Singular Value Decomposition

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cf. Eigen decomposition
$$A = Q[\searrow]Q^T$$
QR decomposition
$$A = Q[\searrow]$$

Goal: Another matrix decomposition (SVD)
for low-rank matrix approximation

See note on "least square fit" & *Numerical Recipes* Sec. 2.6

Rank of a Matrix

- **$N \times M$ matrix A as a mapping: $R^M \rightarrow R^N$**

$$M \begin{bmatrix} 1 \\ x \\ \\ \end{bmatrix} \quad \boxed{x\left(\in R^M\right) \xrightarrow[A]{} b = Ax\left(\in R^N\right)} \quad \begin{bmatrix} 1 \\ b \\ \\ \end{bmatrix} N$$
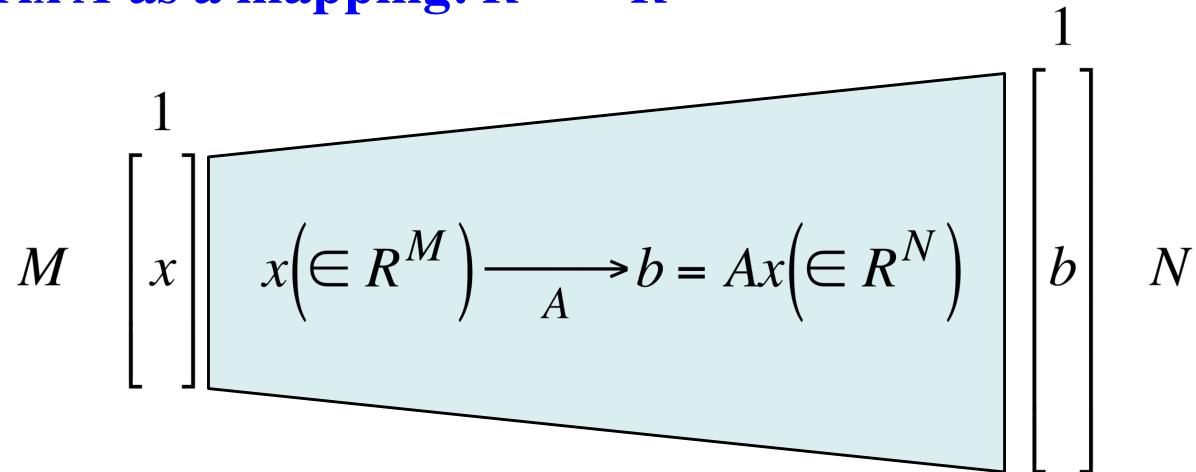
- **Range of A: Vector space $\{b = Ax | \forall x\}$**

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

$$b = A^{\forall} x = \sum_{v=1}^{m} c_v |v\rangle$$

Low Rank Approximations of a Matrix

- **Rank-1 approximation:** $NM \rightarrow N + M$

$$N \begin{bmatrix} & M & \\ & \psi & \\ & & \end{bmatrix} \cong \begin{bmatrix} u \\ \\ \end{bmatrix} \overbrace{\begin{bmatrix} N\times 1 & 1\times M \\ & v & \end{bmatrix}}^{N\times M} \qquad |u\rangle\langle v|\forall x\rangle \propto |u\rangle$$

- **Rank-2 approximation:** $NM \rightarrow 2(N + M)$

$$\begin{bmatrix} \\ \psi \\ \\ \end{bmatrix} \cong \begin{bmatrix} u_1 \\ \\ \end{bmatrix} w_1 \begin{bmatrix} v_1 \end{bmatrix} + \begin{bmatrix} u_2 \\ \\ \end{bmatrix} w_2 \begin{bmatrix} v_2 \end{bmatrix}$$

- **Rank-m ($m \ll N, M$) approximation:** $NM \rightarrow m(N + M)$

$$\begin{bmatrix} \\ \psi \\ \\ \end{bmatrix} \cong \sum_{\nu=1}^{m} \begin{bmatrix} u_\nu \\ \\ \end{bmatrix} w_\nu \begin{bmatrix} v_\nu \end{bmatrix}$$

Singular Value Decomposition

- **Problem:** Optimal approximation of an $N{\times}M$ matrix ψ of rank-m ($m \ll N$)?
- **Theorem:** An $N{\times}M$ matrix ψ (assume $N \geq M$) can be decomposed as

$$\psi = UDV^T = \sum_{\nu=1}^{M} U_{i\nu} d_\nu V_{j\nu} = \sum_{\nu=1}^{M} u_i^{(\nu)} d_\nu v_j^{(\nu)}$$

where $U \in R^N{\times}R^M$ & $V \in R^M{\times}R^M$ are column orthogonal & D is diagonal

$$U^T U = V^T V = I_M$$

See appendix on polar & singular decompositions

- **Theorem:** Sort the SVD diagonal elements in descending order, $d_1 \geq d_2 \geq ... \geq d_M \geq 0$, & retain the first m terms

$$\psi^{(m)} \equiv \sum_{\nu=1}^{m} u^{(\nu)} d_\nu v^{(\nu)T}$$

which is optimal among $\forall$rank-m matrices in the 2-norm sense with the error

$$\min_{rank(A)=m} \left\| A - \psi \right\|_2 = \left\| \psi^{(m)} - \psi \right\|_2 = d_{m+1}$$

Use the program!

cf. singular.c & svdcmp.c   cc -o singular singular.c svdcmp.c -lm

SVD for Image Compression
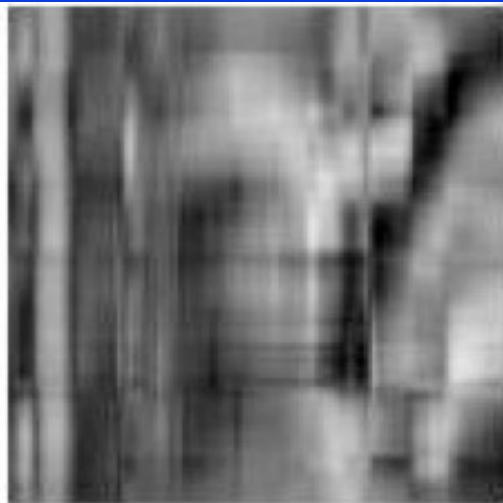
Original Image   5 Iterations   10 Iterations
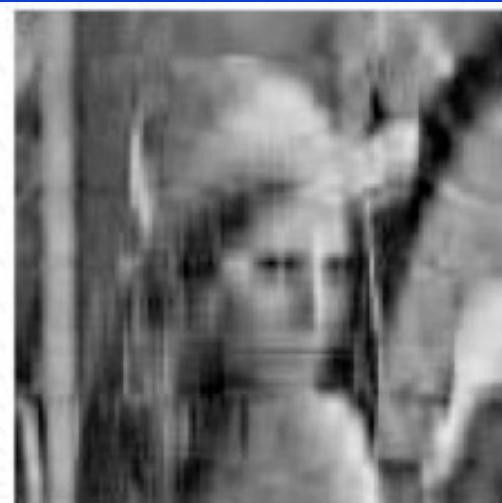
D. Richards & A. Abrahamsen

20 Iterations   60 Iterations   100 Iterations

SVD in Data Mining

Given Point Set
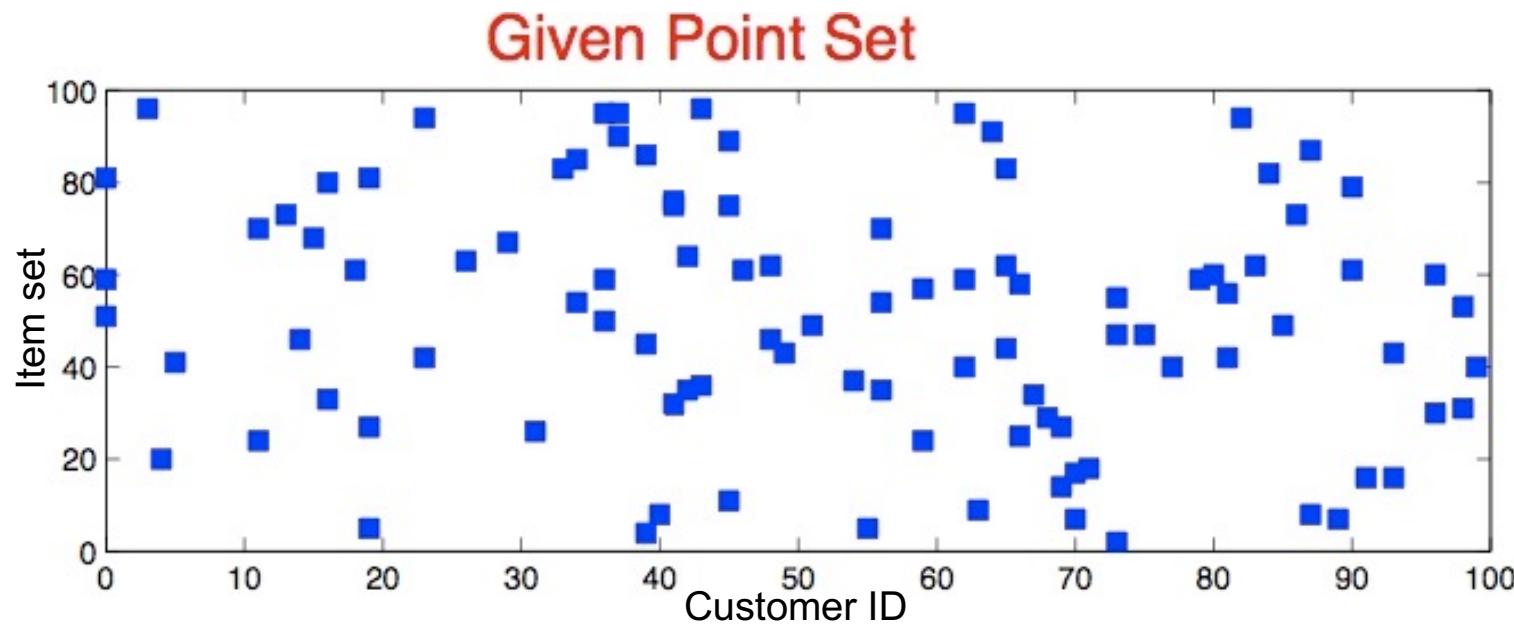
Approximating Attributes by Representative Vectors

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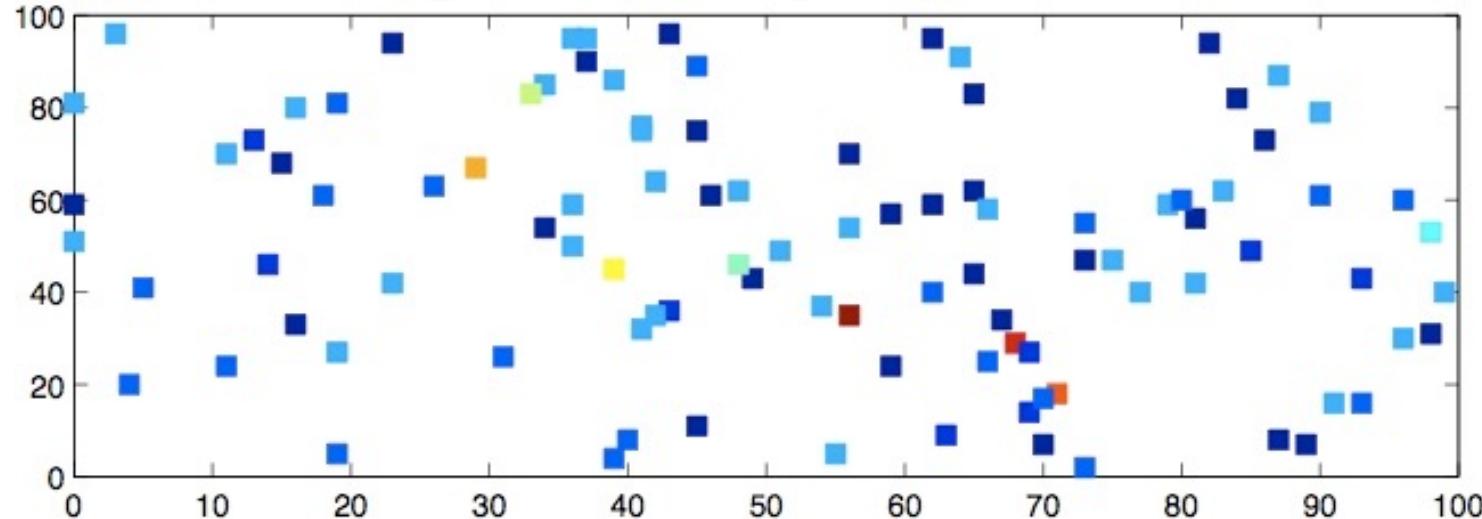
Reduced Density Matrix

- **Quantum system coupled to an environment**

  | B: Block | E: Environment |

  $$\{|i\rangle = \psi_i(x)|i = 1, \ldots, N\} \quad \{|j\rangle = \phi_i(X)|j = 1, \ldots, M\}$$

- **∀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**

  $$\left\langle \forall A \right\rangle = \sum_i \sum_j \psi_{ij}^* \langle j|\langle i|A \sum_{i'} \sum_{j'} \psi_{i'j'}|i'\rangle|j'\rangle$$

  $$= \sum_i \sum_j \sum_{i'} \sum_{j'} \psi_{i'j'}\psi_{ij}^* \langle i|A|i'\rangle \underbrace{\langle j|j'\rangle}_{\delta_{jj'}}$$

  $$= \sum_i \sum_{i'} \sum_j \psi_{i'j}\psi_{ij}^* \langle i|A|i'\rangle \equiv \sum_i \sum_{i'} \rho_{i'i}A_{ii'} = \text{tr}_B(\rho A)$$

  Arbitrary operator in the block

  $$\rho_{i'i} \equiv \sum_j \psi_{i'j}\psi_{ij}^* \qquad A_{ii'} \equiv \langle i|A|i'\rangle$$

Low-Rank Approx. to Reduced Density Matrix

$$\psi \cong \psi^{(m)} = \sum_{\nu=1}^{m} u^{(\nu)} d_\nu v^{(\nu)T} \qquad \psi_{ij}^{(m)} = \sum_{\nu=1}^{m} u_i^{(\nu)} d_\nu v_j^{(\nu)}$$

$$\rho = \psi\psi^T \cong \psi^{(m)}\psi^{(m)T} = \sum_{\nu=1}^{m} \sum_{\nu'=1}^{m} u^{(\nu)} d_\nu \left(v^{(\nu)T} v^{(\nu')} \right) d_{\nu'} u^{(\nu')T}$$

$$= \sum_{\nu=1}^{m} \sum_{\nu'=1}^{m} u^{(\nu)} d_\nu \left(\delta_{\nu\nu'} \right) d_{\nu'} u^{(\nu')T} = \sum_{\nu=1}^{m} u^{(\nu)} d_\nu^2 u^{(\nu)T} \equiv \rho^{(m)}$$

$$\rho_{ii'}^{(m)} = \sum_{\nu=1}^{m} u_i^{(\nu)} d_\nu^2 u_{i'}^{(\nu)}$$

- **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.**

S. R. White, *Phys. Rev. B* **48**, 10345 ('93);
G. K.-L. Chan & S. Sharma, *Annu. Rev. Phys. Chem.* **62**, 465 ('11) (Eqs. 3-10)

More SVD in quantum chemistry

J. F. Gonthier & M. Head-Gordon, *J. Chem. Phys.* **147**, 144110 ('17)

Entanglement Entropy & Quantum Computing

- **Entanglement entropy:** A measure of quantum entanglement between two subsystems. If a state describing two subsystems A and B is a *separable* state $|\Psi_{AB}\rangle = |\phi_A\rangle|\phi_B\rangle$ (*i.e.*, tensor product), then the reduced density matrix $\rho_A = \text{Tr}_B|\Psi_{AB}\rangle\langle\Psi_{AB}| = |\phi_A\rangle\langle\phi_A|$ is a *pure state*. Thus, the entropy of the state is zero. A reduced density matrix having a non-zero entropy is therefore a signal of the existence of entanglement in the system.

- **Area law:** A quantum state satisfies an *area law* if the leading term of the entanglement entropy grows at most proportionally with the *boundary* between the two partitions. Area laws are remarkably common for ground states of local *gapped* quantum many-body systems. *It greatly reduces the complexity of quantum many-body systems. The density matrix renormalization group and matrix product states, for example, implicitly rely on such area laws*. https://en.wikipedia.org/wiki/Entropy_of_entanglement

Measurement-driven entanglement transition in hybrid quantum circuits

"With increasing measurement rate, the volume law phase is unstable to a disentangled area law phase, passing through a single entanglement transition at a critical rate of measurement."
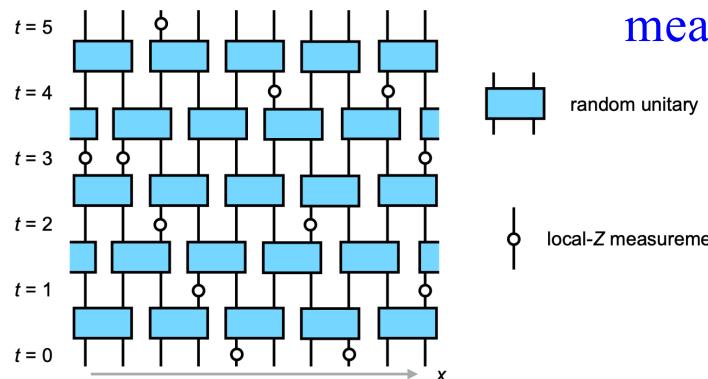
Y. Li *et al.*, *Phys. Rev. B* **100**, 134306 ('19)

$t = 5$
$t = 4$
$t = 3$
$t = 2$
$t = 1$
$t = 0$

random unitary

local-Z measurement

x

SVD for 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**
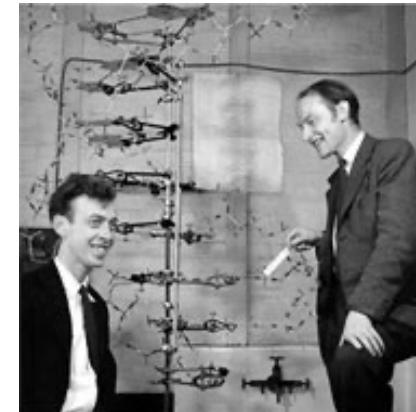
- **Quantum tunneling current for rapid DNA sequencing?**

Lagerqvist *et al.*, *Nano Letters* ('06)
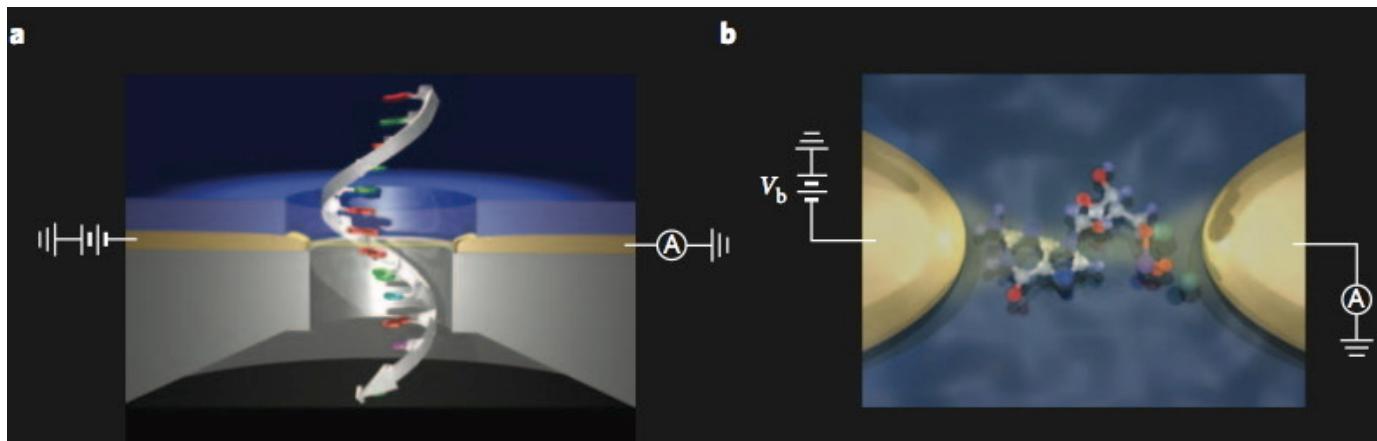
Tsutsui *et al.*, *Nature Nanotechnology* ('10)
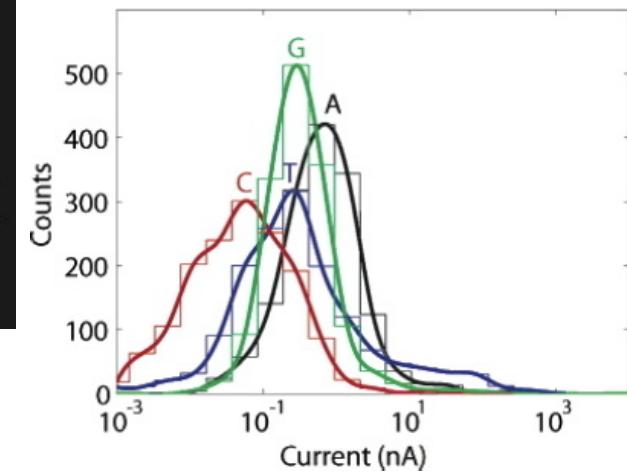
- **Tunneling current alone cannot distinguish the 4 nucleotides (A, C, G, T)**

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**
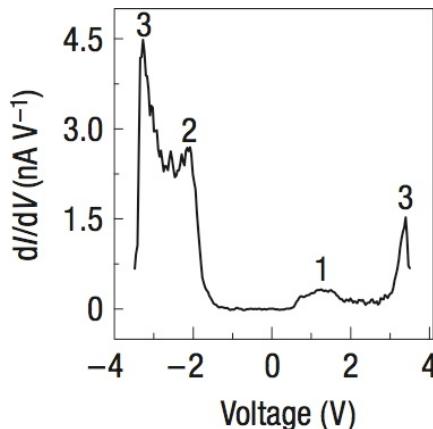
Shapir *et al.*,
Nature Materials ('08)
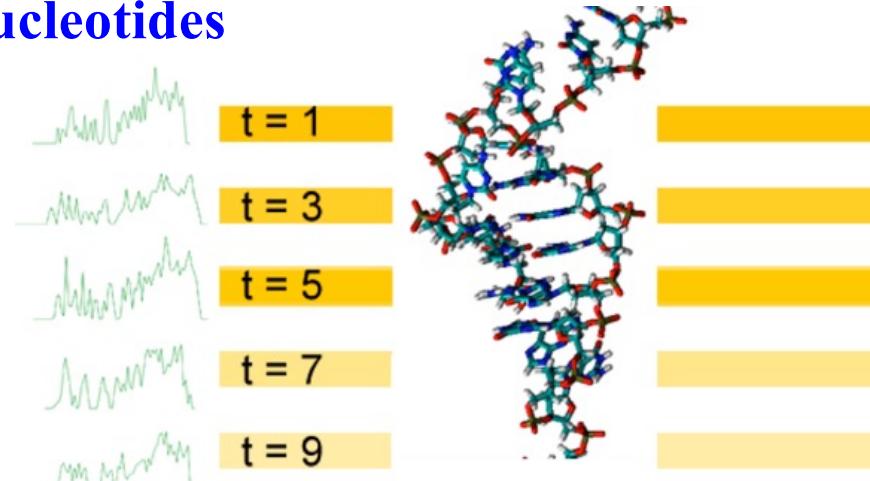
- **Principal component analysis (PCA) & fuzzy c-means clustering clearly distinguish the 4 nucleotides**
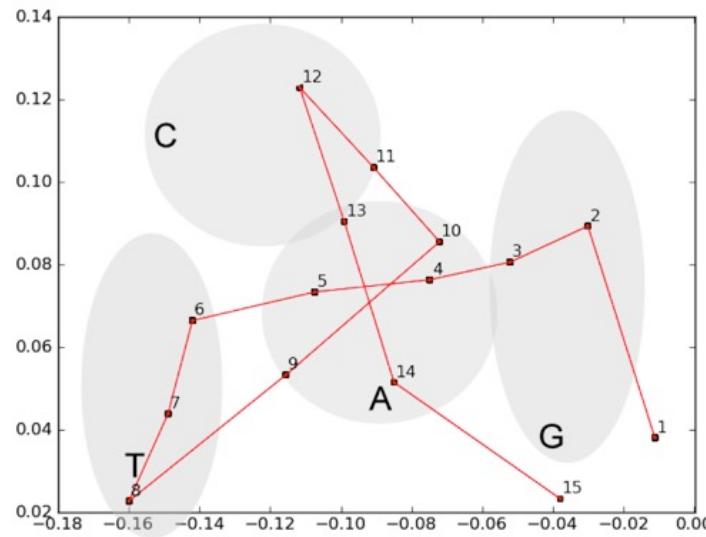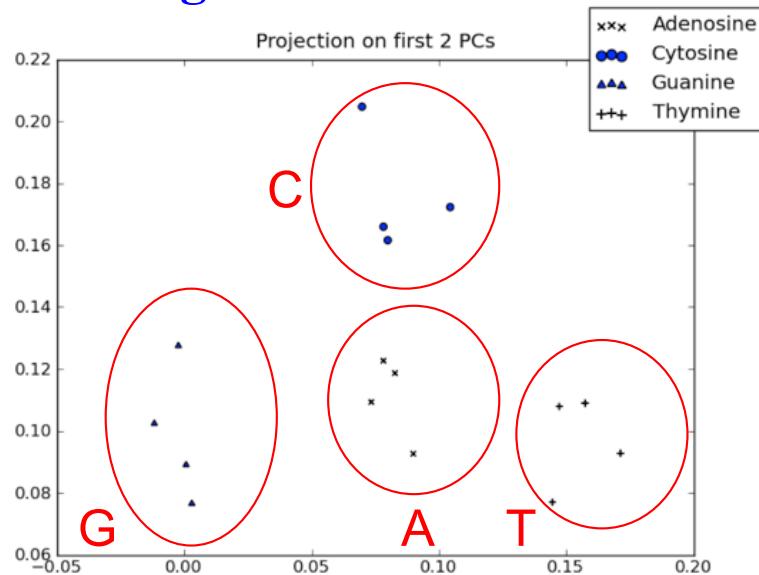
H. Yuen *et al.*, *IJCS* **4**, 352 ('10)

http://www.henryyuen.net/

- **Viterbi algorithm for even higher-accuracy sequencing**   See Henry's landmark discovery

SVD *vs*. PCA (in Economics)

- **SVD of *N* (number of companies) × *T* (number of time points) of stock-price time series**

$$\underset{T \times N}{\Xi^T} = \underset{T \times N}{U} \; \underset{N \times N}{\Sigma} \; \underset{N \times N}{V^T}$$

- **Stock correlation matrix**

$$\underset{N \times N}{C} = \underset{N \times T}{\Xi} \; \underset{T \times N}{\Xi^T}$$

Apply it in your area!

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

$$C = \Xi\Xi^T$$
$$= V\Sigma \overset{I}{\overbrace{U^T U}} \Sigma V^T$$
$$= V\Sigma^2 V^T$$

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

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

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

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

$$\sum_{k=1}^{N} \lambda_k = N$$

$\rho(\lambda)$

RMT

$\lambda_2 = 4.56$ $\quad$ $\lambda_1 = 10.46$

Probability Density

Eigenvalue λ

N stock prices

T time points

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