Canonical forms of MPS

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Exercise (a): Complete the function that transforms MPSs into canonical forms

There is a function **`canonForm_Ex.m`** which is zipped together with this document. The function is designed to transform the input MPS `M` into left-, right-, and bond-canonical forms, depending on the index `id` of the target bond.

Moreover, one can also set criteria `Nkeep` and `Skeep`, for truncating small singular values and the corresponding singular vectors at each SVD. (Note that we do not consider degeneracies near the truncation threshold in this application, in contrast to iterative diagonalization.)

Read the documentation of the function for the details of its input and output properties.

The main computational parts of `canonForm_Ex` are missing; search for the keyword "TODO" to identify missing parts. **Complete the function.** You will notice that the function is wrapped by `try` ... `catch e` ... `end`, which is usefull for debugging.

To test whether the function is correctly implemented, let's consider the following example. First, define a random MPS `M`.

```
clear

N = 50; % number of sites
d = 3; % local space dimension
D = 30; % bond dimension

M = cell(1,N); % MPS; M{n} is the tensor at site n

for itN = (1:N)
    % assign individual tensors
    % leg order: left, right, bottom
    if itN == 1
    % left end; left leg is of size 1
        M{itN} = rand(1,D,d);
    elseif itN == N
    % right end; right leg is of size 1
        M{itN} = rand(D,1,d);
    else
        M{itN} = rand(D,D,d);
    end
end
```

Obtain the left-canonical form of `M`. We do not truncate singular values and vectors, by setting `Nkeep` = `[]` and `Skeep` = `0`.

```
[M_L,S_L] = canonForm_Ex(M,numel(M),[],0);
```

```
S_L
```

```
S_L = 1.8985e+69
```

Since `M` is not normalized from the outset, the norm S is not `1`; it's actually very huge!

We see that the sizes of the leftmost tensors have decreased after bringing into the left-canonical form.

```
M(1:5)
```

ans = 1×5 cell

	1	2	3	4	5
1	1×30×3 double	30×30×3 dou...	30×30×3 dou...	30×30×3 dou...	30×30×3 dou...

```
M_L(1:5)
```

ans = 1×5 cell

	1	2	3	4	5
1	1×3×3 double	3×9×3 double	9×27×3 double	27×30×3 dou...	30×30×3 dou...

Indeed, in this example, `M(1:3)` were redundantly large, so they could be compactified just via the thin SVD.

Compute the overlap between the transformed MPS (with the norm S pulled out) and the original one. It should be equal to the norm of the MPS.

```
Tovl = 1; % overlap
for itN = (1:N)
    Tovl = updateLeft(Tovl,2,M{itN},[],[],M_L{itN});
end
Tovl/S_L
```

```
ans = 1.0000
```

We can use `updateLeft` also to "close the zipper" from right, after permuting the left and right legs of the ket and bra tensors.

```
Tovl = 1; % overlap
for itN = (N:-1:1)
    Tovl = updateLeft(Tovl,2,permute(M{itN},[2 1 3]), ...
        [],[],permute(M_L{itN},[2 1 3]));
end
Tovl/S_L
```

```
ans = 1.0000
```

We can further bring `M_L` into the right-canonical form.

```
[M_R,S_R] = canonForm_Ex(M_L,0,[],0);
Tovl = 1; % overlap
for itN = (1:N)
    Tovl = updateLeft(Tovl,2,M{itN},[],[],M_R{itN});
end
Tovl/S_R
```

```
ans = 1.8985e+69
```

Now also the right-most tensors are compactified.

```
M(end-4:end)
```

ans = 1×5 cell

	1	2	3	4	5
1	30×30×3 dou...	30×30×3 dou...	30×30×3 dou...	30×30×3 dou...	30×1×3 double

```
M_R(end-4:end)
```

ans = 1×5 cell

	1	2	3	4	5
1	30×30×3 dou...	30×27×3 dou...	27×9×3 double	9×3×3 double	3×1×3 double

As the last check, let's consider the bond-canonical form.

```
[M_B,S_B] = canonForm_Ex(M,25,[],0);
Tovl = 1; % overlap
for itN = (1:N)
    Tovl = updateLeft(Tovl,2,M{itN},[],[],M_B{itN});
    if itN == 25
        Tovl = Tovl*diag(S_B);
    end
end
```

Here the overlap should equal to the squared norm, since the diagonal matrix of singular values is contracted in the middle.

```
Tovl/(S_L^2)
```

```
ans = 1.0000
```

Exercise (b): Truncate bond dimensions

Before solving this Exercise, it is necessary to solve Exercise 1 above, since we will use the function `canonForm_Ex.m` that brings the MPS into canonical forms.

In this Exercise, we will compare how the truncation of the bond space affects the norm of the MPS, for different canonical forms. Let's generate a random MPS again.

```
clear

N = 50; % number of sites
d = 3; % local space dimension
D = 30; % bond dimension

M = cell(1,N); % MPS; M{n} is the tensor at site n

for itN = (1:N)
```

```
    % assign individual tensors
    % leg order: left, right, bottom
    if itN == 1
    % left end; left leg is of size 1
        M{itN} = rand(1,D,d);
    elseif itN == N
    % right end; right leg is of size 1
        M{itN} = rand(D,1,d);
    else
        M{itN} = rand(D,D,d);
    end
end
```

Make a round trip, by first bringing `M` to the left- and then to the right-canonical form.

```
M = canonForm_Ex(M,numel(M),[],0); % left-canonical
M = canonForm_Ex(M,0,[],0); % right-canonical
```

With this right-canonical MPS `M` as the input to `canonForm_Ex.m`, apply the transformation into (i) left-canonical form, (ii) right-canonical form, and (iii) bond-canonical form for the bond between `M{25}` and `M{26}`, with different values of `Nkeep` < `D` = `30`, while keeping `Skeep` = `0`. How does the norm change? Can you explain the result?