Theory of low rank approximations

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Theorem 1. *Let $A \in \mathbb{R}^{m \times n}$ for $m \geq n$ be a matrix with the SVD decomposition $A = U\Sigma V^T$. Then the best approximation of A in Frobenious norm is given by*

$$A_k = argmin \|X - A\|_F$$

where we restrict X such that $rank(X) = k$. The best approximation is on the form

$$A_k = \sum_{i=1}^{k} \sigma_i(A) \boldsymbol{u}_i \boldsymbol{v}_i^T$$

Proof. As the Frobenious norm of a matrix A is given by $\|A\|_F = (\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2)^{\frac{1}{2}}$ we have that

$$\begin{aligned} \|A\|_F^2 &= \|U\Sigma V^T\|_F^2 \\ &= \|\Sigma\|_F^2 \\ &= \sum_{i=1}^{n} \sigma_i(A)^2 \end{aligned}$$

Furthermore by Von Neumanns trace inequality we have that

$$| < A, B >_F | \leq \sum_{i=1}^{n} \sigma_i(A) \sigma_i(B)$$

Hence we can find the lower bound for the Frobenious norm

$$\begin{aligned} \|X - A\|_F^2 &= < X - A, X - A >_F \\ &= \|A\|_F^2 - 2 < A, X >_F + \|X\|_F^2 \\ &\geq \sum_{i=1}^{n} \sigma_i(A)^2 - 2 \sum_{i=1}^{n} \sigma_i(A) \sigma_i(X) + \sum_{i=1}^{n} \sigma_i(X)^2 \\ &= \sum_{i=1}^{n} (\sigma_i(A) - \sigma_i(X))^2 \end{aligned}$$

where it should be noted that this part is heavily inspired by [p. 58 Mirsky][1].

If $\sigma_1(A) \geq \sigma_2(A) \geq \cdots \geq \sigma_n(A)$ and X is of rank k, then it is evident that we attain the lower bound when we have X such that $\sigma_i(A) = \sigma_i(X)$ for $i = 1, \cdots, k$ and hence the lower bound is

$$\|X - A\|_F^2 \geq \sum_{i=k+1}^{n} \sigma_i(A)^2$$

It is then trivial to show that the lower bound is attained by $A_k = \sum_{i=1}^{k} \sigma_i(A) \boldsymbol{u}_i \boldsymbol{v}_i^T = U_k \Sigma_k V_k^T$

$$\begin{aligned}
\|A_k - A\|_F^2 &= \|U_k \Sigma_k V_k^T - U \Sigma V^T\|_F^2 \\
&= \|U \Sigma_k V^T - U \Sigma V^T\|_F^2 \\
&= \|\Sigma_k - \Sigma\|_F^2 \\
&= \sum_{i=1}^{k} (\sigma_i(A) - \sigma_i(A))^2 + \sum_{i=k+1}^{n} \sigma_i(A)^2 \\
&= \sum_{i=k+1}^{n} \sigma_i(A)^2
\end{aligned}$$

Hence A_k is the best approximation of rank k in the Frobenious norm. □

Theorem 2. *Let $A \approx P_k B_k Q_k^T$ be the approximation of $A \in \mathbb{R}^{m \times n}, n \leq m$ by Lanczos bidiagonalization, where B is lower bidiagonal. Then the columns of Q_k, P_k are orthonormal.*

Proof. We will in the proceeding proof refer to the notation used to describe the Lanczos bidiagonalization in [2]. Lets first show that

$$\begin{aligned}
< u_1, u_2 > = 0 \\
< v_1, v_2 > = 0
\end{aligned}$$

$\|u_1\|_2 = \|v_1\|_2 = 1$ is true by how the algorithm is initialized, from this we also can see that $\alpha_1 = v_1^T A^T u_1 = u_1^T A v_1$. Hence we have

$$\begin{aligned}
< u_1, u_2 > &= \frac{1}{\beta_2} u_1^T (A v_1 - \alpha_1 u_1) \\
&= \frac{1}{\beta_2} (\alpha_1 - \alpha_1 u_1^T u_1) = 0 \\
< v_1, v_2 > &= \frac{1}{\alpha_2} v_1^T (A^T u_2 - \beta_2 v_1) \\
&= \frac{1}{\alpha_2} (v_1^T A^T u_2 - v_1^T A^T u_2 v_1^T v_1) = 0,
\end{aligned}$$

where we in the last line used that $\beta_2 = u_2^T A v_1 - \alpha_1 u_2^T u_1 = u_2^T A v_1$. It could also be shown that $< u_2, u_2 >=< v_2, v_2 >= 1$, but this follows directly from the algorithm, as we normalize u_2, v_2 using α_2, β_2.

We will now proceed with an induction hypothesis. Lets assume that, for some l such that $1 < l < k$ we have that

$$\begin{aligned} &< u_i, u_j > = \delta_{i,j} \\ &< v_i, v_j > = \delta_{i,j} \text{ for } 1 \leq i, j \leq l. \end{aligned}$$

We then prove that from this assumption, orthogonality holds in general, for $l < i, j \leq k$. From the assumption we see the following (for $1 \leq i, j \leq l$)

$$\alpha_i = v_i^T A^T u_i - \beta_i v_i^T v_{i-1} = v_i^T A^T u_i$$

We have

$$\begin{aligned} < u_i, u_{j+1} > &= \frac{1}{\beta_{j+1}} u_i^T (A v_j - \alpha_j u_j) \\ &\overset{(i=j=l)}{=} \frac{1}{\beta_{l+1}} (u_l^T A v_l - \alpha_l u_l^T u_l) = \frac{1}{\beta_{l+1}} (\alpha_l - \alpha_l) = 0 \end{aligned}$$

$$\begin{aligned} < v_i, v_{j+1} > &= \frac{1}{\alpha_{j+1}} v_i^T (A^T u_{j+1} - \beta_{j+1} v_j) \\ &= \frac{1}{\alpha_{j+1}} (v_i^T A^T u_{j+1} - u_{j+1}^T A v_j v_i^T v_j - \alpha_j u_{j+1}^T u_j v_i^T v_j) \\ &\overset{(i=j=l)}{=} \frac{1}{\alpha_{l+1}} (v_l^T A^T u_{l+1} - u_{l+1}^T A v_l - \alpha_l u_{l+1}^T u_l) \\ &= \frac{\alpha_l}{\alpha_{l+1}} u_{l+1}^T u_l = 0 \end{aligned}$$

hence we have shown that the vectors u_{l+1}, v_{l+1} is orthogonal to its preceeding $u_i, v_i, i \leq l$. They are also normalized

$$
\begin{aligned}
< v_i, v_{j+1} > &= \frac{1}{\alpha_{j+1}}(v_i^T A^T u_{j+1} - u_{j+1}^T A v_j v_i^T v_j - \alpha_j u_{j+1}^T u_j v_i^T v_j) \\
&\overset{(i=j+1=l+1)}{=} \frac{1}{\alpha_{l+1}}(v_{l+1}^T A^T u_{l+1} - u_{l+1}^T A v_l v_{l+1}^T v_l - \alpha_l u_{l+1}^T u_l v_{l+1}^T v_l) \\
&= \frac{1}{\alpha_{l+1}}(v_{l+1}^T A^T u_{l+1}) = \frac{1}{\alpha_{l+1}}(v_{l+1}^T(\alpha_{l+1} v_{l+1} + \beta_{l+1} v_l)) = \frac{\alpha_{l+1}}{\alpha_{l+1}} = 1
\end{aligned}
$$

$$
\begin{aligned}
< u_i, u_{j+1} > &= \frac{1}{\beta_{j+1}}(\alpha_i v_i^T v_j + \beta_i v_{i-1}^T v_j - \alpha_j u_i^T u_j) \\
&\overset{(i=j+1=l+1)}{=} \frac{1}{\beta_{l+1}}(\alpha_{l+1} v_{l+1}^T v_l + \beta_{l+1} v_l^T v_l - \alpha_l u_{l+1}^T u_l) \\
&= \frac{\beta_{l+1}}{\beta_{l+1}} = 1
\end{aligned}
$$

To conclude, we have shown that the assumption is indeed true for $l = 2$. And when assuming orthogonality for $u_i, v_i, i \leq l$ orthogonality follows for u_{l+1}, v_{l+1}. Hence, by induction, $P_k := [u_1, \cdots, u_k], Q_k := [v_1, \cdots, v_k]$ have orthonormal columns. $\square$

Theorem 3. *Let $U \in \mathbb{R}^{m\times k}$ with orthogonal columns and $B \in \mathbb{R}^{m\times m}$ be skew symmetric, i.e. that $B^T = -B$. Then for*

$$\bar{U} = cay(B)U$$

$\bar{U}$ has orthogonal columns.

Proof. Lets first show that the terms of the Cayley transform commutes

$$
\begin{aligned}
(I - \frac{1}{2}B)^{-1}(I + \frac{1}{2}B) &= (I - \frac{1}{2}B)^{-1}((I - \frac{1}{2}B)(-1) + 2I) \\
&= 2(I - \frac{1}{2}B)^{-1} \\
&= (I + \frac{1}{2}B)(I - \frac{1}{2}B)^{-1}
\end{aligned}
$$

Which enables us to prove that $\mathrm{cay}(B)$ is orthogonal when B is skew symmetric

$$
\begin{aligned}
\mathrm{cay}(B)^T \mathrm{cay}(B) &= (I + \frac{1}{2}B)^T (I - \frac{1}{2}B)^{-T} (I - \frac{1}{2}B)^{-1} (I + \frac{1}{2}B) \\
&= (I - \frac{1}{2}B)(I + \frac{1}{2}B)^{-1}(I - \frac{1}{2}B)^{-1}(I + \frac{1}{2}B) \\
&= (I + \frac{1}{2}B)^{-1}(I - \frac{1}{2}B)(I - \frac{1}{2}B)^{-1}(I + \frac{1}{2}B) \\
&= I
\end{aligned}
$$

This gives us the following

$$
\begin{aligned}
\bar{U}^T\bar{U} &= U^T \text{cay}(B)^T \text{cay}(B) U \\
&= U^T U
\end{aligned}
$$

As U has orthonormal columns, then it follows that $\bar{U}$ has orthonormal columns. $\square$

Theorem 4. *Let $C = [F_U, -U], D = [U, F_U], C, D \in \mathbb{R}^{m\times 2k}$, and $F_U = U^\perp R_{2,2}$ be the QR-factorization. Then the Cayley transformation of CD^T could be expressed as*

$$
cay(CD^T) = I + [U, U^\perp]\begin{bmatrix} 0 & -R_{2,2}^T \\ R_{2,2} & 0 \end{bmatrix}\left(I - \frac{1}{2}\begin{bmatrix} 0 & -R_{2,2}^T \\ R_{2,2} & 0 \end{bmatrix}\right)^{-1}[U, U^\perp]^T.
$$

Proof. Analytic functions such as the cayley transformation have power series expansions for a suitable choice of coefficients α, on the form

$$
\text{cay}(B) = \sum_{i=0}^{\infty}\alpha_i B^i
$$

And for $B = CD^T$ it is possible to show that, if we can rewrite the power series as

$$
\phi(B) = \alpha_0 I + C\sum_{i=1}^{\infty}\alpha_i (D^T C)^{i-1} D^T
$$

then we can write the Cayley transform as

$$
\text{cay}(CD^T) = I + C(I + \frac{1}{2}D^T C)^{-1} D^T.
$$

With the given QR-decomposition of F_U we can write CD^T on the form

$$
CD^T = [U, U^\perp]\underbrace{\begin{bmatrix} 0 & -R_{2,2}^T \\ R_{2,2} & 0 \end{bmatrix}}_{=R}[U, U^\perp]^T.
$$

Let now $W = [U, U^\perp] \in \mathbb{R}^{m\times 2k}$ and $R \in \mathbb{R}^{2k\times 2k}$ be the above matrix with the upper diagonal QR-terms $R_{2,2}$. We can then show that the middle terms collapse when taking powers of B, i.e. that

$$
\begin{aligned}
B^i &= W\underbrace{RW^TWR}_{=R^2}W^T \cdots W\underbrace{RW^TWR}_{=R^2}W^T \\
&= WR^{i-2}\underbrace{RW^TWR}_{=R^2}W^T \\
&= WR^iW^T
\end{aligned}
$$

this is a fact, as we have

$$
\begin{aligned}
WRW^TWRW^T &= WR\begin{bmatrix} I & U^TU^\perp \\ U^\perp U^T & I \end{bmatrix} RW^T \\
&= W\begin{bmatrix} -R_{2,2}^TR_{2,2} & 0 \\ 0 & -R_{2,2}^TR_{2,2} \end{bmatrix} W^T \\
&= WR^2W^T.
\end{aligned}
$$

This enables us to construct a power series in a similar fashion as above

$$
\begin{aligned}
\mathrm{cay}(B) = \phi(B) &= \alpha_0 I + W\sum_{i=1}^{\infty}\alpha_i R^i W^T \\
&= \alpha_0 I + W(\phi(R) - I)W^T \\
&= \alpha_0 I + WR(I - \frac{1}{2}R)^{-1}W^T
\end{aligned}
$$

Where we used that

$$
\begin{aligned}
\phi(R) - I &= (I + \frac{1}{2}R)(I - \frac{1}{2}R)^{-1} - I && (1) \\
&= (I + \frac{1}{2}R - I + \frac{1}{2}R)(I - \frac{1}{2}R)^{-1} && (2) \\
&= R(I - \frac{1}{2}R)^{-1} && (3)
\end{aligned}
$$

which yields the expression we set out to prove

$$
\mathrm{cay}(CD^T) = I + [U, U^\perp]\begin{bmatrix} 0 & -R_{2,2}^T \\ R_{2,2} & 0 \end{bmatrix}\left(I + \frac{1}{2}\begin{bmatrix} 0 & -R_{2,2}^T \\ R_{2,2} & 0 \end{bmatrix}\right)^{-1}[U, U^\perp]^T.
$$

$\square$

References

[1] L. Mirsky. Symmetric gauge functions and unitraily invariant norms. *The Quarterly Journal of Mathematics*, 11(1):50–59, 01 1960. ISSN 0033-5606. doi: 10.1093/qmath/11.1.50. URL https://doi.org/10.1093/qmath/11.1.50.

[2] Horst Simon. Low rank matrix approximation using the lanczos bidiagonalization process with applications. *SIAM Journal on Scientific Computing*, 21, 10 1997. doi: 10.1137/S1064827597327309.