## 3.4 The MCTDH and MCTDHF Approximations

Building on the results for abstract variational approximations in §3.2, we now turn to practically important and intensively studied approximations by specifying the approximation manifolds $\mathcal{M}$. To motivate the definition, we consider model reductions for finite-dimensional objects.

### 3.4.1 Singular value decomposition for matrices (SVD)

Consider a matrix $A \in \mathbb{R}^{n \times n}$.

Theorem: Every complex $n \times n$-matrix $A$ can be written as the product

$$A = USV^H = S \times_1 U \times_2 V = \sum_{i,j=1}^{n} s_{ij} u_i v_j^H =$$
$$= \sum_{i=1}^{n} \sigma_i u_i v_i^H ,$$

where $S = \mathrm{diag}(\sigma_1, \dots, \sigma_n)$, $B^H := \overline{B}^T$, $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$, $U = (u_1, \dots, u_n)$, $V = (v_1, \dots, v_n)$ ... are unitary $n \times n$ matrices, $\sigma_i$ ... "singular values", $u_i$ ... left singular vectors, $v_i$ ... right singular vectors.

Proof: [26, 27]

Theorem: (Approximation properties of SVD):

For a given matrix $A \in \mathbb{C}^{n\times n}$, the truncated SVD

$$A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^H$$

gives the best approximation of A of rank k

w.r.t. the spectral norm,

$$\|A\|_2 := \max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2},$$

i.e. $\min_{\mathrm{rank}(B)=k} \|A - B\|_2 = \|A - A_k\| = \sigma_{k+1}$.

The same holds for the Frobenius norm,

$$\|A\|_F := \left(\sum_{i,j=1}^{n} |a_{ij}|^2\right)^{1/2},$$

with

$$\|A - A_k\|_F = \left(\sum_{j=k+1}^{n} \sigma_j^2\right)^{1/2}$$

Proof: [26, 27]

Now, instead of requiring best approximation, we alternatively propose to use a variational principle:

Compute $Y \in \mathcal{M}_r$,

$\mathcal{M}_r := \{ Y = USV^H : U, V \in \mathbb{C}^{n\times r}$ unitary, $S \in \mathbb{C}^{r\times r} \}$

such that

$$\langle \delta Y | \dot{Y} - \dot{A} \rangle_F = 0 \quad \forall \delta Y \in T_Y \mathcal{M}_r . \qquad (*)$$

The inner product $\langle \cdot | \cdot \rangle_F$ is that associated with the Frobenius norm, $\langle A | B \rangle_F = \mathrm{tr}(A^H B) = \sum_{i,j=1}^{n} \bar{a}_{ij} b_{ij}$.

$T_Y \mathcal{M}_r = \{ \delta Y = \delta U S V^H + U \delta S V^H + US(\delta V)^H :$
$\delta U, \delta V \in \mathbb{C}^{n\times r}, \delta S \in \mathbb{C}^{r\times r} \}$

To derive differential equations for $U, S, V$ from $(*)$, we furthermore impose

$$\dot{U}^H U = \dot{V}^H V = 0 .$$

Now, choose

1) $\delta Y = u_i v_j^H$:

$$\langle \delta Y | \dot{Y} - \dot{A} \rangle_F = \langle u_i v_j^H | \sum_{k,l=1}^{r} ( \dot{s}_{kl} u_k v_l^H + s_{kl} \dot{u}_k v_l^H + \dots$$

$$\dots + s_{kl} u_k \dot{v}_l^H ) - \dot{A} \rangle_F =$$

$$= \langle u_i | \sum_{k=1}^{r} ( \dot{s}_{kj} u_k + s_{kj} \dot{u}_k ) - \dot{A} v_j \rangle = \dot{s}_{ij} - u_i^H \dot{A} v_j \equiv 0$$

2) $\delta Y = \sum_{j=1}^{r} s_{ij}\, \delta u_i\, v_j^H, \quad \delta u_i \perp \{u_1, \dots, u_r\}$

$$\langle \delta Y \,|\, \dot{Y} - \dot{A} \rangle_F = \Big\langle \sum_{j=1}^{r} s_{ij}\, \delta u_i\, v_j^H \,\Big|\, \cdots$$

$$\cdots \Big|\, \sum_{k,l=1}^{r} \left( \dot{s}_{kl}\, u_k v_l^H + s_{kl}\, \dot{u}_k v_l^H + s_{kl}\, u_k \dot{v}_l^H \right) - \dot{A} \Big\rangle_F =$$

$$= \sum_{j=1}^{r} \bar{s}_{ij} \Big\langle \delta u_i \,\Big|\, \sum_{k=1}^{r} \left( \dot{s}_{kj}\, u_k + s_{kj}\, \dot{u}_k \right) - \dot{A} v_j \Big\rangle =$$

$$= \Big\langle \delta u_i \,\Big|\, \sum_{j,k=1}^{r} \bar{s}_{ij}\, s_{kj}\, \dot{u}_k - \sum_{j=1}^{r} \bar{s}_{ij}\, \dot{A} v_j \Big\rangle = 0$$

Define $P_U := \sum_{j=1}^{r} u_j u_j^H$, $P_U^\perp := I - P_U$

(and analogously $P_V, P_V^\perp$). Then

$$P_U^\perp \dot{U} S S^H = P_U^\perp \dot{A} V S^H$$

$$\dot{U} = P_U^\perp \dot{A} V S^{-1}$$

Analogously,

$$\dot{V} = P_V^\perp \dot{A}^H U S^{-H}$$

The resulting equations of motion are

$$\dot{S} = U^H \dot{A} V$$

$$\dot{U} = P_U^\perp \dot{A} V S^{-1}$$

$$\dot{V} = P_V^\perp \dot{A}^H U S^{-H}$$

Note: The right-hand-side only contains $\dot{A}$, which may be significantly sparser than $A$!

The procedure has been denoted as "dynamical low rank approximation" [28].
The approximation can be shown to be quasi-optimal on the approximation manifold, and the error grows only linearly in $t$ under certain assumptions. The results are shown together with numerical examples at

http://www.othmar-koch.org/slides_dlra.pdf

The approach can be generalized to higher order tensors $\mathcal{A} \in \mathbb{C}^{N_1 \times \cdots \times N_f}$,

$$\mathcal{A}(t) \approx \mathcal{U}(t) = S \times_1 \phi^{(1)} \times_2 \cdots \times_f \phi^{(f)} =$$

$$= \sum_{j_1=1}^{n_1} \cdots \sum_{j_f=1}^{n_f} s_{j_1 \cdots j_f}(t)\, \phi_{j_1}^{(1)}(t) \otimes_1 \cdots \otimes_{f-1} \phi_{j_f}^{(f)}(t)$$

The tensor $\mathcal{U}$ is given in the form of a "Tucker decomposition" of "low rank"

Remark: There are different concepts of tensor rank, which for order $> 2$ do not coincide!

The tensor-DLRA equations of motion, approximation results and numerical examples are given in

http://www.othmar-koch.org/slides_dlra.pdf