AM 205: lecture 8

- Last time: Cholesky factorization, QR factorization
- Today: how to compute the QR factorization, the Singular Value Decomposition

QR Factorization

Recall that solving linear least-squares via the normal equations requires solving a system with the matrix $A^T A$

But using the normal equations directly is problematic since $\text{cond}(A^T A) = \text{cond}(A)^2$ (this is a consequence of the SVD)

The QR approach avoids this condition-number-squaring effect and is much more numerically stable!

QR Factorization

How do we compute the QR Factorization?

There are three main methods

- Gram–Schmidt Orthogonalization
- Householder Triangularization
- Givens Rotations

We will cover Gram–Schmidt and Givens rotations in class

Gram–Schmidt Orthogonalization

Suppose $A \in \mathbb{R}^{m \times n}$, $m \geq n$

One way to picture the QR factorization is to construct a sequence of orthonormal vectors $q_1, q_2, \ldots$ such that

$$\text{span}\{q_1, q_2, \ldots, q_j\} = \text{span}\{a_{(:,1)}, a_{(:,2)}, \ldots, a_{(:,j)}\}, \quad j = 1, \ldots, n$$

We seek coefficients r_{ij} such that

$$\begin{aligned} a_{(:,1)} &= r_{11} q_1, \\ a_{(:,2)} &= r_{12} q_1 + r_{22} q_2, \\ &\vdots \\ a_{(:,n)} &= r_{1n} q_1 + r_{2n} q_2 + \cdots + r_{nn} q_n. \end{aligned}$$

This can be done via the Gram–Schmidt process, as we'll discuss shortly

Gram–Schmidt Orthogonalization

In matrix form we have:

$$\left[\begin{array}{c|c|c|c} & & & \\ a_{(:,1)} & a_{(:,2)} & \cdots & a_{(:,n)} \\ & & & \end{array}\right] = \left[\begin{array}{c|c|c|c} & & & \\ q_1 & q_2 & \cdots & q_n \\ & & & \end{array}\right] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}$$

This gives $A = \hat{Q}\hat{R}$ for $\hat{Q} \in \mathbb{R}^{m \times n}$, $\hat{R} \in \mathbb{R}^{n \times n}$

This is called the reduced QR factorization of A, which is slightly different from the definition we gave earlier

Note that for $m > n$, $\hat{Q}^T\hat{Q} = \mathrm{I}$, but $\hat{Q}\hat{Q}^T \neq \mathrm{I}$ (the latter is why the full QR is sometimes nice)

Full vs Reduced QR Factorization

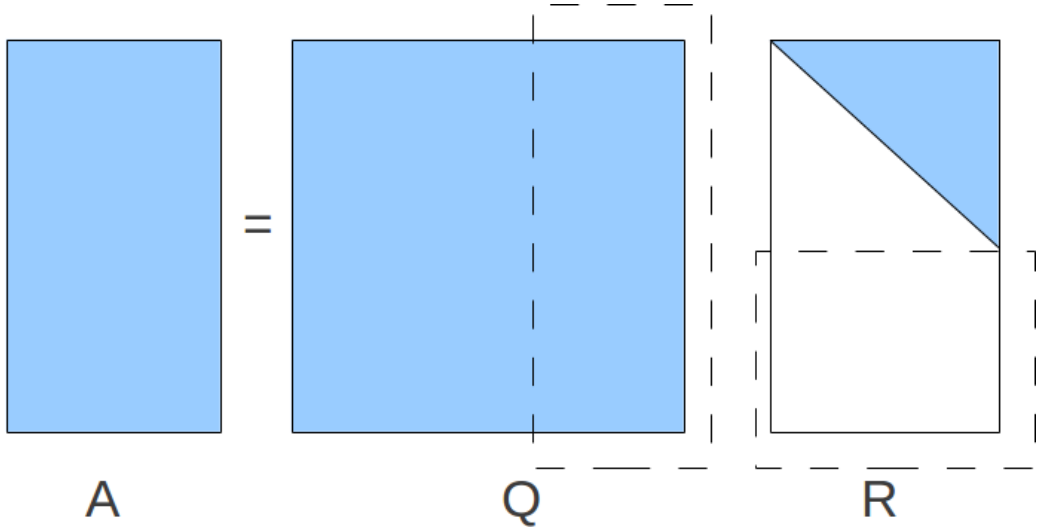
The full QR factorization (defined earlier)

$$A = QR$$

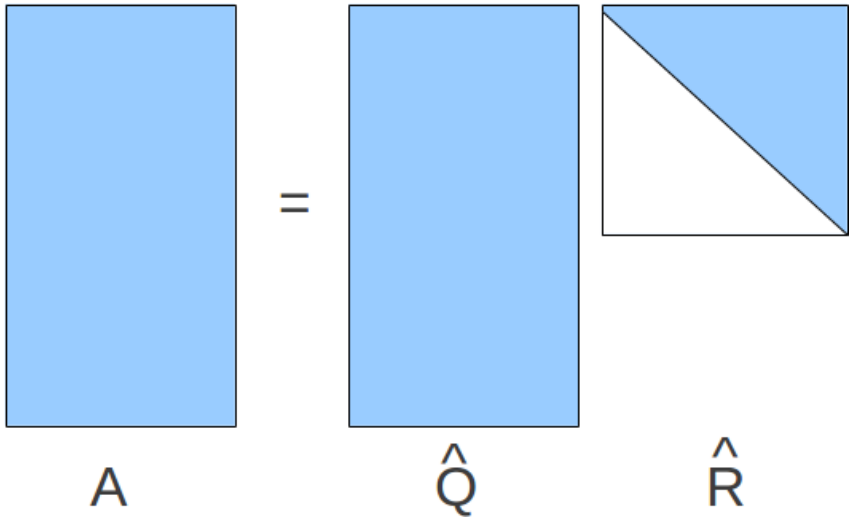
is obtained by appending $m - n$ arbitrary orthonormal columns to $\hat{Q}$ to make it an $m \times m$ orthogonal matrix

We also need to append rows of zeros to $\hat{R}$ to "silence" the last $m - n$ columns of Q, to obtain $R = \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix}$

Full vs Reduced QR Factorization



Full QR



Reduced QR

Full vs Reduced QR Factorization

Exercise: Show that the linear least-squares solution is given by $\hat{R}x = \hat{Q}^T b$ by plugging $A = \hat{Q}\hat{R}$ into the Normal Equations

This is equivalent to the least-squares result we showed earlier using the full QR factorization, since $c_1 = \hat{Q}^T b$

Full versus Reduced QR Factorization

In Python, `numpy.linalg.qr` gives the reduced QR factorization by default

```
Python 2.7.8 (default, Jul 13 2014, 17:11:32)
[GCC 4.2.1 Compatible Apple LLVM 5.1 (clang-503.0.40)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy as np
>>> a=np.random.random((5,3))
>>> (q,r)=np.linalg.qr(a)
>>> q
array([[-0.07519839, -0.74962369,  0.041629  ],
       [-0.25383796, -0.42804369, -0.24484042],
       [-0.78686491,  0.40126393, -0.21414012],
       [-0.06631853, -0.17513071, -0.79738432],
       [-0.55349522, -0.25131537,  0.5065989 ]])
>>> r
array([[-1.17660526, -0.58996516, -1.49606297],
       [ 0.        , -0.34262421, -0.72248544],
       [ 0.        ,  0.        , -0.35192857]])
```

Full versus Reduced QR Factorization

In Python, supplying the `mode='complete'` option gives the complete QR factorization

```
Python 2.7.8 (default, Jul 13 2014, 17:11:32)
[GCC 4.2.1 Compatible Apple LLVM 5.1 (clang-503.0.40)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy as np
>>> a=np.random.random((5,3))
>>> (q,r)=np.linalg.qr(a,mode='complete')
>>> q
array([[-0.07519839, -0.74962369,  0.041629  ,  0.12584638, -0.64408015],
       [-0.25383796, -0.42804369, -0.24484042, -0.74729789,  0.3659835 ],
       [-0.78686491,  0.40126393, -0.21414012, -0.09167938, -0.40690266],
       [-0.06631853, -0.17513071, -0.79738432,  0.51140185,  0.25995667],
       [-0.55349522, -0.25131537,  0.5065989 ,  0.3946791 ,  0.46697922]])
>>> r
array([[-1.17660526, -0.58996516, -1.49606297],
       [ 0.        , -0.34262421, -0.72248544],
       [ 0.        ,  0.        , -0.35192857],
       [ 0.        ,  0.        ,  0.        ],
       [ 0.        ,  0.        ,  0.        ]])
```

Gram–Schmidt Orthogonalization

Returning to the Gram–Schmidt process, how do we compute the q_i, $i = 1, \ldots, n$?

In the jth step, find a unit vector $q_j \in \text{span}\{a_{(:,1)}, a_{(:,2)}, \ldots, a_{(:,j)}\}$ that is orthogonal to $\text{span}\{q_1, q_n, \ldots, q_{j-1}\}$

We set

$$v_j \equiv a_{(:,j)} - (q_1^T a_{(:,j)})q_1 - \cdots - (q_{j-1}^T a_{(:,j)})q_{j-1},$$

and then $q_j \equiv v_j / \|v_j\|_2$ satisfies our requirements

We can now determine the required values of r_{ij}

Gram–Schmidt Orthogonalization

We then write our set of equations for the q_i as

$$\begin{aligned} q_1 &= \frac{a_{(:,1)}}{r_{11}}, \\ q_2 &= \frac{a_{(:,2)} - r_{12} q_1}{r_{22}}, \\ &\vdots \\ q_n &= \frac{a_{(:,n)} - \sum_{i=1}^{n-1} r_{in} q_i}{r_{nn}}. \end{aligned}$$

Then from the definition of q_j, we see that

$$\begin{aligned} r_{ij} &= q_i^T a_{(:,j)}, \qquad\qquad i \neq j \\ |r_{jj}| &= \|a_{(:,j)} - \sum_{i=1}^{j-1} r_{ij} q_i\|_2 \end{aligned}$$

The sign of r_{jj} is not determined uniquely, *e.g.* we could choose $r_{jj} > 0$ for each j

Classical Gram–Schmidt Process

The Gram–Schmidt algorithm we have described is provided in the pseudocode below

1: **for** $j = 1 : n$ **do**
2: $\quad v_j = a_{(:,j)}$
3: $\quad$ **for** $i = 1 : j - 1$ **do**
4: $\quad\quad r_{ij} = q_i^T a_{(:,j)}$
5: $\quad\quad v_j = v_j - r_{ij} q_i$
6: $\quad$ **end for**
7: $\quad r_{jj} = \|v_j\|_2$
8: $\quad q_j = v_j / r_{jj}$
9: **end for**

This is referred to the classical Gram–Schmidt (CGS) method

Gram–Schmidt Orthogonalization

The only way the Gram–Schmidt process can "fail" is if $|r_{jj}| = \|v_j\|_2 = 0$ for some j

This can only happen if $a_{(:,j)} = \sum_{i=1}^{j-1} r_{ij} q_i$ for some j, *i.e.* if $a_{(:,j)} \in \text{span}\{q_1, q_n, \ldots, q_{j-1}\} = \text{span}\{a_{(:,1)}, a_{(:,2)}, \ldots, a_{(:,j-1)}\}$

This means that columns of A are linearly dependent

Therefore, Gram–Schmidt fails $\implies$ cols. of A linearly dependent

Gram–Schmidt Orthogonalization

Equivalently, by contrapositive: cols. of A linearly independent $\implies$ Gram–Schmidt succeeds

Theorem: Every $A \in \mathbb{R}^{m \times n} (m \geq n)$ of full rank has a unique reduced QR factorization $A = \hat{Q}\hat{R}$ with $r_{ii} > 0$

The only non-uniqueness in the Gram–Schmidt process was in the sign of r_{ii}, hence $\hat{Q}\hat{R}$ is unique if $r_{ii} > 0$

Gram–Schmidt Orthogonalization

Theorem: Every $A \in \mathbb{R}^{m \times n} (m \geq n)$ has a full QR factorization.

Case 1: A has full rank

- We compute the reduced QR factorization from above
- To make Q square we pad $\hat{Q}$ with $m - n$ arbitrary orthonormal columns
- We also pad $\hat{R}$ with $m - n$ rows of zeros to get R

Case 2: A doesn't have full rank

- At some point in computing the reduced QR factorization, we encounter $\|v_j\|_2 = 0$
- At this point we pick an arbitrary q_j orthogonal to $\text{span}\{q_1, q_2, \ldots, q_{j-1}\}$ and then proceed as in Case 1

Modified Gram–Schmidt Process

The classical Gram–Schmidt process is numerically unstable!
(sensitive to rounding error, orthogonality of the q_j degrades)

The algorithm can be reformulated to give the modified Gram–Schmidt process, which is numerically more robust

Key idea: when each new q_j is computed, orthogonalize each remaining column of A against it

Modified Gram–Schmidt Process

Modified Gram–Schmidt (MGS):

1: **for** $i = 1 : n$ **do**
2: $\quad v_i = a_{(:,i)}$
3: **end for**
4: **for** $i = 1 : n$ **do**
5: $\quad r_{ii} = \|v_i\|_2$
6: $\quad q_i = v_i / r_{ii}$
7: $\quad$ **for** $j = i + 1 : n$ **do**
8: $\quad\quad r_{ij} = q_i^T v_j$
9: $\quad\quad v_j = v_j - r_{ij} q_i$
10: $\quad$ **end for**
11: **end for**

Modified Gram–Schmidt Process

Key difference between MGS and CGS:

- In CGS we compute orthogonalization coefficients r_{ij} wrt the "raw" vector $a_{(:,j)}$
- In MGS we remove components of $a_{(:,j)}$ in $\text{span}\{q_1, q_2, \ldots, q_{i-1}\}$ before computing r_{ij}

This makes no difference mathematically: In exact arithmetic components in $\text{span}\{q_1, q_2, \ldots, q_{i-1}\}$ are annihilated by q_i^T

But in practice it reduces degradation of orthogonality of the q_j
$\Longrightarrow$ superior numerical stability of MGS over CGS

Operation Count

Work in MGS is dominated by lines 8 and 9, the innermost loop:

$$\begin{aligned} r_{ij} &= q_i^T v_j \\ v_j &= v_j - r_{ij} q_i \end{aligned}$$

First line requires m multiplications, $m-1$ additions; second line requires m multiplications, m subtractions

Hence $\sim 4m$ operations per single inner iteration

Hence total number of operations is asymptotic to

$$\sum_{i=1}^{n} \sum_{j=i+1}^{n} 4m \sim 4m \sum_{i=1}^{n} i \sim 2mn^2$$

Alternative QR computation methods

The QR factorization can also be computed using Householder triangularization and Givens rotations.

Both methods take the approach of applying a sequence of orthogonal matrices $Q_1, Q_2, Q_3, \ldots$ to the matrix that successively remove terms below the diagonal (similar to the method employed by the LU factorization).

We will discuss Givens rotations.

A Givens rotation

For $i < j$ and an angle θ, the elements of the $m \times m$ Givens rotation matrix $G(i, j, \theta)$ are

$$\begin{aligned} g_{ii} = c, \qquad g_{jj} = c, \qquad g_{ij} = s, \qquad g_{ji} = -s, \\ g_{kk} = 1 \quad \text{for } k \neq i, j, \\ g_{kl} = 0 \quad \text{otherwise,} \end{aligned} \tag{1}$$

where $c = \cos\theta$ and $s = \sin\theta$.

A Givens rotation

Hence the matrix has the form

$$G(i,j,\theta) = \begin{pmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & c & \dots & s & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & -s & \dots & c & \dots & 0 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{pmatrix}$$

It applies a rotation within the space spanned by the ith and jth coordinates

Effection of a Givens rotation

Consider a $m \times n$ rectangular matrix A where $m \geq n$

Suppose that a_1 and a_2 are in the ith and jth positions in a particular column of A

Restricting to just ith and jth dimensions, a Givens rotation $G(i, j, \theta)$ for a particular angle θ can be applied so that

$$\begin{pmatrix} c & s \\ -s & c \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \alpha \\ 0 \end{pmatrix},$$

where α is non-zero, and the jth component is eliminated

Stable computation

α is given by $\sqrt{a_1^2 + a_2^2}$. We could compute

$$c = a_1/\sqrt{a_1^2 + a_2^2}, \qquad s = a_2/\sqrt{a_1^2 + a_2^2}$$

but this is susceptible to underflow/overflow if α is very small.

A better procedure is as follows:

- if $|a_1| > |a_2|$, set $t = \tan\theta = a_2/a_1$, and hence $c = \frac{1}{\sqrt{1+t^2}}, s = ct$.
- if $|a_2| \geq |a_1|$, set $\tau = \cot\theta = a_1/a_2$, and hence $s = \frac{1}{\sqrt{1+\tau^2}}, c = s\tau$.

Givens rotation algorithm

To perform the Givens procedure on a dense $m \times n$ rectangular matrix A where $m \geq n$, the following algorithm can be used:

1: $R = A, Q = I$
2: **for** $k = 1 : n$ **do**
3: **for** $j = m : k + 1$ **do**
4: Construct $G = G(j - 1, j, \theta)$ to eliminate a_{jk}
5: $A = GA$
6: $Q = QG^T$
7: **end for**
8: **end for**

Givens rotation advantages

In general, for dense matrices, Givens rotations are not as efficient as the other two approaches (Gram–Schmidt and Householder)

However, they are advantageous for sparse matrices, since non-zero entries can be eliminated one-by-one. They are also amenable to parallelization. Consider the 6×6 matrix:

$$\begin{pmatrix} \times & \times & \times & \times & \times & \times \\ 5 & \times & \times & \times & \times & \times \\ 4 & 6 & \times & \times & \times & \times \\ 3 & 5 & 7 & \times & \times & \times \\ 2 & 4 & 6 & 8 & \times & \times \\ 1 & 3 & 5 & 7 & 9 & \times \end{pmatrix}$$

The numbers represent the steps at which a particular matrix entry can be eliminated. *e.g.* on step 3, elements $(4, 1)$ and $(6, 2)$ can be eliminated concurrently using $G(3, 4, \theta_a)$ and $G(5, 6, \theta_b)$, respectively, since these two matrices operate on different rows.

Singular Value Decomposition

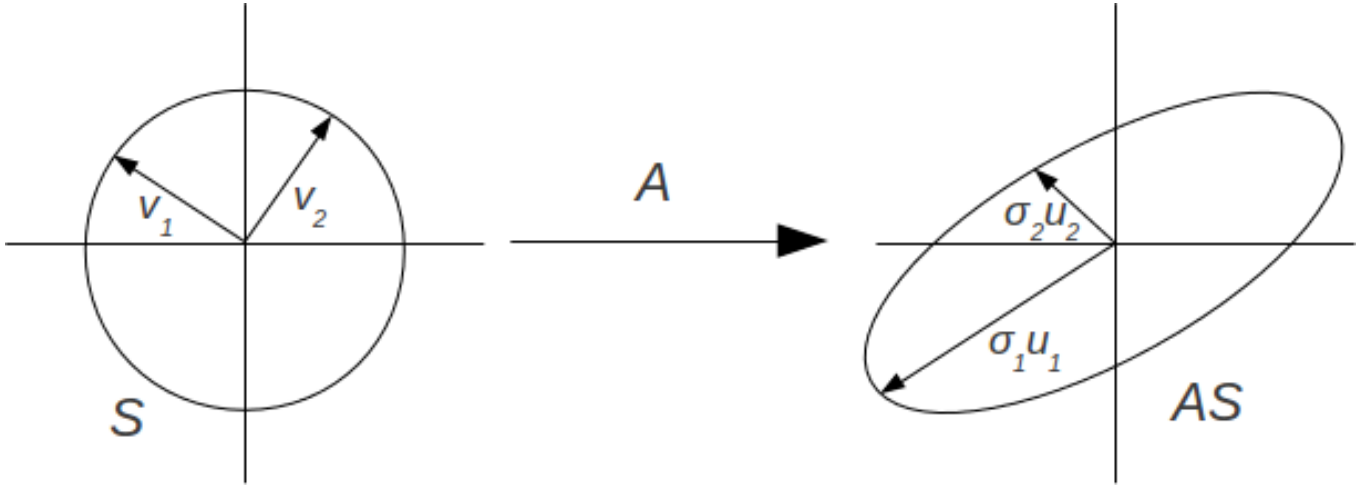
The Singular Value Decomposition (SVD) is a very useful matrix factorization

Motivation for SVD: image of the unit sphere, S, from any $m \times n$ matrix is a hyperellipse

A hyperellipse is obtained by stretching the unit sphere in $\mathbb{R}^m$ by factors $\sigma_1, \ldots, \sigma_m$ in orthogonal directions $u_1, \ldots, u_m$

Singular Value Decomposition

For $A \in \mathbb{R}^{2\times 2}$, we have



Singular Value Decomposition

Based on this picture, we make some definitions:

- Singular values: $\sigma_1, \sigma_2, \ldots, \sigma_n \geq 0$ (we typically assume $\sigma_1 \geq \sigma_2 \geq \ldots$)
- Left singular vectors: $\{u_1, u_2, \ldots, u_n\}$, unit vectors in directions of principal semiaxes of AS
- Right singular vectors: $\{v_1, v_2, \ldots, v_n\}$, preimages of the u_i so that $Av_i = \sigma_i u_i$, $i = 1, \ldots, n$

(The names "left" and "right" come from the formula for the SVD below)

Singular Value Decomposition

The key equation above is that

$$Av_i = \sigma_i u_i, \quad i = 1, \ldots, n$$

Writing this out in matrix form we get

$$\begin{bmatrix} \\ A \\ \\ \end{bmatrix} \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix} = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix}$$

Or more compactly:

$$AV = \widehat{U}\widehat{\Sigma}$$

Singular Value Decomposition

Here

- $\widehat{\Sigma} \in \mathbb{R}^{n \times n}$ is diagonal with non-negative, real entries
- $\widehat{U} \in \mathbb{R}^{m \times n}$ with orthonormal columns
- $V \in \mathbb{R}^{n \times n}$ with orthonormal columns

Therefore V is an orthogonal matrix ($V^T V = VV^T = \mathrm{I}$), so that we have the reduced SVD for $A \in \mathbb{R}^{m \times n}$:

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

Singular Value Decomposition

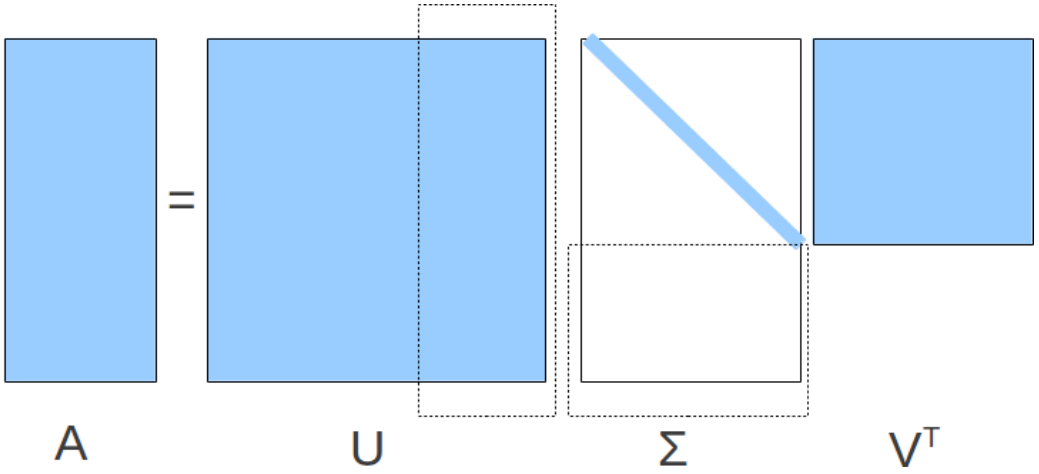
Just as with QR, we can pad the columns of $\widehat{U}$ with $m - n$ arbitrary orthogonal vectors to obtain $U \in \mathbb{R}^{m \times m}$

We then need to "silence" these arbitrary columns by adding rows of zeros to $\widehat{\Sigma}$ to obtain Σ

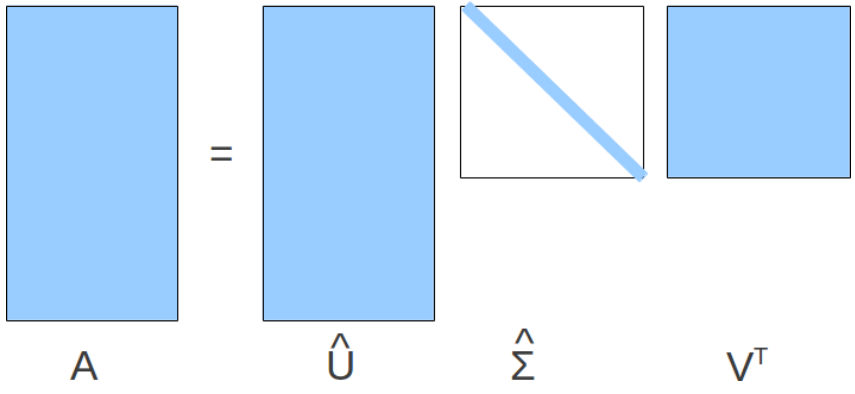
This gives the full SVD for $A \in \mathbb{R}^{m \times n}$:

$$A = U \Sigma V^T$$

Full vs Reduced SVD



Full SVD



Reduced SVD

Singular Value Decomposition

Theorem: Every matrix $A \in \mathbb{R}^{m \times n}$ has a full singular value decomposition. Furthermore:

- The σ_j are uniquely determined
- If A is square and the σ_j are distinct, the $\{u_j\}$ and $\{v_j\}$ are uniquely determined up to sign

Singular Value Decomposition

This theorem justifies the statement that the image of the unit sphere under any $m \times n$ matrix is a hyperellipse

Consider $A = U\Sigma V^T$ (full SVD) applied to the unit sphere, S, in $\mathbb{R}^n$:

1. The orthogonal map V^T preserves S
2. Σ stretches S into a hyperellipse aligned with the canonical axes e_j
3. U rotates or reflects the hyperellipse without changing its shape

SVD in Python

Python's `numpy.linalg.svd` function computes the full SVD of a matrix

```
Python 2.7.8 (default, Jul 13 2014, 17:11:32)
[GCC 4.2.1 Compatible Apple LLVM 5.1 (clang-503.0.40)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy as np
>>> a=np.random.random((4,2))
>>> (u,s,v)=np.linalg.svd(a)
>>> u
array([[-0.38627868,  0.3967265 , -0.44444737, -0.70417569],
       [-0.4748846 , -0.845594  , -0.23412286, -0.06813139],
       [-0.47511682,  0.05263149,  0.84419597, -0.24254299],
       [-0.63208972,  0.35328288, -0.18704595,  0.663828  ]])
>>> s
array([ 1.56149162,  0.24419604])
>>> v
array([[-0.67766849, -0.73536754],
       [-0.73536754,  0.67766849]])
```

SVD in Python

The `full_matrices=0` option computes the reduced SVD

```
Python 2.7.8 (default, Jul 13 2014, 17:11:32)
[GCC 4.2.1 Compatible Apple LLVM 5.1 (clang-503.0.40)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy as np
>>> a=np.random.random((4,2))
>>> (u,s,v)=np.linalg.svd(a,full_matrices=0)
>>> u
array([[-0.38627868,  0.3967265 ],
       [-0.4748846 , -0.845594  ],
       [-0.47511682,  0.05263149],
       [-0.63208972,  0.35328288]])
>>> s
array([ 1.56149162,  0.24419604])
>>> v
array([[-0.67766849, -0.73536754],
       [-0.73536754,  0.67766849]])
```

Matrix Properties via the SVD

- The rank of A is r, the number of nonzero singular values[1]

Proof: In the full SVD $A = U\Sigma V^T$, U and V^T have full rank, hence it follows from linear algebra that $\text{rank}(A) = \text{rank}(\Sigma)$

- $\text{image}(A) = \text{span}\{u_1, \ldots, u_r\}$ and $\text{null}(A) = \text{span}\{v_{r+1}, \ldots, v_n\}$

Proof: This follows from $A = U\Sigma V^T$ and

$$\begin{aligned} \text{image}(\Sigma) &= \text{span}\{e_1, \ldots, e_r\} \in \mathbb{R}^m \\ \text{null}(\Sigma) &= \text{span}\{e_{r+1}, \ldots, e_n\} \in \mathbb{R}^n \end{aligned}$$

[1] This also gives us a good way to define rank in finite precision: the number of singular values larger than some (small) tolerance

Matrix Properties via the SVD

- $\|A\|_2 = \sigma_1$

Proof: Recall that $\|A\|_2 \equiv \max_{\|v\|_2=1} \|Av\|_2$. Geometrically, we see that $\|Av\|_2$ is maximized if $v = v_1$ and $Av = \sigma_1 u_1$.

- The singular values of A are the square roots of the eigenvalues of $A^T A$ or AA^T

Proof: (Analogous for AA^T)

$$A^T A = (U\Sigma V^T)^T (U\Sigma V^T) = V\Sigma U^T U\Sigma V^T = V(\Sigma^T \Sigma)V^T,$$

hence $(A^T A)V = V(\Sigma^T \Sigma)$, or $(A^T A)v_{(:,j)} = \sigma_j^2 v_{(:,j)}$

Matrix Properties via the SVD

The pseudoinverse, A^+, can be defined more generally in terms of the SVD

Define pseudoinverse of a scalar σ to be $1/\sigma$ if $\sigma \neq 0$ and zero otherwise

Define pseudoinverse of a (possibly rectangular) diagonal matrix as transpose of the matrix and taking pseudoinverse of each entry

Pseudoinverse of $A \in \mathbb{R}^{m \times n}$ is defined as

$$A^+ = V \Sigma^+ U^T$$

A^+ exists for any matrix A, and it captures our definitions of pseudoinverse from previously

Matrix Properties via the SVD

We generalize the condition number to rectangular matrices via the definition $\kappa(A) = \|A\|\|A^+\|$

We can use the SVD to compute the 2-norm condition number:

- $\|A\|_2 = \sigma_{\text{max}}$
- Largest singular value of A^+ is $1/\sigma_{\text{min}}$ so that $\|A^+\|_2 = 1/\sigma_{\text{min}}$

Hence $\kappa(A) = \sigma_{\text{max}}/\sigma_{\text{min}}$

Matrix Properties via the SVD

These results indicate the importance of the SVD, both theoretically and as a computational tool

Algorithms for calculating the SVD are an important topic in Numerical Linear Algebra, but outside scope of this course

Requires $\sim 4mn^2 - \frac{4}{3}n^3$ operations

For more details on algorithms, see Trefethen & Bau, or Golub & van Loan