Graph Kernels

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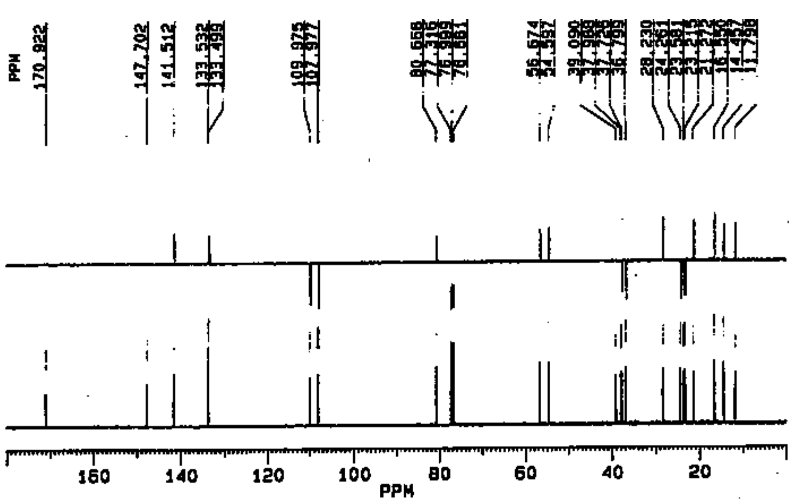
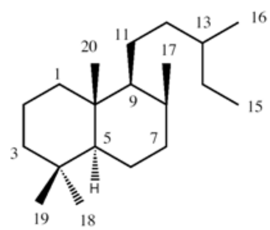
^{13}C NMR Spectrum



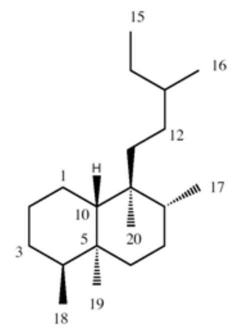
Diterpenes

bicyclic

skeleton-type labdan



skeleton-type clerodan



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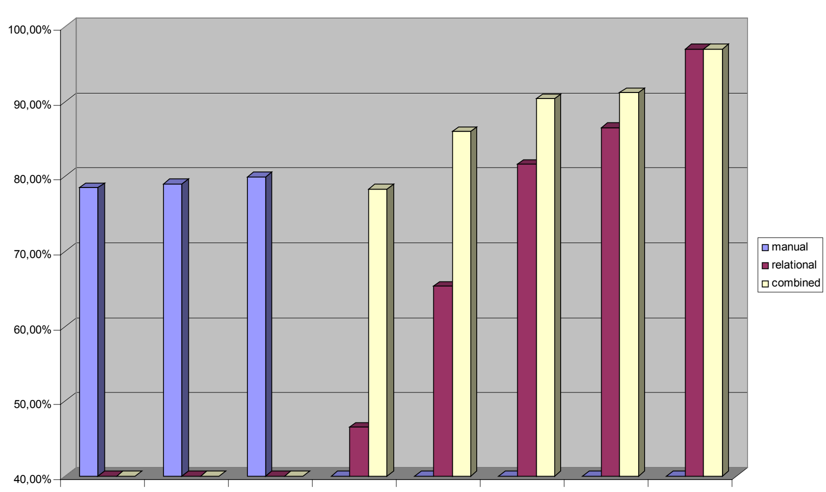
Empirical Results



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Kernels for Unreal Data

Graph Edit Distance / Matching Metric

Convolution Kernels

Instance Space has Graph Structure

Kernels on Strings / Trees

Kernels for Structured Data

Labelled Directed Graphs

$G = (\mathcal{V}, \mathcal{E}, label)$

$\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V} \quad label : \mathcal{V} \to \mathcal{L}$

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Labelled Directed Graphs

$$G = (\mathcal{V}, \mathcal{E}, label)$$

$$\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V} \quad label : \mathcal{V} \to \mathcal{L}$$

$$[L]_{r,i} = \begin{cases} 1 & \text{if } l_r = label(v_i) \\ 0 & \text{otherwise} \end{cases}$$

$$[E]_{i,j} = \begin{cases} 1 & \text{if } (v_i, v_j) \in \mathcal{E} \\ 0 & \text{otherwise} \end{cases}$$

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Basic Idea

$\langle LL^\top, L'L'^\top \rangle$

E E^n

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$\{\langle LE^iL^\top, L'E'^jL'^\top \rangle\}_{i,j}$

Kernels for LDGs

$\{\langle LE^iL^\top, L'E'^jL'^\top \rangle\}_{i,j}$

$$k_n(G, G') = \sum_{i,j=0}^{n} \lambda_i \lambda_j \langle LE^iL^\top, LE'^jL'^\top \rangle$$

Kernels for LDGs

$$\left\{\left\langle LE^i L^\top, L'E'^j L'^\top\right\rangle\right\}_{i,j}$$

$$k_n(G, G') = \sum_{i,j=0}^{n} \lambda_i \lambda_j \left\langle LE^i L^\top, LE'^j L'^\top\right\rangle$$

$\lim_{n\to\infty} k_n(G, G')$

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Absolute Convergent Kernel

If

$$\sum_{i=0}^{n} \lambda_i a^i$$

is absolute convergent for $n \to \infty$ and

$$\lim_{i\to\infty} \lambda_i i^2 a^i = 0$$

then k_n is absolute convergent for $n \to \infty$.

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Absolute Convergent Kernel

If

$$\sum_{i=0}^{n} \lambda_i a^i$$

$$a \geq \max_G \min\{\Delta^+(G), \Delta^-(G)\}$$
$$\Delta^+(G) = max\{|\delta^+(v)|, v \in \mathcal{V}\}$$
$$\Delta^-(G) = max\{|\delta^-(c)|, v \in \mathcal{V}\}$$

is absolute convergent for $n \to \infty$ and

$$\lim_{i \to \infty} \lambda_i i^2 a^i = 0$$

then k_n is absolute convergent for $n \to \infty$.

Convergence Proof

$$\left\langle L \left(\lim_{n \to \infty} \sum_{i=0}^{n} \lambda_i E^i \right) L^\top, L' \left(\lim_{m \to \infty} \sum_{j=0}^{m} \lambda_j E'^j \right) L'^\top \right\rangle =$$

Convergence Proof

$$\left\langle L \left(\lim_{n\to\infty} \sum_{i=0}^{n} \lambda_i E^i \right) L^\top, L' \left(\lim_{m\to\infty} \sum_{j=0}^{m} \lambda_j E'^j \right) L'^\top \right\rangle =$$

$$\left\langle \lim_{n\to\infty} \sum_{i=0}^{n} \lambda_i L E^i L^\top, \lim_{m\to\infty} \sum_{j=0}^{m} \lambda_j L' E'^j L'^\top \right\rangle =$$

Convergence Proof

$$\left\langle L \left(\lim_{n\to\infty} \sum_{i=0}^{n} \lambda_i E^i \right) L^\top, L' \left(\lim_{m\to\infty} \sum_{j=0}^{m} \lambda_j E'^j \right) L'^\top \right\rangle =$$

$$\left\langle \lim_{n\to\infty} \sum_{i=0}^{n} \lambda_i L E^i L^\top, \lim_{m\to\infty} \sum_{j=0}^{m} \lambda_j L' E'^j L'^\top \right\rangle =$$

$$\lim_{n\to\infty} \sum_{i=0}^{n} \sum_{j=0}^{i} \lambda_i \lambda_{i-j} \left\langle L E^i L^\top, L' E'^{i-j} L'^\top \right\rangle =$$

Convergence Proof

$$\left\langle L\left(\lim_{n\to\infty}\sum_{i=0}^{n}\lambda_i E^i\right)L^\top, L'\left(\lim_{m\to\infty}\sum_{j=0}^{m}\lambda_j E'^j\right)L'^\top\right\rangle =$$

$$\left\langle \lim_{n\to\infty}\sum_{i=0}^{n}\lambda_i L E^i L^\top, \lim_{m\to\infty}\sum_{j=0}^{m}\lambda_j L' E'^j L'^\top\right\rangle =$$

$$\lim_{n\to\infty}\sum_{i=0}^{n}\sum_{j=0}^{i}\lambda_i\lambda_{i-j}\left\langle L E^i L^\top, L' E'^{i-j} L'^\top\right\rangle =$$

$$\lim_{n\to\infty}\sum_{i,j=0}^{n}\lambda_i\lambda_j\left\langle L E^i L^\top, L' E'^j L'^\top\right\rangle = k_\infty(G,G')$$

qed

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Example 1: Geometric *k*

$$\lambda_i = \gamma^i$$

$$\lim_{n\to\infty}\sum_{i=0}^{n}\gamma^i = \frac{1}{1-\gamma}$$

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Example 1: Geometric *k*

$$\lambda_i = \gamma^i \qquad \lim_{n\to\infty}\sum_{i=0}^{n}\gamma^i = \frac{1}{1-\gamma}$$

$$geom(\gamma, E) = \lim_{n\to\infty}\sum_{i=0}^{n}\gamma^i E^i$$

$$k_{geom}(G, G') = \left\langle L\,geom(\gamma, E)L^\top, L'\,geom(\gamma, E')L'^\top\right\rangle$$

Example 2: Exponential *k*

$$\lambda_i = \frac{\beta^i}{i!} \qquad \lim_{n\to\infty}\sum_{i=0}^{n}\frac{\beta^i}{i!} = e^\beta$$

Example 2: Exponential *k*

$\lambda_i = \frac{\beta^i}{i!}$

$$\lim_{n\to\infty} \sum_{i=0}^{n} \frac{\beta^i}{i!} = e^{\beta}$$

$$\lim_{n\to\infty} \sum_{i=0}^{n} \lambda_i E^i = \lim_{n\to\infty} \sum_{i=0}^{n} \frac{(\beta E)^i}{i!} = e^{\beta E}$$

$$k_{exp}(G, G') = \left\langle L e^{\beta E} L^{\top}, L' e^{\beta E'} L'^{\top} \right\rangle$$

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Efficient Computation

$$e^{\beta E} = \lim_{n\to\infty} \sum_{i=0}^{n} \frac{(\beta E)^i}{i!}$$

$$E = T^{-1} D T$$

$$E^n = (T^{-1} D T)^n = T^{-1} D^n T$$

$$e^{\beta E} = T^{-1} e^{\beta D} T$$

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Thank You !

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