Orthonormal Vectors

- A set S of nonzero vectors are *orthonormal* if, for every **x** and **y** in S, we have dot(**x**,**y**)=0 (orthogonality) and for every **x** in S we have $||\mathbf{x}||_2=1$ (length is 1).

The QR Algorithm

- The QR algorithm for finding eigenvalues is based on the QR factorisation we learnt in the least squares part of the course
- Recall the QR factorization represents a matrix A as:

$$A = QR$$

  where Q is a matrix whose columns are orthonormal, and R is an upper triangular matrix.
- Recall that $Q^H Q = I$ and $Q^{-1} = Q^H$.
- Q is termed a *unitary* matrix.

QR Algorithm without Shifts

$A_0 = A$

for k=1,2,…

$Q_k R_k = A_k$

$A_{k+1} = R_k Q_k$

end

Since:

$$A_{k+1} = R_k Q_k = Q_k^{-1} A_k Q_k$$

then A_k and A_{k+1} are similar and so have the same eigenvalues.

A_{k+1} tends to an upper triangular matrix with the same eigenvalues as A. These eigenvalues lie along the main diagonal of A_{k+1}.

QR Algorithm with Shift

$A_0 = A$
for k=1,2,…
    $s = A_k(n,n)$
    $Q_k R_k = A_k - sI$
    $A_{k+1} = R_k Q_k + sI$
end

Since:

$$A_{k+1} = R_k Q_k + sI$$
$$= Q_k^{-1}(A_k - sI)Q_k + sI$$
$$= Q_k^{-1} A_k Q_k$$

so once again A_k and A_{k+1} are similar and so have the same eigenvalues.

The shift operation subtracts s from each eigenvalue of A, and speeds up convergence.

MATLAB Code for QR Algorithm

- Let A be an n× n matrix

  n = size(A,1);

  I = eye(n,n);

  s = A(n,n); [Q,R] = qr(A-s*I); A = R*Q+s*I
- Use the up arrow key in MATLAB to iterate or put a loop round the last line.

Deflation

- The eigenvalue at A(n,n) will converge first.
- Then we set s=A(n-1,n-1) and continue the iteration until the eigenvalue at A(n-1,n-1) converges.
- Then set s=A(n-2,n-2) and continue the iteration until the eigenvalue at A(n-2,n-2) converges, and so on.
- This process is called *deflation*.

Computational Methods
CMSC/AMSC/MAPL 460

EigenValue decomposition
Singular Value Decomposition

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Eigenvalue sensitivity

$$A = X \Lambda X^{-1}$$

$$\Lambda = X^{-1} A X$$

$$\Lambda + \delta\Lambda = X^{-1}(A + \delta A)X$$

$$\delta\Lambda = X^{-1}\delta A X$$

$$\|\delta\Lambda\| \leq \|X^{-1}\|\|X\|\|\delta A\| = \kappa(X)\|\delta A\|$$

The sensitivity of the eigenvalues is estimated by the condition number of the matrix of eigenvectors.

The SVD

- **Definition:** Every matrix A of dimensions $m \times n$ ($m \geq n$) can be decomposed as

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

- where
  - U has dimension $m \times m$ and $U^*U = I$,
  - Σ has dimension $m \times n$,
    the only nonzeros are on the main diagonal, and they are nonnegative real numbers $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n$,
  - V has dimension $n \times n$ and $V^* V = I$.

Relation with the Eigenvalue Decomposition

- Let $A = U \Sigma V^*$. Then

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

$$= V\Sigma^* U^* \, U\Sigma V^* = V\Sigma^2 V^*$$

- This tells us that the singular value decomposition of A is related to the Eigenvalue decomposition of $A^* A$
- Recall eigen value decomposition $A = (X \Lambda X^*)$
  - So V which contains the right singular vectors of A has the right eigenvectors of $A^* A$
  - Σ^2 are the eigenvalues of $A^* A$
  - The **singular values** σ_i of A are the square roots of the **eigenvalues** of $A^* A$.

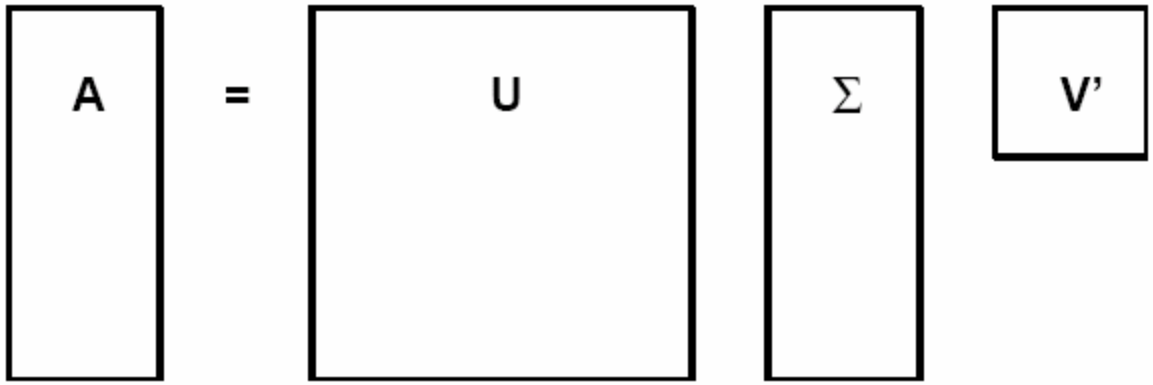
Relation with the Eigenvalue Decomposition (2)

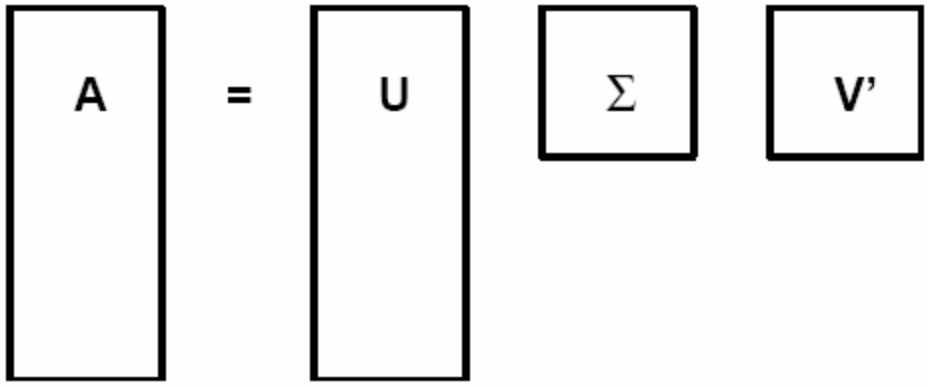
- Let $A = U \Sigma V$. Then

$$A A^* = (U\Sigma V^*)\,(U\Sigma V^*)^*$$
$$= U\Sigma V^* V\Sigma^* U^* = U\Sigma^2 U^*$$

- This tells us that the singular value decomposition of A is related to the Eigenvalue decomposition of AA^*
- Recall eigen value decomposition $A = (X \Lambda X^*)$
  - So U contains the the **left singular vectors** of A, which are also the left eigenvectors of AA^*
  - Σ^2 are the eigenvalues of AA^* *and* the **singular values** σ_i of A are the square roots of the **eigenvalues** of AA^*

Economy-sized SVD





Computing the SVD

- The algorithm is a variant on algorithms for computing eigendecompositions.
  - rather complicated, so better to use a high-quality existing code rather than writing your own.
- In Matlab: [U,S,V] = svd(A)
- The cost is $O(mn^2)$ when $m \geq n$. The constant is of order 10.

Uses of the SVD

- Recall to solve least squares problems we could look at the normal equations ($A^*Ax=A^*b$)
  - So, SVD is closely related to solution of least-squares
  - Used for solving ill conditioned least-squares
- Used for creating low-rank approximations
- Both applications are related

SVD and reduced rank approximation

- $\mathbf{Ax}=\mathbf{b}$ $\mathbf{A}$ is $m\times n$, $\mathbf{x}$ is $n\times 1$ and $\mathbf{b}$ is $m\times 1$.
- $\mathbf{A}=\mathbf{USV}^t$ where $\mathbf{U}$ is m×m, $\mathbf{S}$ is m×n and $\mathbf{V}$ is $n\times n$
- $\mathbf{USV}^t\,\mathbf{x}=\mathbf{b}$. So $\mathbf{SV}^t\,\mathbf{x}=\mathbf{U}^t\mathbf{b}$
- If $\mathbf{A}$ has rank r, then r singular values are significant

$$\mathbf{V}^t\mathbf{x}= \mathrm{diag}(\sigma_1^{-1},\ldots,\sigma_r^{-1},0,\ldots,0)\mathbf{U}^t\mathbf{b}$$

$$\mathbf{x}= \mathbf{V}\,\mathrm{diag}(\sigma_1^{-1},\ldots,\sigma_r^{-1},0,\ldots,0)\mathbf{U}^t\mathbf{b}$$

$$\mathbf{x}_r = \sum_{i=1}^{r} \frac{\mathbf{u}_i^t\mathbf{b}}{\sigma_i}\mathbf{v}_i \qquad \sigma_r > \varepsilon,\quad \sigma_{r+1} \le \varepsilon$$

- We can truncate r at any value and achieve "reduced-rank" approximation to the matrix
- For ordered signular values, this gives the "best reduced rank approximation"

SVD and pseudo inverse

- Pseudoinverse $\mathbf{A}^{+}=\mathbf{V}\ \mathrm{diag}(\sigma_1^{-1},\ldots,\sigma_r^{-1},0,\ldots,0)\ \mathbf{U}^t$
  - $\mathbf{A}^{+}$ is a $n\times m$ matrix.
  - If rank $(\mathbf{A}) = n$ then $\mathbf{A}^{+}=(\mathbf{A}^t\mathbf{A})^{-1}\mathbf{A}$
  - If $\mathbf{A}$ is square $\mathbf{A}^{+}=\mathbf{A}^{-1}$

Well posed problems

- Hadamard postulated that for a problem to be "well posed"

1. Solution must exist
2. It must be unique
3. Small changes to input data should cause small changes to solution

- Many problems in science and computer vision result in "ill-posed" problems.
  - Numerically it is common to have condition 3 violated.
  - Recall from the SVD $\mathbf{x} = \sum_{i=1}^{n} \frac{\mathbf{u}_i^t \mathbf{b}}{\sigma_i} \mathbf{v}_i \qquad \sigma_r > \varepsilon, \quad \sigma_{r+1} \leq \varepsilon$

    If the σ are close to zero small changes in the "data" vector **b** cause big changes in **x**.
- Converting ill-posed problem to well-posed one is called *regularization*.

SVD and Regularization

- Pseudoinverse provides one means of regularization
- Another is to solve $(\mathbf{A}+\varepsilon\mathbf{I})\mathbf{x}=\mathbf{b}$ $\mathbf{x} = \sum_{i=1}^{n} \frac{\sigma_i}{\varepsilon + \sigma_i^2}(\mathbf{u}_i^t \mathbf{b})\mathbf{v}_i$
- Solution of the regular problem requires minimizing of $\|\mathbf{Ax-b}\|^2$
- Solving this modified problemcorresponds to minimizing

$$\|\mathbf{Ax-b}\|^2 + \varepsilon\|\mathbf{x}\|^2$$

- Philosophy – pay a "penalty" of $O(\varepsilon)$ to ensure solution does not blow up.
- In practice we may know that the data has an uncertainty of a certain magnitude … so it makes sense to optimize with this constraint.
- Ill-posed problems are also called "ill-conditioned"