## VII.E. The singular value decomposition (SVD)

In this section we describe a generalization of the Spectral Theorem to non-normal operators, and even to transformations between different vector spaces. This is a computationally useful generalization, with applications to data fitting and data compression in particular. It is used in many branches of science, in statistics, and even machine learning. As we develop the underlying mathematics, we will encounter two closely associated constructions: the polar decomposition and pseudoinverse, in each case presenting the version for operators followed by that for matrices.

To begin, let $(V,\langle\cdot, \cdot\rangle)$ be an $n$-dimensional inner-product space, $T: V \rightarrow V$ an operator. By Spectral Theorem III, if $T$ is normal then it has a unitary eigenbasis $\mathcal{B}$, with complex eigenvalues $\sigma_{1}, \ldots, \sigma_{s}$. In particular, $T$ is unitary iff these $\left|\sigma_{i}\right|=1$ (since preserving lengths of a unitary eigenbasis is equivalent to preserving lengths of all vectors), and self-adjoint iff the $\sigma_{i}$ are real (Exercise (1)).

So (for instance) a normal operator $T$ is both unitary and selfadjoint iff $T$ has only +1 and -1 as eigenvalues - which is to say, $T$ is an orthogonal reflection, acting on $V=W \oplus W^{\perp}$ by $\operatorname{Id}_{W}$ on $W$ and $-\mathrm{Id}_{W^{\perp}}$ on $W^{\perp}$. But the broader point here is that we should have in mind the following "table of analogies":

| operators | numbers |
| :---: | :---: |
| normal | $\mathbb{C}$ |
| unitary | $S^{1}$ |
| self-adjoint | $\mathbb{R}$ |
| ?? | $\mathbb{R}_{\geq 0}$ |

where $S^{1} \subset \mathbb{C}$ is the unit circle.
So, how do we complete the table?
VII.E.1. DEFINITION. $T$ is positive (resp. strictly positive) if it is normal, with all eigenvalues in $\mathbb{R}_{\geq 0}$ (resp. $\mathbb{R}_{>0}$ ).

Since they are unitarily diagonalizable with real eigenvalues, positive operators are self-adjoint. Given a self-adjoint (or normal) operator $T$, any $\vec{v} \in V$ is a sum of orthogonal eigenvectors $\vec{w}_{j}$ with eigenvalues $\sigma_{j}$; so

$$
\langle\vec{v}, T \vec{v}\rangle=\sum_{i, j}\left\langle\vec{w}_{i}, T \vec{w}_{j}\right\rangle=\sum_{i . j} \sigma_{j}\left\langle\vec{w}_{i}, \vec{w}_{j}\right\rangle=\sum_{j} \sigma_{j}\left\|\vec{w}_{j}\right\|^{2}
$$

is in $\mathbb{R}_{\geq 0}$ for all $\vec{v}$ if and only if $T$ is positive. If $V$ is complex, the condition that $\langle\vec{v}, T \vec{v}\rangle \geq 0(\forall \vec{v})$ on its own gives self-adjointness (Exercise VII.D.7), hence positivity, of $T$. (If $V$ is real, this condition alone isn't enough.)
VII.E.2. EXAMPLE. Orthogonal projections are positive, since they are self-adjoint with eigenvalues 0 and 1 .

Polar decomposition. A nonzero complex number can be written (in "polar form") as a product $r e^{i \theta}$, for unique $r \in \mathbb{R}_{>0}$ and $e^{i \theta} \in S^{1}$. If $T$ is a normal operator, then it has a unitary eigenbasis $\mathcal{B}=\left\{\hat{v}_{1}, \ldots, \hat{v}_{n}\right\}$, with $[T]_{\mathcal{B}}=\operatorname{diag}\left\{r_{1} e^{i \theta_{1}}, \ldots, r_{n} e^{i \theta_{n}}\right\}\left(r_{i} \in\right.$ $\mathbb{R}_{\geq 0}$ ); and defining $|T|, U$ by $[|T|]_{\mathcal{B}}=\operatorname{diag}\left\{r_{1}, \ldots, r_{n}\right\}$ and $[U]_{\mathcal{B}}=$ $\operatorname{diag}\left\{e^{i \theta_{1}}, \ldots, e^{i \theta_{n}}\right\}$, we have $T=U|T|$ with $U$ unitary and $|T|$ positive, and $U|T|=|T| U$. One might expect such "polar decompositions" of operators to stop there. But there exists an analogue for arbitrary transformations, one that will lead on to the SVD as well!

To formulate this general polar decomposition, let $T: V \rightarrow V$ be an arbitrary linear transformation. Notice that $T^{\dagger} T$ is self-adjoint (since $\left.\left(T^{\dagger} T\right)^{\dagger}=T^{\dagger} T^{\dagger \dagger}=T^{\dagger} T\right)$ and, in fact, positive:

$$
\left\langle\vec{v}, T^{\dagger} T \vec{v}\right\rangle=\langle T \vec{v}, T \vec{v}\rangle \geq 0,
$$

since $\langle\cdot, \cdot\rangle$ is an inner product. So we have a unitary $\mathcal{B}$ with $\left[T^{\dagger} T\right]_{\mathcal{B}}=$ $\operatorname{diag}\left\{\lambda_{1}, \ldots, \lambda_{n}\right\}$, and all $\lambda_{i} \in \mathbb{R}_{\geq 0}$. (Henceforth we impose the convention that $\lambda_{1} \geq \lambda_{2} \geq \ldots \geq \lambda_{n}$.) Taking nonnegative square roots $\mu_{i}=\sqrt{\lambda_{i}} \in \mathbb{R}_{\geq 0}$, we define a new operator $|T|$ by $[|T|]_{\mathcal{B}}=$ $\operatorname{diag}\left\{\mu_{1}, \ldots, \mu_{n}\right\} ;$ clearly $|T|^{2}=T^{\dagger} T$, and $|T|$ is positive.
VII.E.3. THEOREM. There exists a unitary operator $U$ such that

$$
T=U|T|
$$

This "polar decomposition" is unique exactly when $T$ is invertible. Moreover, $U$ and $|T|$ commute exactly when $T$ is normal.

PROOF. We have $\left.\|T \vec{v}\|^{2}=\langle T \vec{v}, T \vec{v}\rangle=\left\langle\vec{v}, T^{\dagger} T \vec{v}\right\rangle=\left.\langle\vec{v}| T\right|^{2,} \vec{v}\right\rangle=$ $\langle | T|\vec{v},|T| \vec{v}\rangle=\||T| \vec{v}\|^{2}$ since $|T|$ is self-adjoint. Consequently $T$ and $|T|$ have the same kernel, hence (by Rank + Nullity) the same rank; so while their images (as subspaces of $V$ ) may differ, they have the same dimension. Moreover, mapping $|T| \vec{w} \mapsto T \vec{w}$ gives a welldefined linear transformation from $\mathrm{im}|T|$ to $\mathrm{im} T$.

By Spectral Theorem I, $V=\operatorname{im}|T| \stackrel{\perp}{\oplus} \operatorname{ker}|T|$. So $\operatorname{dim}(\operatorname{ker}|T|)=$ $\operatorname{dim}\left((\operatorname{im} T)^{\perp}\right)$, and we fix an invertible transformation $U^{\prime}: \operatorname{ker}|T| \rightarrow$ $(\operatorname{im} T)^{\perp}$ sending some choice of unitary basis to another unitary basis. Writing $\vec{v}=|T| \vec{w}+\vec{v}^{\prime}$ (with $|T| \vec{v}^{\prime}=\overrightarrow{0}$ ), we now define

$$
U: \underbrace{\operatorname{im}|T|^{\perp} \operatorname{ker}|T|}_{V} \rightarrow \underbrace{\operatorname{im} T \stackrel{\perp}{\oplus}(\operatorname{im} T)^{\perp}}_{V}
$$

by $U \vec{v}:=T \vec{w}+U^{\prime} \vec{v}^{\prime}$. Since $\left\|T \vec{w}+U^{\prime} \vec{v}^{\prime}\right\|^{2}=\|T \vec{w}\|^{2}+\left\|U^{\prime} \vec{v}^{\prime}\right\|^{2}=$ $\||T| \vec{w}\|^{2}+\left\|\vec{v}^{\prime}\right\|^{2}=\|\vec{v}\|^{2}, U$ is unitary; and taking $\vec{v}=|T| \vec{w}$ gives $U|T| \vec{w}=T \vec{w}(\forall \vec{w} \in V)$.

Now if $T$ is invertible, then so is $|T|\left(\right.$ all $\left.\mu_{i}>0\right) \Longrightarrow U=T|T|^{-1}$. If it isn't, then $\operatorname{ker}|T| \neq\{0\}$ and non-uniqueness enters in the choice of $U^{\prime}$.

Finally, if $U$ and $|T|$ commute, then they simultaneously unitarily diagonalize, and therefore so does $T$, making $T$ normal. If $T$ is normal, we have constructed $U$ and $|T|$ above, and they commute.
VII.E.4. Example. Consider $V=\mathbb{R}^{4}$ with the dot product, and

$$
A=[T]_{\hat{e}}=\left(\begin{array}{cccc}
2 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0
\end{array}\right)
$$

Since $A$ has a Jordan block, we know it is not diagonalizable; and so $T$ is not normal. However,

$$
\left[T^{\dagger} T\right]_{\hat{\mathcal{~}}}={ }^{t} A A=\left(\begin{array}{cccc}
4 & 0 & 0 & 0 \\
0 & 2 & 1 & 0 \\
0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0
\end{array}\right)=P_{\mathcal{B}} \mathscr{D} P_{\mathcal{B}}^{-1}
$$

with $\mathcal{B}:=\left\{\hat{e}_{1}, \hat{e}_{2}+\varphi_{-} \hat{e}_{3}, \hat{e}_{2}-\varphi_{+} \hat{e}_{3}, \hat{e}_{4}\right\}$ and $\mathscr{D}:=\operatorname{diag}\left\{4, \eta_{+}, \eta_{-}, 0\right\}$ (where $\varphi_{ \pm}:=\frac{ \pm 1+\sqrt{5}}{2}$ and $\eta_{ \pm}:=\frac{3 \pm \sqrt{5}}{2}=\varphi_{ \pm}^{2}$ ). Taking the positive square $\operatorname{root} \mathscr{D}^{\frac{1}{2}}:=\operatorname{diag}\left\{2, \varphi_{+}, \varphi_{-}, 0\right\}$, we get

$$
[|T|]_{\hat{e}}=|A|:=P_{\mathcal{B}} \mathscr{D}^{\frac{1}{2}} P_{\mathcal{B}}^{-1}=\left(\begin{array}{cccc}
2 & 0 & 0 & 0 \\
0 & \frac{3}{\sqrt{5}} & \frac{1}{\sqrt{5}} & 0 \\
0 & \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} & 0 \\
0 & 0 & 0 & 0
\end{array}\right) .
$$

On $W:=\operatorname{span}\left\{\hat{e}_{1}, \hat{e}_{2}, \hat{e}_{3}\right\}=\operatorname{im} T=\operatorname{im}|T|$, we must have $\left.U\right|_{W}=$ $\left.T\right|_{W}\left(\left.|T|\right|_{W}\right)^{-1}$; while on $\operatorname{span}\left\{\hat{e}_{4}\right\}=W^{\perp}, U$ can be taken to act by any scalar of norm 1 . Therefore

$$
[U]_{\hat{e}}=Q:=\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\
0 & \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} & 0 \\
0 & 0 & 0 & e^{i \theta}
\end{array}\right)
$$

and $A=Q|A|$. Geometrically, $|A|$ dilates the $\mathcal{B}$-coordinates of a vector, then $Q$ performs a rotation.

SVD for endomorphisms. ${ }^{26}$ Now let $|T|$ be the (unique) positive square root of $T^{\dagger} T$ as above, and $\mathcal{B}=\left\{\hat{v}_{1}, \ldots, \hat{v}_{n}\right\}$ the unitary basis of $V$ under which $[|T|]_{\mathcal{B}}=\operatorname{diag}\left\{\mu_{1}, \ldots, \mu_{n}\right\}$.
VII.E.5. DEfinition. These $\left\{\mu_{i}\right\}$ are called the singular values of $T$.

[^0]Writing $T=U|T|$ and $\hat{w}_{i}:=U \hat{v}_{i}, U^{\dagger} U=\operatorname{Id}_{V} \Longrightarrow\left\langle\hat{w}_{i}, \hat{w}_{j}\right\rangle=$ $\left\langle U^{\dagger} U \hat{v}_{i}, \hat{v}_{j}\right\rangle=\left\langle\hat{v}_{i}, \hat{v}_{j}\right\rangle=\delta_{i j} \Longrightarrow \mathcal{C}:=\left\{\hat{w}_{1}, \ldots, \hat{w}_{n}\right\}=U(\mathcal{B})$ is unitary. For $\vec{v} \in V$, we have
(VII.E.6)

$$
\begin{aligned}
T \vec{v} & =U|T| \sum_{i=1}^{n}\left\langle\hat{v}_{i}, \vec{v}\right\rangle \hat{v}_{i}=\sum_{i=1}^{n}\left\langle\hat{v}_{i}, \vec{v}\right\rangle U|T| \hat{v}_{i} \\
& =\sum_{i=1}^{n} \mu_{i}\left\langle\hat{v}_{i}, \vec{v}\right\rangle U \hat{v}_{i}=\sum_{i=1}^{n} \mu_{i}\left\langle\hat{v}_{i}, \vec{v}\right\rangle \hat{w}_{i} .
\end{aligned}
$$

Viewing $\left\langle\hat{v}_{i}, \cdot\right\rangle=: \ell_{\hat{v}_{i}}: V \rightarrow \mathbb{C}$ as a linear functional, and $\hat{w}_{i}: \mathbb{C} \rightarrow V$ as a map (sending $\alpha \in \mathbb{C}$ to $\alpha \hat{w}_{i}$ ), (VII.E.6) becomes
(VII.E.7)

$$
T=\sum_{i=1}^{n} \mu_{i} \hat{w}_{i} \circ \ell_{\hat{v}_{i}} .
$$

How does this look in matrix terms? Let $\mathcal{A}$ be an arbitrary ${ }^{27}$ unitary basis of $V$, and set $A:=[T]_{\mathcal{A}}$. Using $\{1\}$ as a basis of $\mathbb{C}$, (VII.E.7) yields

$$
\begin{equation*}
A=\sum_{i=1}^{n} \mu_{i \mathcal{A}}\left[\hat{w}_{i}\right]_{\{1\}\{1\}}\left[\ell_{\hat{v}_{i}}\right]_{\mathcal{A}}=\sum_{i=1}^{n} \mu_{i}\left[\hat{w}_{i}\right]_{\mathcal{A}}\left[\hat{v}_{i}\right]_{\mathcal{A}}^{*} . \tag{VII.E.8}
\end{equation*}
$$

Here $\left[\hat{w}_{i}\right]_{\mathcal{A}}\left[\hat{v}_{i}\right]_{\mathcal{A}}^{*}$ is a $(n \times 1) \cdot(1 \times n)$ matrix product, yielding an $n \times n$ matrix of rank one. So (VII.E.7) (resp. (VII.E.8)) decompose $T$ (resp. $A$ ) into a sum of rank-one endomorphisms (resp. matrices) weighted by the singular values. This is a first version of the singular value decomposition.
VII.E.9. REMARK. If $T$ is positive, we can take $U=\operatorname{Id}_{V}$, so that $\hat{w}_{i} \circ \ell_{\hat{v}_{i}}=\hat{v}_{i} \circ \ell_{\hat{v}_{i}}=: \operatorname{Pr}_{\hat{v}_{i}}$ is the orthogonal projection onto span $\left\{\hat{v}_{i}\right\}$. Thus (VII.E.7) merely restates Spectral Theorem I in this case. In fact, if $T$ is normal, then $T, T^{\dagger} T$, and $|T|$ simultaneously diagonalize. If $\tilde{\mu}_{1}, \ldots, \tilde{\mu}_{n}$ are the eigenvalues of $T$, then we evidently have $\mu_{i}=\left|\tilde{\mu}_{i}\right| ; U$ may then be defined by $[U]_{\mathcal{B}}=\operatorname{diag}\left\{\tilde{\mu}_{i} / \mu_{i}\right\}$ (with $0 / 0$ interpreted as 1). Thus (VII.E.7) reads $T=\sum_{i=1}^{n} \tilde{\mu}_{i} \operatorname{Pr}_{\hat{v}_{i}}$, which restates Spectral Theorem III. So in this sense, the SVD generalizes the results in §VII.D.

[^1]Now since $U$ sends $\mathcal{B}$ to $\mathcal{C}$, we have
and thus

$$
{ }_{\mathcal{C}}[T]_{\mathcal{B}}=\underbrace{\left.\mathcal{C}^{[U]}\right]_{\mathcal{B}}}_{\mathbb{I}_{n}}[|T|]_{\mathcal{B}}=\operatorname{diag}\left\{\mu_{1}, \ldots, \mu_{n}\right\}=: D
$$

$$
\begin{equation*}
A=[T]_{\mathcal{A}}={ }_{\mathcal{A}}[\mathbb{I}]_{\mathcal{C} \mathcal{C}}[T]_{\mathcal{B} \mathcal{B}}[I]_{\mathcal{A}}=: S_{1} D S_{2}, \tag{VII.E.10}
\end{equation*}
$$

with $S_{1}$ and $S_{2}$ unitary matrices (as they change between unitary bases). Roughly speaking, (VII.E.10) presents $A$ as a composition of the form "rotation, ${ }^{28}$ dilation, rotation".
VII.E.11. Theorem. Any $A \in M_{n}(\mathbb{C})$ can be presented as a product $S_{1} D S_{2}$, where $D$ is a diagonal matrix with entries in $\mathbb{R}_{\geq 0}$, and $S_{i} S_{i}^{*}=\mathbb{I}_{n}$. The diagonal entries of $D$, called the singular values of $A$, are unique. If they are distinct, nonzero, and in decreasing order, then $\left(S_{1}, S_{2}\right)$ are unique modulo rescaling $\rightsquigarrow\left(S_{1} \Delta, \Delta^{-1} S_{2}\right)$ by a unitary diagonal matrix $\Delta .{ }^{29}$

Proof. Existence was deduced above. We have $D^{*}=D$ hence

$$
A^{*} A=S_{2}^{*} D^{*} S_{1}^{*} S_{1} D S_{2}=S_{2}^{*} D^{2} S_{2}
$$

which is (with respect to the dot product) a unitary diagonalization of the Hermitian matrix $A^{*} A$. So $D^{2}$, hence $D$, is unique; and if the diagonal entries are distinct, then the unitary eigenbasis $(\Longrightarrow$ columns of $S_{2}^{*}$ ) is determined up to $e^{i \theta}$ scaling factors. If no singular values are $0, D$ is invertible and $S_{1}=A S_{2}^{*} D^{-1}$.
VII.E.12. EXAMPLE. Let's look at the operator

$$
T=\frac{d}{d t}: \mathcal{P}_{2}(\mathbb{R}) \rightarrow \mathcal{P}_{2}(\mathbb{R})
$$

with $\langle f, g\rangle:=\int_{-1}^{1} f(t) g(t) d t$. This is a non-diagonalizable (hence non-normal) nilpotent transformation. We compute its singular values - which are not all zero, even though 0 is the only eigenvalue of $T$ - and the bases $\mathcal{B}$ and $\mathcal{C}$.

[^2]To compute $T^{\dagger}$ we will need an o.n. basis $\mathcal{A}$ : Gram-Schmidt on $\left\{1, t, t^{2}\right\}$ yields $\mathcal{A}:=\left\{\frac{1}{\sqrt{2}}, \sqrt{\frac{3}{2}} t, \frac{3}{2} \sqrt{\frac{5}{2}}\left(t^{2}-\frac{1}{3}\right)\right\}$ and

$$
\begin{array}{r}
{[T]_{\mathcal{A}}=\left(\begin{array}{ccc}
0 & \sqrt{3} & 0 \\
0 & 0 & \sqrt{15} \\
0 & 0 & 0
\end{array}\right) \Longrightarrow\left[T^{+}\right]_{\mathcal{A}}=[T]_{\mathcal{A}}^{*}=\left(\begin{array}{ccc}
0 & 0 & 0 \\
\sqrt{3} & 0 & 0 \\
0 & \sqrt{15} & 0
\end{array}\right)} \\
\Longrightarrow\left[T^{\dagger} T\right]_{\mathcal{A}}=\left(\begin{array}{ccc}
0 & 0 & 0 \\
0 & 3 & 0 \\
0 & 0 & 15
\end{array}\right) \Longrightarrow[|T|]_{\mathcal{A}}=\left(\begin{array}{ccc}
0 & 0 & 0 \\
0 & \sqrt{3} & 0 \\
0 & 0 & \sqrt{15}
\end{array}\right)
\end{array}
$$

$\Longrightarrow$ singular values (in decreasing order) are $\sqrt{15}, \sqrt{3}, 0$, and

$$
\mathcal{B}=\left\{\frac{3}{2} \sqrt{\frac{5}{2}}\left(t^{2}-\frac{1}{3}\right), \sqrt{\frac{3}{2}} t, \frac{1}{\sqrt{2}}\right\}=:\left\{\hat{v}_{1}, \hat{v}_{2}, \hat{v}_{3}\right\}
$$

Now $\operatorname{im}(|T|)=\operatorname{span}\left\{\hat{v}_{1}, \hat{v}_{2}\right\}, \operatorname{ker}(|T|)=\operatorname{span}\left\{\hat{v}_{3}\right\}=\operatorname{ker}(T), \operatorname{im}(T)=$ $\operatorname{span}\left\{\hat{v}_{2}, \hat{v}_{3}\right\}$, and $\operatorname{im}(T)^{\perp}=\operatorname{span}\left\{\hat{v}_{1}\right\}$. So we define

$$
U: \operatorname{span}\left\{\hat{v}_{1}, \hat{v}_{2}\right\} \stackrel{\perp}{\oplus} \operatorname{span}\left\{\hat{v}_{3}\right\} \longrightarrow \operatorname{span}\left\{\hat{v}_{2}, \hat{v}_{3}\right\} \stackrel{\perp}{\oplus} \operatorname{span}\left\{\hat{v}_{1}\right\}
$$

by sending $\hat{v}_{1}=|T|\left(\frac{1}{\sqrt{15}} \hat{v}_{1}\right) \mapsto T\left(\frac{1}{\sqrt{15}} \hat{v}_{1}\right)=\hat{v}_{2}, \hat{v}_{2}=|T|\left(\frac{1}{\sqrt{3}} \hat{v}_{2}\right) \mapsto$ $T\left(\frac{1}{\sqrt{3}} \hat{v}_{2}\right)=\hat{v}_{3}$, and $\hat{v}_{3} \mapsto \hat{v}_{1}$. We then have

$$
[U]_{\mathcal{A}}=\left(\begin{array}{lll}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0
\end{array}\right)
$$

and $\mathcal{C}=U(\mathcal{B})=\left\{\hat{v}_{2}, \hat{v}_{3}, \hat{v}_{1}\right\}$. The ${ }^{30}$ SVD of $A=[T]_{\mathcal{A}}$ thus reads (noting that $\mathcal{A}=\left\{\hat{v}_{3}, \hat{v}_{2}, \hat{v}_{1}\right\}$ )

$$
A=S_{1} D S_{2}=\left(\begin{array}{lll}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 1
\end{array}\right)\left(\begin{array}{ccc}
\sqrt{15} & 0 & 0 \\
0 & \sqrt{3} & 0 \\
0 & 0 & 0
\end{array}\right)\left(\begin{array}{lll}
0 & 0 & 1 \\
0 & 1 & 0 \\
1 & 0 & 0
\end{array}\right) .
$$

VII.E.13. CAUTION. Even if $T$ is diagonalizable, it may not be unitarily diagonalizable (i.e. normal), and only in the latter case are $T^{\prime}$ 's singular values the absolute values of $T^{\prime}$ s eigenvalues (Rem. VII.E.9).
${ }^{30}$ Of course, even over $\mathbb{R}$ it isn't quite unique: one can play with the signs in $S_{1}$ and $S_{2}$.

SVD for transformations. We now turn to the more general form of the SVD. Let $T: V \rightarrow W$ be a linear transformation between finitedimensional inner-product spaces, and fix unitary bases $\mathcal{A}$ resp. $\mathcal{A}^{\prime}$ of $V$ resp. $W$. Write $n=\operatorname{dim} V, m=\operatorname{dim} W$.
VII.E.14. Lemma. The transformation $T^{\dagger}: W \rightarrow V$ defined by

$$
\mathcal{A}\left[T^{\dagger}\right]_{\mathcal{A}^{\prime}}=\left(\mathcal{A}^{\prime}[T]_{\mathcal{A}}\right)^{*}
$$

is the unique operator satisfying

$$
\begin{equation*}
\left\langle T^{\dagger} \vec{w}, \vec{v}\right\rangle=\langle\vec{w}, T \vec{v}\rangle \tag{VII.E.15}
\end{equation*}
$$

for all $\vec{v} \in V, \vec{w} \in W$. We call it the adjoint of $T$.
Proof. Since $\mathcal{A}, \mathcal{A}^{\prime}$ are unitary, (VII.E.15) is equivalent to

$$
\left[T^{\dagger} \vec{w}\right]_{\mathcal{A}}^{*}[\vec{v}]_{\mathcal{A}}=[\vec{w}]_{\mathcal{A}^{\prime}}^{*}[T \vec{v}]_{\mathcal{A}^{\prime}}
$$

and thus to $[\vec{w}]_{\mathcal{A}^{\prime}}^{*}\left(\mathcal{A}^{[ }\left[T^{\dagger}\right]_{\mathcal{A}^{\prime}}\right)^{*}[\vec{v}]_{\mathcal{A}}=[\vec{w}]_{\mathcal{A}^{\prime} \mathcal{A}^{\prime}}^{*}[T]_{\mathcal{A}}[\vec{v}]_{\mathcal{A}}$.
VII.E.16. LEMMA. We have $V=\operatorname{ker}(T) \stackrel{\perp}{\oplus} \operatorname{im}\left(T^{\dagger}\right)$ and $W=\operatorname{im}(T) \stackrel{\perp}{\oplus}$ $\operatorname{ker}\left(T^{\dagger}\right)$, with $T$ (resp. $\left.T^{\dagger}\right)$ restricting to an isomorphism from $\operatorname{im}\left(T^{\dagger}\right) \rightarrow$ $\left.\operatorname{im}(T) \operatorname{resp} . \operatorname{im}(T) \rightarrow \operatorname{im}\left(T^{\dagger}\right)\right)$.

Proof. By Lemma VII.E.14, $T$ and $T^{\dagger}$ have the same rank $r$, so Rank + Nullity $\Longrightarrow$

$$
\left\{\begin{array}{rl}
\operatorname{dim}(\operatorname{ker} T)+\operatorname{dim}\left(\operatorname{im} T^{\dagger}\right) & =(n-r)+r=n=\operatorname{dim} V \\
\operatorname{dim}(\operatorname{im} T)+\operatorname{dim}\left(\operatorname{ker} T^{\dagger}\right) & =r+(m-r)
\end{array}=m=\operatorname{dim} W .\right.
$$

For $\vec{v} \in \operatorname{ker}(T),\left\langle\vec{v}, T^{\dagger} \vec{w}\right\rangle=\langle T \vec{v}, \vec{w}\rangle=\langle\overrightarrow{0}, \vec{w}\rangle=0 \Longrightarrow \operatorname{ker}(T) \perp$ $\operatorname{im}\left(T^{\dagger}\right) \Longrightarrow \operatorname{ker}(T) \cap \operatorname{im}\left(T^{\dagger}\right)=\left.\{0\} \Longrightarrow T\right|_{\mathrm{im}\left(T^{\dagger}\right)}$ is injective. This proves the assertions about $V$ and $T$; those for $W$ and $T^{\dagger}$ follow by symmetry.

The compositions $T^{\dagger} T: V \rightarrow V$ and $T T^{\dagger}: W \rightarrow W$ are clearly positive (argue as above), and preserve the $\stackrel{\perp}{\oplus}$ 's in Lemma VII.E.16. So $T^{\dagger} T\left(\right.$ resp. $\left.T T^{\dagger}\right)$ is an automorphism of $\operatorname{im}\left(T^{\dagger}\right)($ resp. $\operatorname{im}(T))$ " $\stackrel{\perp}{\oplus}$ the zero map on $\operatorname{ker}(T)\left(\right.$ resp. $\left.\operatorname{ker}\left(T^{\dagger}\right)\right)$. The same remarks apply to
the positive operator $\sqrt{T^{\dagger} T}$ (resp. $\sqrt{T T^{\dagger}}$ ), and there exists a unitary basis $\mathcal{B}=\left\{\hat{v}_{1}, \ldots, \hat{v}_{n}\right\}$ of $V$ with $\left[\sqrt{T^{+} T}\right]_{\mathcal{B}}=\operatorname{diag}\left\{\mu_{1}, \ldots, \mu_{r}, 0, \ldots, 0\right\}$ and $\mu_{1} \geq \mu_{2} \geq \ldots \geq \mu_{r}>0$.
VII.E.17. Definition. These $\left\{\mu_{i}\right\}$ are called the (nonzero) singular values of $T$.

In particular, $\left\{\hat{v}_{1}, \ldots, \hat{v}_{r}\right\} \subset \operatorname{im}\left(T^{\dagger}\right)$ and $\left\{\hat{v}_{r+1}, \ldots, \hat{v}_{n}\right\} \subset \operatorname{ker}(T) ;$ and we define $\left\{\hat{w}_{1}, \ldots, \hat{w}_{r}\right\} \subset \operatorname{im}(T)$ by $\hat{w}_{i}:=\frac{1}{\mu_{i}} T \hat{v}_{i}$. Since

$$
\left\langle\hat{w}_{i}, \hat{w}_{j}\right\rangle=\frac{1}{\mu_{i} \mu_{j}}\left\langle T \hat{v}_{i}, T \hat{v}_{j}\right\rangle=\frac{1}{\mu_{i} \mu_{j}}\left\langle T^{\dagger} T \hat{v}_{i}, \hat{v}_{j}\right\rangle=\frac{\mu_{i}^{2}}{\mu_{i} \mu_{j}}\left\langle\hat{v}_{i}, \hat{v}_{j}\right\rangle=\frac{\mu_{i}}{\mu_{j}} \delta_{i j}=\delta_{i j}
$$

this gives a unitary basis of $\operatorname{im}(T)$, which we complete to a unitary basis $\mathcal{C} \subset W$ by choosing $\left\{\hat{w}_{r+1}, \ldots, \hat{w}_{m}\right\} \subset \operatorname{ker}\left(T^{\dagger}\right)$. This proves
VII.E.18. THEOREM (Abstract SVD). There exist unitary bases $\mathcal{B} \subset$ $V, \mathcal{C} \subset W$ such that ${ }^{31}$
(VII.E.19)

$$
\mathcal{C}[T]_{\mathcal{B}}=\operatorname{diag}_{m \times n}\left\{\mu_{1}, \ldots, \mu_{r}, 0, \ldots, 0\right\}
$$

with $\mu_{1} \geq \ldots \geq \mu_{r}>0$, and $r=\operatorname{rank}(T)$.
VII.E.20. REMARK. (i) $\mathcal{C}$ is an eigenbasis for $\sqrt{T T^{\dagger}}$, and its nonzero eigenvalues are also the $\left\{\mu_{i}\right\}_{i=1}^{r}: T T^{\dagger} \hat{w}_{i}=\frac{1}{\mu_{i}} T T^{\dagger} T \hat{v}_{i}=\frac{1}{\mu_{i}} T\left(\mu_{i}^{2} \hat{v}_{i}\right)=$ $\mu_{i}^{2} \hat{w}_{i}$.
(ii) Suppose that $\mathcal{B}^{\prime} \subset V, \mathcal{C}^{\prime} \subset W$ are unitary bases such that $\mathcal{C}^{\prime}[T]_{\mathcal{B}^{\prime}}=\operatorname{diag}_{m \times n}\left\{\mu_{1}^{\prime}, \ldots, \mu_{s}^{\prime}, 0 \ldots, 0\right\}$ (with $\mu_{1}^{\prime} \geq \cdots \geq \mu_{r}^{\prime}>0$ ): then $s=r$ and $\mu_{i}^{\prime}=\mu_{i}(\forall i)$. This is because $\mathcal{B}_{\mathcal{B}^{\prime}}\left[T^{+} T\right]_{\mathcal{B}^{\prime}}={ }_{\mathcal{B}^{\prime}}\left[T^{\dagger}\right]_{\mathcal{C}^{\prime} \mathcal{C}^{\prime}}[T]_{\mathcal{B}^{\prime}}=$ $\left(\mathcal{C}^{\prime}[T]_{\mathcal{B}^{\prime}}\right)^{*} \mathcal{C}^{\prime}[T]_{\mathcal{B}^{\prime}}=\operatorname{diag}_{m \times n}\left\{\left(\mu_{1}^{\prime}\right)^{2}, \ldots,\left(\mu_{r}^{\prime}\right)^{2}, 0 \ldots, 0\right\}$, so that $\left\{\mu_{i}^{\prime}\right\}$ are the eigenvalues of $\sqrt{T^{\dagger} T}$. So the (nonzero) singular values are the unique positive numbers that can appear in (VII.E.19).
(iii) Moreover, if the $\mu_{i}$ are distinct and $T$ is injective (resp. surjective), the elements of $\mathcal{B}^{\prime}$ (resp. $\mathcal{C}^{\prime}$ ) are $e^{i \theta}$-multiples of the elements of $\mathcal{B}$ (resp. $\mathcal{C}$ ).
VII.E.21. DEfinition. The pseudoinverse of $T$ is the transformation $T^{\sim}: W \rightarrow V$ given by 0 on $\operatorname{ker}\left(T^{\dagger}\right)$ and inverting $T$ on $\operatorname{im}(T)$.

[^3]VII.E.22. COROLLARY. $\mathcal{B}\left[T^{\sim}\right]_{\mathcal{C}}=\operatorname{diag}_{n \times m}\left\{\mu_{1}^{-1}, \ldots, \mu_{r}^{-1}, 0, \ldots, 0\right\}$.

Note that if $T$ is invertible, then $T^{\sim}=T^{-1}$.
VII.E.23. Corollary. $T^{\sim} T: V \rightarrow V$ is the orthogonal projection $\operatorname{Pr}_{\mathrm{im}\left(T^{\dagger}\right)}$ and $T T^{\sim}: W \rightarrow W$ is $\operatorname{Pr}_{\operatorname{im}(T)}$.

SVD for $m \times n$ matrices. The matrix version of Theorem VII.E. 18 has been called the fundamental theorem of matrix algebra. Its efficient computer implementation for large matrices has been the subject of countless articles in numerical analysis. While we won't say anything about these algorithms, they are more efficient (and accurate) than the orthogonal diagonalization of $A^{*} A$, which remains our algorithm of choice here.
VII.E.24. THEOREM (Matrix SVD). Let $A$ be an arbitrary $m \times n m a-$ trix of rank $r$, with complex entries. Then there exist unitary matrices $P \in M_{m}(\mathbb{C}), Q \in M_{n}(\mathbb{C})$ and real numbers $\mu_{1} \geq \ldots \geq \mu_{r}>0$, such that ${ }^{32}$
(VII.E.25)

$$
A=P \Delta Q^{*}=\left(\hat{p}_{1} \cdots \hat{p}_{m}\right) \operatorname{diag}_{m \times n}\left\{\mu_{1}, \ldots, \mu_{r}, 0, \ldots, 0\right\}\left(\hat{q}_{1} \cdots \hat{q}_{n}\right)^{*}
$$

(and $A^{*}=Q^{t} \Delta P^{*}$ ). The map from $\mathbb{C}^{n} \rightarrow \mathbb{C}^{m}$ given by $\vec{x} \mapsto A \vec{x}$ breaks into two components under the orthogonal direct sum decompositions

$$
\begin{array}{cl}
\mathbb{C}^{n}=V_{\mathrm{col}}\left(A^{*}\right) \stackrel{\perp}{\oplus} \operatorname{Nul}(A) & \longrightarrow \\
\quad V_{\mathrm{col}}(A) \stackrel{\perp}{\oplus} \operatorname{Nul}\left(A^{*}\right)=\mathbb{C}^{m} \\
\operatorname{span}\left\{\hat{q}_{1}, \ldots, \hat{q}_{r}\right\} & \operatorname{span}\left\{\hat{p}_{1}, \ldots, \hat{p}_{r}\right\}
\end{array}
$$

Namely, it is given by $\hat{q}_{j} \stackrel{A}{\longmapsto} \mu_{j} \hat{p}_{j}(j=1, \ldots, r)$ on the first summands and by zero on the second. (The reverse map given by $A^{*}$ sends $\hat{p}_{j} \mapsto \mu_{j} \hat{q}_{j}$.) The nonzero singular values $\mu_{j}$ are the positive square roots of the nonzero eigenvalues of $A^{*} A\left(\right.$ resp. $\left.A A^{*}\right)$, for which the columns of $Q$ (resp. P) give unitary eigenbases.

[^4]Proof. Apply Theorem VII.E. 18 to the setting: $V=\mathbb{C}^{n}$ with $\langle\cdot, \cdot\rangle=\operatorname{dot}$ product and $\mathcal{A}=\hat{e} ; W=\mathbb{C}^{m}$ with $\langle\cdot, \cdot\rangle=\operatorname{dot}$ product and $\mathcal{A}^{\prime}=\hat{e} ; T: V \rightarrow W$ such that $A=\mathcal{A}^{\prime}[T]_{\mathcal{A}}$. Then

$$
\mathcal{A}^{\prime}[T]_{\mathcal{A}}=\mathcal{A}^{\prime}\left[\operatorname{Id}_{W}\right]_{\mathcal{C} \mathcal{C}}[T]_{\mathcal{B} \mathcal{B}}\left[\operatorname{Id}_{V}\right]_{\mathcal{A}}
$$

is $A=P_{\mathcal{C}} \Delta P_{\mathcal{B}}^{*}$ (and we put $P:=P_{\mathcal{C}}, Q:=P_{\mathcal{B}}$ ). The remaining details are immediate from the "abstract" analysis.
VII.E.26. DEfinition. The pseudoinverse of $A$ is the $n \times m$ matrix

$$
A^{\sim}:={ }_{\mathcal{A}}\left[T^{\sim}\right]_{\mathcal{A}^{\prime}}=Q \Delta^{\sim} P^{*},
$$

where $\Delta^{\sim}=\operatorname{diag}_{n \times m}\left\{\mu_{1}^{-1}, \ldots, \mu_{r}^{-1}, 0, \ldots, 0\right\}$.
VII.E.27. COROLLARY. $A^{\sim} A=\left[P r_{V_{\text {col }}\left(A^{*}\right)}\right]_{\hat{e}}$ and $A A^{\sim}=\left[\operatorname{Pr}_{V_{\text {col }}(A)}\right]_{\hat{e}}$ are matrices of orthogonal projections (under the dot product).
VII.E.28. REMARK. In all of this, if $A$ is real then $A^{*}={ }^{t} A \Longrightarrow$ $V_{\text {col }}\left(A^{*}\right)=V_{\text {row }}(A)$. In this case, we can take $P, Q$ orthogonal, and $A=P \Delta^{t} Q$ with the $\left\{\hat{q}_{i}\right\}$ appearing as the rows of ${ }^{t} Q$. Some matrix algebra texts call $V_{\text {row }}(A), V_{\text {col }}(A), \operatorname{Nul}(A)$, and $\operatorname{Nul}\left({ }^{t} A\right)$ the "four fundamental subspaces" in the context of the SVD.
VII.E.29. ExAMPLE. Consider the rank 1 matrix

$$
A=\left(\begin{array}{ll}
1 & -1 \\
1 & -1 \\
2 & -2
\end{array}\right)
$$

We have

$$
{ }^{t} A A=\left(\begin{array}{cc}
6 & -6 \\
-6 & 6
\end{array}\right)=Q \operatorname{diag}\left\{\mu_{1}^{2}, 0\right\}^{t} Q
$$

with $\mu_{1}=\sqrt{12}$ and $Q=\frac{1}{\sqrt{2}}\left(\begin{array}{cc}1 & 1 \\ -1 & 1\end{array}\right)$. Now

$$
\hat{p}_{1}=\frac{1}{\mu_{1}} A \hat{q}_{1}=\frac{1}{\sqrt{6}}\left(\begin{array}{l}
1 \\
1 \\
2
\end{array}\right)
$$

while $\hat{p}_{2}, \hat{p}_{3}$ have to be an o.n. basis of $\operatorname{Nul}\left({ }^{t} A\right)$. So

$$
A=\left(\begin{array}{ccc}
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\
\frac{2}{\sqrt{6}} & 0 & \frac{-1}{\sqrt{3}}
\end{array}\right)\left(\begin{array}{cc}
\sqrt{12} & 0 \\
0 & 0 \\
0 & 0
\end{array}\right)\left(\begin{array}{cc}
\frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{array}\right)
$$

is a SVD, and

$$
\begin{gathered}
A^{\sim}=\left(\begin{array}{cc}
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
\frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{array}\right)\left(\begin{array}{ccc}
\frac{1}{\sqrt{12}} & 0 & 0 \\
0 & 0 & 0
\end{array}\right)\left(\begin{array}{ccc}
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} \\
\frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\
\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{-1}{\sqrt{3}}
\end{array}\right) \\
=\frac{1}{12}\left(\begin{array}{ccc}
1 & 1 & 2 \\
-1 & -1 & -2
\end{array}\right)
\end{gathered}
$$

the pseudoinverse. So for instance $A^{\sim} A=\frac{1}{2}\left(\begin{array}{cc}1 & -1 \\ -1 & 1\end{array}\right)$ does indeed orthogonally project onto $V_{\text {row }}(A)=\operatorname{span}\left\{\binom{1}{-1}\right\}$.

Applications to least squares and linear regression. Let $T: V \rightarrow$ $W$ be an arbitrary linear transformation, with $V=\mathbb{C}^{n}$ and $W=\mathbb{C}^{m}$ equipped with the dot product, and $A:={ }_{\hat{e}}[T]_{\hat{e}}$. Write $\vec{v} \in V, \vec{w} \in W$ and $[\vec{v}]_{\hat{e}}=\vec{x},[\vec{w}]_{\hat{e}}=\vec{y}$.
VII.E.30. DEFINITION. For any fixed $\vec{w} \in W$, a least-squares solution (LSS) to $T \vec{v}=\vec{w}$ (or equivalently $A \vec{x}=\vec{y}$ ) is any $\widetilde{v} \in V$ minimizing $\|T \widetilde{v}-\vec{w}\|$. The minimal LSS $\widetilde{v}_{\min }$ is the (unique) LSS minimizing $\|\widetilde{v}\|$.

The minimum distance from $\vec{w}$ to $\mathrm{im}(T)$ is, of course, the distance from $\vec{w}$ to the orthogonal projection $\widetilde{w}:=\operatorname{Pr}_{i m(T)} \vec{w}$,

and so $\tilde{v}$ is just any solution to

$$
\begin{equation*}
T \widetilde{v}=\widetilde{w}(\Longleftrightarrow A \widetilde{x}=\widetilde{y}) \tag{VII.E.31}
\end{equation*}
$$

VII.E.32. THEOREM. (i) The least-squares solutions of $T \vec{v}=\vec{w}$ are the solutions of the normal equations

$$
\begin{equation*}
T^{\dagger} T \widetilde{v}=T^{\dagger} \vec{w}\left(\Longleftrightarrow A^{*} A \widetilde{x}=A^{*} \vec{y}\right) \tag{VII.E.33}
\end{equation*}
$$

(ii) The minimal LSS of $T \vec{v}=\vec{w}$ is

$$
\begin{equation*}
\widetilde{v}_{\text {min }}=T^{\sim} \vec{w} . \tag{VII.E.34}
\end{equation*}
$$

Proof. (i) Since $\operatorname{im}(T)^{\perp}=\operatorname{ker}\left(T^{\dagger}\right)$, $\widetilde{v}$ satisfies (VII.E.33) $\Longleftrightarrow$ $\vec{w}-T \widetilde{v} \in \operatorname{im}(T)^{\perp} \Longleftrightarrow \widetilde{v}$ satisfies (VII.E.31).
(ii) By Corollary VII.E.23, $\widetilde{w}=T T^{\sim} \vec{w}$. So $\widetilde{v}$ satisfies (VII.E.31) $\Longleftrightarrow \vec{\kappa}:=\widetilde{v}-T^{\sim} \vec{w} \in \operatorname{ker}(T)$. But $\operatorname{im}\left(T^{\sim}\right)=\operatorname{im}\left(T^{\dagger}\right)$ is $\perp$ to $\operatorname{ker}(T)$ $\Longrightarrow\|\widetilde{v}\|^{2}=\left\|T^{\sim} \vec{w}\right\|^{2}+\|\vec{\kappa}\|^{2}$. Clearly then $\|\tilde{v}\|$ is minimized by $\vec{\kappa}=\overrightarrow{0}$.

Now $T^{\dagger} T$ is invertible iff $T$ is 1-to- 1 (cf. Exercise (2)), in which case $\widetilde{v}\left(=\widetilde{v}_{\text {min }}\right)$ is unique and the normal equations become

$$
\begin{equation*}
\widetilde{v}=\left(T^{\dagger} T\right)^{-1} T^{\dagger} \widetilde{w}\left(\Longleftrightarrow \widetilde{x}=\left(A^{*} A\right)^{-1} A^{*} \vec{y}\right) \tag{VII.E.35}
\end{equation*}
$$

If $\operatorname{ker}(T) \neq\{0\}$, then (VII.E.33) is less convenient and (VII.E.34) seems the better result. But it turns out that if $A$ is large, computationally (VII.E.34) is more useful than the normal equations regardless of invertibility of $A^{*} A$. This is because the SVD gives

$$
\begin{equation*}
\tilde{x}_{\min }=A^{\sim} \vec{y}=Q \Delta^{\sim} P^{*} \vec{y}, \tag{VII.E.36}
\end{equation*}
$$

and $\Delta^{\sim}$ involves inverting the $\left\{\mu_{i}\right\}$ whereas $\left(A^{*} A\right)^{-1}$ involves inverting the $\left\{\mu_{i}^{2}\right\}$. If some nonzero $\mu_{i}{ }^{\prime}$ s differ by orders of magnitude, the computation of $\left(A^{*} A\right)^{-1}$ will therefore introduce significantly more error than (VII.E.36). That said, the normal equations are typically simpler for small examples, as we'll now see.
VII.E.37. EXAMPLE. We find the LSS for the linear system $A \vec{x}=\vec{y}$, where

$$
A=\left(\begin{array}{cc}
1 & -1 \\
1 & 0 \\
1 & 1 \\
1 & 2
\end{array}\right), \vec{y}=\left(\begin{array}{c}
2 \\
0 \\
-2 \\
1
\end{array}\right)
$$

Compute

$$
\begin{aligned}
{ }^{t} A A & =\left(\begin{array}{ll}
4 & 2 \\
2 & 6
\end{array}\right), \quad\left({ }^{t} A A\right)^{-1}=\frac{1}{10}\left(\begin{array}{cc}
3 & -1 \\
-1 & 2
\end{array}\right) \\
& \Longrightarrow \widetilde{x}=\left({ }^{t} A A\right)^{-1 t} A \vec{y}=\frac{1}{2}\binom{1}{-1}
\end{aligned}
$$

Writing $\mu_{ \pm}^{2}=5 \pm \sqrt{5}$, the SVD is

$$
A=\left(\begin{array}{cccc}
\frac{3-\sqrt{5}}{2 \sqrt{10}} & \frac{3+\sqrt{5}}{2 \sqrt{10}} & -\frac{1}{2} & \frac{1}{2 \sqrt{5}} \\
\frac{1-\sqrt{5}}{2 \sqrt{10}} & \frac{1+\sqrt{5}}{2 \sqrt{10}} & \frac{1}{2} & \frac{-3}{2 \sqrt{5}} \\
\frac{-1-\sqrt{5}}{2 \sqrt{10}} & \frac{-1+\sqrt{5}}{2 \sqrt{10}} & \frac{1}{2} & \frac{3}{2 \sqrt{5}} \\
\frac{-3-\sqrt{5}}{2 \sqrt{10}} & \frac{-3+\sqrt{5}}{2 \sqrt{10}} & -\frac{1}{2} & \frac{1}{2 \sqrt{5}}
\end{array}\right)\left(\begin{array}{cc}
\mu_{+} & 0 \\
0 & \mu_{-} \\
0 & 0 \\
0 & 0
\end{array}\right)\left(\begin{array}{cc}
\frac{1-\sqrt{5}}{\sqrt{2} \mu^{2}} & -\frac{\sqrt{2}}{\mu_{-}} \\
\frac{1+\sqrt{5}}{\sqrt{2} \mu_{+}} & -\frac{\sqrt{2}}{\mu_{+}}
\end{array}\right)
$$

and replacing the middle factor by $\Delta^{\sim}=\operatorname{diag}_{4 \times 2}\left\{\mu_{+}^{-1}, \mu_{-}^{-1}\right\}$ gives

$$
A^{\sim}=\frac{1}{10}\left(\begin{array}{cccc}
4 & 3 & 2 & 1 \\
-3 & -1 & 1 & 3
\end{array}\right)
$$

But using $A^{\sim}=\left({ }^{t} A A\right)^{-1 t} A$ (see Exercise (2) below) is much easier!
This example can be seen as a data fitting (linear regression) problem: the line $Y=x_{1}+x_{2} X$ minimizing the sum of squares of vertical errors in

is $Y=\frac{1}{2}-\frac{1}{2} X$.
VII.E.38. EXAMPLE. Having entered the sports business, a certain crop-sciences company in St. Louis is engaged in trying to grow a better baseball player. They've tracked a few little-leaguers and got the data

which suggests a parabola ${ }^{33}$

$$
Y=f(X)=b_{0}+b_{1} X+b_{2} X^{2}
$$

So write

$$
\begin{aligned}
& Y_{1}=b_{0}+b_{1} X_{1}+b_{2} X_{1}^{2}+\varepsilon_{1} \\
& Y_{2}=b_{0}+b_{1} X_{2}+b_{2} X_{2}^{2}+\varepsilon_{2} \\
& Y_{3}=b_{0}+b_{1} X_{3}+b_{2} X_{3}^{2}+\varepsilon_{3} \\
& Y_{4}=b_{0}+b_{1} X_{4}+b_{2} X_{4}^{2}+\varepsilon_{4}
\end{aligned}
$$

which translates to $\vec{Y}=A \vec{b}+\vec{\varepsilon}$, where

$$
A=\left(\begin{array}{lll}
1 & X_{1} & X_{1}^{2} \\
1 & X_{2} & X_{2}^{2} \\
1 & X_{3} & X_{3}^{2} \\
1 & X_{4} & X_{4}^{2}
\end{array}\right)=\left(\begin{array}{lll}
1 & 0 & 0 \\
1 & 1 & 1 \\
1 & 2 & 4 \\
1 & 3 & 9
\end{array}\right)
$$

Minimizing $\|\vec{\varepsilon}\|=\|A \vec{b}-\vec{Y}\|$ just means solving $A \widetilde{b}=\widetilde{Y}$, or equivalently

$$
{ }^{t} A A \widetilde{b}={ }^{t} A \vec{Y}
$$

[^5]which is
\[

\left($$
\begin{array}{ccc}
4 & 6 & 14 \\
6 & 14 & 36 \\
14 & 36 & 98
\end{array}
$$\right)\left($$
\begin{array}{c}
\tilde{b}_{0} \\
\tilde{b}_{1} \\
\tilde{b}_{2}
\end{array}
$$\right)=\left($$
\begin{array}{c}
9 \\
15 \\
33
\end{array}
$$\right) \underset{\mathrm{RREF}}{\Longrightarrow} \widetilde{\beta}=\left($$
\begin{array}{r}
1.05 \\
2.55 \\
-0.75
\end{array}
$$\right) .
\]

So using $f(X)=1.05+2.55 X-0.75 X^{2} \Longrightarrow 0=f^{\prime}(X)=2.55-$ $1.5 X$ is maximized at $X=1.7$. Therefore the ideal distance from the Arch for raising baseball stars must be 17 miles. Because our data wasn't questionable at all and our sample size was YUGE.

Applications to data compression. One of the many other computational applications of the SVD is called principal component analysis. Suppose in a country of $N=1$ million internet users, you want to target ads (or fake news) based on online behavior, where the number $M$ of possible clicks or purchases is also very large. Assume however that only $k$ (cultural, demographic, etc.) attributes of a person generally determine this behavior: that is, there exists an $N \times k$ "attribute matrix" and a $k \times M$ "behavior matrix" whose product is roughly $A$, the $N \times M$ matrix of raw user data. In other words, we expect $A$ to be well-approximated by a rank $k$ matrix, with $k$ much smaller than $M$ and $N$.

The SVD in the first form we encountered (cf. (VII.E.8)) extends to non-square matrices: in view of (VII.E.25),

$$
\begin{equation*}
A=\sum_{\ell=1}^{r} \mu_{\ell} \cdot \underset{N \times 1}{\hat{p}_{\ell}} \cdot \underset{\substack{\hat{q}_{\ell}^{*}}}{\hat{N}^{*}} \tag{VII.E.39}
\end{equation*}
$$

where $r=\operatorname{rank}(A)$. It turns out that

$$
\begin{equation*}
A_{k}:=\sum_{\ell=1}^{k} \mu_{\ell} \cdot \hat{p}_{\ell} \cdot \hat{q}_{\ell}^{*} \tag{VII.E.40}
\end{equation*}
$$

is the "best" rank $k$ approximation to $A$ (in the sense of minimizing the operator norm ${ }^{34}\left\|A-A_{k}\right\|$ among all rank $k M \times N$ matrices). In the situation just described, we'd expect $A_{k}$ to be very close ${ }^{34}\|M\|:=\max _{\|\vec{v}\|=1}\|M \vec{v}\| ;$ in fact, $\left\|A-A_{k}\right\|=\mu_{k+1}$. In addition, (VII.E.40) minimizes the "stupid" matrix norm $\|M\|:=\left(\sum_{i, j} M_{i j}\right)^{\frac{1}{2}}$ for $A-A_{k}$.
to $A$, while requiring us to record only $k(1+M+N)$ numbers (the $\mu_{\ell}$ and entries of $\hat{p}_{\ell}, \hat{q}_{\ell}$ for $\left.\ell=1, \ldots, k\right)$, a significant data compression vs. the $M N$ entries of $A$. The formulas (VII.E.39)-(VII.E.40) are close in spirit to (discrete) Fourier analysis, which breaks a function down into its constituent frequency components - viz., $A_{i j}=$ $\sum_{\ell, \ell^{\prime}} \alpha_{\ell, \ell^{\prime}} e^{2 \pi \sqrt{-1}} \frac{i \ell}{M} e^{2 \pi \sqrt{-1}} \frac{j \ell^{\prime}}{N}$. But the SVD allows for many fewer terms in (VII.E.40), since the $\hat{p}_{\ell}, \hat{q}_{\ell}$ are not fixed trigonometric functions, but rather "adapted to" the matrix $A$. On the other hand, the discrete Fourier transform doesn't require recording $\hat{p}_{\ell}$ and $\hat{q}_{\ell}$, so has that advantage. Fortunately for computational applications, MATLAB has efficient algorithms for both!

## Exercises

(1) (a) Show that if a normal operator $T: V \rightarrow V$ has real eigenvalues, then it is self-adjoint.
(b) More generally, for a normal operator $T$ with eigenvalues $\left\{\lambda_{i}\right\}$, what are the eigenvalues of $T^{+}$?
(2) (a) Show that $T$ is 1 -to- 1 iff $T^{\dagger} T$ is invertible.
(b) Show that if $T$ is 1-to-1, then $T^{\sim}=\left(T^{\dagger} T\right)^{-1} T^{\dagger}$. (So in this case, (VII.E.34) and (VII.E.35) are "the same". However, the two formulas $\left(A^{*} A\right)^{-1} A^{*}$ and $Q \Delta^{\sim} P^{*}$ for $A^{\sim}$ really do have different strengths.)
(3) As luck would have it, at time $t=0$ bullies stuffed your backpack full of radioactive material from the Bridgeton landfill. Your legal team thinks there are two substances in there, with half-lives of one and five days respectively, but all they can do is measure the overall masses $M_{1}, M_{2}, \ldots, M_{n}$ of the backpack at the end of days $1,2 \ldots, n$. (The bullies also superglued it shut, you see.) Measurements have error, so you need to formulate a linear regression model in order to determine the original masses $A, B$ of the two substances at time $t=0$. This should involve an $n \times 2$ matrix.
(4) Find a polar decomposition for

$$
A=\left(\begin{array}{ccc}
20 & 4 & 0 \\
0 & 0 & 1 \\
4 & 20 & 0
\end{array}\right)
$$

(5) Calculate the matrix SVD for

$$
A=\left(\begin{array}{cccc}
1 & 1 & 1 & 1 \\
1 & 0 & -2 & 1 \\
1 & -1 & 1 & 1
\end{array}\right)
$$

(6) Calculate the minimal least-squares solution of the system

$$
\begin{aligned}
x_{1}+x_{2} & =1 \\
x_{1}+x_{2} & =2 \\
-x_{1}-x_{2} & =0
\end{aligned}
$$


[^0]:    ${ }^{26}$ The reader may of course replace "unitary" and C by "orthonormal" /"orthogonal" and $\mathbb{R}$ in what follows.

[^1]:    ${ }^{27}$ What you should actually have in mind here is, in the case where $V=\mathbb{C}^{n}$ with dot product, the standard basis $\hat{e}$.

[^2]:    ${ }^{28}$ More precisely, "rotation" here can mean a complicated sequence of rotations and reflections.
    ${ }^{29}$ If $A \in M_{n}(\mathbb{R})$, then the above construction shows that $S_{1}$ and $S_{2}$ can be taken to be real (orthogonal); and such $S_{i}$ are unique modulo rescaling by $\Delta$ real diagonal unitary, i.e. with diagonal entries $\pm 1$.

[^3]:    ${ }^{31}$ The notation means an $m \times n$ matrix, whose entries are zero except for $(j, j)^{\text {th }}$ entries for $1 \leq j \leq r(\leq m, n)$.

[^4]:    ${ }^{32}$ Here $\hat{p}_{1}, \ldots, \hat{p}_{m}$ and $\hat{q}_{1}, \ldots, \hat{q}_{n}$ are the column vectors of $P$ and $Q$. They are unitary bases for $\mathbb{C}^{m}$ and $\mathbb{C}^{n}$ under the dot product. The orthogonal direct sum decompositions further below are also with respect to the dot product.

[^5]:    ${ }^{33}$ More seriously, rather than looking at the shape of the data set, one should try to base the form of $f$ on physical principle (see for instance Exercise (2) below).

