

Overview

- The singular value decomposition (SVD)
 - Motivation
 - Theorem
- Another essential diagram: SVD finds orthonormal bases for $C(\mathbf{A})$, $N(\mathbf{A}^T)$, $C(\mathbf{A}^T)$, $N(\mathbf{A})$
- SVD computation
- Rank-1 expansion of a matrix
- Matrix norm
- SVD in image compression, analysis
- The pseudo-inverse

- Motivation: FTLA does not specify bases for $C(\mathbf{A})$, $N(\mathbf{A}^T)$, $C(\mathbf{A}^T)$, $N(\mathbf{A})$.
- Question: Is there some “natural” basis for the fundamental matrix subspaces?
- Consider linear mapping: $\mathbf{f}: \mathbb{R}^n \rightarrow \mathbb{R}^m$, $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$, $\mathbf{A} \in \mathbb{R}^{m \times n}$
 - The input \mathbf{x} is given in the identity matrix basis, $\mathbf{x} = \mathbf{I}_n \mathbf{x}$
 - The output $\mathbf{b} = \mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$ is also obtained in the identity matrix basis, $\mathbf{y} = \mathbf{I}_m \mathbf{y}$
 - In these basis the effect of \mathbf{A} might be costly to compute

$$\mathbf{b} = x_1 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \cdots + x_n \mathbf{a}_n \Rightarrow b_i = x_1 a_{i1} + x_2 a_{i2} + \cdots + x_n a_{i,n}.$$

- What would be simpler? One possibility: a simple scaling of each component suggested by

$$\mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} = \mathbf{D}\mathbf{x} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_m)\mathbf{x} = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_m \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} \Rightarrow b_i = \lambda_i x_i$$



- Seek different bases for domain, codomain of $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$, $f(\mathbf{x}) = \mathbf{A}\mathbf{x}$, $\mathbf{A} \in \mathbb{R}^{m \times n}$
 - an orthonormal basis \mathbf{V} in \mathbb{R}^n , $\mathbf{V} \in \mathbb{R}^{n \times n}$, $\mathbf{V}\mathbf{V}^T = \mathbf{V}^T\mathbf{V} = \mathbf{I}_n$

$$\mathbf{I}\mathbf{x} = \mathbf{V}\mathbf{y} \Rightarrow \mathbf{y} = \mathbf{V}^T\mathbf{x}$$

- an orthonormal basis \mathbf{U} in \mathbb{R}^m , $\mathbf{U} \in \mathbb{R}^{m \times m}$, $\mathbf{U}\mathbf{U}^T = \mathbf{U}^T\mathbf{U} = \mathbf{I}_m$

$$\mathbf{I}\mathbf{b} = \mathbf{U}\mathbf{c} \Rightarrow \mathbf{c} = \mathbf{U}^T\mathbf{b}$$

- impose that the effect of \mathbf{A} in the new bases is a simple component scaling

$$\mathbf{c} = \mathbf{\Sigma}\mathbf{y} \Rightarrow \mathbf{U}^T\mathbf{b} = \mathbf{\Sigma}\mathbf{V}^T\mathbf{x} \Rightarrow \mathbf{b} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T\mathbf{x} \Rightarrow$$

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

- Note that $\mathbf{\Sigma} \in \mathbb{R}^{m \times n}$

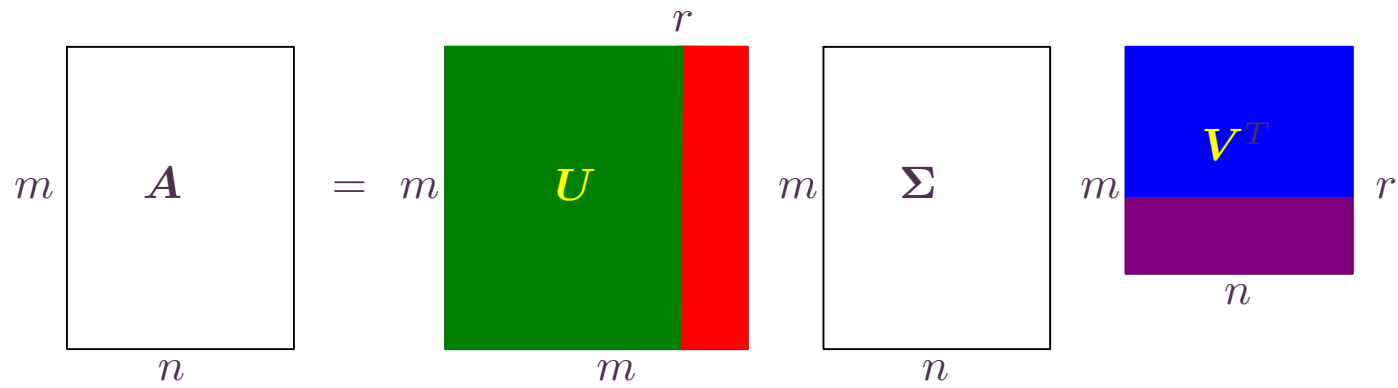
Theorem. (SVD) For any $A \in \mathbb{R}^{m \times n}$, $A = U \Sigma V^T$, with $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$ orthogonal, $\Sigma \in \mathbb{R}_+^{m \times n}$ pseudo-diagonal $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, \dots, 0)$, $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$, $r \leq \min(m, n)$

The SVD is determined by eigendecomposition of $A^T A$, and $A A^T$

- $A^T A = (U \Sigma V^T)^T (U \Sigma V^T) = V (\Sigma^T \Sigma) V^T$, an eigendecomposition of $A^T A$. The columns of V are eigenvectors of $A^T A$ and called *right singular vectors* of A
- $A A^T = (U \Sigma V^T)(U \Sigma^T V^T)^T = U (\Sigma \Sigma^T) U^T$, an eigendecomposition of $A A^T$. The columns of U are eigenvectors of $A A^T$ and called *left singular vectors* of A
- The matrix Σ has zero elements except for the diagonal that contains σ_i , the *singular values* of A , computed as the square roots of the eigenvalues of $A^T A$ (or $A A^T$)



- SVD of $\mathbf{A} \in \mathbb{R}^{m \times n}$ reveals: $\text{rank}(\mathbf{A})$, bases for $\mathcal{C}(\mathbf{A})$, $\mathcal{N}(\mathbf{A}^T)$, $\mathcal{C}(\mathbf{A}^T)$, $\mathcal{N}(\mathbf{A})$



$$\mathbf{A} = \begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_r & \mathbf{u}_{r+1} & \dots & \mathbf{u}_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_r & & & \\ & & & 0 & & \\ & & & & \ddots & \end{bmatrix} \begin{bmatrix} \mathbf{v}_1^T \\ \vdots \\ \mathbf{v}_r^T \\ \mathbf{v}_{r+1}^T \\ \vdots \\ \mathbf{v}_n^T \end{bmatrix}$$

- From $A = U\Sigma V^T$ deduce $AA^T = U\Sigma^2 U^T$, $A^T A = V\Sigma^2 V^T$, hence U is the eigenvector matrix of AA^T , and V is the eigenvector matrix of $A^T A$
- SVD computation is available in Julia, Octave, Matlab, Mathematica ...

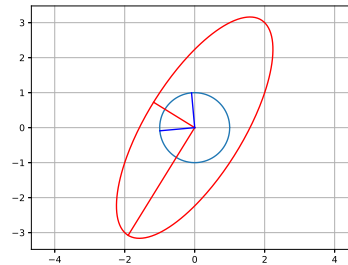
```
∴ short(x) = round(x,digits=6);
```

```
∴ A=[2 -1; -3 1]; F=svd(A); U=F.U; Σ=Diagonal(F.S); Vt=F.Vt; short.([A U*Σ*Vt])
```

```
∴ short.([U Σ Vt'])
```

```
∴
```

- SVD of $A = \begin{bmatrix} 2 & -1 \\ 3 & 1 \end{bmatrix}$ diagram, $f(x) = Ax$



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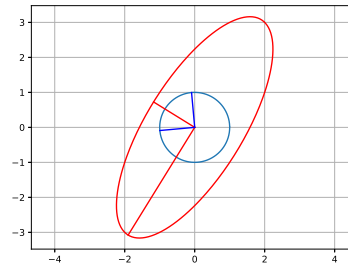
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```

$$\begin{bmatrix} 2.0 & -1.0 & 2.0 & -1.0 \\ -3.0 & 1.0 & -3.0 & 1.0 \end{bmatrix} \quad (1)$$

```
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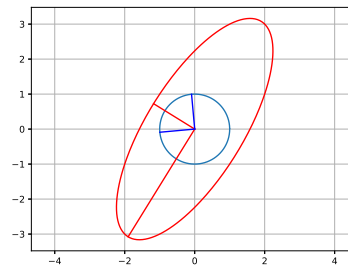
$$\begin{bmatrix} 2.0 & -1.0 & 2.0 & -1.0 \\ -3.0 & 1.0 & -3.0 & 1.0 \end{bmatrix} \quad (2)$$

```
∴ short.([U Σ Vt'])
```

$$\begin{bmatrix} -0.576048 & 0.817416 & 3.864328 & 0.0 & -0.932722 & -0.360597 \\ 0.817416 & 0.576048 & 0.0 & 0.258777 & 0.360597 & -0.932722 \end{bmatrix} \quad (3)$$

```
∴
```

- SVD of $A = \begin{bmatrix} 2 & -1 \\ 3 & 1 \end{bmatrix}$ diagram, $f(x) = Ax$



- $A = U\Sigma V^T$, carry out block multiplication

$$A = \begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_r & \mathbf{u}_{r+1} & \dots & \mathbf{u}_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & & & & \\ & \ddots & & & & \\ & & \sigma_r & & & \\ & & & 0 & & \\ & & & & \ddots & \end{bmatrix} \begin{bmatrix} \mathbf{v}_1^T \\ \vdots \\ \mathbf{v}_r^T \\ \mathbf{v}_{r+1}^T \\ \vdots \\ \mathbf{v}_n^T \end{bmatrix} \Rightarrow$$

$$A = \begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_r & \mathbf{u}_{r+1} & \dots & \mathbf{u}_m \end{bmatrix} \begin{bmatrix} \sigma_1 \mathbf{v}_1^T \\ \vdots \\ \sigma_r \mathbf{v}_r^T \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix} = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \dots + \sigma_r \mathbf{u}_r \mathbf{v}_r^T$$

- The above is known as a “rank-one” expansion since $\text{rank}(\mathbf{u}_k \mathbf{v}_k^T) = 1$. Note that $\mathbf{u}_k \mathbf{v}_k^T \in \mathbb{R}^{m \times n}$ and is a matrix whose columns are n scalings of \mathbf{u}_k
- SVD theorem: $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$, Often $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_k \gg \sigma_{k+1} \geq \dots \geq \sigma_r > 0$

- U, V specify intrinsic directions within $\mathbb{R}^m, \mathbb{R}^n$ along which A acts as scaling transformation
- Applying linear mapping to the v_1 vector, $f(v_1) = Av_1$

$$Av_1 = \left(\sum_{i=1}^p \sigma_i u_i v_i^T \right) v_1 = \sum_{i=1}^p \sigma_i u_i (v_i^T v_1) = \sigma_1 u_1$$

- Direction most amplified by $f(x) = Ax$ is v_1 and the result is the vector $\sigma_1 u_1$
- Define a matrix norm as the largest amplification factor

$$\|A\|_2 = \max_{\|x\|_2=1} \|Ax\|_2.$$

- The largest singular value σ_1 is the matrix 2-norm

$$\sigma_1 = \max_{\|x\|_2=1} \|Ax\|_2.$$

- Full SVD

$$\mathbf{A} = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^T, r \leq \min(m, n).$$

- Truncated SVD

$$\mathbf{A} \cong \mathbf{A}_p = \sum_{i=1}^p \sigma_i \mathbf{u}_i \mathbf{v}_i^T.$$

- Many applications, e.g., image compression



Figure 1. Successive SVD approximations of Andy Warhol's painting, *Marilyn Diptych* (~1960), with $k = 10, 20, 40$ rank-one updates.

- Consider $x_1, x_2: \mathbb{R} \rightarrow \mathbb{R}$, data streams in time of inputs $x_1(t)$ and outputs $x_2(t)$
- Is there some function f linking outputs to inputs? $f(x_1(t)) = x_2(t)$
- Seek answer by first asking: is x_2 *correlated* to x_1 ?
- Introduce mean values

$$\mu_1 \cong \bar{x}_1 = \frac{1}{N} \sum_{i=1}^N x_1(t_i) = E[x_1], \mu_2 \cong \bar{x}_2 = \frac{1}{N} \sum_{i=1}^N x_2(t_i) = E[x_2].$$

- E is the *expectation*, a linear mapping, $E: \mathbb{R}^N \rightarrow \mathbb{R}$ whose associated matrix is

$$\mathbf{E} = \frac{1}{N} [1 \ 1 \ \dots \ 1].$$

- Shift data such that $\bar{x}_1 = \bar{x}_2 = 0$. Define correlation coefficient

$$\rho(x_1, x_2) = \frac{E[x_1 x_2]}{\sigma_1 \sigma_2} = \frac{E[x_1 x_2]}{\sqrt{E[x_1^2] E[x_2^2]}} = \frac{\mathbf{x}_1^T \mathbf{x}_2}{\|\mathbf{x}_1\| \|\mathbf{x}_2\|}.$$

- *uncorrelated*, if $\rho = 0$; *correlated*, if $\rho = 1$; *anti-correlated*, if $\rho = -1$.

- Correlated signals

```
∴ t=0:0.01:1; x1=1.0*t; x2=t.^2; rho=transpose(x1)*x2/norm(x1)/norm(x2)
```

```
∴
```

- Uncorrelated signals

```
∴ m=size(x1)[1]; x3=2*(rand(m,1).-0.5)[: ,1]; rho=transpose(x1)*x3/norm(x1)/norm(x3)
```

```
∴
```

- Anticorrelated signals

```
∴ x4=-t.^2; rho=transpose(x1)*x4/norm(x1)/norm(x4)
```

- Correlated signals

```
∴ t=0:0.01:1; x1=1.0*t; x2=t.^2; rho=transpose(x1)*x2/norm(x1)/norm(x2)
```

```
0.968249831385581
```

```
∴
```

- Uncorrelated signals

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∴ m=size(x1)[1]; x3=2*(rand(m,1).-0.5)[: ,1]; rho=transpose(x1)*x3/norm(x1)/norm(x3)
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```
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```
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```
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```

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```
∴ m=size(x1)[1]; x3=2*(rand(m,1).-0.5)[:,1]; rho=transpose(x1)*x3/norm(x1)/norm(x3)
```

```
0.040354121344516436
```

```
∴
```

- Anticorrelated signals

```
∴ x4=-t.^2; rho=transpose(x1)*x4/norm(x1)/norm(x4)
```

- Are input and output parameters $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$ well chosen?
- Perhaps components are redundant, a more economical description might be

$$\mathbf{u} \in \mathbb{R}^q, \mathbf{v} \in \mathbb{R}^p, p < m, q < n$$

- Extend idea from correlation coefficient: take N measurements

$$\mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_n] \in \mathbb{R}^{N \times n}, \mathbf{Y} = [\mathbf{y}_1 \ \mathbf{y}_2 \ \dots \ \mathbf{y}_n] \in \mathbb{R}^{N \times m}.$$

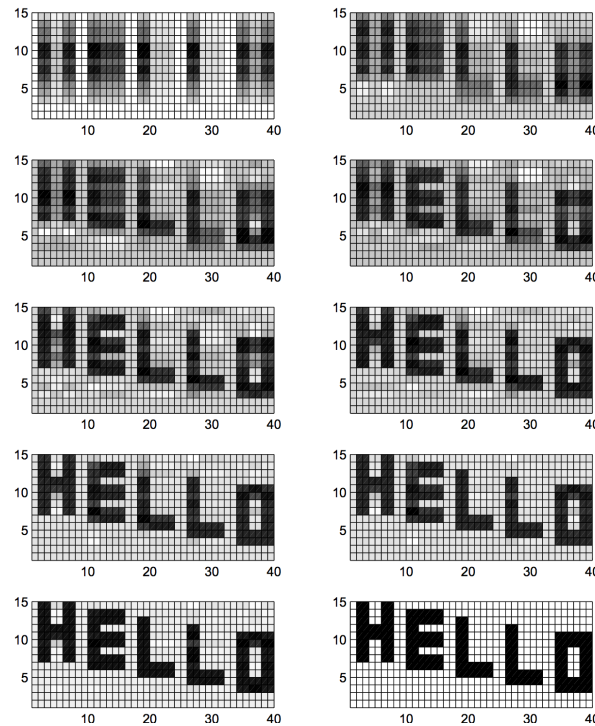
- Choose origin such that $E[\mathbf{x}] = \mathbf{0}$, $E[\mathbf{y}] = \mathbf{0}$.
- *Covariance matrix* (generalization of single variable *variance*)

$$\mathbf{C}_X = \mathbf{X}^T \mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix} [\mathbf{x}_1 \ \mathbf{x}_2 \ \dots \ \mathbf{x}_n] = \begin{bmatrix} \mathbf{x}_1^T \mathbf{x}_1 & \mathbf{x}_1^T \mathbf{x}_2 & \dots & \mathbf{x}_1^T \mathbf{x}_n \\ \mathbf{x}_2^T \mathbf{x}_1 & \mathbf{x}_2^T \mathbf{x}_2 & \dots & \mathbf{x}_2^T \mathbf{x}_n \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{x}_n^T \mathbf{x}_1 & \mathbf{x}_n^T \mathbf{x}_2 & \dots & \mathbf{x}_n^T \mathbf{x}_n \end{bmatrix}$$

- SVDs: $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$, $\mathbf{C}_\mathbf{X} = \mathbf{X}^T\mathbf{X} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$, $\mathbf{\Lambda} = \mathbf{\Sigma}^T\mathbf{\Sigma}$
- Take first q column vectors of \mathbf{V} , $\mathbf{V}_q = [\mathbf{v}_1 \dots \mathbf{v}_q]$, $q < n$

$$\mathbf{x} = \mathbf{V}_q \mathbf{u} = [\mathbf{v}_1 \ \mathbf{v}_2 \ \dots \ \mathbf{v}_q] \mathbf{u}.$$

- System description in terms of $\mathbf{u} \in \mathbb{R}^q$ is more economical than that in terms of $\mathbf{x} \in \mathbb{R}^n$
- In image compression, successive pixel columns are correlated and reduced descriptions are possible



- Consider linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$, $\mathbf{A} \in \mathbb{R}^{m \times m}$, $\text{rank}(\mathbf{A}) = m$. SVD solution steps:
 1. Compute the SVD, $\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \mathbf{A}$;
 2. Find the coordinates of \mathbf{b} in the orthogonal basis \mathbf{U} , $\mathbf{c} = \mathbf{U}^T \mathbf{b}$;
 3. Scale the coordinates of \mathbf{c} by the inverse of the singular values $y_i = c_i / \sigma_i$, $i = 1, \dots, m$, such that $\mathbf{\Sigma}\mathbf{y} = \mathbf{c}$ is satisfied;
 4. Find the coordinates of \mathbf{y} in basis \mathbf{V}^T , $\mathbf{x} = \mathbf{V}\mathbf{y}$.
- What if $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\text{rank}(\mathbf{A}) = r < m$. If $\mathbf{b} \in C(\mathbf{A})$ above procedure still works with a simple modification of step 3 with i going now from 1 to r
 1. $\mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \mathbf{A}$;
 2. $\mathbf{c} = \mathbf{U}^T \mathbf{b}$;
 3. $y_i = c_i / \sigma_i$, $i = 1, \dots, r$
 4. $\mathbf{x} = \mathbf{V}\mathbf{y}$.
- If $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\text{rank}(\mathbf{A}) = r < m$. If $\mathbf{b} \notin C(\mathbf{A})$, the above steps give the best approximation of \mathbf{b} by linear combination of columns of \mathbf{A} in the 2-norm

- Since the steps to solve a linear system or find best approximation are identical define a matrix A^+ that carries out all steps:

$$(U \Sigma V^T) x = b \Leftrightarrow U (\Sigma V^T x) = b$$

$$(\Sigma V^T x) = U^T b \Leftrightarrow \Sigma (V^T x) = U^T b$$

- Recall $\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_r, 0, \dots, 0)$. Define $\Sigma^+ = \text{diag}(1/\sigma_1, 1/\sigma_2, \dots, 1/\sigma_r, 0, \dots, 0)$

$$V^T x = \Sigma^+ U^T b$$

$$x = V \Sigma^+ U^T b$$

- Gather all above steps into a single matrix $A^+ = V \Sigma^+ U^T$ called the *pseudo-inverse* of A .
- The solution then to a linear system (either exact solution or best approximation) is

$$x = A^+ b$$

- In Julia, Matlab, Octave, above procedure is implemented through $x=A \setminus b$.