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3.) TSP Hamiltonian

Note $x_{\alpha j} \in \{0,1\}$

let $\hat{H} = \hat{H}_a + \hat{H}_b + \hat{H}_c + \hat{H}_d$

a.) $\hat{H}_a$ will penalize (increase energy) for cities that appear more than once in the path

$$\boxed{\hat{H}_a = \sum_{\alpha=0}^{n-1} \left(1 - \sum_{j=0}^{n-1} x_{\alpha,j}\right)^2}$$

This is similar to the scheduling problem we discussed in lecture.

b.) $\hat{H}_b$ will penalize for timesteps that have more than one city

$$\boxed{\hat{H}_b = \sum_{j=0}^{n-1} \left(1 - \sum_{\alpha=0}^{n-1} x_{\alpha,j}\right)^2}$$

c.) $\hat{H}_c$ penalizes if the edge between two cities is not in the graph G.

$$\boxed{\hat{H}_c = \sum_{j=0}^{n-2} \left( \sum_{\alpha \in \{x_{\alpha,j}=1\}} \sum_{\beta \in \{x_{\beta,j+1} = 1\}} \gamma \, \mathbb{1}_{\{E(\alpha,\beta) \notin G\}} \right)}$$

where $\gamma \in \mathbb{R}$ is a tunable hyperparameter for scaling the magnitude of the penalty. The indicator function:

$$\mathbb{1}_{\{E(\alpha,\beta) \notin G\}} = \begin{cases} 1 & \text{if } E(\alpha,\beta) \notin G \text{ (edge does not exist)} \\ 0 & \text{if } E(\alpha,\beta) \in G \text{ (edge exists)} \end{cases}$$

N.b.: The notation $\sum\limits_{\alpha \in \{x_{\alpha,j} = 1\}}$ is the sum over cities, $\alpha$,

(cont.) →

3.) c) (cont.)
at time step $j$, for which $x_{\alpha,j} = 1$.

d.) $\hat{H}_d$ penalizes paths that are too long i.e. drives system towards shortest path.
Note: $W_{\alpha,\beta}$ = length (cost) of edge from city $\alpha$ to $\beta$.

$$\boxed{\begin{gathered}\hat{H}_d = \sum_{j=0}^{n-2} \left( \sum_{\alpha \in \{x_{\alpha,j} = 1\}} \sum_{\beta \in \{x_{\beta,j+1} = 1\}} \lambda_{\alpha,\beta} \right) \\ \text{where } \lambda_{\alpha,\beta} = \begin{cases} W_{\alpha,\beta} & \text{if } E(\alpha,\beta) \in G \\ \max(W_{l,m}) & \text{if } E(\alpha,\beta) \notin G \\ & \forall\, l,m \text{ such that } E(l,m) \in G. \end{cases}\end{gathered}}$$

In other words, if edge $E(\alpha,\beta) \in G$, $\lambda_{\alpha,\beta}$ will be the distance to travel from $\alpha$ to $\beta$.
However, if $E(\alpha,\beta) \notin G$, we still need to penalize the path in some way, & since $W_{\alpha,\beta}$ does not exist, we penalize the system by setting $\lambda_{\alpha,\beta}$ to equal the largest distance in the entire graph, G. That way, a path of entirely imaginary edges is ensured to get a penalty from this term that is larger than a real path of the same number of time steps.

Now, $\hat{H} = \hat{H}_a + \hat{H}_b + \hat{H}_c + \hat{H}_d$ represents the TSP Hamiltonian.