An Introduction to PCA

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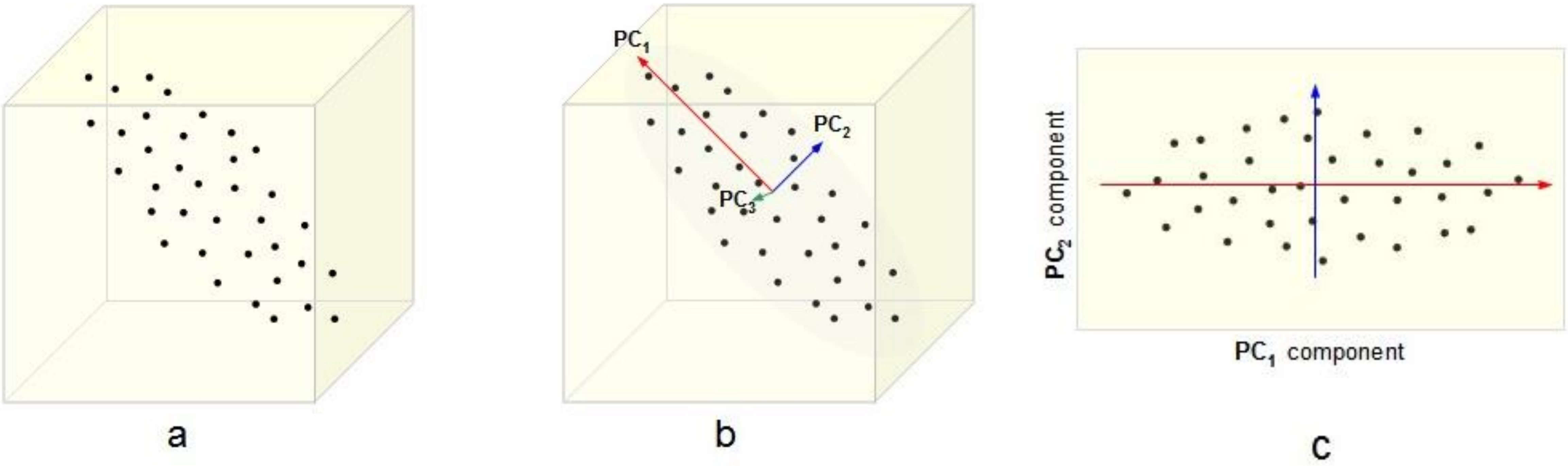
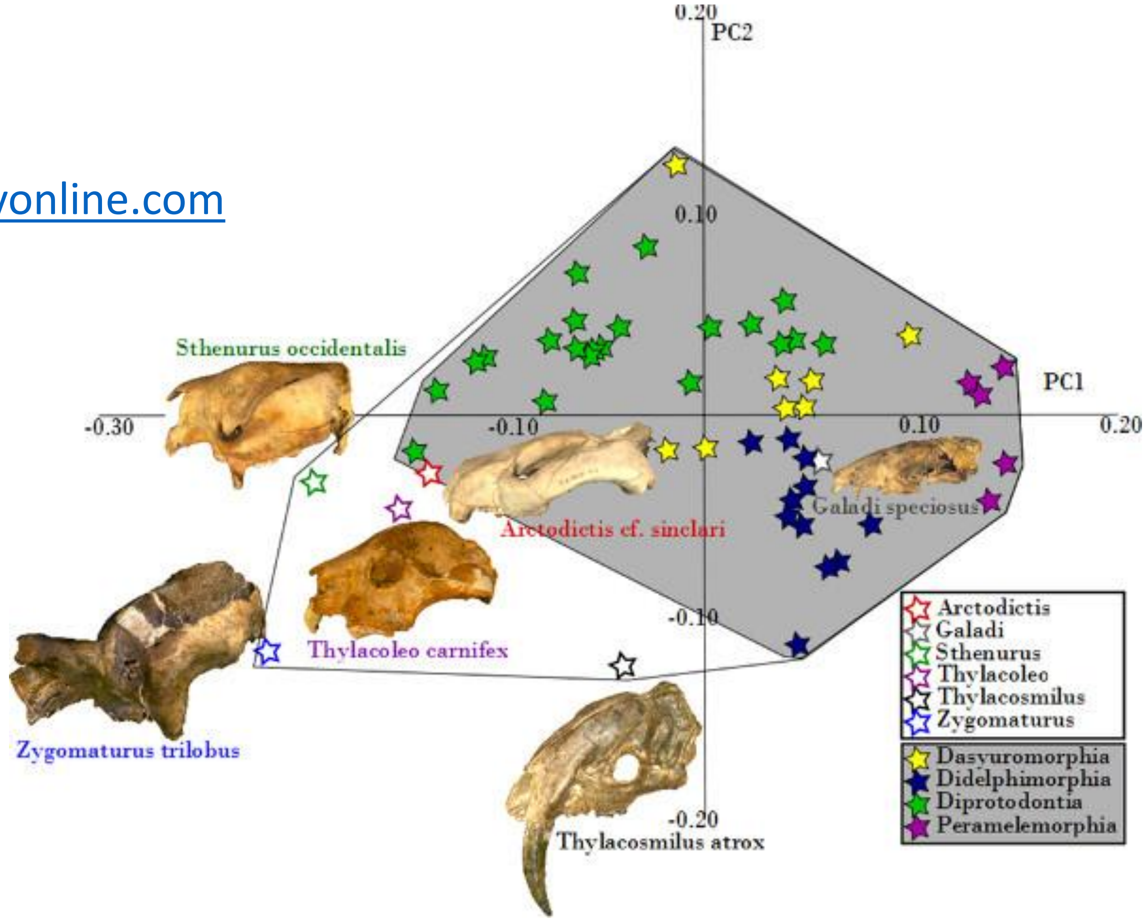
Dimensionality reduction



Picture taken from http://cnx.org/resources/269e78e2506cdbdc7f45ca17bb7d83491ce0c644/pca.jpg

An application

Picture taken from
http://www.palaeontologyonline.com



Many more applications: solving system of linear equations, computing pseudoinverse, building block of many other algorithms…

Singular Value Decomposition (SVD)

$$M = U\,\Sigma V^T$$

- U, V – orthonormal column matrices
- Σ – positive diagonal matrix
- $\sigma_1 \geq \cdots \geq \sigma_m$ - singular values
- Intuitive repsn. of transformation; unique
- For symmetric matrices, $U = \pm V$
- U eigenvectors of MM^T

Construction of SVD

- $v_1 = \underset{v:\|v\|_2=1}{\operatorname{argmax}} \|Mv\|_2$

$$v_{i+1} = \underset{\substack{v:\|v\|_2=1 \\ v\perp v_1,\cdots,v_i}}{\operatorname{argmax}} \|Mv\|_2$$

- $u_1 = \frac{Mv_1}{\|Mv_1\|_2}$

$$u_{i+1} = \frac{Mv_{i+1}}{\|Mv_{i+1}\|_2}$$

- $\sigma_1 = \|Mv_1\|_2$

$$\sigma_{i+1} = \|Mv_{i+1}\|_2$$

Relation to various norms

- Spectral norm/Operator norm : $\|M\|_2 \coloneqq \max_{v:\|v\|_2=1} \|Mv\|_2 = \sigma_1$

- Frobenius norm : $\|M\|_F \coloneqq \sqrt{\left(\sum_{i,j} M_{ij}^2\right)} = \sqrt{\sum_i \sigma_i^2}$

- Schatten norms : $\|M\|_{S_p} \coloneqq \left(\sum_i \sigma_i^p\right)^{1/p}$

A simple application

Lemma: If M is square and has orthonormal columns then it also has orthonormal rows.

Proof:

$$\|Mv\|_2 = 1 \;\forall\; v \in \mathbb{R}^n$$

$$\Rightarrow \sigma_i = 1 \;\forall\; i$$

$$\Rightarrow \|u^T M\|_2 = 1 \;\forall\; u \in \mathbb{R}^n$$

$\Rightarrow$Rows of M are orthonormal.

Eckart-Young-Mirsky Theorem

Let $M = U\Sigma V^T$ be the SVD of M. Then, for any rank-k matrix A, we have:

$$\|M - A\|_2 \geq \left\|M - U_k \Sigma_k V_k^T\right\|_2 = \sigma_{k+1}$$

$$\|M - A\|_F \geq \left\|M - U_k \Sigma_k V_k^T\right\|_F = \sqrt{\sum_{i=k+1}^{m} \sigma_i^2}$$

Proof of Eckart-Young-Mirsky Theorem

- Since $\mathrm{rank}(A) \leq \mathrm{k}$, $\dim(\mathrm{null}(A)) \geq \mathrm{n} - \mathrm{k}$.

- Since $\dim(\mathrm{null}(A)) + \dim\left(\mathrm{range}(\mathrm{V}_{\mathrm{k}+1})\right) \geq n - k + k + 1 = n + 1$,
there exists $\mathrm{x} \in null(A) \cap range(V_{k+1})$.

- $\|(M - A)x\|_2^2 = \sum_{i=1}^{k+1} \sigma_i^2 < x, v_i >^2 \geq \sigma_{k+1}^2 \sum_{i=1}^{k+1} < x, v_i >^2 = \sigma_{k+1}^2$

Proof of Eckart-Young-Mirsky Theorem

Frobenius norm for rank-1 case

$$\min_{u,v} \|M - uv^T\|_F^2$$

Stationary points: $$(M - uv^T)v = 0$$
$$u^T(M - uv^T) = 0$$

$\Rightarrow u, v$ are singular vectors of M

Optimality $\Rightarrow u, v$ are top singular vectors!

Perturbation questions

It is often the case that data is corrupted, and we observe

$$M = L + N$$

where L is the desired matrix and N is noise.

Would like to answer questions such as

- How large is $\left(\sigma_k(M) - \sigma_k(L)\right)$?
- How far are $\mathrm{u_k(M)}$ and$\mathrm{u_k(L)}$?

Perturbation inequalities

$$M = L + N$$

- Weyl's inequalities

$$|\sigma_k(M) - \sigma_k(L)| \leq \|N\|_2$$

- Davis Kahan theorem

$$\left\|(\mathrm{U_k(M)})_{\perp}^{T}\mathrm{U_k(L)}\right\|_2 \leq \frac{\|N\|_2}{|\sigma_k(L) - \sigma_{k+1}(L)|}$$

An exercise

- Suppose L is a rank- k matrix and $\mathrm{M} = \mathrm{L} + \mathrm{N}$. Then,

$$\|L - P_k(M)\|_2 \leq 2\|N\|_2.$$

Proof: $\|L - P_k(M)\|_2 \leq \|M - L\|_2 + \|M - P_k(M)\|_2$

$$\leq 2\|M - L\|_2 \quad \leq 2\|N\|_2.$$

A similar argument gives $\|L - P_k(M)\|_F \leq 2\|N\|_F$.

Another exercise

- Suppose L is a rank- k matrix and $\mathrm{M} = \mathrm{L} + \mathrm{N}$. Then,

$$\|L - P_k(M)\|_F \leq 2\sqrt{2k}\,\|N\|_2.$$

Proof: Let U be the (at most $2k$) left singular vectors of $\mathrm{L} - \mathrm{P_k}(\mathrm{M})$.

$$\|L - P_k(M)\|_F^2 = Tr\left(U^T\big(L - P_k(M)\big)\big(L - P_k(M)\big)^T U\right)$$

Write $L - P_k(M) = L - M + M - P_k(M)$, and use

$$Tr(U^T A B^T U) \leq 2k\|A\|_2\|B\|_2$$

Summary

- SVD/PCA is a fundamental tool in many settings
- Perturbation analysis is crucial for these purposes
- Tight results known for perturbation in $\|\cdot\|_2$ and $\|\cdot\|_F$ norms
- Coming up later: perturbation bounds in $\|\cdot\|_\infty$norm

References

- Linear Algebra Done Right, by Sheldon Axler
- Matrix Computations, by Gene Golub and Charles Van Loan
- https://terrytao.wordpress.com/2010/01/12/254a-notes-3a-eigenvalues-and-sums-of-hermitian-matrices/