Goal: Another matrix decomposition (SVD) for low-rank matrix approximation
Rank of a Matrix

- \( N \times M \) matrix \( A \) as a mapping: \( R^M \rightarrow R^N \)

\[
\begin{bmatrix}
1 \\
M \\
x
\end{bmatrix}
\xrightarrow{A}
\begin{bmatrix}
x \in R^M \end{bmatrix}
\rightarrow
\begin{bmatrix}
b \\
N
\end{bmatrix}
= A \begin{bmatrix}
x \in R^N \end{bmatrix}
\]

- **Range of \( A \):** Vector space \( \{ b = Ax | \forall x \} \)

- **Rank of \( A \):** Number of linearly-independent vectors in the range, *i.e.*, how many linearly-independent \( N \)-element vectors are there in the range, such that

\[
b = A \forall x = \sum_{\nu=1}^{m} c_{\nu} | \nu \rangle
\]
Low Rank Approximations of a Matrix

- **Rank-1 approximation:** $NM \rightarrow N + M$
  \[
  \begin{bmatrix}
  M \\
  N
  \end{bmatrix}
  \approx
  \begin{bmatrix}
  u \\
  v
  \end{bmatrix}
  \]

- **Rank-2 approximation:** $NM \rightarrow 2(N + M)$
  \[
  \begin{bmatrix}
  \psi \\
  u_1 \end{bmatrix}
  \approx
  \begin{bmatrix}
  u_1 \\
  v_1
  \end{bmatrix}w_1
  +
  \begin{bmatrix}
  u_2 \\
  v_2
  \end{bmatrix}w_2
  \]

- **Rank-$m$ ($m \ll N, M$) approximation:** $NM \rightarrow m(N + M)$
  \[
  \begin{bmatrix}
  \psi \\
  \end{bmatrix}
  \approx
  \sum_{\nu=1}^{m}
  \begin{bmatrix}
  u_\nu \\
  \end{bmatrix}w_\nu
  \]
  \[
  +
  \begin{bmatrix}
  v_\nu \\
  \end{bmatrix}
  \]

Singular Value Decomposition

- **Problem:** Optimal approximation of an $N \times M$ matrix $\psi$ of rank-$m$ ($m \ll N$)?
- **Theorem:** An $N \times M$ matrix $\psi$ (assume $N \geq M$) can be decomposed as
  \[
  \psi = UDV^T = \sum_{v=1}^{M} U_{i,v} d_v V_{j,v} = \sum_{v=1}^{M} u_i^{(v)} d_v v_j^{(v)}
  \]
  where $U \in \mathbb{R}^{N \times M}$ & $V \in \mathbb{R}^{M \times M}$ are column orthogonal & $D$ is diagonal

\[
U^T U = V^T V = I_M
\]

- **Theorem:** Sort the SVD diagonal elements in descending order $d_1 \geq d_2 \geq ...$ & retain the first $m$ terms
  \[
  \psi^{(m)} = \sum_{v=1}^{m} u_i^{(v)} d_v v_j^{(v)T}
  \]
  which is optimal among $\forall$ rank-$m$ matrices in the 2-norm sense with the error
  \[
  \min_{\text{rank}(A)=m} \| A - \psi \|_2 = \| \psi^{(m)} - \psi \|_2 = d_{m+1}
  \]
  cf. `singular.c` & `svdcmp.c`
SVD for Image Compression

Original Image

5 Iterations

10 Iterations

D. Richards & A. Abrahamsen

20 Iterations

60 Iterations

100 Iterations
SVD in Data Mining

Given Point Set

Approximating Attributes by Representative Vectors

N. Ramakrishnan & A. Y. Grama
Reduced Density Matrix

- Quantum system coupled to an environment

\[
\{ |i\rangle = \psi_i(x) |i = 1, \ldots, N \} \quad \{ |j\rangle = \phi_j(X) |j = 1, \ldots, M \}
\]

- Quantum state of block + environment

\[
|\psi\rangle = \sum_{i=1}^{N} \sum_{j=1}^{M} \psi_{ij} |i\rangle |j\rangle \quad \text{or} \quad \Psi(x, X) = \sum_{i=1}^{N} \sum_{j=1}^{M} \psi_{ij} \psi_i(x) \phi_j(X)
\]

- Reduced density matrix

\[
\langle \forall A \rangle = \sum_{i} \sum_{j} \psi_{ij}^* \langle j | A \sum_{i'} \sum_{j'} \psi_{i'j'} | i' \rangle |j'\rangle
\]

Arbitrary operator in the block

\[
= \sum_{i} \sum_{j} \sum_{i'} \sum_{j'} \psi_{i'j'} \psi_{ij}^* \langle j | A | i' \rangle \langle i | i' \rangle |j\rangle |j'\rangle
\]

\[
= \sum_{i} \sum_{i'} \sum_{j} \psi_{i'j} \psi_{ij}^* \langle i | A | i' \rangle = \sum_{i} \sum_{i'} \rho_{i'i} A_{i'i'} = \text{tr}_B(\rho A)
\]

\[
\rho_{i'i} = \sum_{j} \psi_{i'j} \psi_{ij}^* \quad A_{ii'} \equiv \langle i | A | i' \rangle
\]
Low-Rank Approx. to Reduced Density Matrix

\[ \psi \equiv \psi^{(m)} = \sum_{\nu=1}^{m} u^{(\nu)} d_{\nu} v^{(\nu)T} \]
\[ \psi_{ij}^{(m)} = \sum_{\nu=1}^{m} u_{i}^{(\nu)} d_{\nu} v_{j}^{(\nu)} \]
\[ \rho = \psi \psi^{T} \equiv \psi^{(m)} \psi^{(m)T} = \sum_{\nu=1}^{m} \sum_{\nu'=1}^{m} u^{(\nu)} d_{\nu} \left( v^{(\nu)T} v^{(\nu')} \right) d_{\nu'} u^{(\nu')T} \]
\[ = \sum_{\nu=1}^{m} \sum_{\nu'=1}^{m} u^{(\nu)} d_{\nu} \left( \delta_{\nu\nu'} \right) d_{\nu'} u^{(\nu')T} = \sum_{\nu=1}^{m} u^{(\nu)} d_{\nu}^2 u^{(\nu)T} \equiv \rho^{(m)} \]
\[ \rho_{ii}^{(m)} = \sum_{\nu=1}^{m} u_{i}^{(\nu)} d_{\nu}^2 u_{i'}^{(\nu)} \]

- Density matrix renormalization group = systematic procedure to accurately obtain a quantum ground state:
  1. Incrementally add environment to a block
  2. Solve the global (= block + environment) ground state
  3. Construct a low-rank approx. to represent the block with reduced d.o.f.

Rapid Genome Sequencing

- $10M Archon X prize for decoding 100 human genomes in 10 days & $10K per genome (http://genomics.xprize.org): Preemptive attack on diseases

- Quantum tunneling current for rapid DNA sequencing?

- Tunneling current alone cannot distinguish the 4 nucleotides (A, C, G, T)

Tsutsui et al., Nature Nanotechnology ('10)

Lagerqvist et al., Nano Letters ('06)
Rapid DNA Sequencing via Data Mining

- Use tunneling current (I)-voltage (V) characteristic (or electronic density-of-states) as the ‘fingerprints’ of the 4 nucleotides

- Principal component analysis (PCA) & fuzzy c-means clustering clearly distinguish the 4 nucleotides

- Viterbi algorithm for even higher-accuracy sequencing

Shapir et al., *Nature Materials* (’08)

H. Yuen et al., *IJCS 4*, 352 (’10)
SVD vs. PCA

- **SVD of** $N$ (number of companies) $\times T$ (number of time points) of stock-price time series

\[
\Xi^T = U \Sigma V^T
\]

- **Stock correlation matrix**

\[
C = \Xi \Xi^T
\]

- **Principal component analysis (PCA):** Eigen decomposition of the correlation matrix

\[
C = \Xi \Xi^T = V \Sigma U^T U \Sigma V^T = V \Sigma^2 V^T
\]

- **Compare the spectrum with that of random matrix theory (RMT) for judging statistical significance**

\[
\rho_{\text{RMT}} = \frac{Q}{2\pi} \sqrt{\frac{(\lambda_+ - \lambda)(\lambda - \lambda_-)}{\lambda}}
\]

\[
\lambda_{\pm} = \left(1 + \frac{1}{\sqrt{Q}}\right)^2
\]

\[
Q = T/(2N) \quad N,T \to \infty
\]

\[
\sum_{k=1}^{N} \lambda_k = N
\]

Y. Kichikawa et al., *Proc. Comp. Sci.* 60, 1836 ('15)