Computational Methods

Eigenvalues and Singular Values

Eigenvalues and Singular Values

- Eigenvalues and singular values describe important aspects of transformations and of data relations
  - Eigenvalues determine the important the degree to which a linear transformation changes the length of transformed vectors
  - Eigenvectors indicate the directions in which the principal change happen
- Eigenvalues are important for many problems in computer science and engineering, including
  - Dimensionality reduction
  - Compression

Eigenvalues

- Eigenvalues λ and eigenvectors x characterize dimensions that are purely stretched by a given linear transformation

$$Ax = \lambda x$$

  - The spectrum of A is the set of its eigenvalues
  - The spectral radius of A is the magnitude of the larges of its eigenvalues
- Eigenvalues characterize the degree to which a linear transformation stretches input vectors
  - Also important for sensitivity analysis of linear problems

Eigenvalues

- A linear transformation has as many eigenvalues and eigenvectors as it has dimensions
  - Eigenvectors might be duplicates
  - Eigenvalues might be complex
- Any data point (vector) can be written as a linear combination of eigenvectors
  - Allows efficient decomposition of vectors

Power Iteration

- The eigenvalue equation is related to the fixed point equations (except with scaling)

$$Ax = \lambda x$$

  - Simplest solution method to find eigenvectors (and eigenvalues) is power iteration
  - characterize dimensions that are purely stretched by a given linear transformation

- Power iteration converges to a scaled version of the eigenvector with the dominant eigenvalue

$$x_{t+1} = Ax_t$$

Power Iteration

- Power iteration converges except if
  - x_0 has no component of the dominant eigenvector
  - There are more than one eigenvector with the same eigenvalue
- Normalized power iteration renormalizes the result x_{t+1} after each iteration

$$y_{k+1} = Ax_k \quad , \quad x_{k+1} = \frac{y_{k+1}}{\|y_{k+1}\|_\infty}$$

  - Converges to dominant eigenvector and dominant eigenvalue

$$\|y_k\|_\infty \rightarrow \lambda_d \quad , \quad x_k \rightarrow \frac{1}{\|v_d\|_\infty} v_d$$

Inverse Iteration

- Inverse iteration is used to find the smallest eigenvalue
- converges except if

$$Ay_{k+1} = x_k \quad , \quad x_{k+1} = \frac{y_{k+1}}{\|y_{k+1}\|_\infty}$$

  - Inverse iteration corresponds to power iteration with the inverse matrix A^{-1}
- Inverse iteration and power iteration can only find the smallest and the largest eigenvalues
  - Need to find a way to determine other eigenvalues and eigenvectors

Characteristic Polynomial

- The determination of eigenvectors and eigenvalues can be transformed into a root finding problem

$$(A-\lambda I)x = 0$$

  - Has a nonzero solution for the eigenvector x if and only if *(A-λ I)* is not singular
  - Eigenvalues of the nonsingular matrix are the roots of the characteristic polynomial

$$\det(A-\lambda I) = 0$$

    - The characteristic polynomial is a polynomial of degree *n*
    - Complex eigenvalues occur in conjugate pairs
- Computation of the characteristic polynomial is complex
  - Can be accelerated by first performing LU factorization

Characteristic Polynomial

- Computing roots of a polynomial of degree larger than 4 cannot always be computed directly and require an iterative solution
- Computing eigenvalues using the characteristic polynomial is numerically not stable and highly complex
  - Computing coefficients of characteristic polynomial requires computation of the determinant
  - Root finding requires iterative solution process
  - Coefficients of characteristic are very sensitive
- Characteristic polynomial is a powerful theoretical tool but not a practical computational approach

Eigenvalue Problems

- Characteristics of eigenvalue problems influence the choice of algorithm
  - All or only some eigenvalues
  - Only eigenvalues or eigenvalues and eigenvectors
  - Dense or sparse matrix
  - Real of complex values
  - Other properties of matrix A

Problem Transformations

- A number of transformations either preserve or have a predictable effect on the eigenvalues
  - Shift: For any scalar σ
    $$Ax = \lambda x \quad \rightarrow \quad (A - \sigma I)x = (\lambda - \sigma)x$$
  - Inversion:
    $$Ax = \lambda x \quad \rightarrow \quad A^{-1}x = \frac{1}{\lambda}x$$
  - Powers:
    $$Ax = \lambda x \quad \rightarrow \quad A^k x = \lambda^k x$$
  - Polynomial: for any polynomial p(t)
    $$Ax = \lambda x \quad \rightarrow \quad p(A)x = p(\lambda)x$$
  - Similarity: for any similar matrix $B = T^{-1}AT$
    $$Bx = \lambda x \quad \rightarrow \quad ATx = \lambda(Tx)$$

Problem Transformations

- Eigenvalues and eigenvectors of diagonal matrices are easy to determine
  - Eigenvalues are the values on the diagonal
  - Eigenvectors are the columns of the identity matrix
- Not all matrices are diagonalizable using similarity transformations
- Eigenvalues of triangular matrices can also be determined easily
  - Eigenvalues are diagonal entries of the matrix
  - Eigenvectors can be computed from $(A - \lambda I)x = 0$

Convergence of Iterations

- Speed of convergence of power iteration and inverse iteration depends on the ratio of two eigenvalues
  - For power iteration, convergence is faster the larger the ratio of the largest and the second largest eigenvalue is
  - For inverse iteration, convergence is faster the smaller the ratio of the smallest and the second smallest eigenvector is
- Shift transformation allows to change the ratio of eigenvalues $\frac{\lambda_1}{\lambda_2} \rightarrow \frac{\lambda_1 - \sigma}{\lambda_2 - \sigma}$
  - Knowledge of eigenvalue of sought after eigenvector would allow to lower this ratio to 0
    - Allows to increase the convergence rate of inverse iteration

Rayleigh Quotient Iteration

- Rayleigh quotient iteration uses the Rayleigh quotient as a shift parameter $\sigma = \frac{x^T A x}{x^T x}$, $(A - \sigma I)$
  - This allows to make the ratio of eigenvalues close to 0 and thus accelerates the convergence of inverse iteration

$$(A - \sigma_k I) y_{k+1} = x_k$$

$$x_{k+1} = \frac{y_{k+1}}{\|y_{k+1}\|_\infty}$$

    - This algorithm is usually called Rayleigh quotient iteration
  - Rayleigh quotient iteration converges usually very fast
    - Each iteration requires a new matrix factorization and is therefore *O(n³)* F

Computing All Eigenvalues

- Power iteration and inverse iteration allow to compute only the largest and the smallest eigenvalues and eigenvectors.
  - To compute the other eigenvalues we need to either
    - Remove the already found eigenvector (and eigenvalue) from the matrix to be able to reapply power or inverse iteration
    - Find a way to find all the eigenvectors simultaneously
  - Removing eigenvectors from the space spanned by a transformation A is called deflation

Deflation

- To remove an eigenvalue (and corresponding eigenvector) we have to find a set of transformations that preserves all other eigenvalues
  - Householder transforms can be used to derive such a transformation H with

    $$Hx_1 = \alpha e_1$$

  - The similarity transform described by H yields a matrix

    $$HAH^{-1} = \begin{pmatrix} \lambda_1 & b^T \\ 0 & B \end{pmatrix}$$

    - Since similarity transforms were used this matrix has the same eigenvalues
    - B has all the eigenvalues of A with the exception of λ_1
  - Power iteration can be applied to this new matrix B

Deflation

- Power iteration with deflation can compute all eigenvalues but requires determining the eigenvector in each iteration
  - Eigenvector in B can be used to compute eigenvector in A

$$x_3 = H^{-1}\begin{pmatrix} \dfrac{b^T y_2}{\lambda_2 - \lambda_1} \\ y_2 \end{pmatrix}$$

  - Alternatively, the eigenvalue could be used directly in A to determine the eigenvector
    - More computationally complex

Simultaneous Iteration

- Simultaneous iteration attempts to simultaneously iterate multiple vectors

$$X_{k+1} = AX_k$$

  - X converges to the space spanned by the p dominant eigenvectors
    - Subspace iteration
  - But X becomes ill-conditioned since all columns in X ultimately converge to the dominant eigenvector
    - Need normalization that keeps vectors well conditioned and non-equal
      - Orthogonal iteration using QR factorization

QR Iteration

- As for least squares (and equation solving) QR factorization allows a factorization of the matrix into components that stay well conditioned

$$Q_{k+1}R_{k+1} = X_k$$

$$X_{k+1} = AQ_{k+1}$$

  - By using Q (a similarity transform) for the iteration, the eigenvalues are preserved and it converges to block triangular form
    - Triangular form if all eigenvalues are real values and distinct

QR Iteration

- To find eigenvalues, QR iteration can be applied directly to A

$$A_k = Q_k^H A_{k-1} Q_k$$

  - Converges to triangular or block triangular matrix containing all eigenvalues as diagonal elements of as eigenvalues of diagonal blocks
    - Can be computed without explicitly performing the product

$$Q_{k+1} R_{k+1} = A_k$$

$$A_{k+1} = R_{k+1} Q_{k+1} (= Q_{k+1}^H A_k Q_{k+1})$$

  - Can be accelerated using shift transformation

Singular Values

- Singular values are related to Eigenvalues and characterize important aspects of the space described by the transformation
  - Nullspace
  - Span
- Singular Value Decomposition divides a transformation A into a sequence of 3 transformations where the second is pure rescaling
  - Scaling parameters are the singular values
  - Columns of the other two transformations are the left and right singular vectors, respectively

Singular Values

- Singular values exist for all transformations A, independent of A being square or not
  - Right singular vectors represent the input vectors that span the orthogonal basis that is being scaled
  - Left singular vectors represent the vectors that the scaled internal basis vectors are transformed into for the output
- Sinuglar values are directly related to the eigenvalues
  - Singular values are the nonnegative square roots of the eigenvalues of AA^T or A^TA
  - Left singular vectors are eigenvectors of AA^T
  - Right singular vectors are eigenvectors of A^TA

Singular Value Decomposition

- Singular value decomposition (SVD) factorizes A

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

  - U is an *mxm* orthogonal matrix of left singular vectors
  - V is an *nxn* orthogonal matrix of right singular vectors
  - Σ is an *mxn* diagonal matrix of singular values
    - Usually Σ is arranged such that the singular values are ordered by magnitude
- Left and right singular vectors are related through the singular values

$$A v_{,i} = \sigma_i u_{,i}$$

$$A^T u_{,i} = \sigma_i v_{,i}$$

Singular Value Decomposition

- Singular value decomposition (SVD) can be computed in different ways
  - Using eigenvalue computation on AA^T
    - Compute eigenvalues of AA^T
    - Determine left singular vectors as eigenvectors for AA^T
    - Determine right singular vectors as eigenvectors for A^TA
    - Leads to some conditioning issues due to the need for matrix multiplication
  - Directly from A by performing Householder transformations and givens rotations until a diagonal matrix is reached
    - Perform QR factorization to achieve triangular matrix
    - Use Householder transforms to achieve bidiagonal shape
    - Use Givens rotations to achieve diagonal form
    - This is usually better conditioned

Singular Value Decomposition

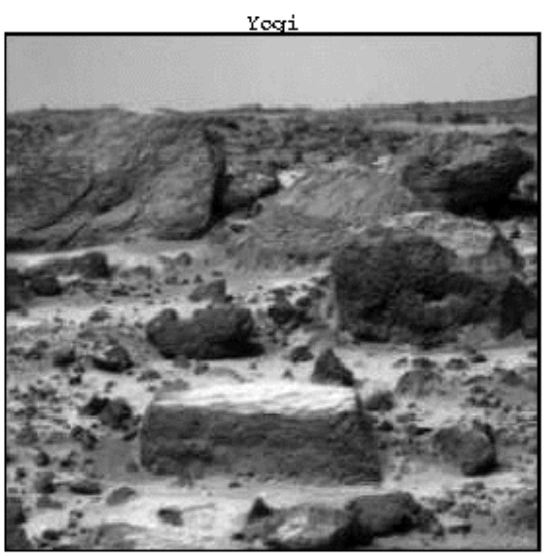
- Singular value decomposition (SVD) can be used for a range of applications
  - Compute least squares solution $Ax \cong b \quad \rightarrow \quad x = \sum_{\sigma_i \neq 0} \frac{u_{,i}^T b}{\sigma_i} v_i$
  - Compute pseudoinverse $A^+ = V\Sigma^+ U^T$
  - Euclidean matrix norm: $\|A\|_2 = \sigma_{\max}$
  - Condition number of a matrix: $cond(A) = \sigma_{\max} / \sigma_{\min}$
  - Matrix rank is equal to the number of non-zero singular values
  - Nullspace of the matrix is spanned by the set of right singular vectors corresponding to singular values of 0
  - Span of a matrix is spanned by the left singular vectors corresponding to non-zero singular values

Singular Value Decomposition

- Singular value decomposition (SVD) is useful in a number of applications
  - Data compression
    - Right singular values transform data into a basis in which it is only scaled
    - Data dimensions with 0 or very small scaling factors are not important for the overall data
    - Wide range of applications:
      - Image compression
      - Dimensionality reduction for data
      - Dimensionality reduction for matrix operations
  - Filtering and noise reduction
    - Most of the time, data has only few important dimensions and noise is most apparent in additional dimensions (with smaller singular values)
    - Ignoring dimensions with small singular values can lead to less noisy data

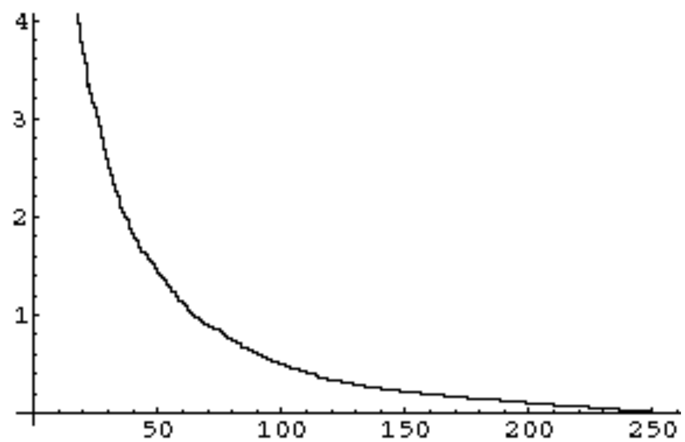
Compression Example

- Image compression is an area where SVD has been used relatively early on
  - Given an image, can we reduce the amount of data that has to be transmitted without loosing too much information
    - Use SVD to find a lower rank approximation of the image that has only limited loss.



Compression Example

- In SVD, the magnitude of the singular values often decreases rapidly after the first few singular values

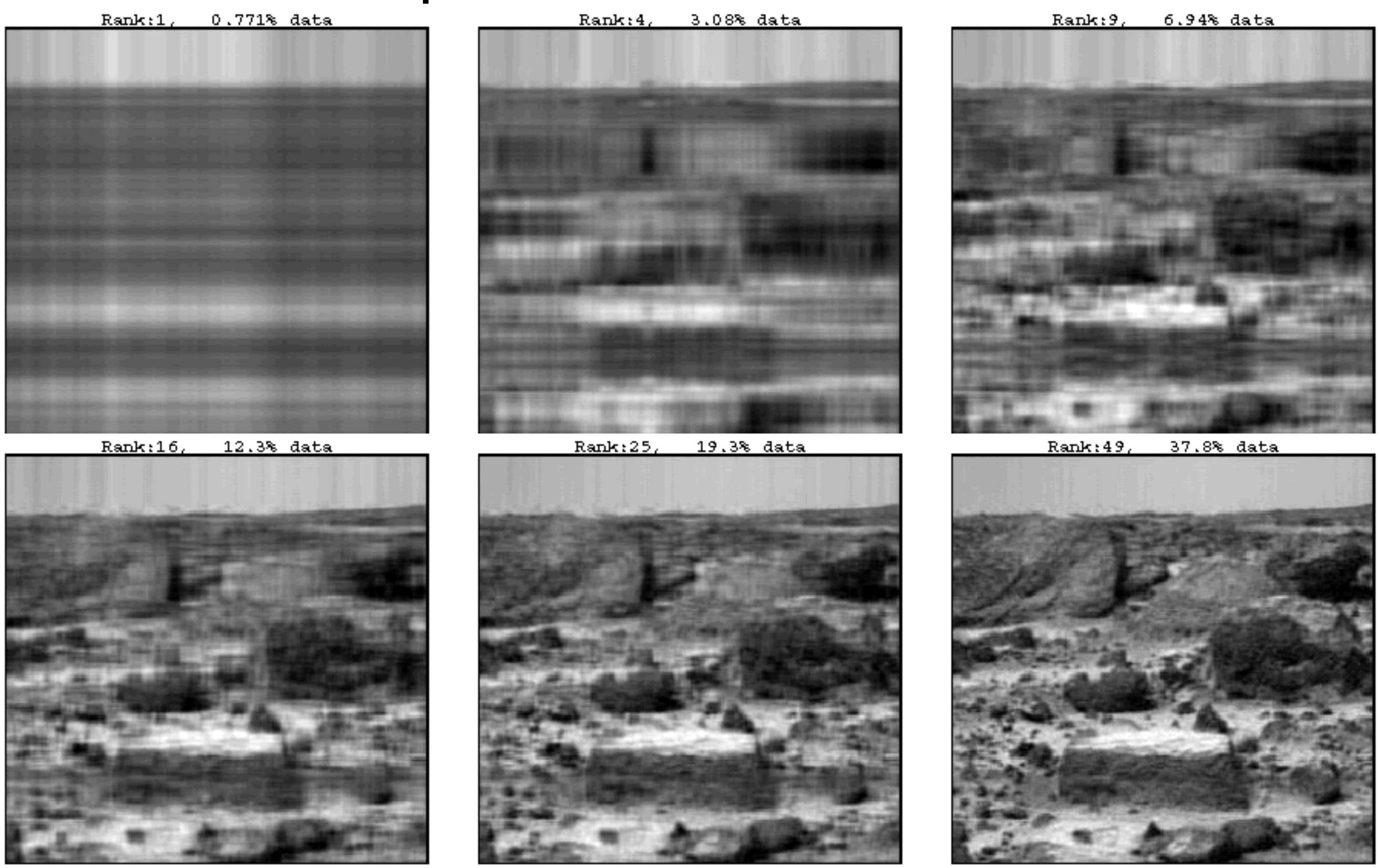


- To compress the image, only keep the *k* largest singular values (and thus singular vectors) to reconstruct the image

$$A \approx U_p \Sigma_p V_p^T$$

Compression Example

- Different compression levels have different loss



Eigenvalues and Singular Values

- Eigenvalues and Eigenvectors capture important properties about linear transformations A
- Eigenvalues and Singular values indicate the importance of particular dimensions of the space
  - Can be used for compression
- Singular values can capture noise characteristics
  - Can be used for filtering of data
  - Can be used to remove noise from data before transformations are applied
- Singular values are also important to analyze problems such as conditioning and sensitivity