CS680, Spring 2020, Assignment 5

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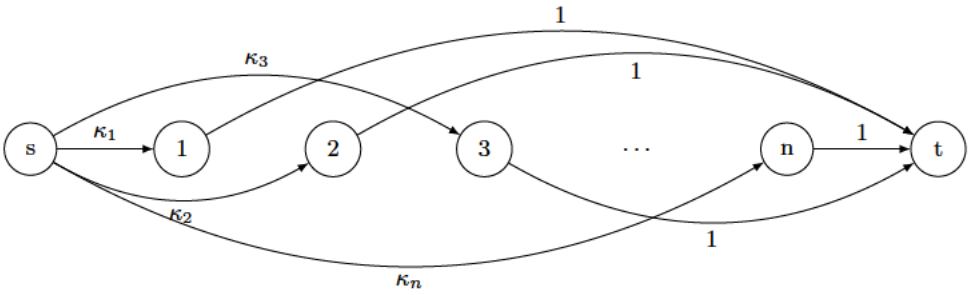
Exercise 1

1. Since the production of kernels is a kernel, $\kappa_{\mathcal{P}}$ is a kernel. And the sum of kernels is still a kernel, therefore, $\kappa_{\mathcal{G}}$ is indeed a kernel.

2. $\kappa_{\mathcal{G}}(x,z)$ $\left[xz*(xz-1)^3*e^{(x\ z)^2/2}*1\right]+\left[xz*e^{|x\ z|}*\tanh(xz+1)*1\right]$

   $\kappa_{\mathcal{G}}(1,-1)$ $8e^{2}$

3. Since we want $\kappa_{\mathcal{G}}$ $\sum_{i}^{n}\kappa_i$, we should have n path from $s\to t$, and each path have a kernel of κ_i.



4. Since we want $\kappa_{\mathcal{G}}$ $\prod_{i}^{n}\kappa_i$, we should only have one path from $s\to t$.

5. $\kappa_{\mathcal{G}_{sub}}(x,z)$ $xz*(xz-1)^3$

6. $\kappa_{\mathcal{G}_{sub}}(x,z)$ $\left[xz*(xz-1)^3*e^{(x\ z)^2/2}\right]+\left[xz*e^{|x\ z|}*\tanh(xz+1)\right]$

7. Use DFS to explore all the path in the graph, the complexity of DFS is $O(|V|+|E|)$. Suppose the graph is stored as adjacency list G, where $G[u]$ is the list of vertexes connect to u. All the kernels on each edge is stored as a matrix w, where $w[u][v]$ represents the kernel on edge $u\to v$. Hence, $w[u][v](\mathbf{x},\mathbf{z})$ will calculate the kernel given $(\mathbf{x},\mathbf{z})$. And we also set the diagonal elements of w as 1. Define a global variable $\kappa_{\mathcal{G}}$ 0 to store the result of calculating graph kernel.

Algorithm 1: DFS

Input: G,s,p,t,κ_p $1,\mathbf{x},\mathbf{z}$

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κ_p   κ_p * (w[p][s](x, z))
if v   t then
    κ_G   κ_G + κ_p
else
    for each vertex v in G[v] do
        DFS(G, v, s, t, κ_p, x, z)
κ_p   κ_p/(w[p][s](x, z))
```

Now we start with DFS$(G, s, s, t, 1, \mathbf{x}, \mathbf{z})$, it will go through all the paths from s to t. $\kappa_{\mathcal{G}}$ will finally store the result.