

Machine Learning for Graphs and some applications to Polymer Science

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In this talk, we will discuss how to compare graphs using graph kernel methods. In a nutshell, even deciding whether two graphs are isomorphic is not trivial, let alone determining a degree of similarity. We will discuss some common techniques, and then apply those to the analysis and design of polymers in chemistry. We will also discuss how to create explanations of decisions based on such algorithms.



Auditório Jacy Monteiro - IME-USP

14:00

Válido como AAC

18 Abr

