

joshua diba meeting notes 7/25

ATIP aggs (miscibility project)

graph could be common features, or kernelization features.

depend on T , cones = reality

have to make T, c dependent? Well, there are models for $K(x_i, x_j)$ learn things all compounds, this already can use bond descriptors/motifs?

propose in eg. dimension have to modify our loss and model to handle this

penalize constant violation to handle $X^T X = I$ constraint?

D - shapes for classes like polymers for PCA plot colored by fraction NH_2
 \rightarrow graph reg.

C, J - do eg. protein by features we can use? for Kernel method,

D - condense for long no. dict. that map color to miscibility outcome

use maps to map color matrix to miscibility matrix

check for missing, dict will do: warning if x missed a color,

to normalize PCA. zero-variance columns \rightarrow false neg. - changed

\rightarrow non-informative, if col has 0 or 1 already normalizing U_i 0 or 1

if U normalize M , U breaks symmetry, do not normalize!

incompatible \Rightarrow impossible \checkmark descent assumption,
 could just keep these missing!! no need to make decision,
 but seems safe.

D - eg. gel \Rightarrow incompatible? check in SI with ex. compound a bit

D - compare to paper's miscibility matrix, we get the same?
 protein surf. ...

C - share Uddel email, upload to Github

D - vector calc. to derive $\nabla_{\theta} \ell$
 \rightarrow gradient descent, read abt gradient descent.

C, J - is $X^T X = I$ constraint ok? not for large X .