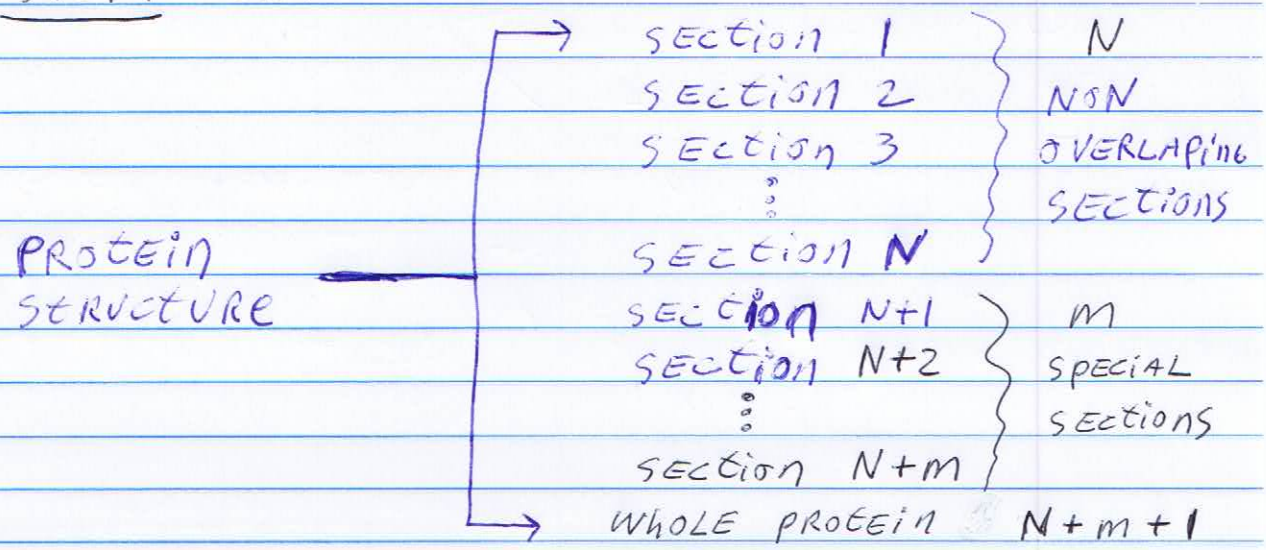
HIERARCHICAL PCA HPCA

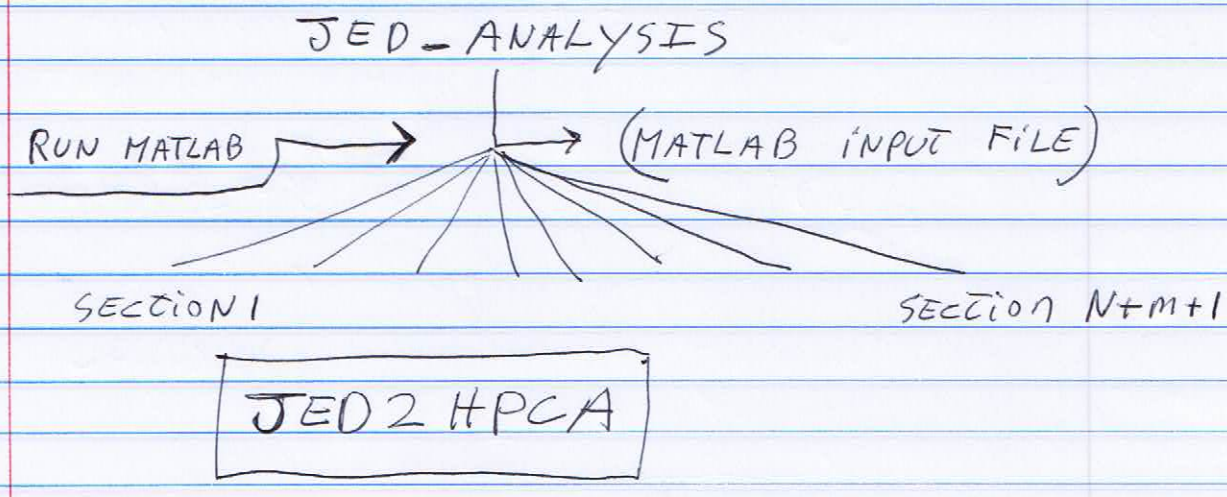
STEP 1 CONSTRUCT SECTIONS



STEP 2 RUN JED ON ALL SECTIONS
TAKE TOP 5 PCA MODES

NOTE: CAN BE SPECIFIED BY USER BASED ON SCREE PLOTS, ETC.

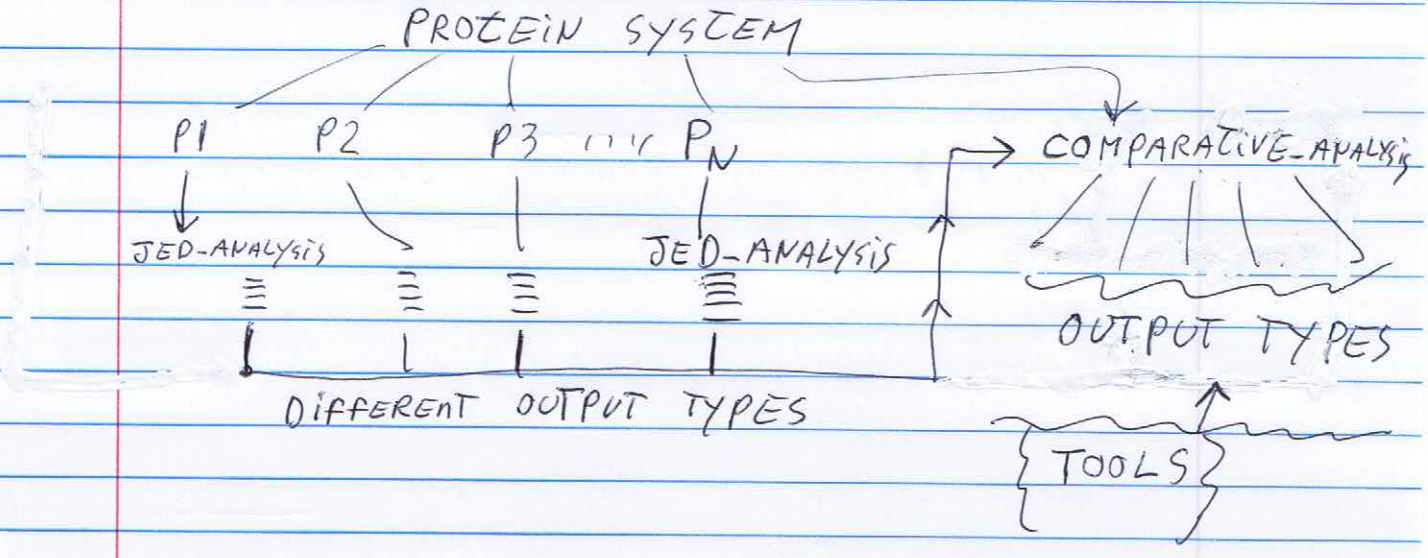
STEP 3 CONSTRUCT INPUT FILE



JED2HPCA

RESULTS FROM JED2HPCA

JED-ANALYSIS



MATHMATICS OF HPCA

LET $|J:S,K\rangle \equiv$ (K-th) cPCA MODE FOR section S

* → COVARIANCE MATRIX

* ORDERING OF OVERLAPPING SECTIONS IS IMPORTANT.
BEST TO PUT SMALLEST → LARGEST
MOST NON-OVERLAPPING BEFORE OVERLAPPING

DEFINE LINEAR INDEXING SCHEME
EXAMPLE 9 sections EACH with 5 MODES.

n	1	2	3	4	5	6	7	8	9	10	11	...	44	45
S,K	1,1	1,2	1,3	1,4	1,5	2,1	2,2	2,3	2,4	2,5	3,1		9,4	9,5

MAP $n \leftrightarrow \{S,K\}_n$ *

APPLY PROJECTION OPERATOR METHOD

$$|v_1\rangle \equiv |J: 1,1\rangle$$

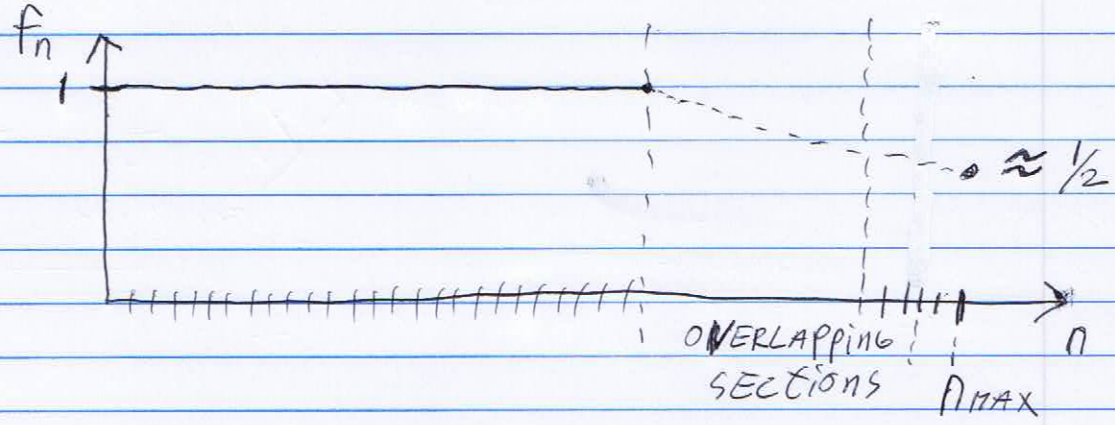
DEFINE $\hat{P}_n \equiv \hat{1} - \sum_{K=1}^{n} |v_K\rangle\langle v_K|$

ITERATIVELY SOLVE:

$$|v_{n+1}\rangle = \frac{\hat{P}_n |J: \{S,K\}_{n+1}\rangle}{\text{NORM}\left[\hat{P}_n |J: \{S,K\}_{n+1}\rangle\right]}$$

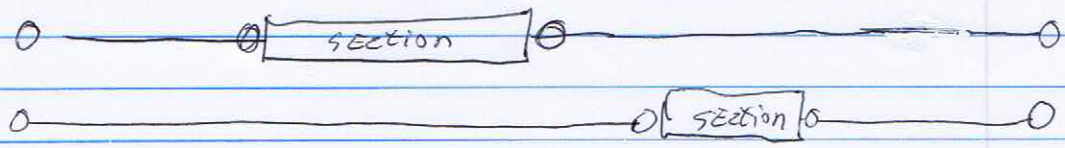
MONITOR OVERLAPS:

$$\text{FRACTION}_n = f_n \equiv \langle v_n | J: \{S,K\}_n\rangle$$

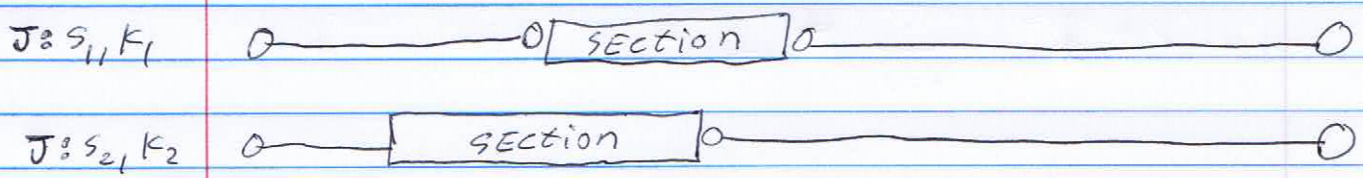


EACH $|v_{n+1}\rangle$ MONITORS AN ORTHOGONAL TYPE OF MOTION TO THE SET $\{|v_K\rangle\}_n \; \forall_{K=1,n}$

NOTE: NON-OVERLAPPING SECTIONS



OVERLAPPING SECTIONS



$\langle J: S_2, K_2 \mid J: S_1, K_1 \rangle \neq 0$ in GENERAL

$\langle v_{n_2} \mid v_{n_1} \rangle = 0$ ALWAYS.

where $n_1 \leftrightarrow \{S_1, K_1\}$ $n_2 \leftrightarrow \{S_2, K_2\}$

BUILD COVARIANCE AND CORRELATION MATRICES

GENERALIZED
INTERNAL COORDINATES: $\{q_n(t)\}$

$$q_n(t) = \langle v_n \mid \vec{C}(t) \rangle$$

$|\vec{C}(t)\rangle \equiv$ CONFORMATION of PROTEIN
→ time FRAME of other indexing

* X, Y, Z COMPONENTS ARE BEING TRACKED!

NEXT CONSTRUCT $\hat{M}$ ← COVARIANCE / CORRELATION

EIGENVALUES / EIGENVECTORS OF $\hat{M}$

$$\{\lambda_n, |v_n\rangle\}$$

CAN LOOK @ INNER PRODUCTS $\langle v_n | v_n \rangle$
COLLAPSED INNER PRODUCTS → $\langle v_s | v_s \rangle$

COMBINED INNER PRODUCTS

OUTER PRODUCTS $\sum_n |U_n\rangle \lambda_n \langle U_n|$

CONSTRUCT $|\varphi_n\rangle = \sum_k \langle k|U_n\rangle |v_k\rangle$

Note $|U_n\rangle = \sum_k \langle k|U_n\rangle |k\rangle$

↑ COMPONENTS of the n-th EIGEN VECTOR

Note: $\langle \varphi_m|\varphi_n\rangle = \sum_j \sum_k \langle v_j| \langle U_m|j\rangle \langle k|U_n\rangle |v_k\rangle$

$\langle v_j|v_k\rangle \equiv \delta_{jk}$

$\langle \varphi_m|\varphi_n\rangle = \sum_k \langle U_m|k\rangle\langle k|U_n\rangle$

$\sum_k |k\rangle\langle k| = 1$

$\langle \varphi_m|\varphi_n\rangle = \langle U_m|U_n\rangle = \delta_{mn}$

$\{|\varphi_n\rangle\} \equiv$ ORTOGONAL SET of modes