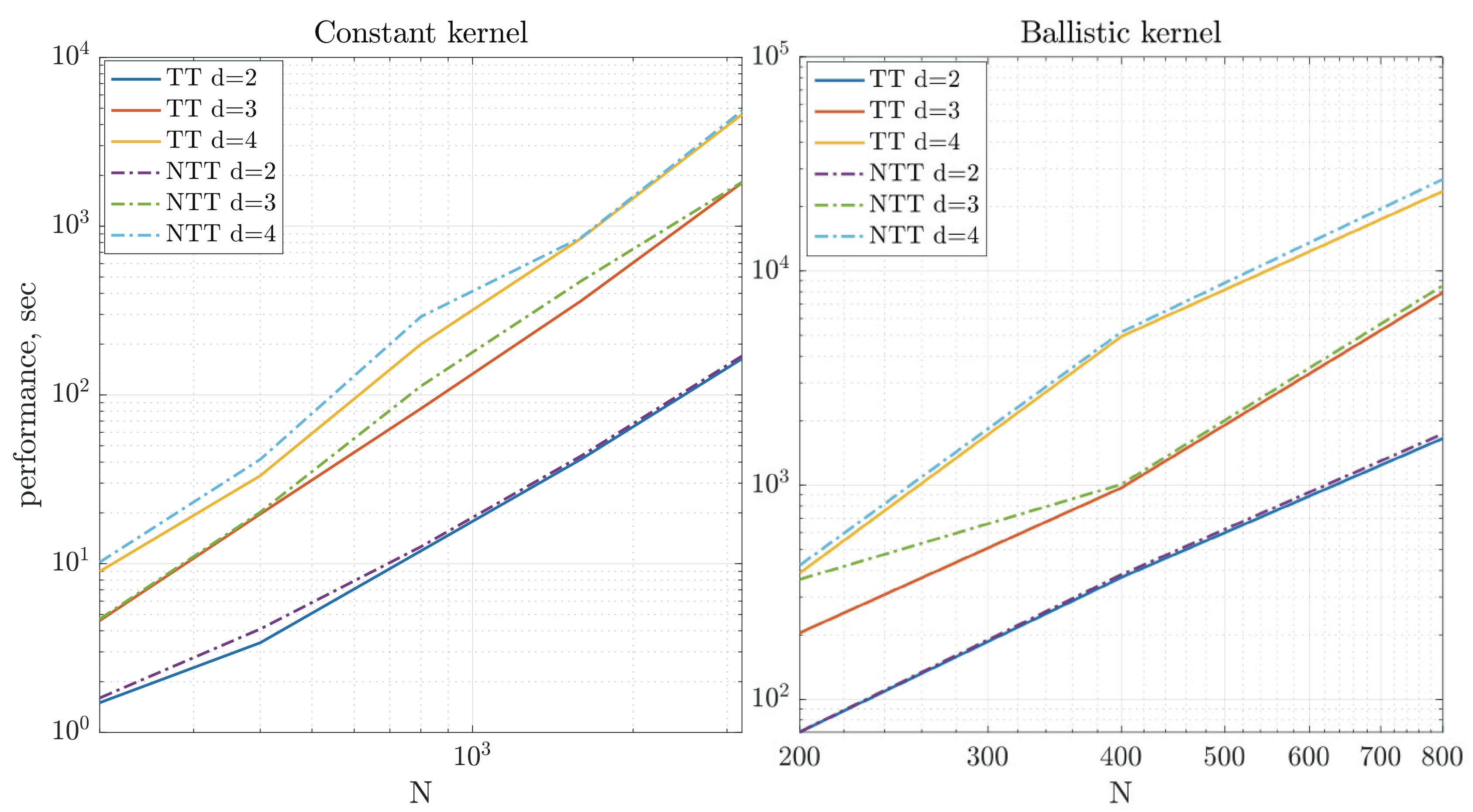

Figure 4. Comparison of the nonnegative TT-based method and standard TT-based scheme for $V_{max} = 40$, $t \in [0, 1]$.

Conclusion

1. New trick allows to effectively introduce nonnegative correction of the solution into the process of numerical integration without to bypass all elements of tensor.
2. Numerical experiments show that correction using the effective method of TT_min approximation add very modest slowdown of the algorithm.
3. Our NTT-corrected method introduce an error below the numerical error of the original tensor-train approximation and the whole numerical scheme.

References

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