

Orthonormal Vectors

- A set S of nonzero vectors are *orthonormal* if, for every \mathbf{x} and \mathbf{y} in S , we have $\text{dot}(\mathbf{x},\mathbf{y})=0$ (orthogonality) and for every \mathbf{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 $k=1,2,\dots$

$$Q_k R_k = A_k$$

$$A_{k+1} = R_k Q_k$$

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 $k=1,2,\dots$

$$s = A_k(n,n)$$

$$Q_k R_k = A_k - sI$$

$$A_{k+1} = R_k Q_k + sI$$

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 $n \times n$ 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

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

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

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

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

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

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 $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n$,
 - V has dimension $n \times n$ and $V^*V = I$.

Relation with the Eigenvalue Decomposition

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

$$\begin{aligned} A^* A &= (U \Sigma V^*)^* U \Sigma V^* \\ &= V \Sigma^* U^* U \Sigma V^* = V \Sigma^2 V^* \end{aligned}$$

- 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

$$\begin{aligned} A A^* &= (U \Sigma V^*) (U \Sigma V^*)^* \\ &= U \Sigma V^* V \Sigma^* U^* = U \Sigma^2 U^* \end{aligned}$$

- 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

$$\begin{array}{|c|} \hline \mathbf{A} \\ \hline \end{array} = \begin{array}{|c|} \hline \mathbf{U} \\ \hline \end{array} \begin{array}{|c|} \hline \mathbf{\Sigma} \\ \hline \end{array} \begin{array}{|c|} \hline \mathbf{V}' \\ \hline \end{array}$$

$$\begin{array}{|c|} \hline \mathbf{A} \\ \hline \end{array} = \begin{array}{|c|} \hline \mathbf{U} \\ \hline \end{array} \begin{array}{|c|} \hline \mathbf{\Sigma} \\ \hline \end{array} \begin{array}{|c|} \hline \mathbf{V}' \\ \hline \end{array}$$

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: $[U,S,V] = \text{svd}(A)$
- 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 $m \times m$, \mathbf{S} is $m \times n$ 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
 $\mathbf{V}^t \mathbf{x}=\text{diag}(\sigma_1^{-1}, \dots, \sigma_r^{-1}, 0, \dots, 0) \mathbf{U}^t \mathbf{b}$
 $\mathbf{x}=\mathbf{V} \text{diag}(\sigma_1^{-1}, \dots, \sigma_r^{-1}, 0, \dots, 0) \mathbf{U}^t \mathbf{b}$
$$\mathbf{x}_r = \sum_{i=1}^r \frac{\mathbf{u}_i^t \mathbf{b}}{\sigma_i} \mathbf{v}_i \quad \sigma_r > \varepsilon, \quad \sigma_{r+1} \leq \varepsilon$$
- We can truncate r at any value and achieve “reduced-rank” approximation to the matrix
- For ordered singular values, this gives the “best reduced rank approximation”

SVD and pseudo inverse

- Pseudoinverse $\mathbf{A}^+ = \mathbf{V} \text{diag}(\sigma_1^{-1}, \dots, \sigma_r^{-1}, 0, \dots, 0) \mathbf{U}^t$
 - \mathbf{A}^+ is a $n \times m$ matrix.
 - If $\text{rank}(\mathbf{A}) = n$ 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 $\mathbf{x} = \sum_{i=1}^n \frac{\mathbf{u}_i^t \mathbf{b}}{\sigma_i} \mathbf{v}_i$ $\sigma_r > \epsilon, \sigma_{r+1} \leq \epsilon$

If the σ are close to zero small changes in the “data” vector \mathbf{b} cause big changes in \mathbf{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 $(\mathbf{A} + \varepsilon \mathbf{I})\mathbf{x} = \mathbf{b}$
- Solution of the regular problem requires minimizing of $\|\mathbf{Ax} - \mathbf{b}\|^2$
- Solving this modified problem corresponds to minimizing

$$\mathbf{x} = \sum_{i=1}^n \frac{\sigma_i}{\varepsilon + \sigma_i^2} (\mathbf{u}_i^t \mathbf{b}) \mathbf{v}_i$$

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

- 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”