II.3 Matrix-factorization

- required for basically any optimization problem
- required for many compression algorithms
- required for finding optimized basis sets

QR decomposition

- Building block of most factorizations.
- Consider $\underline{\underline{A}} \in V_{\mathbb{R}}^{m \times n}$, $m, n \in \mathbb{N}$

  If $m = n$, then there are

  $\underline{\underline{Q}}, \underline{\underline{R}} \in V_{\mathbb{R}}^{m \times m}$ with

  (i) $\underline{\underline{A}} = \underline{\underline{Q}} \cdot \underline{\underline{R}}$

  (ii) $\underline{\underline{Q}}^{-1} = \underline{\underline{Q}}^{\dagger}$

  (iii) $\underline{\underline{R}}$ is upper triangular

- if $\underline{\underline{A}} \in V_{\mathbb{C}}^{m \times n}$, $m \geq n$, then there is $\underline{\underline{Q}} \in V_{\mathbb{C}}^{m \times m}$ unitary matrix with:

$$\underline{\underline{A}} = \underline{\underline{Q}} \begin{bmatrix} \underline{\underline{R}} \\ \underline{\underline{0}} \end{bmatrix}$$

where $\underline{\underline{R}} \in V_{\mathbb{C}}^{n\times n}$ is upper triangular & $\underline{\underline{O}}$ is the $(m-n)\times n$ zero matrix.

Computation of $\underline{\underline{Q}}$ & $\underline{\underline{R}}$

(i) Gram-Schmidt-orthogonalization to columns $\underline{a}_j$ of $\underline{\underline{A}} = \left(\underline{a}_1 \; \underline{a}_2 \; \cdots \; \underline{a}_n\right)$

Idea: compute projectors for some vector $\underline{u}$:

$$\underline{\underline{P}}^{\underline{u}} = \frac{|\underline{u}\rangle\langle \underline{u}|}{\|\underline{u}\|}$$

Iterate:

$$\underline{u}_1 = \frac{\underline{a}_1}{\|\underline{a}_1\|}$$

$$\underline{u}_2 = \left(\underline{\underline{1}} - \underline{\underline{P}}^{\underline{u}_1}\right)\underline{a}_2 = \underline{a}_2 - \frac{\langle \underline{u}_1 | \underline{a}_2\rangle}{\|\underline{u}_2\|}\underline{u}_1$$

$$\underline{u}_3 = \left(\underline{\underline{1}} - \underline{\underline{P}}^{\underline{u}_1} - \underline{\underline{P}}^{\underline{u}_2}\right)\underline{a}_3 = \underline{a}_3 - \frac{\langle \underline{u}_2 | \underline{a}_3\rangle}{\|\underline{u}_2\|}\underline{a}_3 - \frac{\langle \underline{u}_1 | \underline{a}_3\rangle}{\|\underline{u}_1\|}\underline{a}_3$$

$$\vdots$$

$$\underline{u}_k = \left(\underline{\underline{1}} - \sum_{j=1}^{k-1} \underline{\underline{P}}^{\underline{u}_j}\right)\underline{a}_k$$

Then $\underline{e}_k = \frac{\underline{u}_k}{\|\underline{u}_k\|}$ are orthonormal basis & we can express the columns $\underline{a}_j$ in that basis:

$$\underline{a}_k = \sum_{j=1}^{k} \langle \underline{e}_j | \underline{a}_k\rangle \underline{e}_j$$

$$\Rightarrow \quad \underline{\underline{A}} = \underbrace{\begin{pmatrix} - \underline{e}_1 - \\ - \underline{e}_2 - \\ \vdots \\ - \underline{e}_n - \end{pmatrix}}_{\underline{\underline{Q}}} \underbrace{\begin{pmatrix} \langle \underline{e}_1 | \underline{a}_1 \rangle & \langle \underline{e}_1 | \underline{a}_2 \rangle & \cdots & \langle \underline{e}_1 | \underline{a}_n \rangle \\ 0 & \langle \underline{e}_2 | \underline{a}_2 \rangle & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \langle \underline{e}_n | \underline{a}_n \rangle \end{pmatrix}}_{\underline{\underline{R}}}$$

But involvement of inverse $\|\underline{u}_j\|^{-1}$ numerically unstable (finite precision arithmetics!)

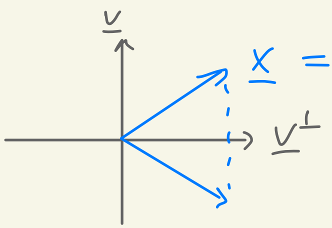
Better: Householder transformations

Basic building block is a reflection of a vector $\underline{x} \in V_{\mathbb{K}}^n$ at a hyperplane generated from a vector $\underline{v} \in V_{\mathbb{K}}^n$:

For $\underline{v} \in V_{\mathbb{K}}^n$ with $\|\underline{v}\| = 1$ define:

$$\underline{\underline{Q}} = \underline{\mathbb{1}} - 2 |\underline{v}\rangle\langle\underline{v}|$$

2D-illustration $\underline{\underline{Q}} \cdot \underline{x}$:



$$\underline{x} = \langle \underline{v} | \underline{x} \rangle |\underline{v}\rangle + \langle \underline{v}^\perp | \underline{x} \rangle |\underline{v}^\perp\rangle$$

Let us choose for some $\underline{x} \in V_{\mathbb{R}}^n$

$$\underline{v} = c^{-1}(\underline{x} - \alpha \underline{e}_1) \quad \text{with } \alpha = \|\underline{x}\| \ \& \ c = \|\underline{x} - \alpha \underline{e}_1\|$$

Then we have

$$\underline{\underline{Q}} \cdot \underline{x} = (\mathbb{1} - 2|\underline{v}\rangle\langle\underline{v}|)\,\underline{x}$$

$$= \underline{x} - 2\langle \underline{v}|\underline{x}\rangle\, \underline{v} = \underline{x}\left(1 - \frac{2}{c}\langle\underline{v}|\underline{x}\rangle\right) + \frac{2\alpha}{c}\langle\underline{v}|\underline{x}\rangle \underline{e}_1$$

using $\langle\underline{v}|\underline{x}\rangle = \dfrac{\langle\underline{x}|\underline{x}\rangle - \alpha\langle\underline{e}_1|\underline{x}\rangle}{c} = \dfrac{\alpha^2 - \alpha\langle\underline{e}_1|\underline{x}\rangle}{c}$

& $c^2 = \langle\underline{x}|\underline{x}\rangle - 2\alpha\langle\underline{x}|\underline{e}_1\rangle + \alpha^2 = 2\left(\alpha^2 - \alpha\langle\underline{x}|\underline{e}_1\rangle\right)$

$$\Rightarrow \underline{\underline{Q}} \cdot \underline{x} = \alpha\, \underline{e}_1$$

Thus we can use $\underline{\underline{Q}} \equiv \underline{\underline{Q}}^{(1)}$ & $\underline{x} = \underline{a}_1$ to transform the first column vector of $\underline{\underline{A}}$:

$$\underline{\underline{Q}}^{(1)} \underline{\underline{A}} = \begin{pmatrix} \alpha_1 & \underline{\underline{Q}}^{(1)}\underline{a}_2 & \cdots \\ 0 & & \\ \vdots & \underline{\underline{A}}^{(1)} & \\ 0 & & \end{pmatrix}$$

applying this construction scheme recursively

using $\tilde{\underline{\underline{Q}}}^{(k)} = \begin{pmatrix} \mathbb{1}_{k-1 \times k-1} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{Q}}^{(k)} \end{pmatrix}$ we obtain

$$\underline{\underline{R}} = \tilde{\underline{\underline{Q}}}^{(n)} \tilde{\underline{\underline{Q}}}^{(n-1)} \cdots \underline{\underline{Q}}^{(1)} \underline{\underline{A}}$$

$\Rightarrow$ defining $\underline{\underline{Q}} = (\underline{\underline{\tilde{Q}}}^{(n)} \cdots \underline{\underline{\tilde{Q}}}^{(1)})^t$ & using unitarity of Householder trafos we get

$$\underline{\underline{A}} = \underline{\underline{Q}} \cdot \underline{\underline{R}}$$

numerical costs:

at k-th iteration we have:

- $(n-(k-1))^2$ multiplications from $|\underline{v}\rangle\langle\underline{v}|$
- $(n-(k-1))^2$ multiplications from $\langle\underline{v}|\underline{a}_j\rangle$

summing over $k=1$ to $k=n-1$ yields $\sim \mathcal{O}(n^3)$

Eigenvalue decomposition (EVD)

$\underline{\underline{A}} \in V_{\mathbb{C}}^{m\times m}$:

$\exists\ \underline{\underline{U}} \in V_{\mathbb{C}}^{m\times m}$ & diagonal matrix $\underline{\underline{D}} \in V_{\mathbb{C}}^{m\times m}$

with $\underline{\underline{A}} = \underline{\underline{U}}\,\underline{\underline{D}}\,\underline{\underline{U}}^{-1}$

If $\underline{\underline{A}} = \underline{\underline{A}}^{+}$ then $\underline{\underline{U}}^{-1} = \underline{\underline{U}}^{+}$ & $\underline{\underline{D}} \in V_{\mathbb{R}}^{m\times m}$

It follows immediately:

$$\underline{\underline{U}} = \begin{pmatrix} | & & | \\ \underline{v}_1 & \cdots & \underline{v}_m \\ | & & | \end{pmatrix} \quad \text{with } \underline{\underline{A}}\,|\underline{v}_i\rangle = \lambda_i |\underline{v}_i\rangle, \quad \lambda_i \in \mathbb{R}$$

The power method

Consider $|\underline{x}\rangle \in V_{\mathbb{C}}^{n \times n}$ & $\langle \underline{x} | \underline{v}_i \rangle = c_i \neq 0$ for all $|\underline{v}_i\rangle$

Expand $|\underline{x}\rangle$ in Basis of $\{ |\underline{v}_i\rangle \}$ & act with $\underline{\underline{A}}$ on $|\underline{x}\rangle$:

$$\underline{\underline{A}} |\underline{x}\rangle = \underline{\underline{A}} \sum_{i=1}^{n} \langle \underline{v}_i | \underline{x} \rangle | \underline{v}_i \rangle$$

$$= \underline{\underline{A}} \left(c_1 |\underline{v}_1\rangle + c_2 |\underline{v}_2\rangle + \dots \right)$$

$$= \lambda_1 \left(c_1 |\underline{v}_1\rangle + \frac{c_2}{c_1} |\underline{v}_2\rangle + \frac{c_3}{c_1} |\underline{v}_3\rangle + \dots \right)$$

assume:

(i) λ_i ordered such that:

$$i > j \Rightarrow \lambda_i \geq \lambda_j$$

(ii) $\underline{\underline{A}}$ non-deg: $i \neq j \Leftrightarrow \lambda_i \neq \lambda_j$

Note: (ii) is rather severe, (i) can always be achieved. (ii) can be resolved by orthogonalization.

Then we have for arbitrary $k \in \mathbb{N}$:

$$\underline{\underline{A}}^k |\underline{x}\rangle = \lambda_1^k \left(c_1 |\underline{v}_1\rangle + \sum_{j=2}^{n} \left(\frac{\lambda_j}{\lambda_1}\right)^k c_j |\underline{v}_j\rangle \right)$$

$$\overset{k\to\infty}{=} \lambda_1^k c_1 |\underline{v}_1\rangle$$

This suggests the following algorithm:

(i) apply $\underline{\underline{A}}$ to $|\underline{x}^j\rangle$ to obtain

$$|\underline{\tilde{x}}^{j+1}\rangle = \underline{\underline{A}} |\underline{x}^j\rangle$$

(ii) normalize to obtain

$$|\underline{x}^{j+1}\rangle = \frac{|\underline{\tilde{x}}^{j+1}\rangle}{\| |\underline{\tilde{x}}^{j+1}\rangle \|}$$

starting with $|\underline{x}^0\rangle \equiv |\underline{x}\rangle$ repeat until

$$\underline{\mathbb{1}} - \langle \underline{x}^{j+1} | \underline{x}^j \rangle < \delta$$

with δ being precision of approx. of eigenvector $|\underline{v}^1\rangle$ belonging to largest eigenvalue.

Drawback:

If we want to get $n > 1$ eigenvalues, we have to restart $n-1$ times orthogonalizing $|\underline{x}^0\rangle$ against all prev. found eigenvectors:

$$|\underline{x}^{0,n}\rangle = |\underline{x}\rangle - \sum_{j=1}^{n-1} \langle \underline{v}_j | \underline{x}\rangle |\underline{v}_j\rangle$$

Simultaneous orthogonalization (SO)

Idea: Do orthogonalization after each application of $\underline{\underline{A}}$ to maintain linear independence.

consider $\underline{\underline{A}}\,|\underline{x}\rangle = \underline{\underline{Q}}^{(1)} \cdot \underline{\underline{R}}^{(1)} |\underline{x}\rangle$

$$\underline{\underline{A}}^2 |\underline{x}\rangle = \underbrace{\underline{\underline{A}} \cdot \underline{\underline{Q}}^{(1)}}_{\underline{\underline{Q}}^{(2)} \cdot \underline{\underline{R}}^{(2)}} \cdot \underline{\underline{R}}^{(1)} |\underline{x}\rangle$$

$$\Rightarrow \underline{\underline{A}}^k |\underline{x}\rangle = \underline{\underline{Q}}^{(k)} \cdot \underline{\underline{R}}^{(k)} \cdot \underline{\underline{R}}^{(k-1)} \cdots \underline{\underline{R}}^{(1)} |\underline{x}\rangle$$

Thus if $\underline{\underline{A}}^k |\underline{x}\rangle$ converges to some $\in V_{\mathbb{C}}^n$, then $\underline{\underline{Q}}^{(k)}$ is matrix of eigenvectors. This can be shown using fact that $\underline{\underline{Q}} \cdot \underline{\underline{A}}$ represents $\underline{\underline{A}}$ in basis obtained from Gram-Schmidt-orthog., such that $\underline{\underline{Q}} \cdot \underline{\underline{A}} |\underline{v}_1\rangle = \lambda_1 |\underline{e}_1\rangle$.

Let us investigate a particular property of the intermediate steps in the simultaneous orthogonalization:

$$\underline{\underline{A}} = \underline{\underline{Q}}^{(1)} \underline{\underline{R}}^{(1)} \Rightarrow \underline{\underline{Q}}^{(1)\dagger} \underline{\underline{A}} = \underline{\underline{R}}^{(1)}$$

$$\underline{\underline{A}}\,\underline{\underline{Q}}^{(1)} = \underline{\underline{Q}}^{(2)} \underline{\underline{R}}^{(2)} \Rightarrow \underline{\underline{Q}}^{(2)\dagger} \underline{\underline{A}}\,\underline{\underline{Q}}^{(1)} = \underline{\underline{R}}^{(2)}$$

$$\vdots$$

$$\underline{\underline{A}}\,\underline{\underline{Q}}^{(k)} = \underline{\underline{Q}}^{(k+1)} \underline{\underline{R}}^{(k+1)} \Rightarrow \underline{\underline{Q}}^{(k+1)\dagger} \underline{\underline{A}}\,\underline{\underline{Q}}^{(k)} = \underline{\underline{R}}^{(k+1)}$$

Note that iterations k & $k+1$ can be connected multiplying $\underline{\underline{R}}^{(k)} \cdot \underline{\underline{R}}^{(k-1)}$ (see yellow marked matrices):

$$\Rightarrow \underline{\underline{R}}^{(k)} \cdot \underline{\underline{R}}^{(k-1)} \cdot \ldots \cdot \underline{\underline{R}}^{(1)} = \underline{\underline{Q}}^{(k)\dagger} \underline{\underline{A}}\,\underline{\underline{Q}}^{(k-1)} \underline{\underline{Q}}^{(k-1)\dagger} \underline{\underline{A}} \cdots \underline{\underline{Q}}^{(1)} \underline{\underline{Q}}^{(1)\dagger} \underline{\underline{A}}$$

$$= \underline{\underline{Q}}^{(k)\dagger} \underline{\underline{A}}^{k}$$

$$\Rightarrow \underline{\underline{A}}^{k} = \underline{\underline{Q}}^{(k)} \cdot \underbrace{\underline{\underline{R}}^{(k)} \cdot \underline{\underline{R}}^{(k-1)} \cdot \ldots \cdot \underline{\underline{R}}^{(1)}}_{\text{upper triangular !}}$$

Since QR-decomposition is unique, this yields the QR-decomposition of k-th power of $\underline{\underline{A}}$!

Thus also: $\underline{\underline{Q}}^{(k)}$ is approx. to matrix of eigenvectors

QR-algorithm (John Francis (1959) / Vera Kublanovskaya (1961))

Sketch of the idea here only:

(i) QR-decompose $\underline{\underline{A}}$: $\underline{\underline{A}} = \underline{\underline{A}}^{(1)} = \underline{\underline{Q}}^{(1)} \cdot \underline{\underline{R}}^{(1)}$

(ii) construct $\underline{\underline{A}}^{(2)} = \underline{\underline{R}}^{(1)} \underline{\underline{Q}}^{(1)}$

(iii) QR-decompose $\underline{\underline{A}}^{(2)} = \underline{\underline{Q}}^{(2)} \underline{\underline{R}}^{(2)}$ & continue from (ii)

note that at k-th iteration:

$$\underline{\underline{A}}^{(k+1)} = \underline{\underline{R}}^{(k)} \underline{\underline{Q}}^{(k)} = \left(\underline{\underline{Q}}^{(k)}\right)^{\dagger} \underbrace{\underline{\underline{Q}}^{(k)} \underline{\underline{R}}^{(k)}}_{\underline{\underline{A}}^{(k)}} \underline{\underline{Q}}^{(k)}$$

$$\Rightarrow \underline{\underline{A}}^{(k+1)} = \left(\underline{\underline{Q}}^{(k)}\right)^{\dagger} \cdots \left(\underline{\underline{Q}}^{(1)}\right)^{\dagger} \underline{\underline{A}}\, \underline{\underline{Q}}^{(1)} \cdots \underline{\underline{Q}}^{(k)}$$

& hence $\underline{\underline{A}}^{(k+1)}$ has the same eigenvalues as $\underline{\underline{A}}$.

The sequence $\underline{\underline{A}}^{(k)}$ can be shown to converge to a triangular matrix. Since eigenvalues λ_k are the roots of the characteristic polynomial fulfilling

$$\det\left(\underline{\underline{A}} - \lambda \mathbb{1}\right) = 0$$

it follows:

If $\underline{\underline{A}}^{(k)}$ is upper triangular, then:

$$\operatorname{diag} \underline{\underline{A}}^{(k)} = (\lambda_1 \dots \lambda_n)$$

the eigenvalues of $\underline{\underline{A}}$.

complexity can be further reduced bringing $\underline{\underline{A}}$ to upper Hessenberg form : $\sim \mathcal{O}(n^3)$

Note:

- There are various special cases such as
  a) $\underline{\underline{A}}$ tri-diagonal
  b) $\underline{\underline{A}}$ hermitian
  c) only $\{\lambda_k\}$ required
  d) only smallest λ_k required

  which drastically speed up computations!

Question: Why does QR-algorithm converges to EVD?

We modify notation:

(i) Denote by $\tilde{\underline{\underline{A}}}^{(k)} = \tilde{\underline{\underline{Q}}}^{(k)} \tilde{\underline{\underline{R}}}^{(k)}$ the matrices obtained in QR-algorithm

(ii) Denote by $\underline{\underline{A}}^{(k)} = \underline{\underline{Q}}^{(k)} \underline{\underline{R}}^{(k)}$ the matrices obtained in SO-algorithm

In QR-algorithm we have:

$$\underline{\underline{A}}^k = \left(\underline{\underline{\tilde{Q}}}^{(1)} \cdot \underline{\underline{\tilde{R}}}^{(1)}\right)^k$$

$$= \underbrace{\underline{\underline{\tilde{Q}}}^{(1)} \cdot \underline{\underline{\tilde{R}}}^{(1)} \cdot \underline{\underline{\tilde{Q}}}^{(1)} \cdot \underline{\underline{\tilde{R}}}^{(1)} \cdot \cdots \cdot \underline{\underline{\tilde{Q}}}^{(1)} \cdot \underline{\underline{\tilde{R}}}^{(1)}}_{k \text{ times}}$$

now $\underline{\underline{\tilde{R}}}^{(1)} \cdot \underline{\underline{\tilde{Q}}}^{(1)}$ are those matrices that are factored in the second iteration of QR-algorithm:

$$\underline{\underline{A}}^k = \underline{\underline{\tilde{Q}}}^{(1)} \underbrace{\underline{\underline{\tilde{Q}}}^{(2)} \underline{\underline{R}}^{(2)} \cdots \underline{\underline{\tilde{Q}}}^{(2)} \underline{\underline{\tilde{R}}}^{(2)}}_{k-1 \text{ times}} \underline{\underline{\tilde{R}}}^{(1)}$$

$$\Rightarrow \underline{\underline{A}}^k = \underline{\underline{\tilde{Q}}}^{(1)} \cdot \underline{\underline{\tilde{Q}}}^{(2)} \cdot \cdots \underline{\underline{\tilde{Q}}}^{(k)} \cdot \underline{\underline{\tilde{R}}}^{(k)} \cdot \underline{\underline{\tilde{R}}}^{(k-1)} \cdot \cdots \cdot \underline{\underline{\tilde{R}}}^{(1)}$$

From SO-algorithm we know:

$$\underline{\underline{A}}^k = \underline{\underline{Q}}^{(k)} \cdot \underline{\underline{R}}^{(k)} \cdot \cdots \cdot \underline{\underline{R}}^{(1)}$$

since $\underline{\underline{\tilde{Q}}}^{(1)} \cdot \underline{\underline{\tilde{Q}}}^{(2)} \cdot \cdots \cdot \underline{\underline{\tilde{Q}}}^{(k)}$ is unitary by construction, we have from uniqueness of QR-decomposition:

$$\underline{\underline{Q}}^{(k)} = \underline{\underline{\tilde{Q}}}^{(1)} \cdot \underline{\underline{\tilde{Q}}}^{(2)} \cdot \cdots \cdot \underline{\underline{Q}}^{(k)}$$

& thus the product of the $\underline{\underline{\tilde{Q}}}^{(j)}$ yield approx. to matrix of eigenvectors of $\underline{\underline{A}}$

Singular value decomposition (SVD)

For every rectangular matrix $\underline{\underline{A}} \in V_{\mathbb{K}}^{m\times n}$ $(m \geq n)$ there exist $\underline{\underline{U}} \in V_{\mathbb{K}}^{m\times n}$, $\underline{\underline{S}}, \underline{\underline{V}} \in V_{\mathbb{K}}^{n\times n}$ with:

(i) $\underline{\underline{A}} = \underline{\underline{U}} \cdot \underline{\underline{S}} \cdot \underline{\underline{V}}$

(ii) $\underline{\underline{U}}^{+} \underline{\underline{U}} = \mathbb{1}_{m\times m}$

(iii) $\underline{\underline{V}} \cdot \underline{\underline{V}}^{+} = \mathbb{1}_{n\times n}$

(iv) $\underline{\underline{S}} = \mathrm{diag}(s_1 \dots s_n)$ with $s_1 \geq s_2 \geq \dots \geq s_n \geq 0$ & $s_j \in \mathbb{R}$

Note: In contrast to EVD here we have:

(i) SVD also exists for rectangular matrices

(ii) s_j are always real

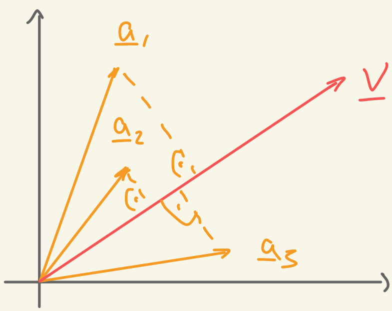
(iii) $\underline{\underline{U}}^{+} \underline{\underline{U}} = \mathbb{1}_{m\times m}$ & $\underline{\underline{V}} \cdot \underline{\underline{V}}^{+} = \mathbb{1}_{n\times n}$ always holds true

Best rank-k approximation

Let us try to develop some intuition for the SVD to appreciate its usefullness.

Consider the least-square minimization problem:

Let $\underline{a}_j \in \mathbb{V}_{\mathbb{K}}^n$, $j \in \{1, \dots, m\}$ be a set of m points. Find the line $\underline{v} \in \mathbb{V}_{\mathbb{K}}^n$ which minimizes the distance of $\underline{v}$ to all $\underline{a}_j$, projecting $\underline{v}$ to the subspaces spanned by $\underline{a}_j$.



$$\underline{v} = \min_{\substack{\underline{x} \in \mathbb{V}_{\mathbb{K}}^n \\ |\underline{x}| = 1}} \sum_{j=1}^{m} \left(\|\underline{a}_j\|^2 - \langle \underline{x} | \underline{a}_j \rangle \right)$$

Note that fixing $\underline{a}_j$, $\sum_{j=1}^{m} \|\underline{a}_j\|$ is constant, so finding $\underline{v}$ is equivalent to maximizing $\sum_{j=1}^{m} \langle \underline{x} | \underline{a}_j \rangle$!

Now let $\underline{\underline{A}} = \begin{pmatrix} - & \underline{a}_1 & - \\ & \vdots & \\ - & \underline{a}_m & - \end{pmatrix} \in \mathbb{V}_{\mathbb{K}}^{m \times n}$.

We define the first singular vector $\underline{v}_1$ via:

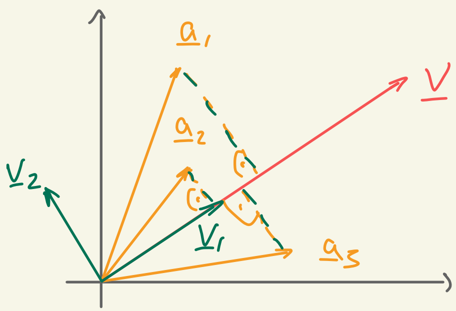
$$\underline{v}_1 = \max_{\substack{\underline{x} \in \mathbb{V}_{\mathbb{K}}^n \\ |\underline{x}| = 1}} |\underline{\underline{A}} | \underline{x} \rangle | = \max_{\substack{\underline{x} \in \mathbb{V}_{\mathbb{K}}^n \\ |\underline{x}| = 1}} \sum_{j=1}^{m} \langle \underline{a}_j | \underline{x} \rangle$$

& $s_1 = |\underline{\underline{A}}\,|\underline{v}_1\rangle|$ as the first singular vector.

Now $|\underline{v}_1\rangle$ spans a subspace, which solves the least squares problem. But what about the residual? We quantify it by finding the solution to the problem:

$$\underline{v}_2 = \max_{\substack{\underline{x} \in V_{/\mathbb{K}}^n \\ |\underline{x}|=1 \\ \langle \underline{v}_1 | \underline{x} \rangle = 0}} |\underline{\underline{A}}\,|\underline{x}\rangle| \quad , \quad s_2 = |\underline{\underline{A}}\,|\underline{v}_2\rangle|$$

In the above sketch:



Continue that process we obtain series:

$\underline{v}_1, \dots, \underline{v}_r$ with $\underline{\underline{A}}\,|\underline{v}_j\rangle$ the solution to the residual least square problem:

$$|\underline{v}_j\rangle = \max_{\substack{\underline{v}_j \in V_{/\mathbb{K}}^n \\ |\underline{v}_j|=1}} |\underline{\underline{A}}\,|\underline{v}_j\rangle| - \sum_{k=1}^{j-1} |\underline{\underline{A}}\,|\underline{v}_k\rangle| \quad \& \quad r \leq n.$$

& the sequence of singular values s_j with: $i < j \Leftrightarrow s_i \geq s_j$.

Consequences for $\underline{\underline{A}} \in V_{\mathbb{K}}^{n \times m}$, $n \geq m$.

(i) For singular vectors $\underline{v}_1, \dots, \underline{v}_k$, $k \leq r$, the subspace $V_k = \mathrm{span}\{\underline{v}_1, \dots, \underline{v}_k\}$ is the best fit k-dimensional subspace to $\underline{\underline{A}}$.

(ii) Since for each $\underline{v}_j$ the norm $|\underline{\underline{A}}|\underline{v}_j\rangle|$ gives the summed squared components along $\underline{v}_j$, it follows immediately:

$$\sum_{j=1}^{m} |\underline{a}_j|^2 = \sum_{j,k=1}^{r} |\langle \underline{v}_k | \underline{a}_j \rangle|^2$$

$$= \sum_{k=1}^{r} |\underline{\underline{A}}|\underline{v}_j\rangle|^2 = \sum_{k=1}^{r} s_k^2$$

On the other hand $|\underline{a}_j|^2 = \sum_{k=1}^{m} |a_{jk}|^2$

Thus the summed, squared singular values yield the Frobenius norm of $\underline{\underline{A}}$:

$$\| \underline{\underline{A}} \|_F = \sum_{k=1}^{r} s_k^2$$

(iii) Since any $\underline{x} \in V_{\mathbb{K}}^n$ can be written as

$$|\underline{x}\rangle = \sum_{j=1}^{r} \langle \underline{v}_j | \underline{x} \rangle |\underline{v}_j\rangle + \langle \underline{v}^{\perp} | \underline{x} \rangle |\underline{v}^{\perp}\rangle$$

Since also $\underline{\underline{A}} |\underline{v}^{\perp}\rangle = 0$, we can define a new set of basis vectors

$$|\underline{u}_j\rangle = \frac{1}{s_j} \underline{\underline{A}} |\underline{v}_j\rangle$$

& it can be shown that:

$$\underline{\underline{A}} = \sum_{j=1}^{r} |\underline{u}_j\rangle\langle \underline{v}_j| \, s_j$$

From (i), (ii) & (iii) it follows:

For a given $k \leq n$, the matrix

$$\underline{\underline{A}}^{(k)} = \sum_{j=1}^{k} |\underline{u}_j\rangle\langle \underline{v}_j| \, s_j$$

is the best rank-k approximation w.r.t. the Frobenius norm:

$$\underline{\underline{A}}^{(k)} = \min_{\underline{\underline{X}} \text{ rank } k} \| \underline{\underline{A}} - \underline{\underline{X}} \|_F$$