Computational Methods
CMSC/AMSC/MAPL 460

EigenValue decomposition
Singular Value Decomposition

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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 $n \times n$ 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*.

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

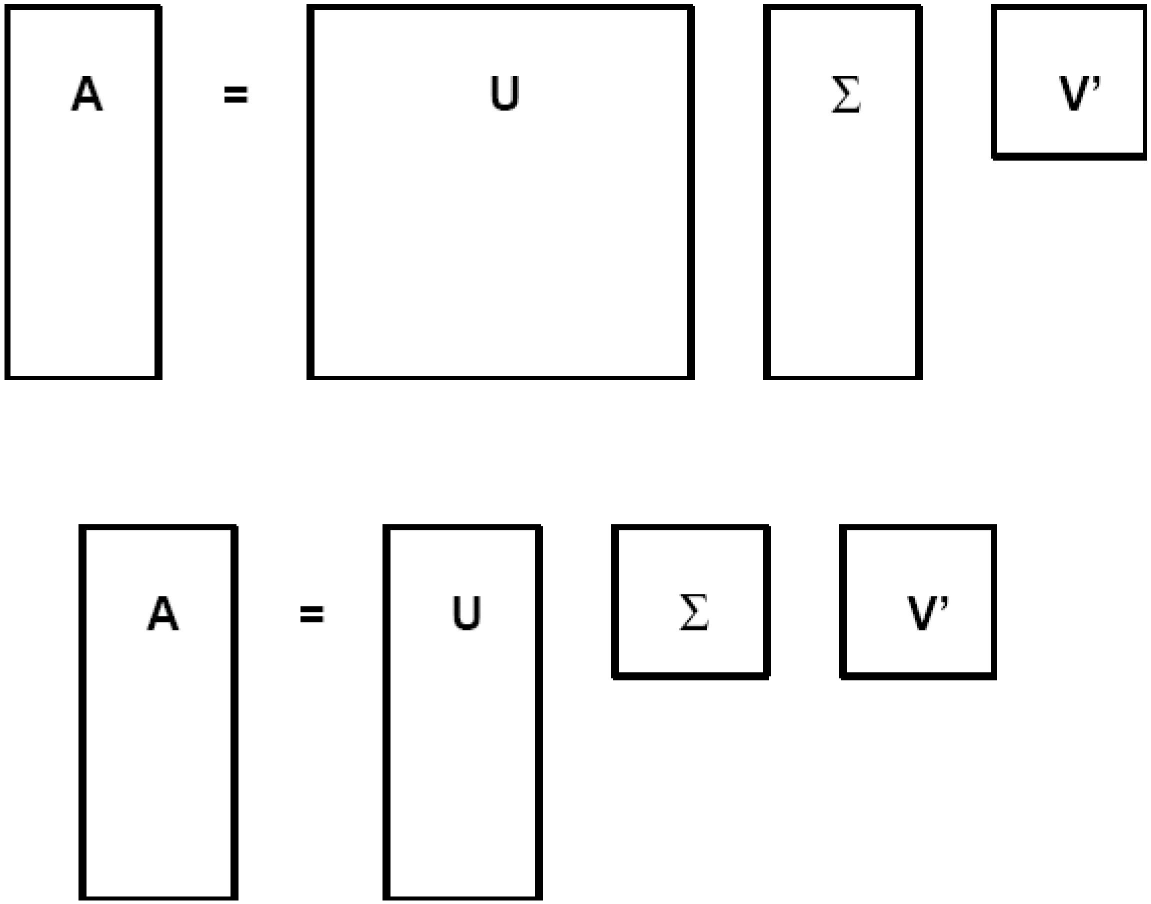
$$A\, A^* = (U\Sigma V^*)\, (U\Sigma V^*)^*$$

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

- 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* *t*he **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

- **Ax=b** **A** is $m\times n$, **x** is $n\times 1$ and **b** is $m\times 1$.
- **A=USV**^{t} where **U** is m×m, **S** is m×n and **V** is $n\times n$
- **USV**^{t} **x=b**. So **SV**^{t} **x=U**^{t}**b**
- If **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

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

  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 $(\mathbf{A}+\varepsilon\mathbf{I})\mathbf{x}=\mathbf{b}$
- Solution of the regular problem requires minimizing of $||\mathbf{Ax}-\mathbf{b}||^2$

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

- Solving this modified problemcorresponds to minimizing

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

- 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"