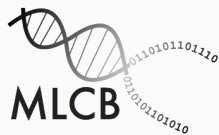


# Kernels for proteins and MMD.

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- Here we want to go through the maths behind the kernels to make sure our implementation is efficient.
- Linear, Weissfeiler-Lehmann kernel

- Not much to optimize there. Just check: [this link](#).

- Computing  $\phi(G)$  needs to be done explicitly and can be done independently prior to computing  $K_{WL} = \phi(G)^T \phi(G')$
- How to compute  $\phi(G)$ ? `networkx` has a function called `weisfeiler_lehman_graph_hash` but it does not return the hash counts at each iteration.

