

TT-toolbox 2.0: Fast multidimensional array operations in TT format

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1 Contributors

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2 What is the TT-format for tensors

Tensor \mathbf{A} is said to be in the TT-format, if

$$A(i_1, i_2, \dots, i_d) = G_1(i_1) \dots G_d(i_d),$$

and $G_k(i_k)$ is a $r_{k-1} \times r_k$ matrix, and $r_0 = r_d = 1$. The approximation in this format is known to be stable and can be based on QR and SVD decompositions. In linear algebra the most important operation is probably matrix-by-vector product. Thus, matrices have to be also represented in TT-format. Vector of length $n_1 \dots n_d$ is said to be in the TT-format, if it has low TT-ranks considered as d -dimensional array (in MATLAB it is just a single call the the `reshape` function. Matrices acting on such vectors have size $M \times N$, where $N = \prod_{k=1}^d n_k$. For simplicity assume they are square, then each element of such matrix can be indexed by $i_1, \dots, i_d, j_1, \dots, j_d$, where multiindex $i_k, k = 1, \dots, d$ corresponds to rows, and $j_k, k = 1, \dots, d$ — to columns of the matrix. The matrix M is said to be in the TT-format if

$$M(i_1, \dots, i_d, j_1, \dots, j_d) = M_1(i_1, j_1) M_2(i_2, j_2) \dots M_d(i_d, j_d),$$

and $M_k(i_k, j_k)$ is a $r_{k-1} \times r_k$ matrix.

3 What is new in version 2.0

TT Toolbox version 2.0 introduces several major innovations compared to version 1.0.

1. New classes `tt_tensor` and `tt_matrix`, which now represent TT-tensors and TT-matrices.
2. Object-oriented approach allowed to overload many standard MATLAB functions, including addition, subtraction, multiplication by number, scalar product, norm, Kronecker products, matrix-by-vector product etc. For details see description below.
3. Complex arithmetic is now fully supported
4. New advanced subroutines are introduced, based on the QTT-DMRG approach: fast approximate matrix-by-vector product, computation of functions of TT-tensors using cross-DMRG algorithm, solution of linear systems via DMRG-solve algorithm and solution of eigenvalue problems via classical DMRG algorithm.
5. Several subroutines to generate basic TT-tensors and TT-matrices: matrices of all ones, identity matrix, random TT-tensors with fixed core sizes

4 Illustration of basic functionality

TT-Toolbox 2.0 has two main classes: `tt_tensor` and `tt_matrix`. The first is a TT-representation of a d -dimensional array in TT-format, and the second — of d -level matrix in TT-format. From old cell-array representations, used in TT-Toolbox 1.0, these representations can be obtained via calls to `tt_tensor` and `tt_matrix` constructors:

```
>> d=5; A=tt_ones(2,d) %Generate a d-dimensional
                        %tensor of all ones
A =
    [2x1 double]
    [2x1 double]
    [2x1 double]
    [2x1 double]
    [2x1 double]
```

And conversion to new format is done via command

```
>> B=tt_tensor(A)
B a 5-dimensional TT-tensor, ranks and mode sizes:
r(1)=1 n(1)=2
r(2)=1 n(2)=2
r(3)=1 n(3)=2
r(4)=1 n(4)=2
r(5)=1 n(5)=2
r(6)=1
```

For matrices in the TT-format situation is analogous, for example,

```
>> e=tt_eye(d,2); %Generate  $2^d \times 2^d$  identity matrix
                    %in TT-format
>> C=tt_matrix(e)
C is a 5-dimensional TT-matrix, ranks and mode sizes:
r(1)=1 n(1)=2 m(1)=2
r(2)=1 n(2)=2 m(2)=2
r(3)=1 n(3)=2 m(3)=2
r(4)=1 n(4)=2 m(4)=2
r(5)=1 n(5)=2 m(5)=2
r(6)=1
```

The conversion operations in the opposite direction are realized via `core` function:

```
>> e=core(C);
>> A=core(B);
```

This helps to keep compatibility with previously developed algorithms. All previous functions are kept in the TT Toolbox 2.0 and can be applied. The `core` command is also overloaded to get a specific core of the TT-decomposition (in the new ordering of indices, it returns a tensor of size $r_{k-1} \times n_k \times r_k$:

```
>> cr=core(B,3); %Get core number 3
>> size(cr)
ans =
      5      2      5
```

For `tt_tensor` and `tt_matrix` classes basic arithmetic operations are defined:

```
>> d=7;
>> v=tt_random(2,d,5); %Generate a random
```

```

                                %d-dimensional tensor
                                %with mode sizes 2 and ranks 5
>> v1=tt_random(2,d,5); %Generate a random
                                %d-dimensional tensor
                                %with mode sizes 2 and ranks 5
>> v=tt_tensor(v); %Make it a TT-tensor
>> v1=tt_tensor(v1);
>> v2=v+2*v1 %Linear combinations

v2 is a 7-dimensional TT-tensor, ranks and mode sizes:
  r(1)=1  n(1)=2
r(2)=10  n(2)=2
r(3)=10  n(3)=2
r(4)=10  n(4)=2
r(5)=10  n(5)=2
r(6)=10  n(6)=2
r(7)=10  n(7)=2
  r(8)=1

```

Note that ranks are added, as expected. The same can be done for matrices with the same syntax.

The computations with TT-tensors are impossible without *TT-rounding*. The tensor is approximated by another TT-tensor with smaller TT-ranks but with prescribed accuracy ε . It is implemented in the `round` command (old syntax is the `tt_compr2` subroutine). For example,

```

>> d=7; v=tt_random(2,d,5); v=tt_tensor(v); v=v+v
v2 is a 7-dimensional TT-tensor, ranks and mode sizes:
  r(1)=1  n(1)=2
r(2)=10  n(2)=2
r(3)=10  n(3)=2
r(4)=10  n(4)=2
r(5)=10  n(5)=2
r(6)=10  n(6)=2
r(7)=10  n(7)=2
  r(8)=1

```

but after rounding ranks are reduced:

```

>> w=round(v,1e-12)
w is a 7-dimensional TT-tensor, ranks and mode sizes:
r(1)=1  n(1)=2
r(2)=2  n(2)=2

```

```

r(3)=4  n(3)=2
r(4)=5  n(4)=2
r(5)=5  n(5)=2
r(6)=4  n(6)=2
r(7)=2  n(7)=2
r(8)=1

```

Note that some ranks are reduced to 4 (maximal possible ranks). To check accuracy, overloaded functions `minus` and `norm` can be used:

```

>> norm(w-v)/norm(w)
ans =
    1.4258e-08

```

The error is only of order of square root of machine precision, since `norm` is computed via scalar products. This will be fixed in future releases of the Toolbox. One can also check particular elements of the tensors w and v . This can be done either via direct indexing:

```

>> em1=w(1,1,2,1,1,1,2)
em1 =
    93.4955
>> em2=v(1,1,2,1,1,1,2)
em2 =
    93.4955
>> em1-em2
ans =
    1.4211e-14

```

This is an indicator of the fact that v and w differ by machine precision. The second options is to use linear index array:

```

>> ind=[1,1,2,1,1,1,2]; em1=w(ind)
em1 =
    93.4955

```

which has to be used if the array is of large or variable dimension, and direct indexing is not possible. Also, taking subsets is also acceptable, for example command

```

>> w1=w(1,:,:,:,:,:);

```

will return TT-tensor $w1$ with the first mode size equal to 1. The `tt_tensor` and `tt_matrix` classes have several constructors. One of the most important is the conversion from the full array, which can be used to detect

TT-structures in given tensors. For example, to get a QTT-representation of a function \sqrt{x} on $[0, 1]$, the following code can be used:

```
>> d=10; n=2^d; h=1.0./(n-1); x=(0:n-1)*h; %Get x
>> x=sqrt(x); x=reshape(x,2*ones(1,d)); %Quantization
>> tt=tt_tensor(x,1e-8)
tt is a 10-dimensional TT-tensor, ranks and mode sizes:
r(1)=1   n(1)=2
r(2)=2   n(2)=2
r(3)=4   n(3)=2
r(4)=6   n(4)=2
r(5)=6   n(5)=2
r(6)=6   n(6)=2
r(7)=6   n(7)=2
r(8)=6   n(8)=2
r(9)=4   n(9)=2
r(10)=2  n(10)=2
r(11)=1
```

To check accuracy, conversion back from TT-format to full format can be used:

```
>> y=full(x); %The result is a d-dimensional tensor
>> y=y(:); norm(y-x(:))/norm(y)
ans =
    7.9424e-10
```

Thus, it is a very accurate approximation. Setting parameter ε to larger values will result in smaller ranks, but lower accuracy.

5 tt_tensor and tt_matrix storage scheme

Class `tt_tensor` contains the following fields:

1. `tt.core` — cores of the TT-decomposition stored in one “long” 1D array
2. `tt.d` — dimension of the array
3. `tt.n` — mode sizes of the array
4. `tt.r` — ranks of the decomposition
5. `tt.ps` — markers for position of the k -the core in array `tt.core`: if `ps=tt.ps`, then k -core can be obtained as

```
>> cr=tt.core; ps=tt.ps; corek=cr(ps(k):ps(k+1)-1);
```

Class `tt_matrix` contains three fields:

1. `ttm.n` — sizes of row indices
2. `ttm.m` — sizes of column indices
3. `ttm.tt` — TT-tensor of the vectorized TT-representation of the matrix

6 Basic functionality

TT-Toolbox supports several basic functions for matrices and vectors. The following operations are supported:

1. `tt=tt_tensor(y,eps)` — construct TT-tensor from full array y with accuracy `eps`.
2. `ttm=tt_matrix(y,eps)` — construct TT-matrix from full array of dimension $n_1 \times n_2 \dots \times n_d \times m_1 \dots \times m_d$ with accuracy `eps`.
3. `tt=tt_tensor(TT)` — constructs TT-tensor from the TT-Toolbox 1.0 format.
4. `ttm=tt_matrix(TTM)` — constructs TT-matrix from the TT-Toolbox 1.0 format.
5. `tt=core(tt,k)`, `ttm=core(ttm,k)` — constructs TT-Toolbox 1.0 format from TT-Toolbox 2.0 format, if parameter k is not specified, and k -th core of the decomposition, if it is specified.
6. `y=full(tt)` — converts TT-tensor `tt` a full array.
7. `y=full(ttm)` — converts TT-matrix `ttm` to a full square matrix.
8. `tt=round(tt,eps)` — approximates given TT-tensor with another TT-tensor with smaller ranks but with prescribed accuracy `eps`.
9. Binary operations `tt1·tt2`, where \cdot can be any operation from the set $\{+, -, .* \}$ (plus, minus, elementwise product). They are implemented when both iterands are either TT-tensors or TT-matrices.
10. `r=rank(tt,k)`, `r=rank(ttm,k)` — returns all ranks of the TT-decomposition if k is not specified, and the k -th rank, if it is given.

11. `sz=size(tt)`, `sz=size(ttm)` — returns the size of the array. For the TT-tensors, it returns d integers, for TT-matrix it returns $d \times 2$ array of integers.
12. `mm=mem(tt)`, `mm=mem(ttm)` — memory required to store the TT-tensor
13. `er=erank(tt)` — effective rank of the TT-tensor.
14. Matrix-by-vector product: $A*b$, where A is a `tt_matrix` and b is a `tt_tensor` of appropriate sizes;
15. Matrix-by-matrix product: $A*B$, where A is a `tt_matrix` and B is a `tt_matrix`.
16. Matrix by full vector product: $A*b$, where A is a `tt_matrix` and b is a full vector of size $\prod_{k=1}^d m_k$.
17. `p=dot(tt1,tt2)` — dot (scalar) product of two TT-tensors
18. `p=norm(tt)` — Frobenius norm of the TT-tensor.
19. `elem=tt(i1,i2,...,id)` — computes element of the TT-tensor in position $i1,i2,...,id$.
20. `elem=tt(ind)`, where `ind` is an integer array of length d return element of the TT-tensor in the position specified by multiindex `ind`.

7 More functions

There are several functions that are helpful in working with TT-tensors and TT-matrices.

21. `ttm=diag(tt)`, `tt=diag(ttm)` — constructs either diagonal TT-matrix from TT-tensor, or takes diagonal of a TT-matrix.
22. `a=kron(b,c)`. For b, c being TT-tensors, it computes outer product of them with number of dimensions equal to the sum of the number of dimensions of b and c . For TT-matrices it computes their Kronecker product in TT-format.
23. `tt=tt_random(d,n,r)` — generate random TT-tensor with dimension d , mode size n , ranks r . n and r can be either numbers (then all dimensions and ranks are the same) or arrays of integers. NOTE: the `tt` is in the OLD format to ensure compatibility. To convert to the new format use `tt_tensor` constructor. In future releases this function will return TT-tensor object.

24. `tt=tt_ones(n,d)` generate tensor with mode sizes n , dimension d of all ones. Returns result in the old format
25. `tt=tt_eye(d,n)` generate identity matrix with dimension d and mode size n . n can be either a number, or integer array. Returns result in the old format.
26. `tt=tt_qlaplace_dd(d)` – generate Laplacian operator with Dirichlet BC on a grid with $2^{d_1} \times 2^{d_2} \times \dots$. Returns result in the old format.
27. `tt=tt_x(d,n)` — returns QTT representation of vector $1 : n^d$ (in the OLD format).

Using these subroutines one can easily implement, say, iterative methods for matrix problems. For example, to implement power method for the maximal eigenvalue for 2D-Laplacian, the following code can be used:

```
%power_iter.m --- simple power iteration
d=10;
mt=tt_qlaplace_dd(d,d);
mt=tt_matrix(mt); %Create 2D Laplacian
                  %on  $2^d \times 2^d$  grid with Dirichlet BC
v=tt_ones(2*d,2);
v=tt_tensor(v); %Create vector of all ones
niter=4000; eps=1e-6;
tic;
for i=1:niter
    v=v/norm(v); v1=mt*v; ev=dot(v1,v);
    v=round(v,eps); %Round to avoid rank growth
    if ( ~mod(i,400) )
        fprintf('iter=%d ev=%d rank=%3.1f \n',i,ev,erank(v))
    end
end
toc
```

This is of course not the best way to compute the maximal eigenvalue and is presented only to illustrate how the Toolbox works. Actual results are

```
>> power_iter
iter=400 ev=7.969962e+00 rank=4.9
iter=800 ev=7.984991e+00 rank=4.6
iter=1200 ev=7.989996e+00 rank=4.6
iter=1600 ev=7.992498e+00 rank=4.6
iter=2000 ev=7.993998e+00 rank=4.4
```

```

iter=2400  ev=7.994999e+00  rank=4.4
iter=2800  ev=7.995714e+00  rank=4.5
iter=3200  ev=7.996249e+00  rank=4.7
iter=3600  ev=7.996666e+00  rank=4.7
iter=4000  ev=7.997000e+00  rank=4.6
Elapsed time is 33.076830 seconds.

```

If we set $d = 20$ then the output is

```

>> power_iter
iter=400  ev=7.969963e+00  rank=4.7
iter=800  ev=7.984991e+00  rank=4.0
iter=1200  ev=7.989996e+00  rank=3.9
iter=1600  ev=7.992498e+00  rank=3.9
iter=2000  ev=7.993999e+00  rank=3.9
iter=2400  ev=7.994999e+00  rank=3.8
iter=2800  ev=7.995714e+00  rank=3.9
iter=3200  ev=7.996249e+00  rank=4.0
iter=3600  ev=7.996666e+00  rank=4.0
iter=4000  ev=7.997000e+00  rank=4.0
Elapsed time is 65.257562 seconds.

```

Timing scales only linear in d . This is the *logarithmic complexity*. The accuracy of the eigenvector can be verified by computing the residue:

```

>> v=v/norm(v); ev=dot(mt*v,v); norm(mt*v-ev*v)/ev
ans =
    2.1651e-04
>>

```

The residue is not good enough due to the very bad eigenvalue solver for this problem.

8 Advanced routines

There are several advanced subroutines for *approximate basic operations*. These include:

1. `y=mvk(a,x,eps,nswp,y,rmax)` — multiplies TT-matrix A by a TT-vector x with accuracy `eps`. TT-tensor y can also be an initial approximation to Ax , `nswp` is the number of DMRG sweeps and `rmax` is the maximal rank of the result (sometimes needed to avoid extensive rank growth).

2. `y=funcrs(tt,fun,eps,y,nswp)` — computes function of a TT-tensor with accuracy `eps` using cross-DMRG method.

‘ Note, that these routines are only efficient for small mode sizes, i.e. for the QTT case ($n = 2$ or sometimes $m = 4$). There are several other subroutines in the subdirectory `exp`, you can try them out! Also, the most brave ones can try one cross approximation algorithm based on element evaluation, contained in the subdirectory `cross`. However, right now they are not as fast as they can be, due to MATLAB indexing (well, they are fast, but not as fast as I think they should be).

As an example, consider computation of the QTT-approximation of \sqrt{x} defined on $[0, 1]$ on a very fine grid, one can use the following code:

```
%funcrs.m: Example of cross-DMRG method
%for computing functions of TT-tensors
d=70; n=2^d; h=1.0./(n-1);
x=tt_x(d,2); %QTT-representation of x with ranks 2
x=tt_tensor(x); %Make it TT-tensor
fun = @(x) sqrt(x);
tic;
tt=funcrs(x,fun,1e-12,x,8);
toc;
```

The computation results are

```
>> fcrs
sweep=1, er=9.34e-02 er_nrm=1.00e+00
sweep=2, er=5.89e-09 er_nrm=3.49e-08
sweep=3, er=2.75e-13 er_nrm=2.98e-08
sweep=4, er=2.75e-13 er_nrm=5.27e-09
sweep=5, er=2.75e-13 er_nrm=2.79e-08
sweep=6, er=2.75e-13 er_nrm=2.79e-08
sweep=7, er=2.75e-13 er_nrm=2.79e-08
Elapsed time is 0.451595 seconds.
```

The convergence criteria for `funcrs` is not a well-developed subject, thus it is safer to perform several sweeps. The solution has very good ranks, which can be verified by calling `erank` command:

```
>> erank(tt)
ans =
    6.2815
```

To check the accuracy of this approximation on 2^{70} points, one can compute integral

$$\int_0^1 \sqrt{x} dx \approx h \sum_{k=1}^n f(x_k).$$

This can be realized via a scalar product of the TT-tensor with tensor of all ones. It should be compared with analytical value $\frac{2}{3}$:

```
>> p=tt_ones(d,2); p=tt_tensor(p); dot(p,tt)*h-2/3
ans =
    -2.3648e-14
```