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Kernel methods for structured data

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Outline

1. Learning with structured data
2. Kernels and convolution kernels
3. Graph kernels
4. Kernel methods for relational learning
5. Dealing with continuous/high dimensional attributes

Part I

Learning with structured data

- Data in propositional supervised learning:
  - Design matrix (input) X: one example per row, one attribute (or codebit) per column
  - Target vector (output) y: one scalar per example (binary, regression, multitask)

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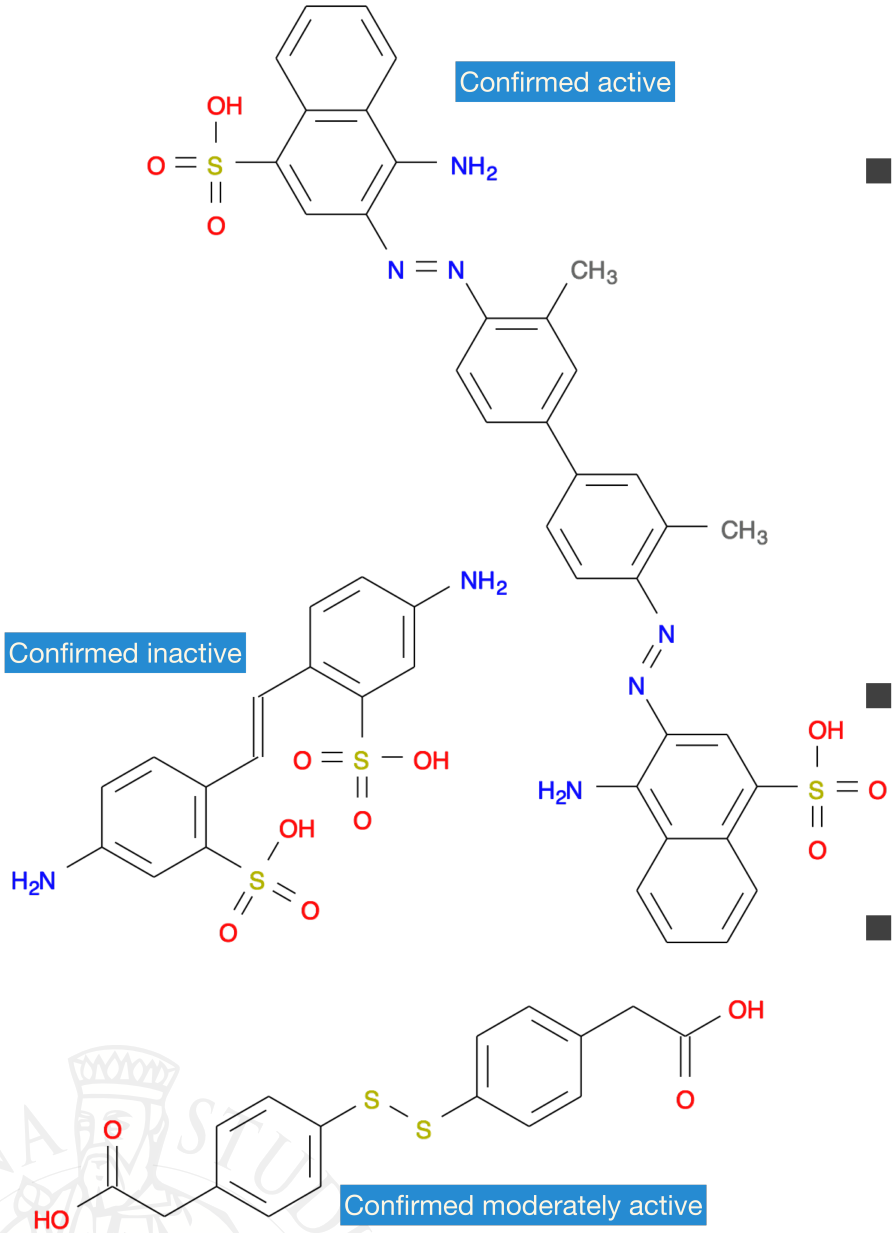
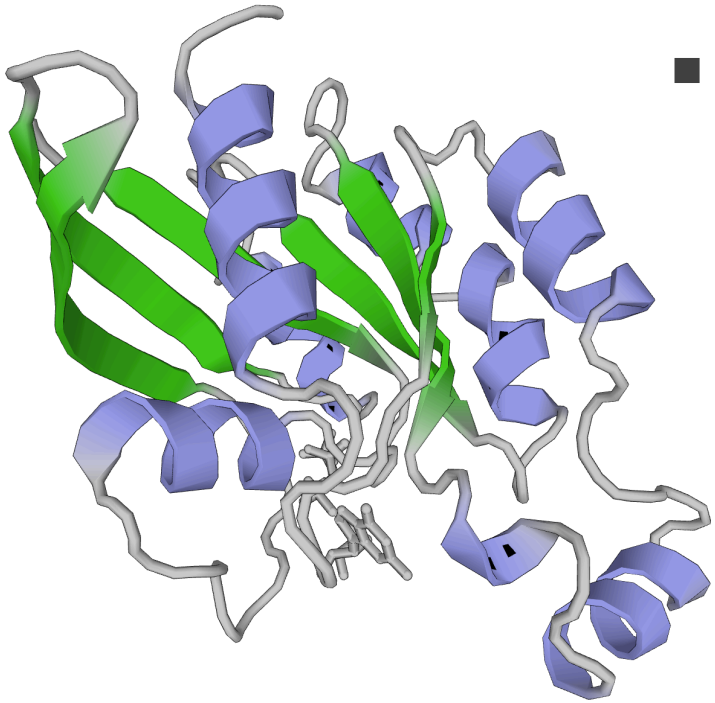
- Data in relational learning:
  - Relational database(s) or equivalent (restricted) first-order logic representations — e.g. learning from interpretations (De Raedt 2008)

Example: Chemoinformatics



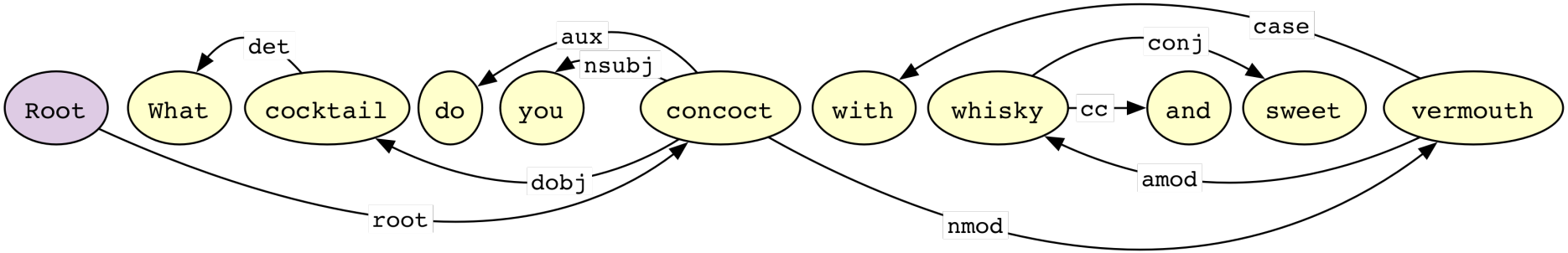
- Each molecule represented as a graph where:
  - Nodes correspond to atoms
  - Edges correspond to bonds
- Attributes may include element, charge, bond type
- Task: many are possible — e.g. active compound in drug design, mutagenicity, biodegradability, etc.

Example: Protein function (Borgwardt et al. 2005b)



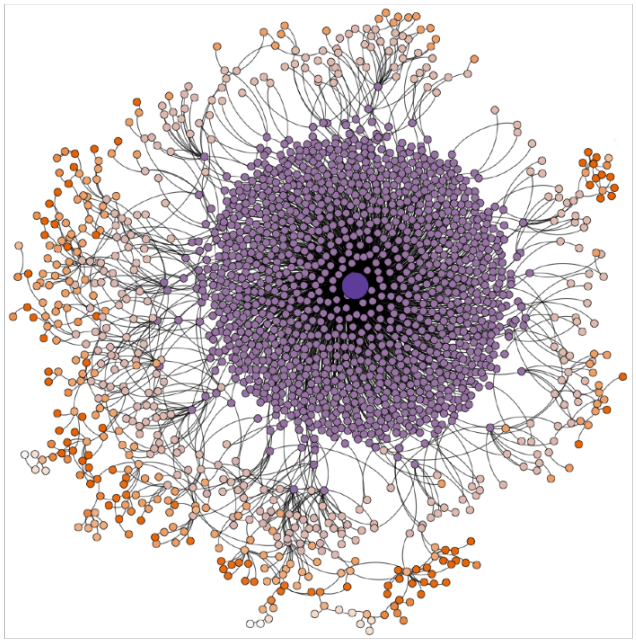
- Each protein represented as a graph where:
  - Nodes correspond to secondary structure elements (SSE)
  - Structural edges (SSE are neighbors in space) and sequential edges (SSE are adjacent in sequence)
- Attributes include physical and chemical information
- Task: discriminate between enzymes and non-enzymes, or categorize according to enzyme type

Example: Sentence classification



- Each sentence represented as a graph where:
  - Nodes correspond to words (possibly represented by word vectors)
  - Edges correspond to the (typed) dependency relation between governors and dependents
- Tasks: many are possible — e.g. classify sentences according to the expected answer, such as *food* (Li et al. 2006); detect weasel sentences (Verbeke et al. 2011), segment scientific abstracts (Verbeke et al. 2012) etc.

Example: sub-community identification (Yanardag et al. 2015)



- Each discussion on reddit represented as a graph where:
  - Nodes correspond to users
  - Edges represent user interactions (e.g. responding to each other's comments)
- Task: Categorize discussions into communities, e.g. question/answer-based community or a discussion-based community

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- In general you can expect interdependencies among output variables
- Thus better accuracy can be achieved by forming features that include these output variables

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- Example: protein secondary structure prediction
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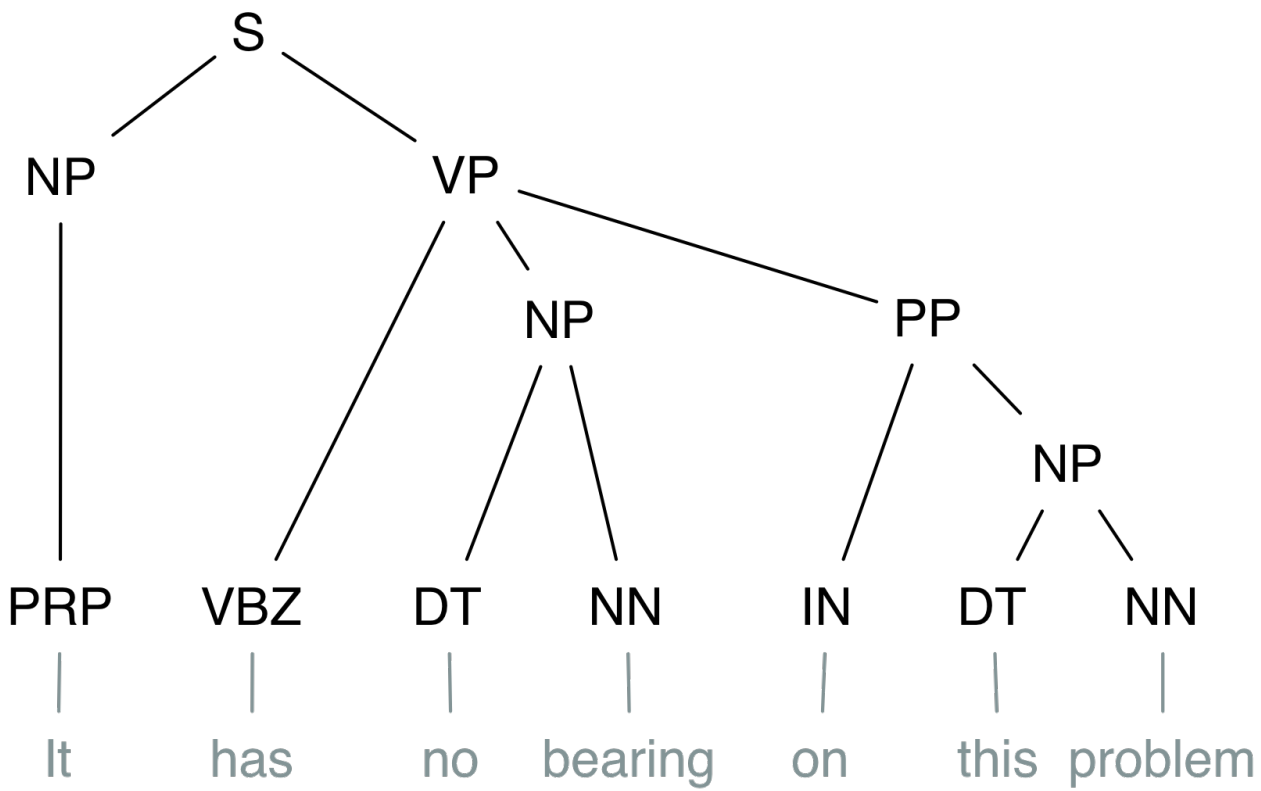
- Example: Part-of-speech tagging
  - Input is a sentence (sequence of words)
    - Output is a corresponding sequence of syntactic categories

PRP	VBZ	DT	NN	IN	DT	NN
It	has	no	bearing	on	this	problem

Example: Natural language parsing

- Each example corresponds to a sentence
- The input is a sequence of words
  - The target is a parse tree for the sentence



Part 2

Kernels and convolution kernels

Basic material only, for details see e.g. (Haussler 1999; Schölkopf et al. 2002; Shawe-Taylor et al. 2004)

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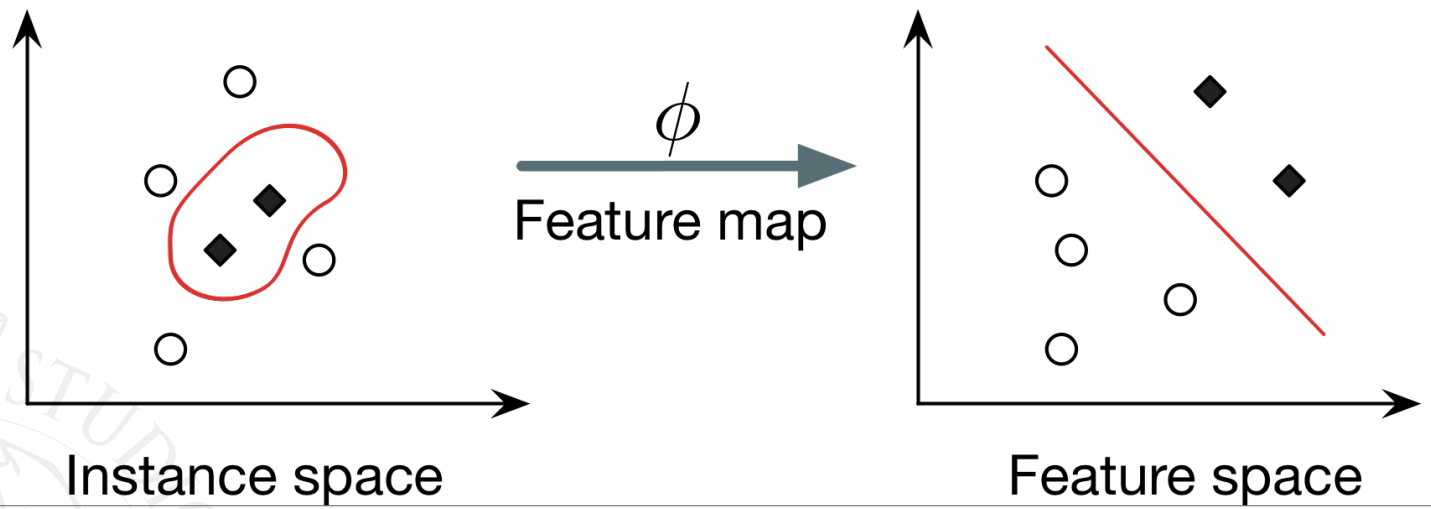

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$$k(x, z) = \langle \phi(x), \phi(z) \rangle \qquad \forall x, z \in \mathcal{X}$$

- Equivalently (Mercer's theorem): k is a valid kernel iff
  - *Symmetric*: $k(x, z) = k(z, x)$
  - *Positive semidefinite*: for every finite set of points, the matrix with entries

$$k_{ij} = k\left(x^{(i)}, x^{(j)}\right)$$

    has no negative eigenvalue

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$$f(x) = \sum_{i=1}^{n} \alpha^{(i)} y^{(i)} k \left(x^{(i)}, x \right) + b$$

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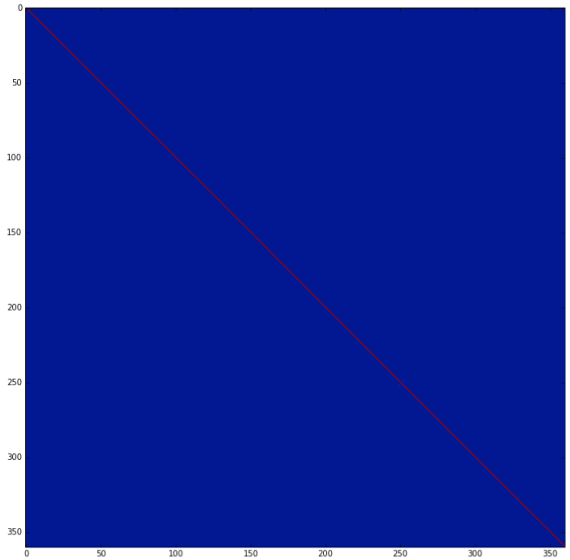
- The purpose of the kernel is to measure the similarity between the test point x and every training example $x^{(i)}$
- The coefficients are the solution of the QP

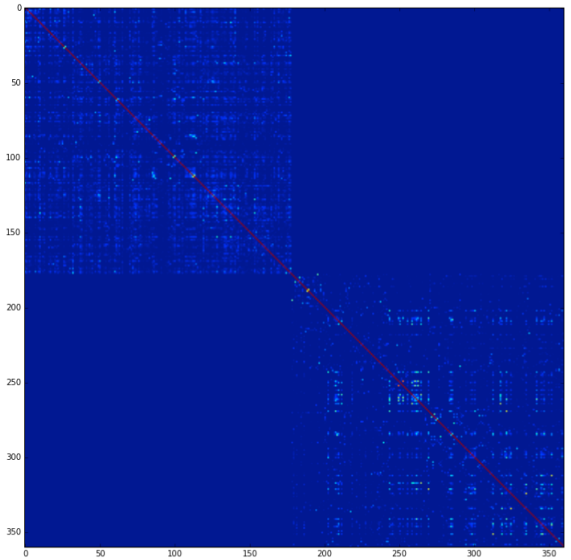
$$\begin{aligned} \min_{\alpha} \quad & \|\alpha\|_1 + \frac{1}{2} \alpha^\intercal Q \alpha \\ \text{subject to:} \quad & 0 \leq \alpha^{(i)} \leq C \qquad i = 1, \ldots, n \\ & \sum_{i=1}^{n} \alpha^{(i)} y^{(i)} = 0 \end{aligned}$$

where $Q = (YY^\intercal) \circ K$ and K is the kernel matrix of $\mathcal{D}$

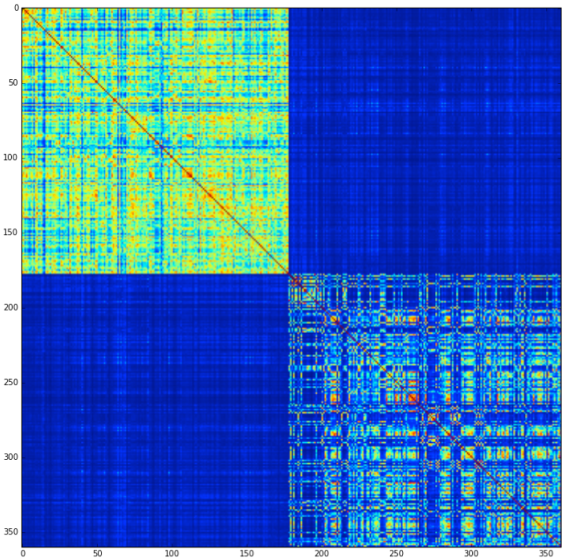
Check that your kernel looks reasonable



Diagonal



Diagonal dominant



Reasonable

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- Performance: Using appropriate kernel functions we may be able to perform nonlinear classification and attain better accuracy (because of lower approximation error)

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- Performance: Using appropriate kernel functions we may be able to perform nonlinear classification and attain better accuracy (because of lower approximation error)
- Efficiency (for small-medium size datasets): we may be able to compute $k(x, z)$ without computing the transformed $\phi(x)$ and $\phi(z)$ explicitly
- Abstraction: The data type of x does not matter anymore and we can apply many existing algorithms to arbitrary objects (in particular, structured ones)

Disadvantages of kernels

- Knowledge: Many different kernels are possible and choosing the correct one may require background knowledge that we don't have

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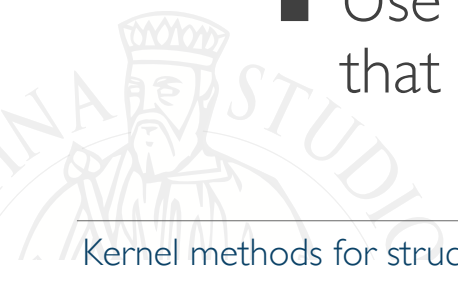
- Efficiency: Solving a quadratic problem is prohibitive for large datasets
- The quadratic problem may be avoided in some cases
  - Approximate the kernel matrix, e.g. using the Nyström method, or restrict to homogeneous kernels (Vedaldi et al. 2012)
  - Use kernels that correspond to very sparse feature vectors that may be obtained explicitly



Closure properties

- Suppose k_1 and k_2 are two valid (positive semi-definite) kernels with $k_j(x, z) = \langle \phi_j(x), \phi_j(z) \rangle$

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- Then the following kernels are also valid:

$$
\begin{aligned}
k_3(x, z) &= k_1(x, z) + k_2(x, z) && \text{(sum)} \\
k_4(x, z) &= k_1(x, z) k_2(x, z) && \text{(product)} \\
k_5(x, z) &= \frac{k_1(x, z)}{\sqrt{k_1(x, x) k_1(z, z)}} && \text{(normalization)}
\end{aligned}
$$

- If k_1 and k_2 are valid kernels then there exists ϕ_1 and ϕ_2 such that

$$k_1(x, z) = \langle \phi_1(x), \phi_1(z) \rangle$$
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Sum and product of kernels

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- $k_1(x, z) + k_2(x, z) = \langle \phi_1(x) \oplus \phi_2(x), \phi_1(z) \oplus \phi_2(z) \rangle$ where $\oplus$ denotes the concatenation operator

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- $k_1(x, z)k_2(x, z) = \langle \phi_1(x) \otimes \phi_2(x), \phi_1(z) \otimes \phi_2(z) \rangle$ where $\otimes$ denotes the Kronecker product

$$a \otimes b = [a_1 b, a_2 b, \cdots, a_p b]$$

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- Easy to prove: if $k(x, z) = \langle \phi(x), \phi(z) \rangle$ define

$$\tilde{\phi}(x) = \frac{\phi(x)}{\|\phi(x)\|}$$

  and check that

$$\tilde{k}(x, z) = \langle \tilde{\phi}(x), \tilde{\phi}(z) \rangle$$

Tensor product and direct sum kernels

- Suppose $\mathcal{X} = \mathcal{X}_1 \times \mathcal{X}_2$

Tensor product and direct sum kernels

- Suppose $\mathcal{X} = \mathcal{X}_1 \times \mathcal{X}_2$
- If κ_d, for $d = 1, \ldots, 2$ are valid kernels on $\mathcal{X}_d \times \mathcal{X}_d$, it is easy to construct valid kernels on tuples, e.g.,
  - Tensor product kernel

$$(\kappa_1 \otimes \kappa_2)((x_1, x_2), (x_2, x_2)) \doteq \kappa_1(x_1, z_1)\kappa_2(x_2, z_2)$$

  - Direct sum kernel

$$(\kappa_1 \oplus \kappa_2)((x_1, x_2), (x_2, x_2)) \doteq \kappa_1(x_1, z_1) + \kappa_2(x_2, z_2)$$

Convolution (or decomposition) kernels (Haussler 1999)

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- For all $x_d \in \mathcal{X}_d, d = 1, \ldots, D$ and $x \in \mathcal{X}$, $(x_1, \ldots, x_D, x) \in R$ iff $x_1, \ldots, x_D$ are the parts of x

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- Notation:

$$R^{-1}(x) \doteq \{(x_1, \ldots, x_D) : (x_1, \ldots, x_D, x) \in R\}$$

Example on strings

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- Let $\mathcal{X} = \Sigma^*$ (the set of all strings over a finite alphabet Σ)
- Let $D = 2$ and $\mathcal{X}_1 = \mathcal{X}_2 = \mathcal{X}$
- Define R so that $(x_1, x_2, x) \in R$ iff x_1 is a prefix of x and x_2 the complementary suffix

$$(\texttt{TATAG}, \texttt{ACGA}, \texttt{TATAGACGA}) \in R$$

$$(\texttt{TAT}, \texttt{ACGA}, \texttt{TATAGACGA}) \notin R$$

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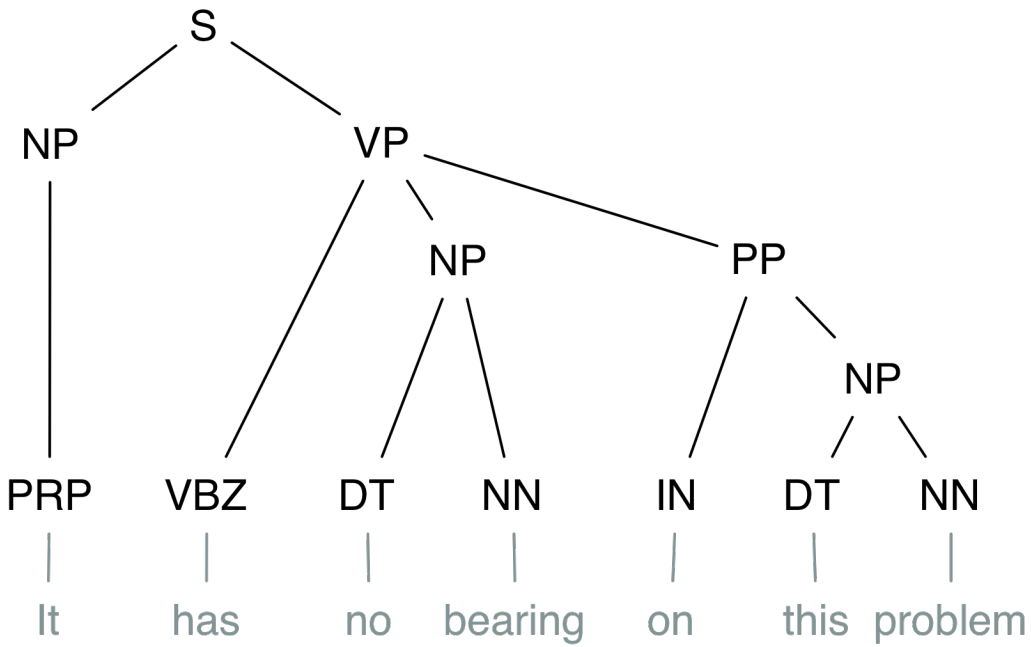
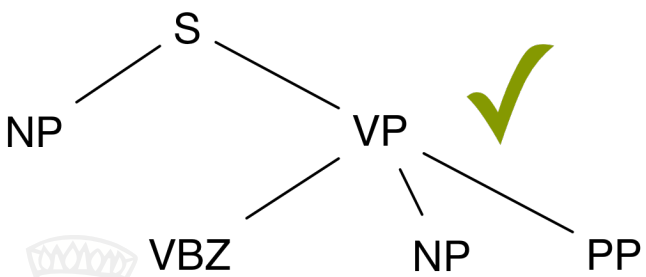
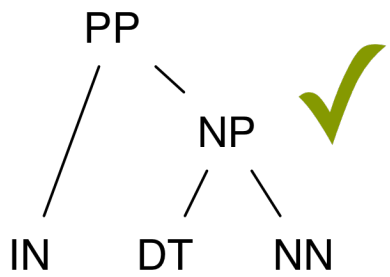
  - Take a complete subtree x' of x
  - Remove some complete subtrees from x'
  - Replace the roots of the removed subtrees
- A co-rooted substree never splits across a production rule

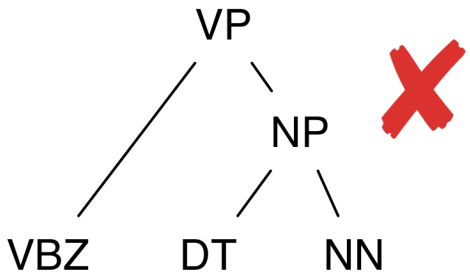
$$(t, x) \in R \quad \text{iff } t \text{ is a co-rooted subtree of } x$$

Co-rooted subtrees (Collins et al. 2001)









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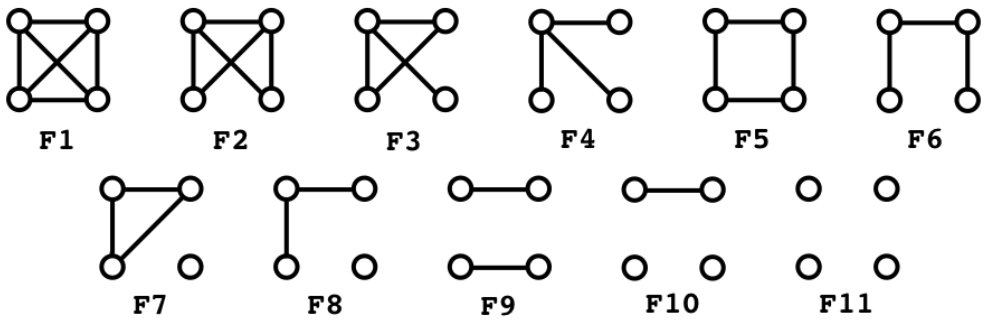
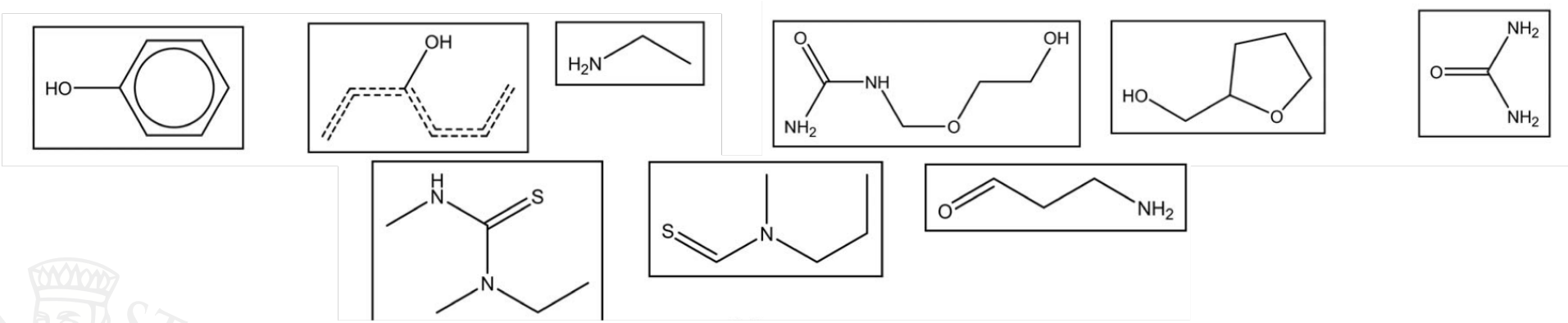
- A path (or walk) π is a sequence of vertices $\pi_1, \ldots, \pi_{|\pi|}$ such that $\pi_j \in V$ and $(\pi_j, \pi_{j+1}) \in E$
- If $\ell : V \mapsto \mathcal{L}$ is the vertex labeling function, the sequence $\ell(\pi_1), \ldots, \ell(\pi_{|\pi|})$ is a labeled path of x

$$(\pi, x) \in R \quad \text{iff } \pi \text{ is a labeled path of } x$$

- Simply: $(g, x) \in R$ iff g is a subgraph of x



All graphlets of 4 nodes (Shervashidze et al. 2009; Yanardag et al. 2015)



Frequent subgraph mining (Deshpande et al. 2005; Wale et al. 2008)

Convolution kernels

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- Suppose we have a valid kernel κ_d over all subspaces $\mathcal{X}_d$ for $d = 1, \ldots, D$
- Then the following kernel is valid over $\mathcal{X}$ (Haussler 1999):

$$K(x, z) = \sum_{\substack{(x_1, \ldots, x_d) \in R^{-1}(x) \\ (z_1, \ldots, z_d) \in R^{-1}(z)}} \prod_{d=1}^{D} \kappa_d(x_d, z_d)$$

Part 3

Graph kernels

Path kernels

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- Labels may be attached to vertices and/or edges
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- Define the path kernel as the *tensor product kernel*

$$\kappa_{\text{path}}(\pi, \pi') = \mathbb{1}\{|\pi| = |\pi'|\} \cdot \prod_{j=1}^{|\pi|} \kappa_{\text{node}}\left(\ell(\pi_j), \ell(\pi'_j)\right) \cdot \prod_{j=1}^{|\pi|-1} \kappa_{\text{edge}}\left(\ell((\pi_j, \pi_{j+1})), \ell((\pi'_j, \pi'_{j+1}))\right)$$

From path kernels to graph kernels

- Random walk kernels count the number of matching walks:

$$K(G, G') = \sum_{\pi \in R^{-1}(G)} \sum_{\pi' \in R^{-1}(G')} \kappa_{\text{path}}(\pi, \pi')$$

where $(\pi, G) \in R$ iff π is a path in G

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- Computing $\phi(G)$ is NP-complete (Gärtner et al. 2003) — proof by reduction to finding a Hamiltonian path

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  where $(\pi, G) \in R$ iff π is a path in G

- Computing $\phi(G)$ is NP-complete (Gärtner et al. 2003) — proof by reduction to finding a Hamiltonian path

- Many possible approaches, we will briefly review the following ideas:
  - Use a marginalized kernel (Kashima et al. 2003)
  - Use product graphs (Gärtner et al. 2003)
  - Use shortest-paths (Borgwardt et al. 2005a)

Marginalized graph kernels

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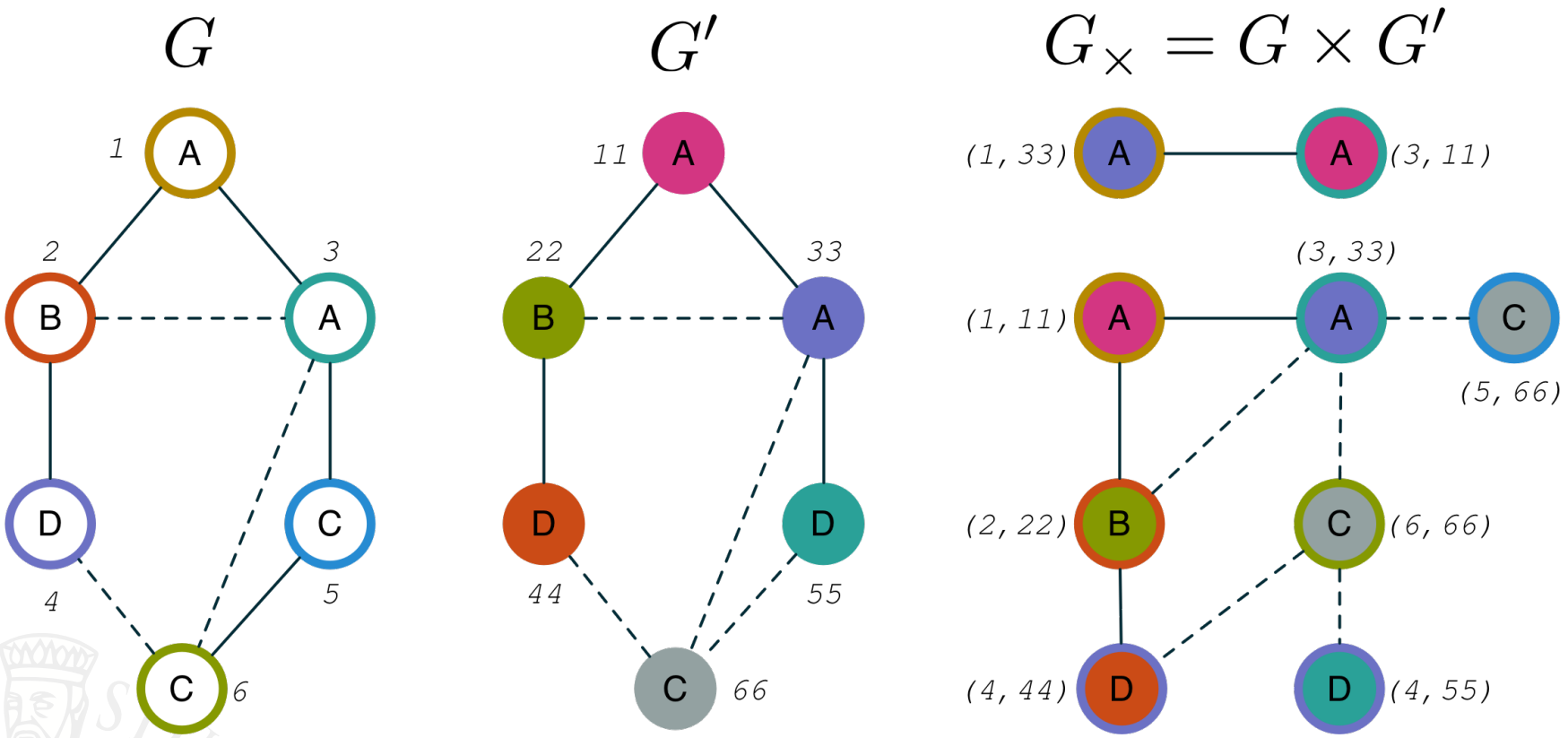
- Define the graph kernel as (Kashima et al. 2003)

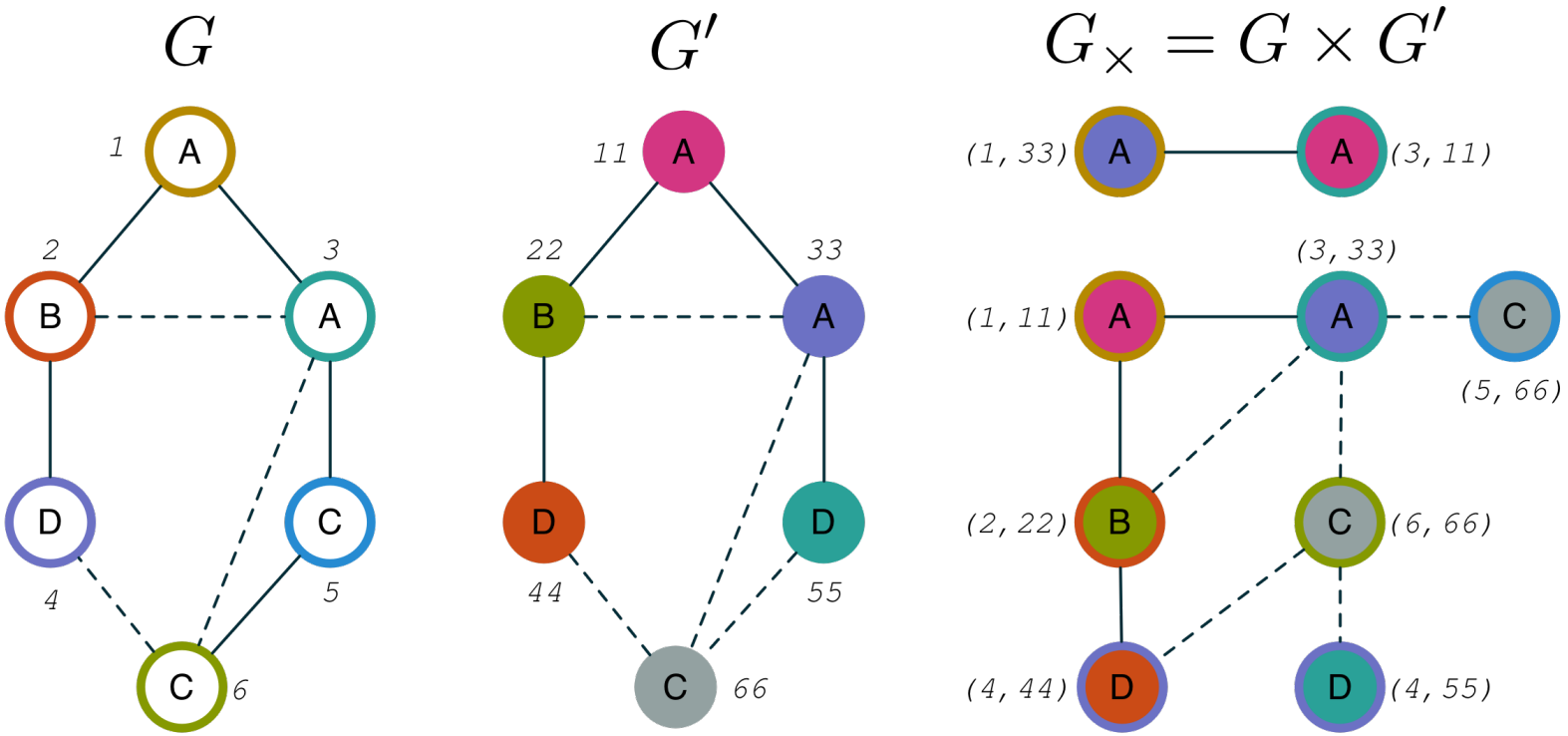
$$k(G, G') = \sum_{\pi} \sum_{\pi'} k_p(\pi, \pi') \, \mathbb{P}(\pi|G) \, \mathbb{P}(\pi'|G')$$

- Given two graphs G and G' they direct product is the graph $G \times G'$

$$V_\times = \{(v, v') \in V \times V' : \ell(v) = \ell(v')\}$$
$$E_\times = \{((u, u'), (v, v')) \in V_\times^2 : (u, v) \in E, (u', v') \in E', \ell(u, v) = \ell(u', v')\}$$

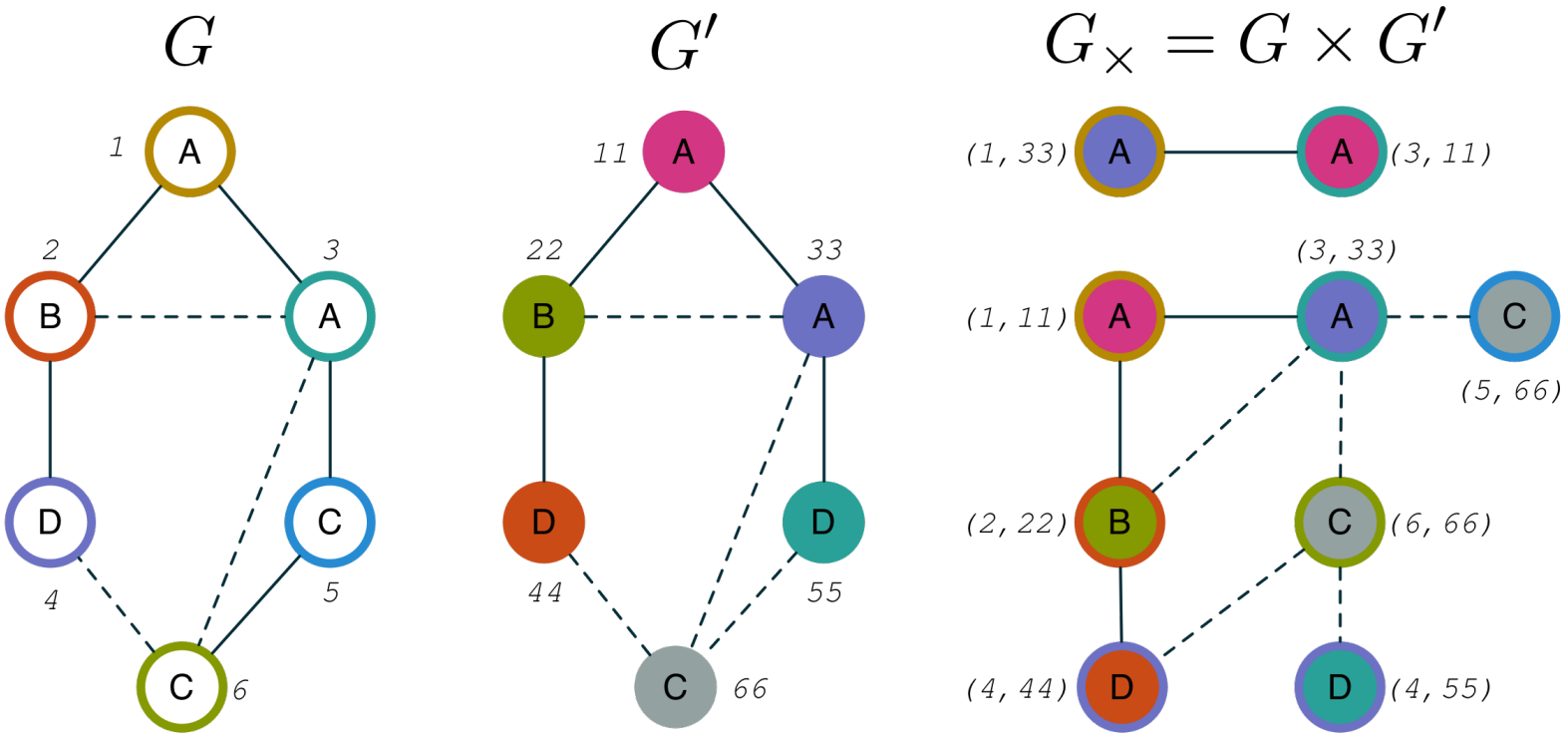


Product graphs



- Main result: There is a bijection between any walk in $G_\times$ and a common walk in G and G' (Gärtner et al. 2003)

Product graphs



- Main result: There is a bijection between any walk in $G_\times$ and a common walk in G and G' (Gärtner et al. 2003)

- Hence the kernel can be computed as

$$K(G, G') = \sum_{i,j \in V_\times} \left[\sum_{n=0}^{\infty} \lambda_n E_\times^n \right]_{ij}$$

- Need to compute

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- Note that any element of E^i is bounded by d^i where d is the maximum degree in G — hence choose $\gamma < 1/d$ obtaining

$$\lim_{n\to\infty} \sum_{i=0}^{n} \gamma^i E_{\times}^i = (I - \gamma E_{\times})^{-1}$$

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Shortest-path graph kernel

- Floyd-Warshall transformation: transform $G = (V, E)$ into $S = (V, \mathcal{E})$ where
  - $(u, v) \in \mathcal{E}$ iff u and v are mutually reachable
  - $\sigma(u, v)$ is the (labeled) shortest path between u and v in G

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- Running time is dominated by the pairwise comparisons, that take $O(V^4)$ — Floyd-Warshall runs in $O(V^3)$

- Two graphs G and G' are isomorphic (written $G \approx G'$) if there exists a bijection $f : V \mapsto V'$ (called an isomorphism) such that $\{u, v\} \in E$ iff $\{f(u), f(v)\} \in E'$

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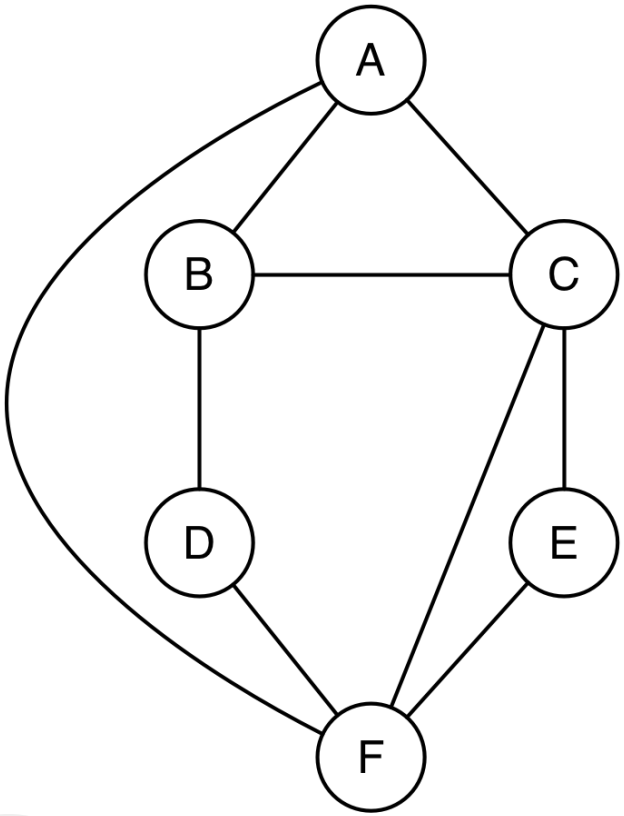
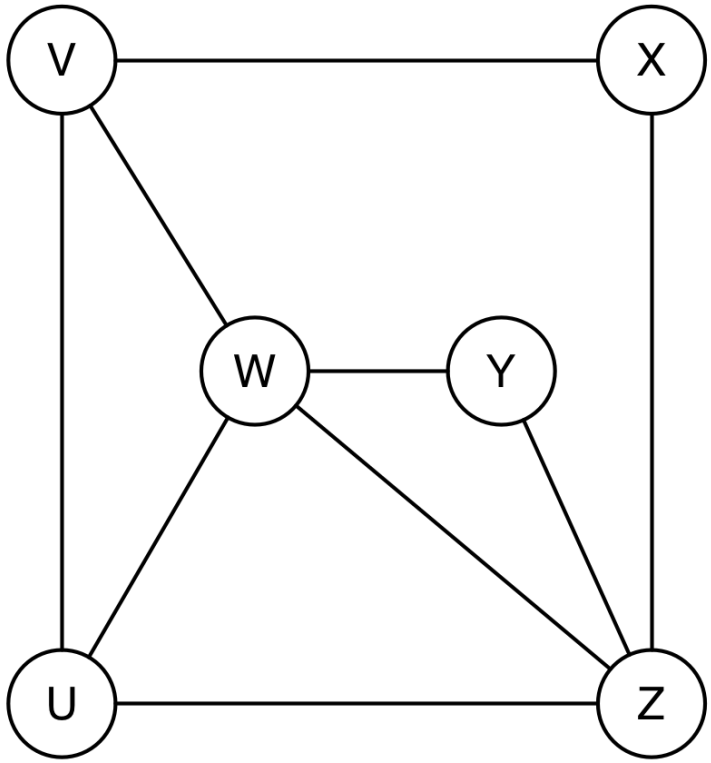
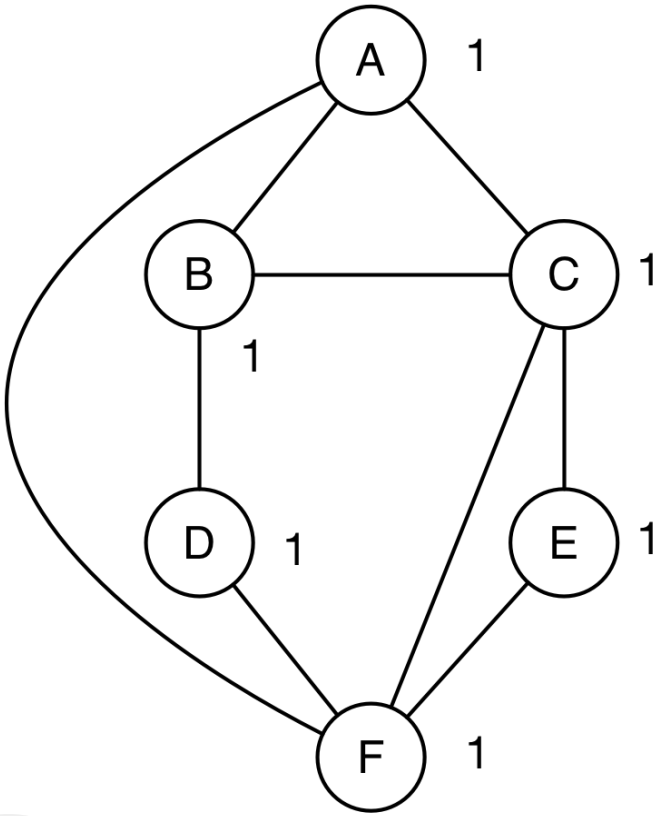
- Very recently found to have quasi-polynomial complexity (Babai 2015)
- Still, practical algorithms employ different strategies, e.g. based on vertex recoloring via propagation mechanisms
- The 1-dimensional Weisfeiler-Lehman test is suitable for deriving a kernel (Shervashidze et al. 2011)

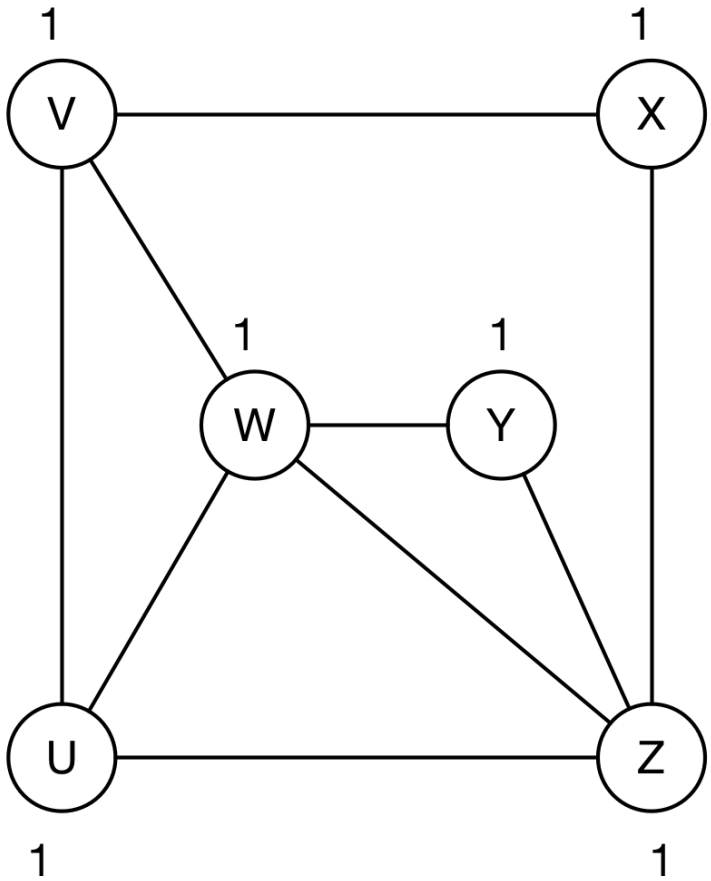
Are these two graphs isomorphic?



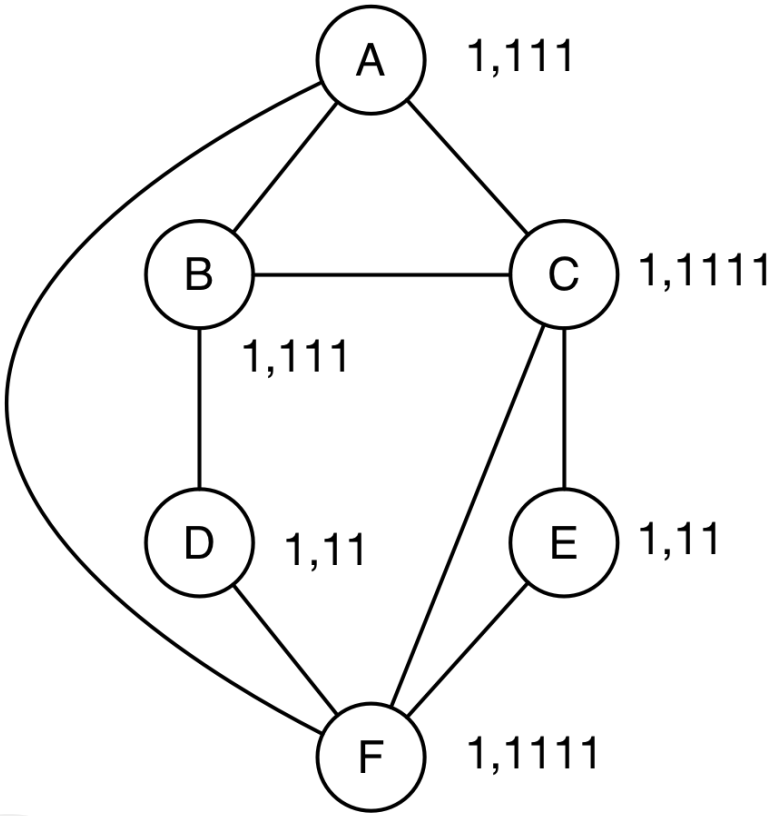


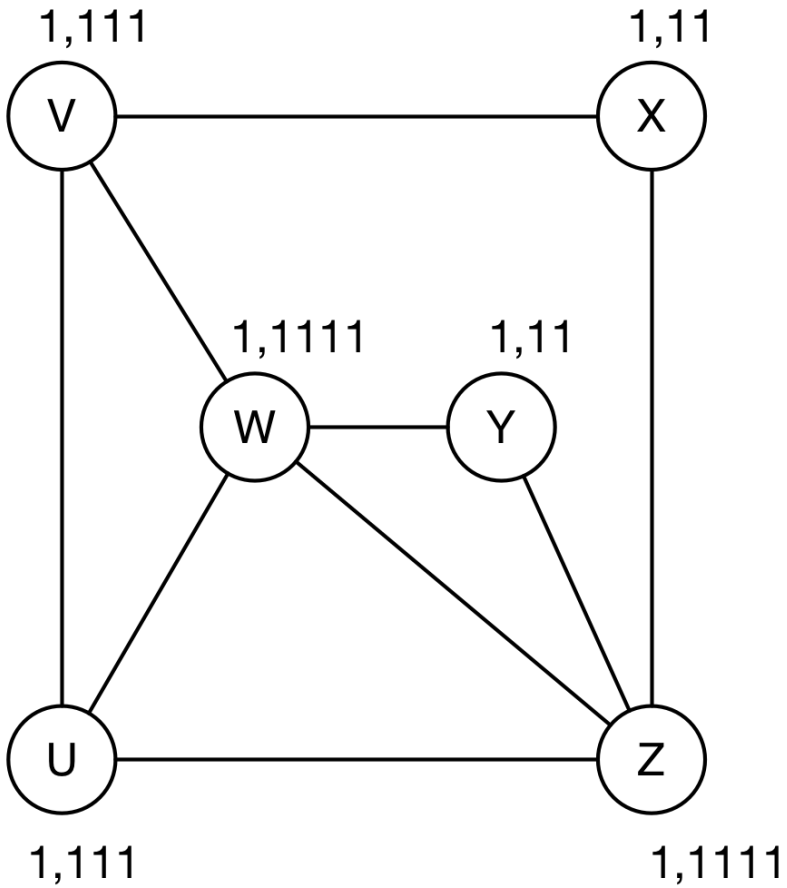
W-L test: start with all ones



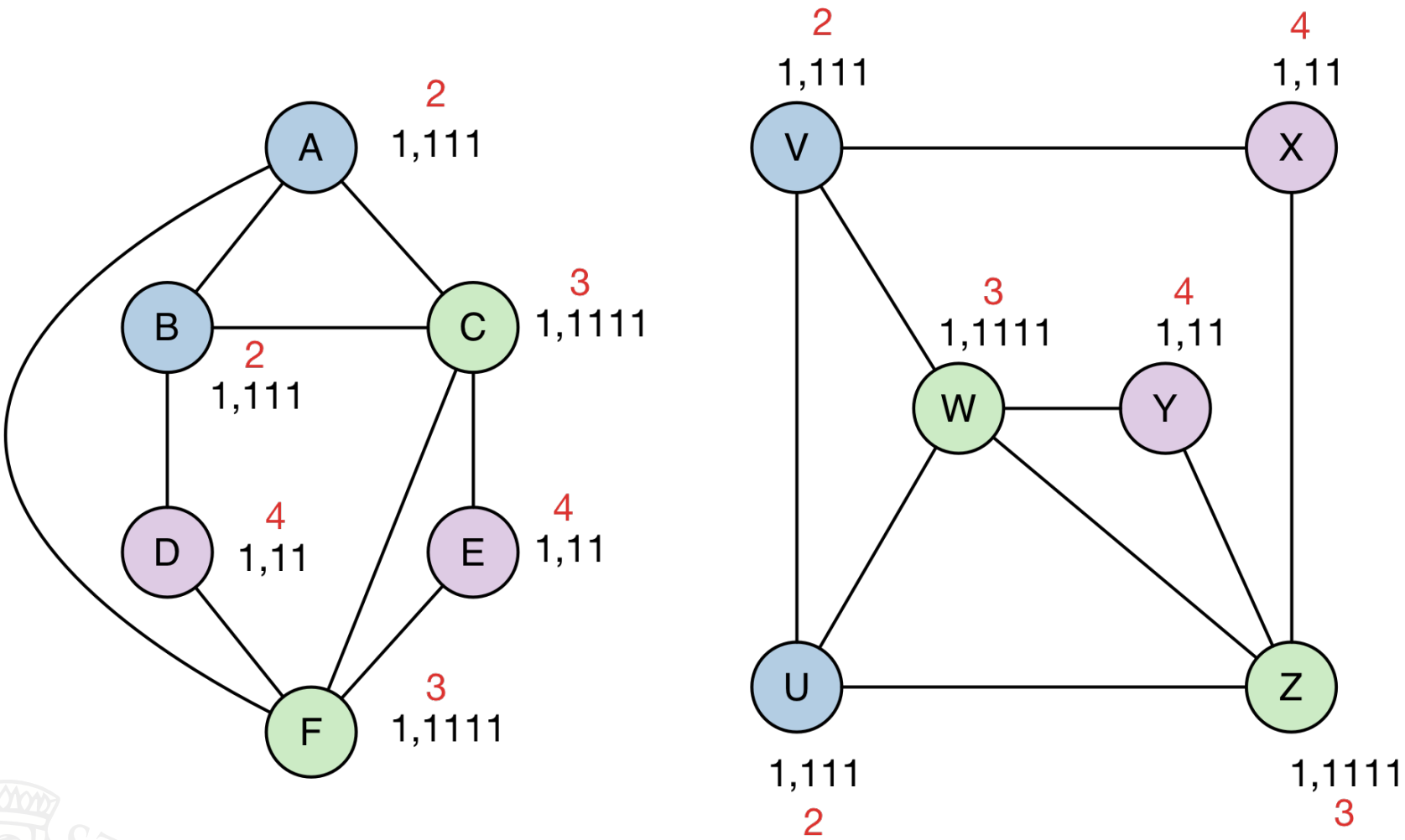


W-L test: propagate

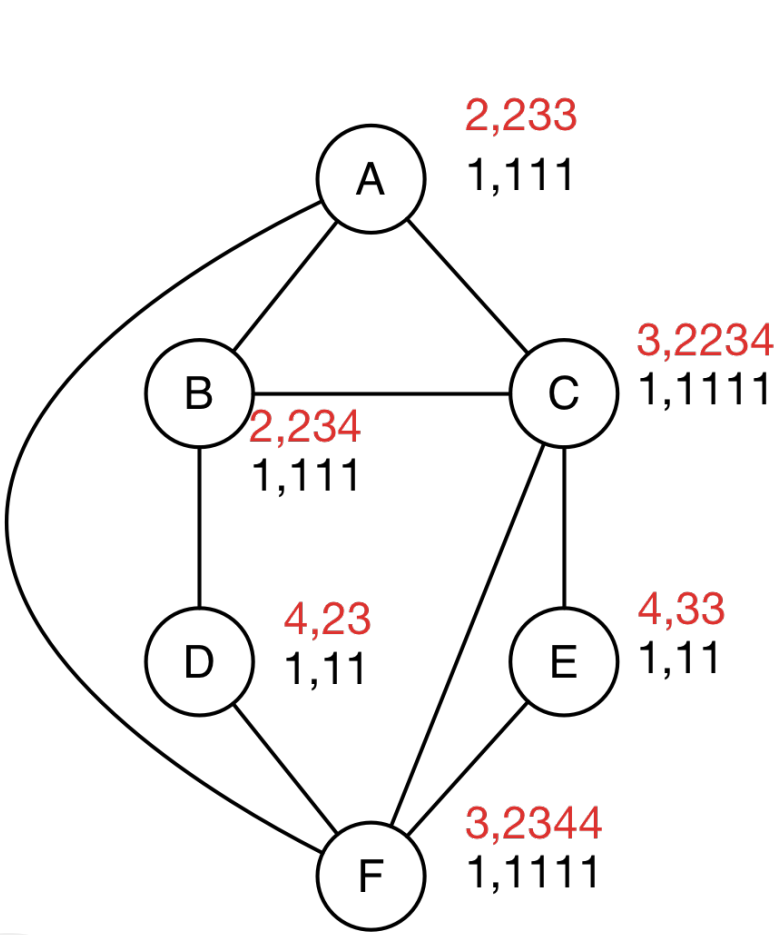


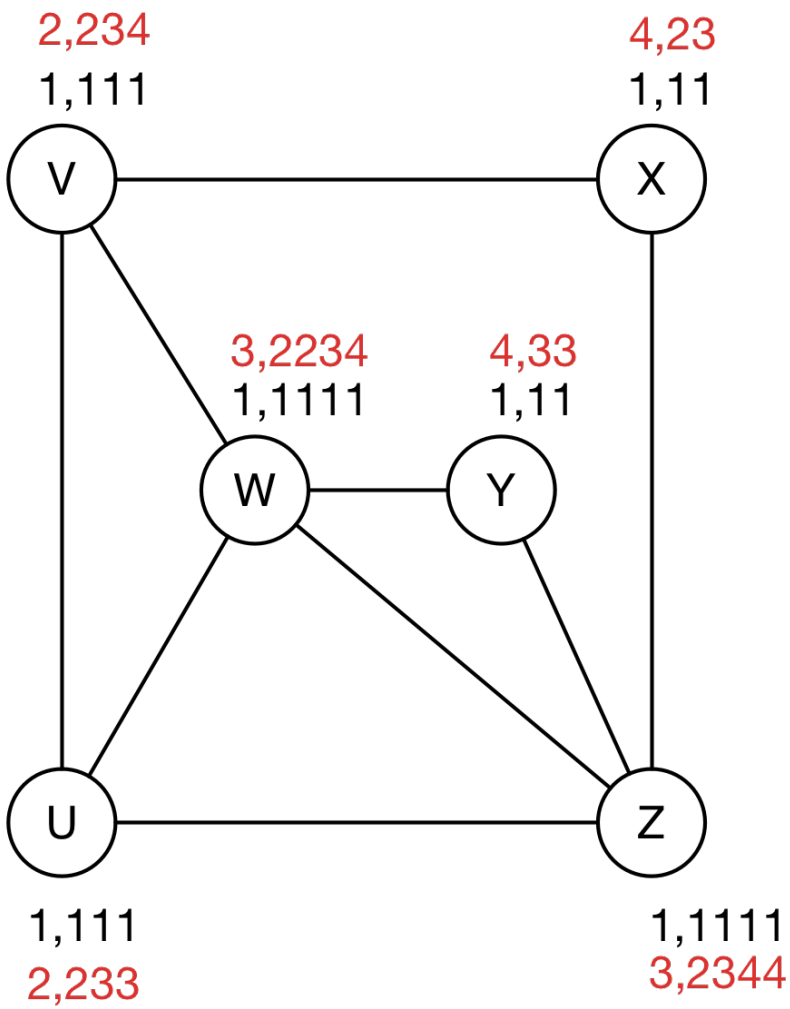


W-L test: recolor

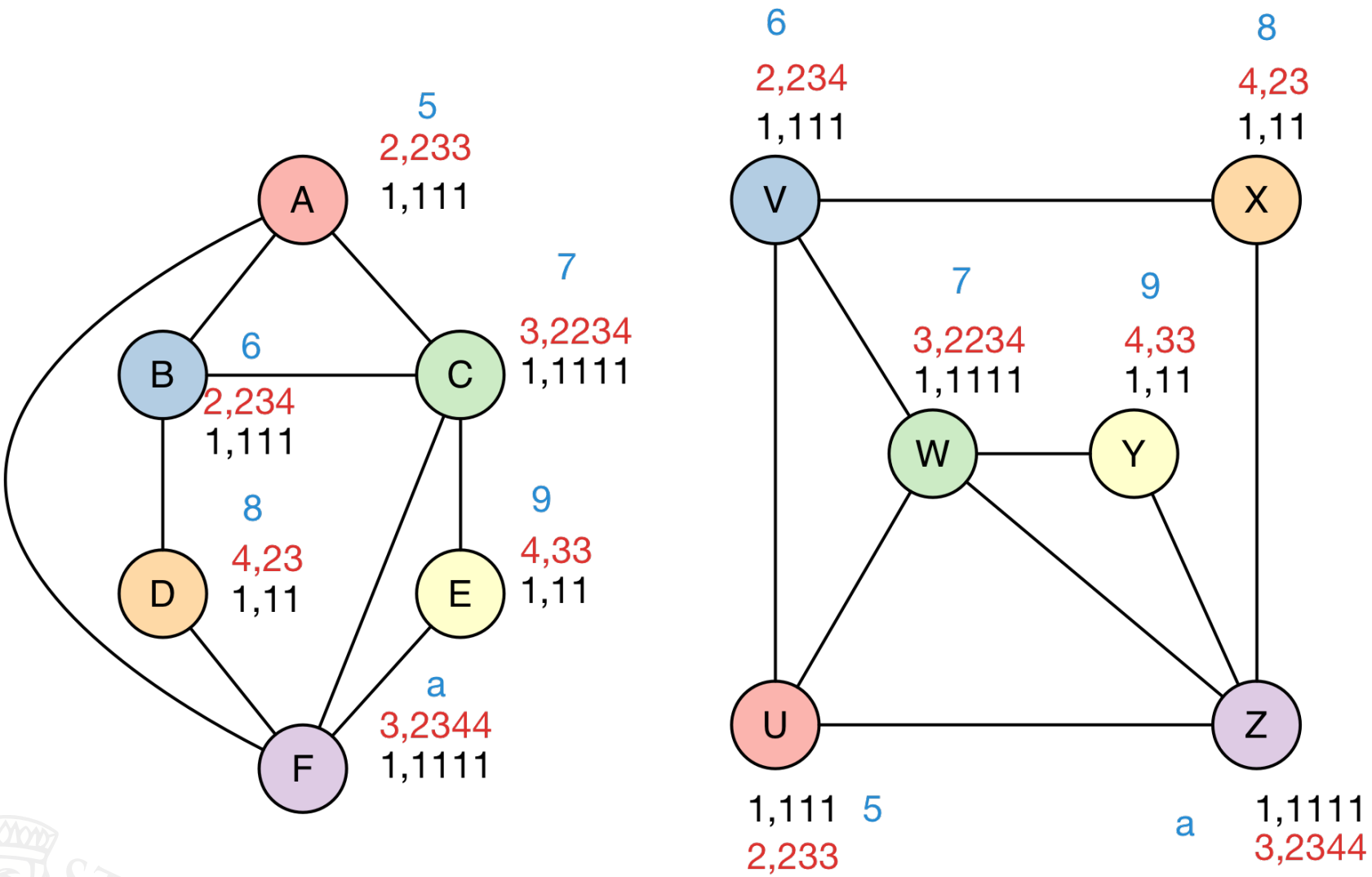


W-L test: propagate again

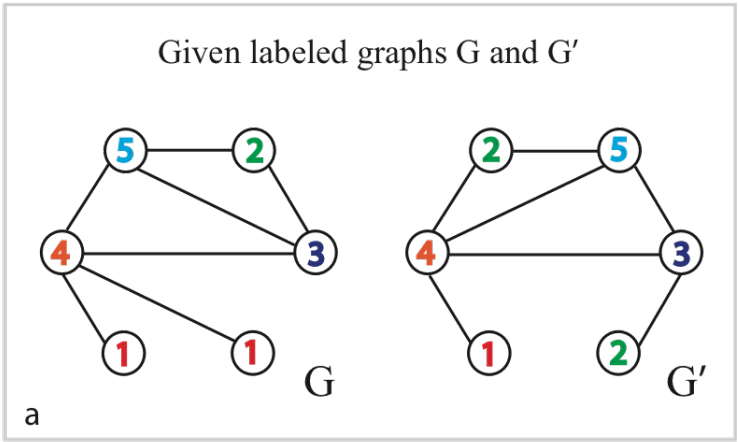


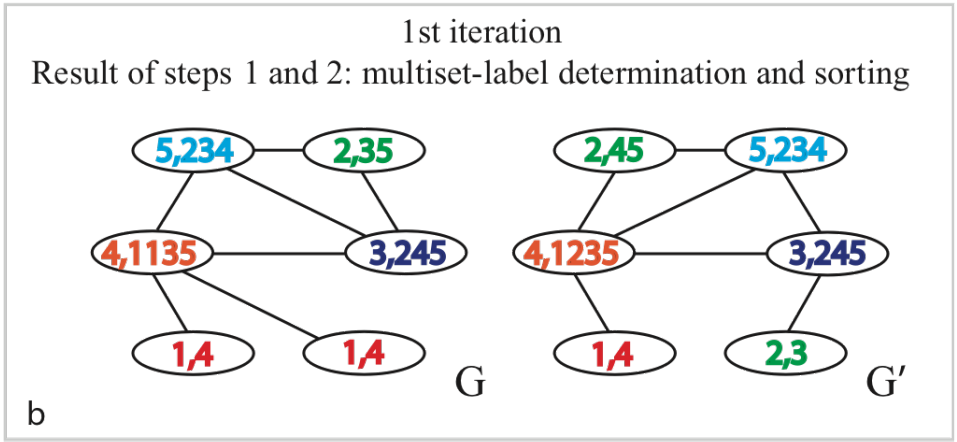


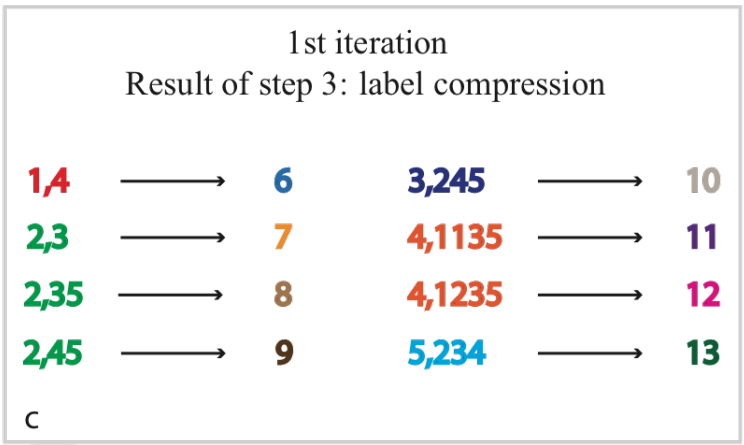
W-L test: recolor again: isomorphic!

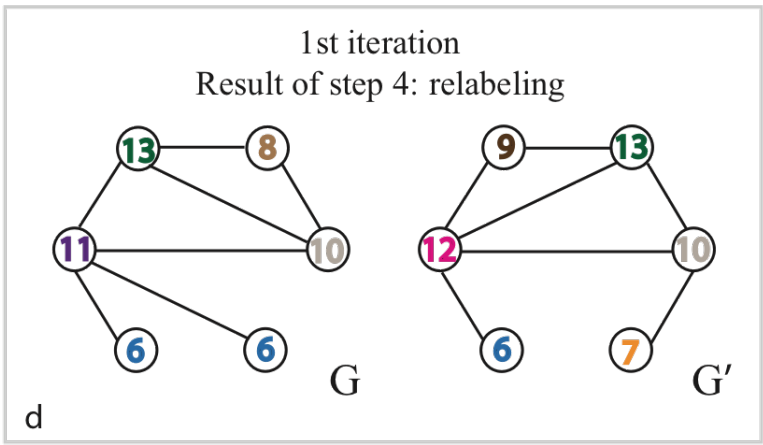


W-L Graph kernel: propagation

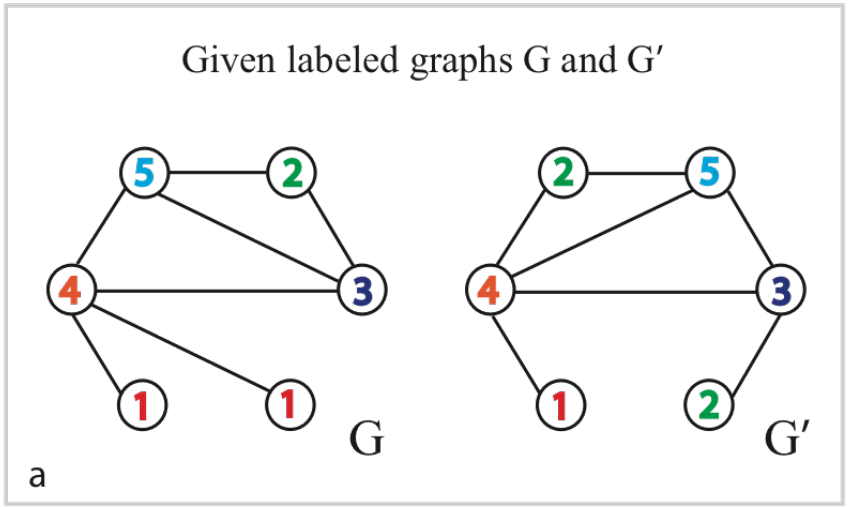


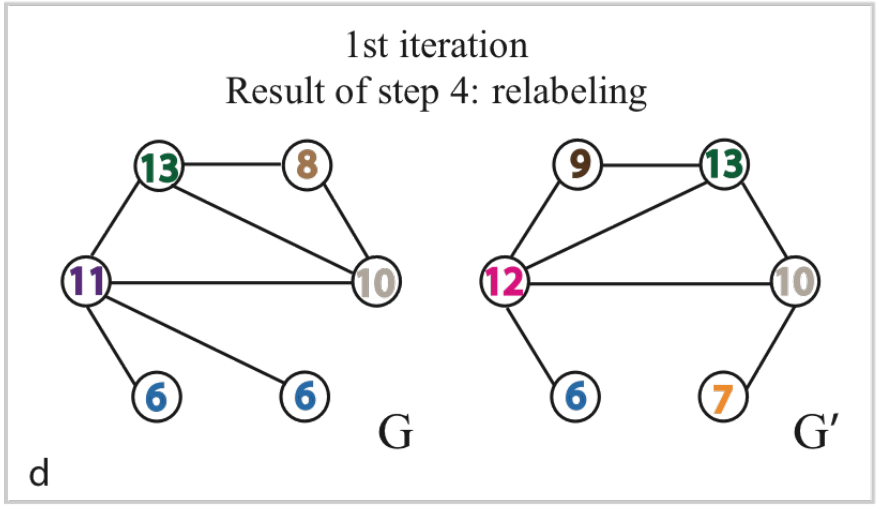






W-L Graph kernel: feature vectors (Shervashidze et al. 2011)





End of the 1st iteration
Feature vector representations of G and G′

$$\varphi^{(1)}_{WLsubtree}(\mathrm{G}) = (2, 1, 1, 1, 1, 2, 0, 1, 0, 1, 1, 0, 1)$$

$$\varphi^{(1)}_{WLsubtree}(\mathrm{G'}) = (\underbrace{1, 2, 1, 1, 1}_{\text{Counts of original node labels}}, \underbrace{1, 1, 0, 1, 1, 0, 1, 1}_{\text{Counts of compressed node labels}})$$

$$k^{(1)}_{WLsubtree}(\mathrm{G},\mathrm{G}') = \langle \varphi^{(1)}_{WLsubtree}(\mathrm{G}), \varphi^{(1)}_{WLsubtree}(\mathrm{G}') \rangle = 11.$$

W-L Graph kernel: Remarks

- Concatenating feature vectors is the same as summing kernels so effectively we have mapped graphs into a sequence of graphs $G_0 = G, G_1, \ldots, G_T$ and computed

$$K_{\text{WL}}(G, G') = \sum_{t=0}^{T} k(G_t, G'_t)$$

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- The number of iterations T is a hyperparameter of the kernel that you have to fix in advance or cross-validate

- The "base kernel" k may be more complicated than just counting the number of common colors, e.g. could use shortest paths

$$K_{\text{WL-sp}}(G, G') = \sum_{t=0}^{T} k_{\text{sp}}(G_t, G'_t)$$

W-L Graph kernel: Results (CPU time)

Data Set	MUTAG	NCI1	NCI109	ENZYMES	D & D
Maximum # nodes	28	111	111	126	5748
Average # nodes	17.93	29.87	29.68	32.63	284.32
# labels	7	37	38	3	82
Number of graphs	188	4110	4127	600	1178
WL subtree	6”	7’20”	7’21”	20”	11’0”
WL edge	3”	1’5”	58”	11”	3 days
WL shortest path	2”	2’20”	2’23”	1’3”	484 days
Ramon & Gärtner	40’6”	81 days	81 days	38 days	103 days
p-random walk	4’42”	5 days	5 days	10’	4 days
Random walk	12”	9 days	9 days	12’19”	48 days
Graphlet count	3”	1’27”	1’27”	25”	30’21”
Shortest path	2”	4’38”	4’39”	5”	23h 17’2”

Table 2: CPU runtime for kernel computation on graph classification benchmark data sets

W-L Graph kernel: Results (accuracy)

Method/Data Set	MUTAG	NCI1	NCI109	ENZYMES	D & D
WL subtree	82.05 ($\pm$0.36)	82.19 ($\pm$ 0.18)	82.46 ($\pm$0.24)	52.22 ($\pm$1.26)	79.78 ($\pm$0.36)
WL edge	81.06 ($\pm$1.95)	84.37 ($\pm$0.30)	84.49 ($\pm$0.20)	53.17 ($\pm$2.04)	77.95 ($\pm$0.70)
WL shortest path	83.78 ($\pm$1.46)	84.55 ($\pm$0.36)	83.53 ($\pm$0.30)	59.05 ($\pm$1.05)	79.43 ($\pm$0.55)
Ramon & Gärtner	85.72 ($\pm$0.49)	61.86 ($\pm$0.27)	61.67 ($\pm$0.21)	13.35 ($\pm$0.87)	57.27 ($\pm$0.07)
p-random walk	79.19 ($\pm$1.09)	58.66 ($\pm$0.28)	58.36 ($\pm$0.94)	27.67 ($\pm$0.95)	66.64 ($\pm$0.83)
Random walk	80.72 ($\pm$0.38)	64.34 ($\pm$0.27)	63.51 ($\pm$ 0.18)	21.68 ($\pm$0.94)	71.70 ($\pm$0.47)
Graphlet count	75.61 ($\pm$0.49)	66.00 ($\pm$0.07)	66.59 ($\pm$0.08)	32.70 ($\pm$1.20)	78.59 ($\pm$0.12)
Shortest path	87.28 ($\pm$0.55)	73.47 ($\pm$0.11)	73.07 ($\pm$0.11)	41.68 ($\pm$1.79)	78.45 ($\pm$0.26)

Table 1: Prediction accuracy ($\pm$ standard deviation) on graph classification benchmark data sets

Neighborhood Subgraph Pairwise Distance Kernel

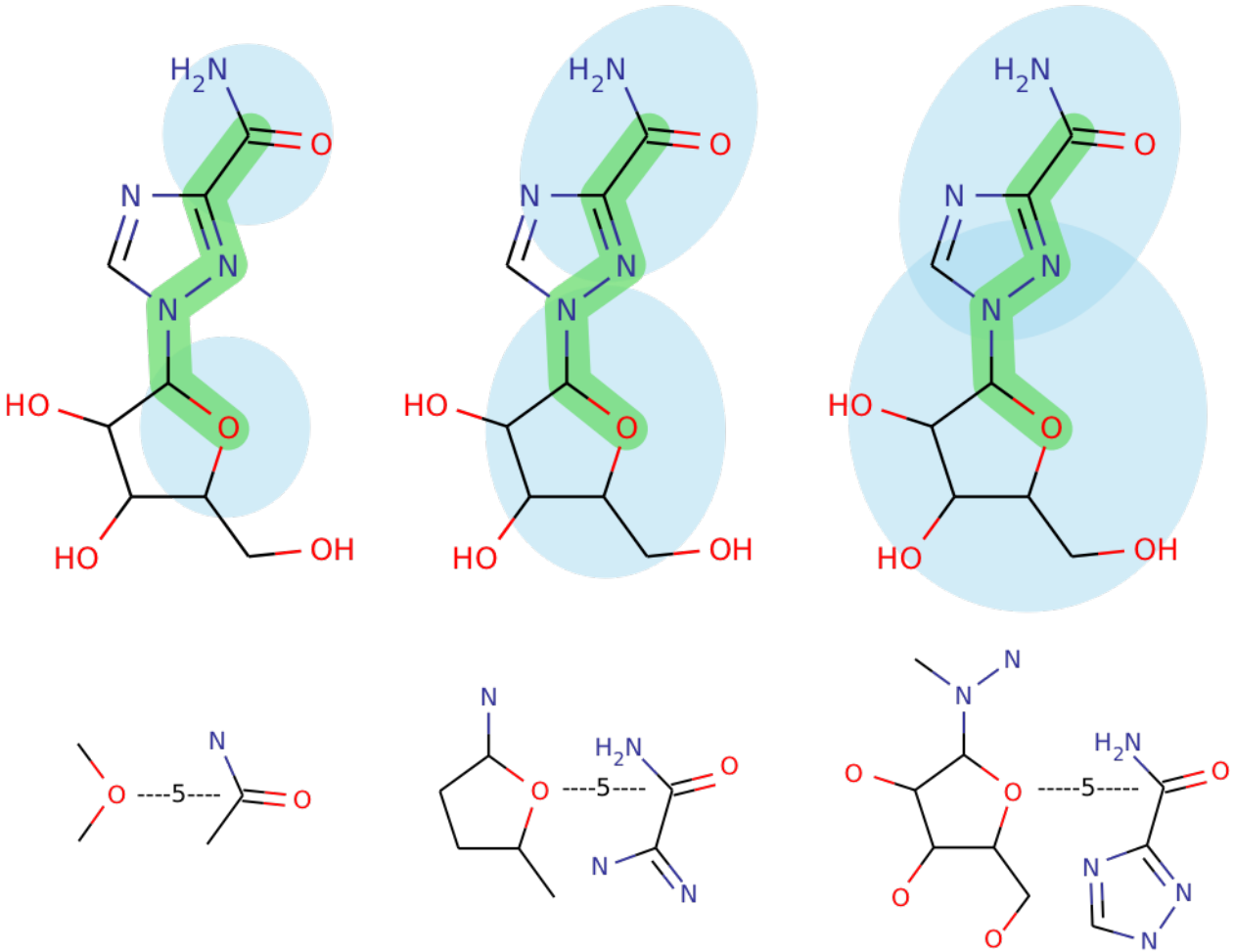
- Convolution kernel based on the relation (Costa et al. 2010)

$$R_{r,d} = \{(\mathcal{N}_r^v(G), \mathcal{N}_r^u(G), G) : \delta_{u,v} = d\}$$

where

- $\delta_{u,v}$ is the shortest-path distance between u and v
- the neighborhood $\mathcal{N}_r^v(G)$ is the subgraph of G induced by all $u \in V$ s.t. $\delta_{u,v} \leq r$

Neighborhood Subgraph Pairwise Distance Kernel



Pairs of neighborhood graphs for radius $r = 1,2,3$ and distance $d = 5$

Neighborhood Subgraph Pairwise Distance Kernel

- $\kappa_{r,d}$ counts the # of common neighborhood subgraphs:

$$\kappa_{r,d}(G, G') = \sum_{\substack{(A,B) \in R_{r,d}^{-1}(G) \\ (A',B') \in R_{r,d}^{-1}(G')}} \mathbb{1}\{A \approx A'\}\,\mathbb{1}\{B \approx B'\}$$

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- Overall kernel:

$$K(G, G') = \sum_{r=0}^{R} \sum_{d=0}^{D} \kappa_{r,d}(G, G')$$

NSPKD Results (CPU time)

Table 2. Net CPU time of graph kernels in seconds

		NCI-60	HIV	PTC	Bursi
	# of mol.	3910	42687	417	4337
	Aug. time	$3.5 \cdot 10^2$	$3.4 \cdot 10^3$	$3.4 \cdot 10^1$	$1.2 \cdot 10^2$
Graph Fragment Kernel (Wale et al. 2008)	GFK(G)	$3.5 \cdot 10^1$	$1.4 \cdot 10^4$	$3.1 \cdot 10^0$	$7.3 \cdot 10^1$
Weighted Decomposition Kernel (Menchetti et al. 2005)	WDK(G)	$1.8 \cdot 10^3$	$1.6 \cdot 10^5$	$8.0 \cdot 10^0$	$1.1 \cdot 10^3$
	WDK(G_a)	$2.3 \cdot 10^3$	$2.3 \cdot 10^5$	$1.4 \cdot 10^1$	$1.5 \cdot 10^3$
Pairwise Maximum Common Subgraphs Kernel (Schietgat et al. 2011)	PMCSK(G)	$2.8 \cdot 10^5$	$3.3 \cdot 10^{4*}$	$6.2 \cdot 10^2$	$3.5 \cdot 10^5$
	PMCSK(G'_a)	$2.8 \cdot 10^5$	$3.3 \cdot 10^{4*}$	$6.3 \cdot 10^2$	$3.5 \cdot 10^5$
Shortest-path Kernel (Shervashidze & Borgwardt, 2009)	PDK(G)	$4.2 \cdot 10^1$	$3.9 \cdot 10^3$	$1.0 \cdot 10^0$	$3.6 \cdot 10^1$
	PDK(G_a)	$7.7 \cdot 10^1$	$4.2 \cdot 10^3$	$2.0 \cdot 10^0$	$5.7 \cdot 10^1$
	NSK(G)	$6.2 \cdot 10^1$	$3.1 \cdot 10^3$	$2.8 \cdot 10^0$	$5.1 \cdot 10^1$
	NSK(G_a)	$3.5 \cdot 10^2$	$6.0 \cdot 10^3$	$1.4 \cdot 10^1$	$2.0 \cdot 10^2$
	NSPDK(G)	$1.2 \cdot 10^2$	$1.0 \cdot 10^4$	$3.4 \cdot 10^0$	$1.1 \cdot 10^2$
	NSPDK(G_a)	$4.6 \cdot 10^2$	$1.9 \cdot 10^4$	$1.6 \cdot 10^1$	$2.9 \cdot 10^2$

* MCSs derived only from the 1503 CA-CM molecules.

NSPKD Results (accuracy)

Table 1. Generalization performance of kernels on unaugmented and augmented molecular graphs

	NCI-60 (avg.)	HIV CA vs. CM	HIV CACM vs. CI	HIV CA vs. CI	PTC (avg.)	Bursi
AUROC (%)						
GFK(G)	77.8 ± 2.3	82.0 ± 4.7	82.8 ± 1.9	93.9 ± 2.6	62.6 ± 10	89.6 ± 0.3
WDK(G)	71.1 ± 2.4	83.1 ± 4.3	82.9 ± 1.8	94.0 ± 3.4	62.1 ± 7.7	88.0 ± 0.4
WDK(G_a)	**80.0 ± 2.3**	84.2 ± 4.3	83.9 ± 1.7	95.0 ± 2.7	65.1 ± 8.7	90.8 ± 0.2
PMCSK(G)	79.6 ± 2.2	**82.6 ± 6.2**	81.8 ± 2.2	93.0 ± 3.7	64.5 ± 8.8	90.5 ± 1.3
PMCSK(G'_a)	**80.3 ± 2.2**	**82.8 ± 6.2**	**83.2 ± 2.1**	93.4 ± 3.4	65.6 ± 8.8	**91.5 ± 1.1**
PDK(G)	73.4 ± 2.6	81.6 ± 4.6	77.7 ± 1.9	92.6 ± 3.2	61.2 ± 9.7	82.7 ± 0.3
PDK(G_a)	77.8 ± 2.4	82.1 ± 4.2	83.4 ± 2.1	94.5 ± 2.4	64.6 ± 9.9	89.3 ± 0.3
NSK(G)	79.1 ± 2.2	**84.2 ± 4.9**	84.3 ± 2.0	95.3 ± 1.5	67.4 ± 9.4	91.6 ± 0.2
NSK(G_a)	79.4 ± 2.2	**84.4 ± 4.5**	84.1 ± 2.2	94.9 ± 2.1	67.1 ± 9.3	**91.8 ± 0.2**
NSPDK(G)	79.5 ± 2.2	**83.9 ± 5.6**	83.8 ± 2.1	**95.6 ± 1.3**	**69.3 ± 9.5**	**91.7 ± 0.3**
NSPDK(G_a)	**80.1 ± 2.2**	**84.1 ± 4.8**	**84.9 ± 2.1**	**95.1 ± 2.0**	**68.9 ± 9.8**	**92.0 ± 0.2**

Part 4

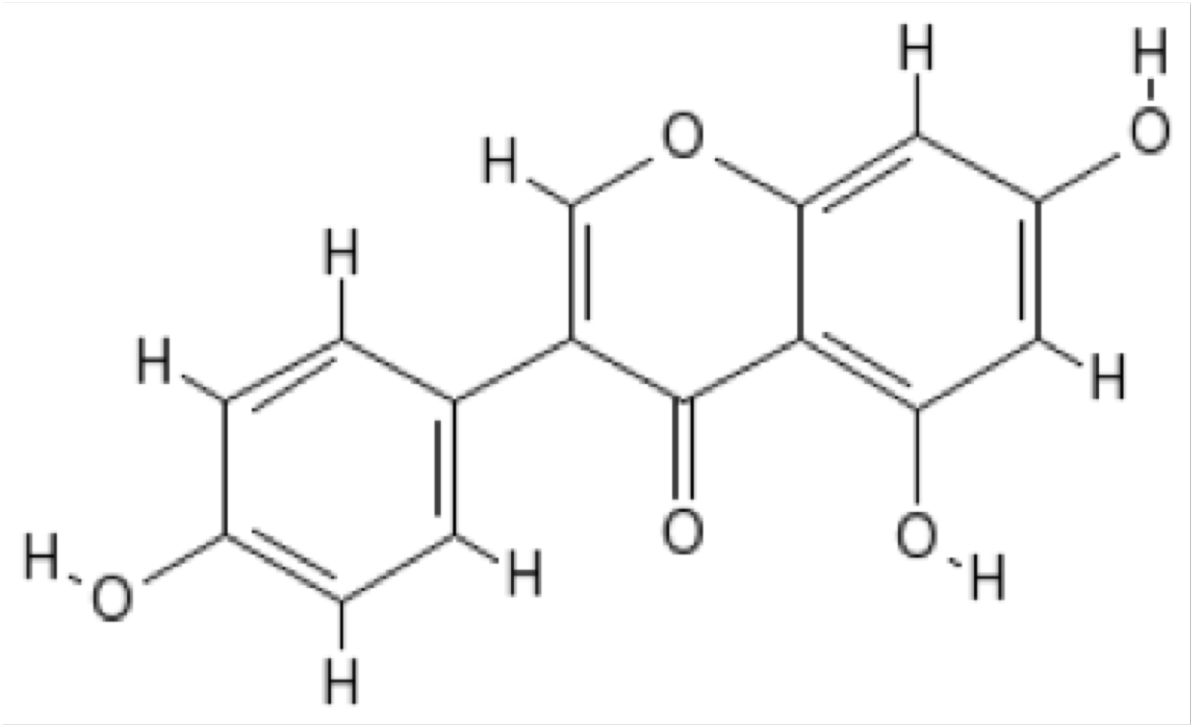
Kernel methods for relational learning

kFOIL (Landwehr et al. 2006, 2010)
kLog (Frasconi et al. 2014)

- Kernel methods in the ILP setting

- Kernel methods in the ILP setting
- Very simple idea:
  - Define a kernel on relational data based on a relational theory
  - Perform structure learning to induce the relational theory
  - This effectively learns the kernel

Relational data example



Examples

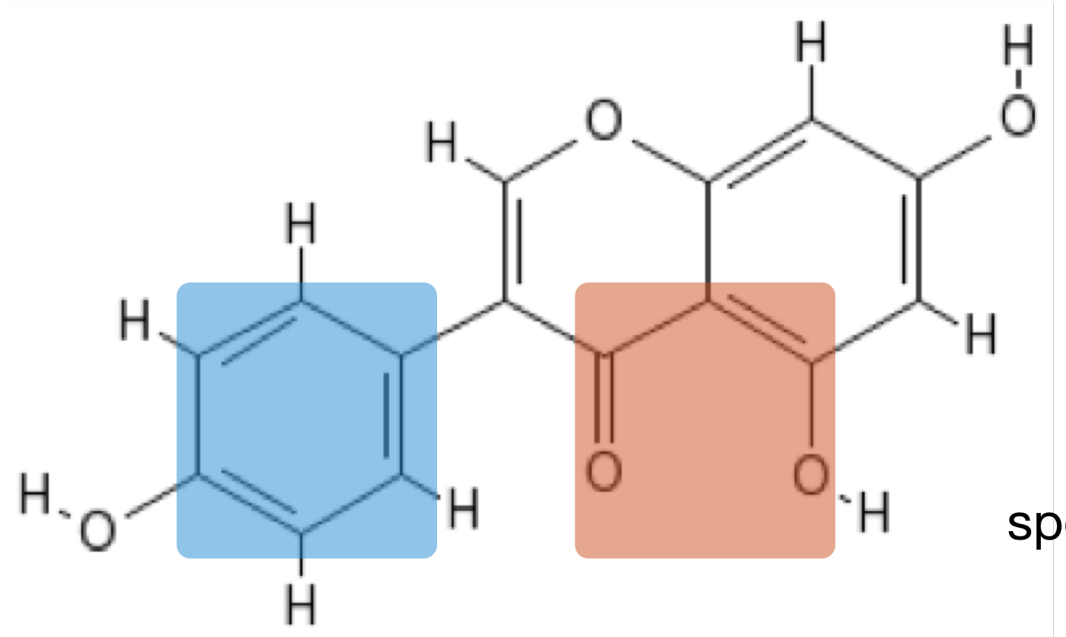
```
pos(m1).
neg(m2).
pos(m3).
pos(m4).
…
```

Background knowlegde

```
molecule(m1).
atom(m1,a11,c).
atom(m1,a12,c).
bond(m1,a11,a12,1).
charge(m1,a11,0.82).
…
```

```
aromatic_ring(M) :-
  bond(M,A,B,7),bond(M,B,C,7),
  bond(M,C,D,7),bond(M,D,E,7),
  bond(M,E,F,7),bond(M,F,A,7).
```

Relational data + theory = features



Clauses match on specific structural features

Theory: set of clauses

```
c1(M,X) :-
  bond(M,A,B,7),bond(M,B,C,7),
  bond(M,C,D,7),bond(M,D,E,7),
  bond(M,E,F,7),bond(M,F,A,7).
```

```
c2(M,X) :-
  atom(M,A,o),bond(M,A,B,2),
  atom(M,B,c),bond(M,B,C,1),
  atom(M,C,c),bond(M,C,D,7),
  atom(M,D,c),bond(M,D,E,1),
  atom(M,E,o).
```

Relational data + theory = features and kernel

- Let $H = \{c_1, \ldots, c_p\}$ be the theory (set of clauses)

Relational data + theory = features and kernel

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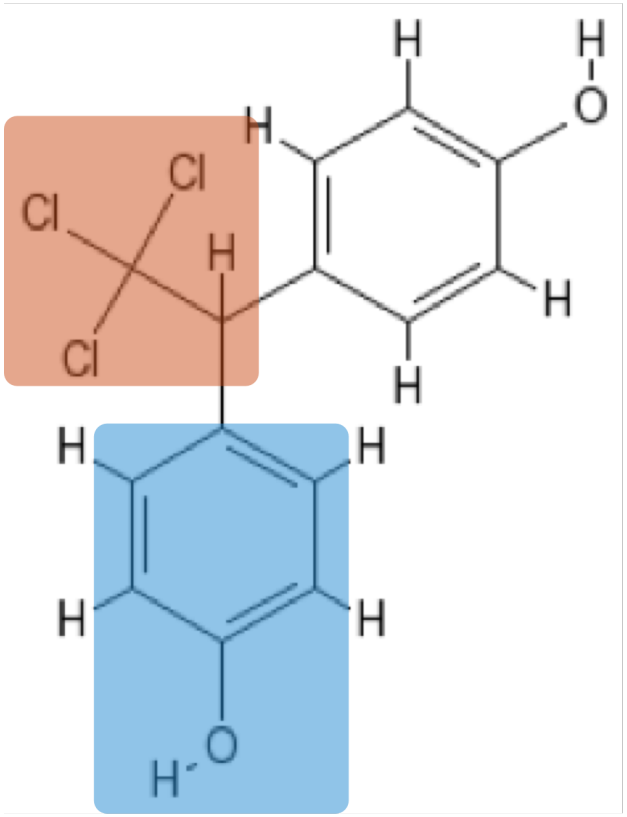
- The kernel is of course

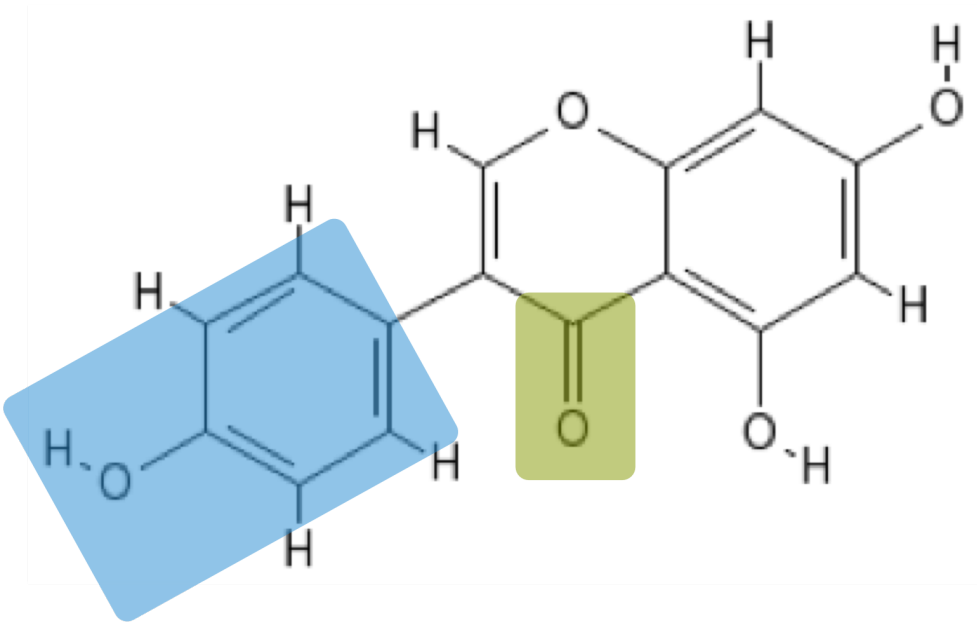
$$k(x, z) = \langle \phi(x), \phi(z) \rangle$$

Example



$\phi(x) = [1, 1, 0]$

Clauses: c1, c2, c3



$\phi(z) = [0, 1, 1]$

$$k(x, z) = \langle [1, 1, 0], [0, 1, 1] \rangle = 1$$

- FOIL style greedy general-to-specific search for clauses

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- Refinement operator: Given a clause c, refine it into c' by finding a minimal specialization in the language of clauses

Searching

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- FOIL style greedy general-to-specific search for clauses
- Refinement operator: Given a clause c, refine it into c' by finding a minimal specialization in the language of clauses
- In traditional ILP the goal is to find a theory that covers all positive examples and no negative example
- In kFOIL the goal is to maximize the accuracy score of a kernel machine based on the kernel defined earlier

- A framework and domain specific language for kernel-based relational learning

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- Embedded in Prolog

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  1. Entity/relationship (E/R) data modeling combined with ideas from *deductive databases*
  2. Graphicalization: Examples (i.e. relational database instances) mapped to (simple) undirected graphs
  3. Graph kernels: construction of feature vectors from graphs

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- Three simple concepts:
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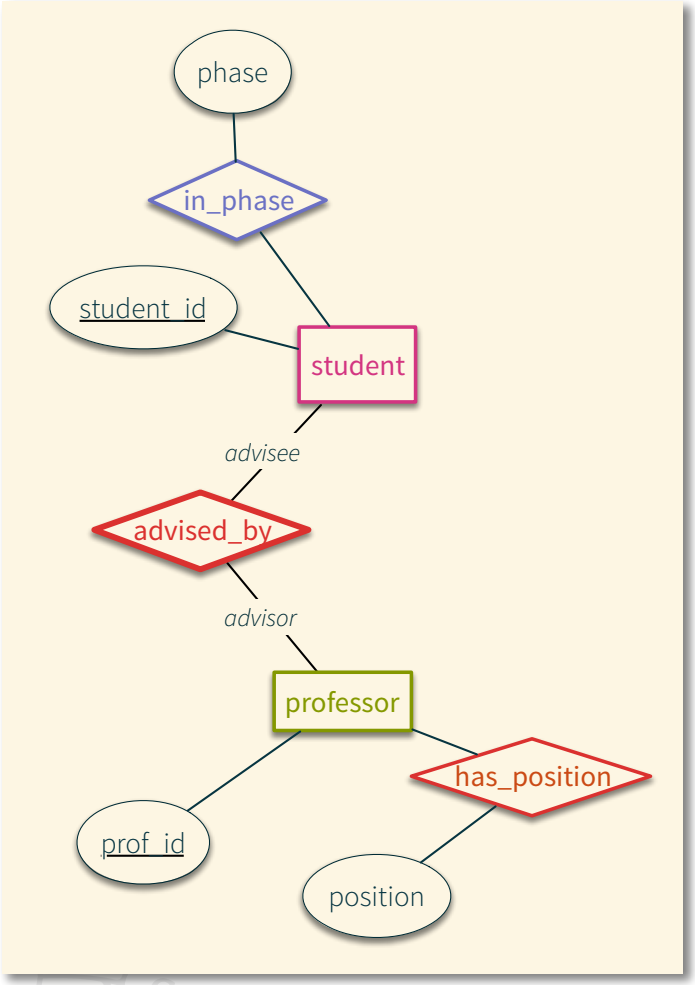
  2. Graphicalization: Examples (i.e. relational database instances) mapped to (simple) undirected graphs
  3. Graph kernels: construction of feature vectors from graphs
- Available: `http://klog.dinfo.unifi.it/`

- Design and maintain complex features in a declarative fashion

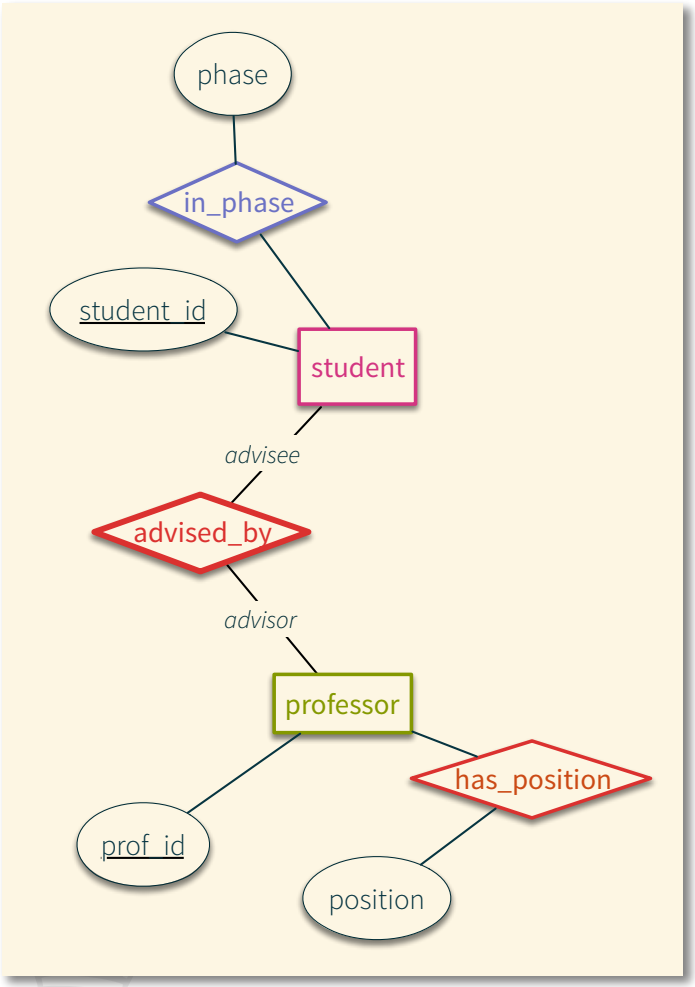
- Design and maintain complex features in a declarative fashion
- Ability to specify several kinds of learning problems, including:
  - classification/regression of structured data
  - entity classification
  - (hyper)link prediction

Modeling the UW-CSE dataset in kLog



- Introduced in (Richardson & Domingos, 2005) to illustrate Markov logic
- Entity/Relationship (E/R) diagram:
  - Boxes are entities
  - Diamonds are relationships
  - Ovals are attributes
  - Underlined attributes are entity identifiers, the other ones are properties

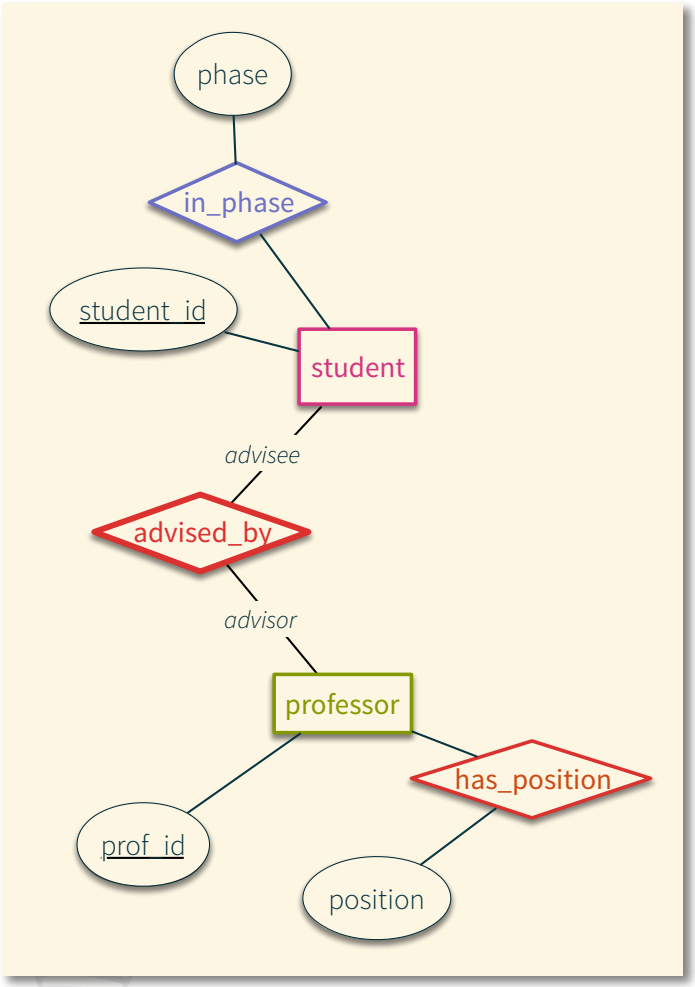
Modeling the UW-CSE dataset in kLog




```
signature student(
    student_id::self
)::extensional.
signature in_phase(
    student_id::student,
    phase::property)::extensional.

signature professor(
   prof_id::self
)::extensional.
signature has_position(
    prof_id::professor,
    position::property
)::extensional.
```

Modeling the UW-CSE dataset in kLog

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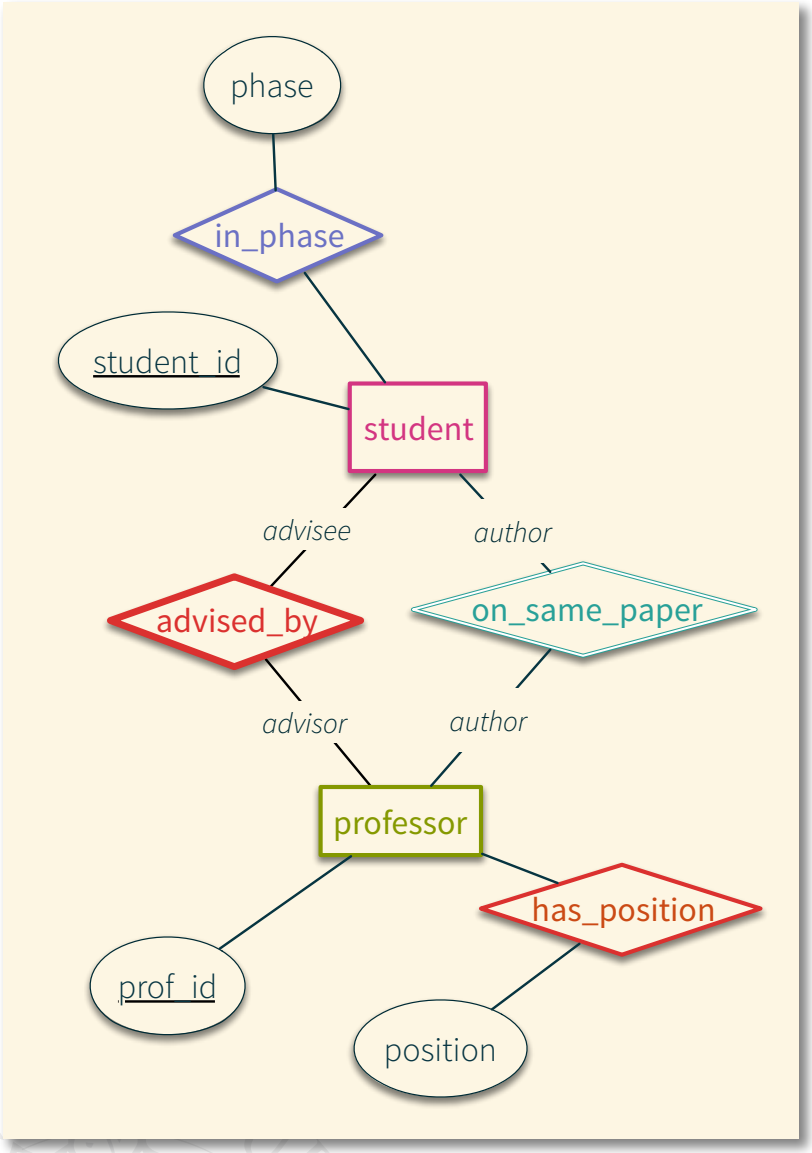
signature professor(
   prof_id::self
)::extensional.
signature has_position(
    prof_id::professor,
    position::property
)::extensional.


signature advised_by(
    student_id::student,
    prof_id::professor
)::extensional.
```

Learning from interpretations: predictors and responses

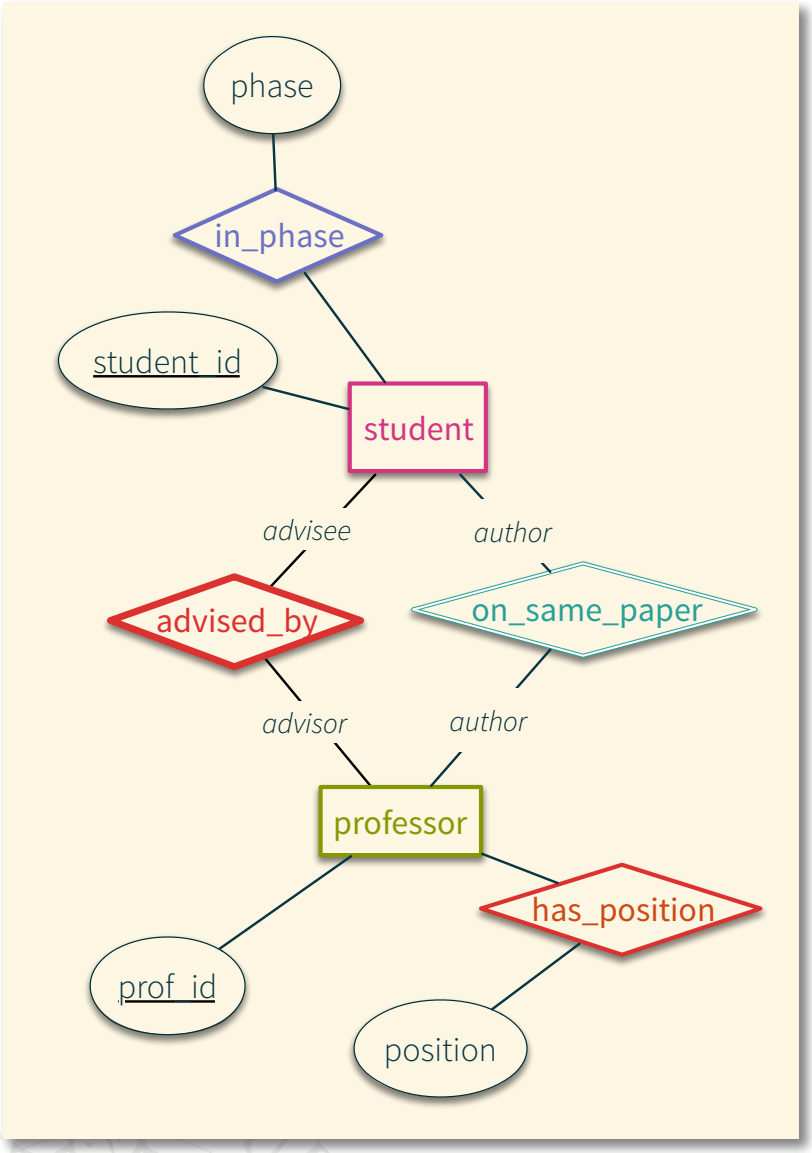
```
student(person311).
student(person14).
...
professor(person7).
professor(person185).
...
has_position(person292,faculty_affiliate).
has_position(person79,faculty).
...
in_phase(person139,post_quals).
in_phase(person333,pre_quals).
...
advised_by(person265,person168).
advised_by(person352,person415).
...
publication(title25,person284).
...
taught_by(course12,person211,autumn_0001).
...
ta(course44,person193,winter_0304).
...
publication(title25,person284).
```

Adding background knowledge: Intensional signatures




```
signature on_same_paper(
    student_id::student,
    prof_id::professor
)::intensional.
```

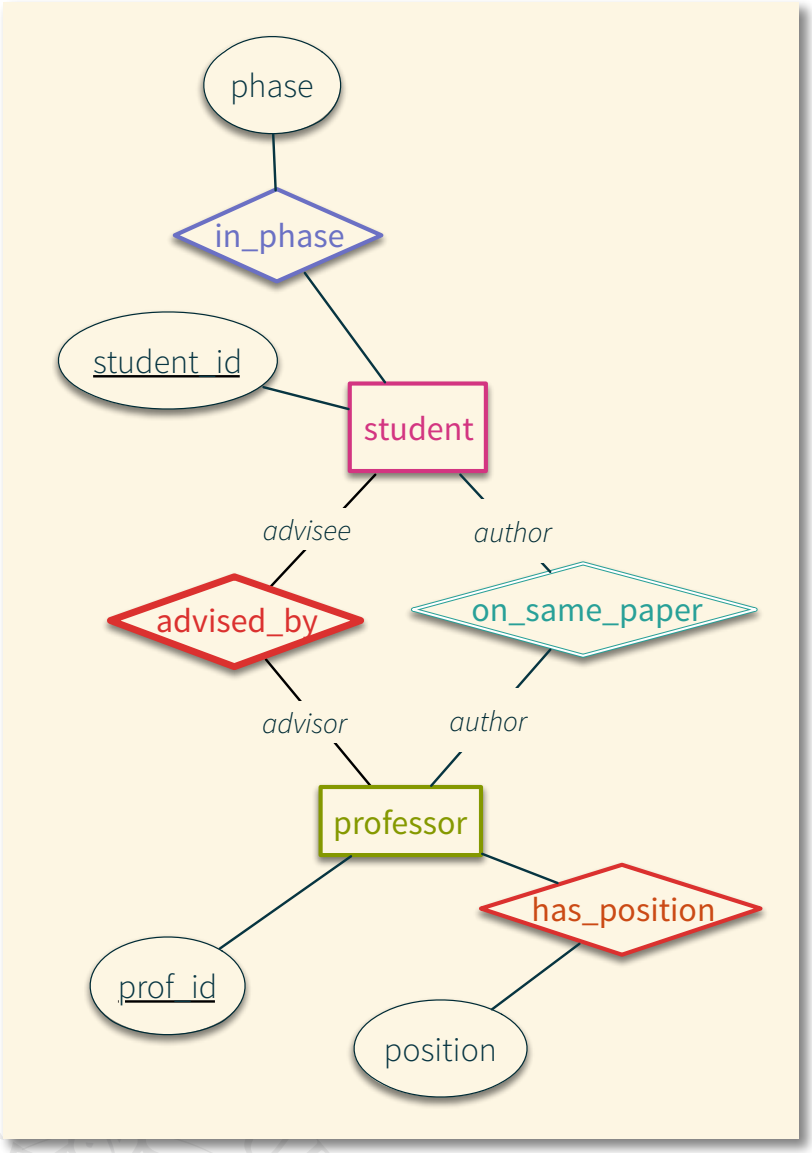
Adding background knowledge: Intensional signatures




```
signature on_same_paper(
   student_id::student,
   prof_id::professor
)::intensional.

on_same_paper(S,P) :-
    student(S), professor(P),
    publication(Pub, S),
    publication(Pub,P).
```

Adding background knowledge: Intensional signatures

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     publication(Pub, S),
     publication(Pub,P).
```
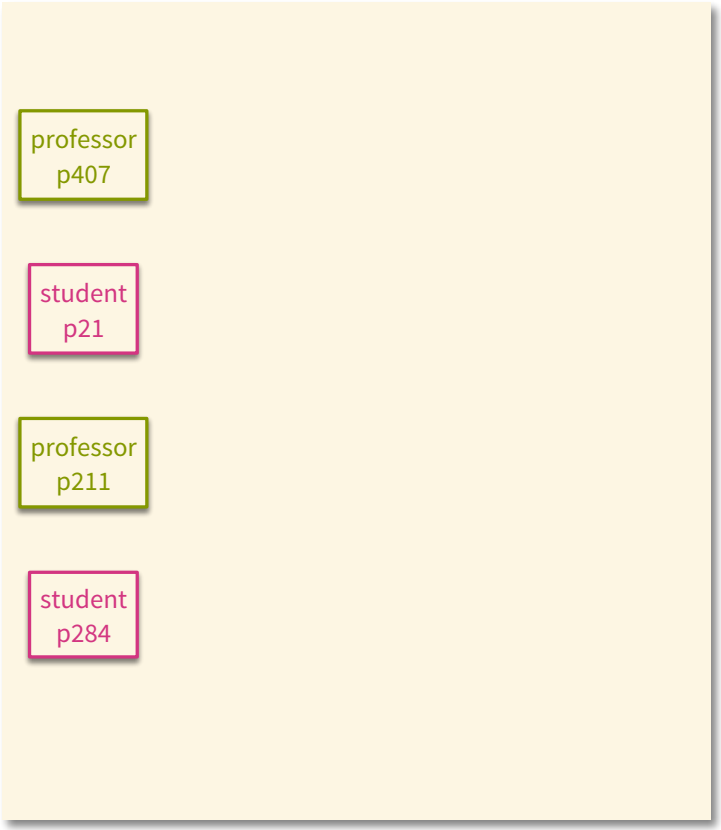
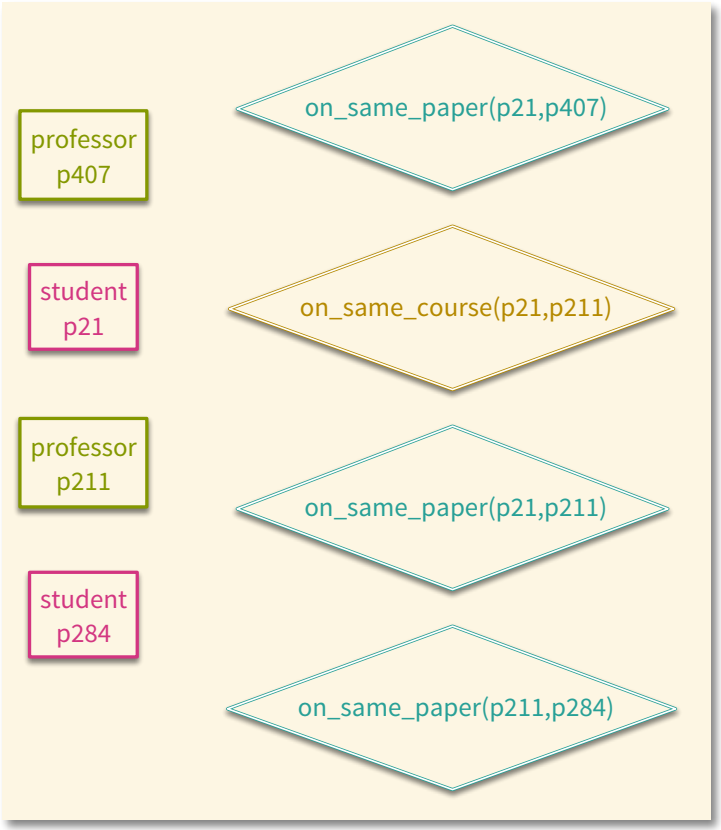

```
signature on_same_course(
   student_id::student,
   prof_id::professor
)::intensional.

on_same_course(S,P) :-
     professor(P), student(S),
     ta(Course,S,Term),
     taught_by(Course,P,Term).
```

Graphicalization: from interpretations to bipartite graphs



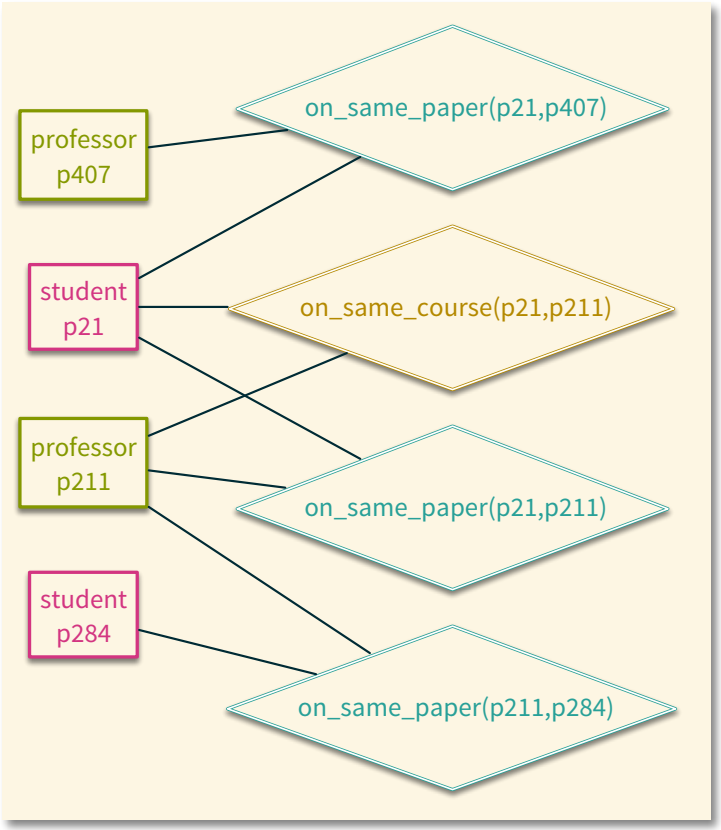
- One square vertex for every entity

Graphicalization: from interpretations to bipartite graphs



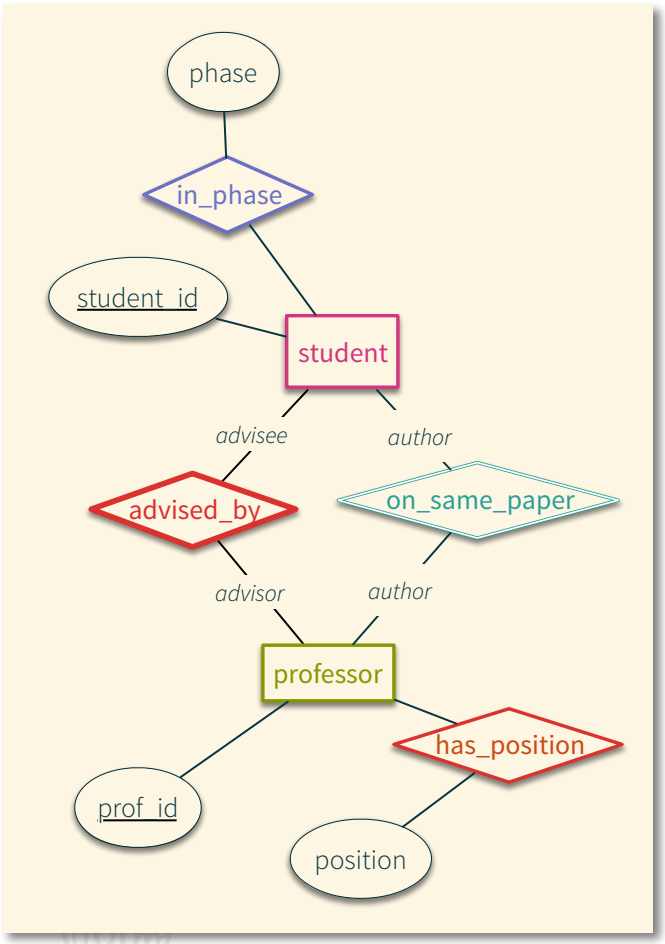
- One square vertex for every entity
- One diamond vertex for every ground relationship

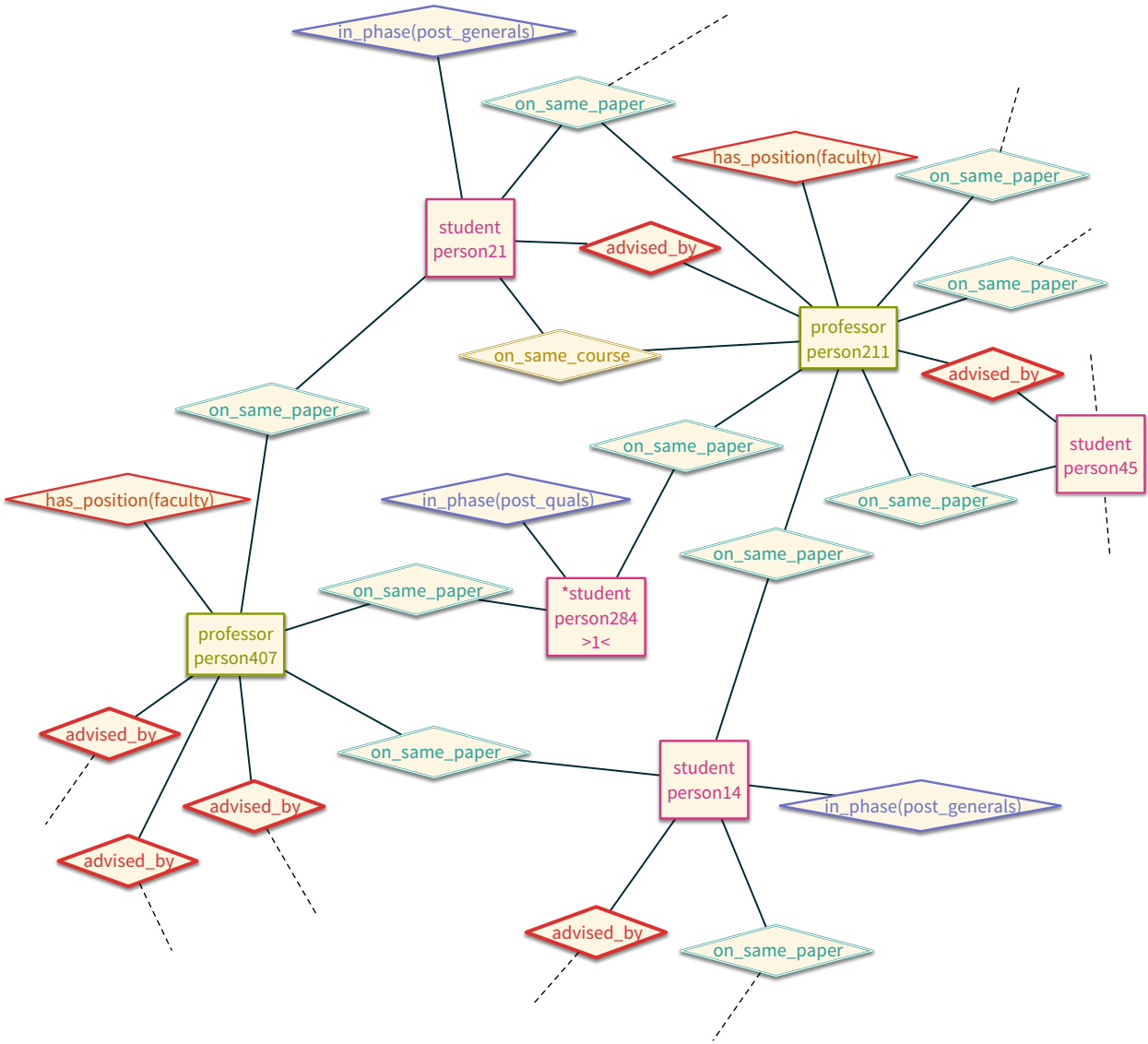
Graphicalization: from interpretations to bipartite graphs



- One square vertex for every entity
- One diamond vertex for every ground relationship
- Add an undirected edge between a square and a diamond if the entity appears in the grounding

Graphicalization in UW-CSE





Using graph kernels to construct features

- In principle, any graph kernel may be adapted and plugged in

Using graph kernels to construct features

- In principle, any graph kernel may be adapted and plugged in
- In practice, kLog uses a generalization of NSPDK (Costa et al. 2010) where:
  - Subgraphs are rooted at certain designated vertices called kernel-points (KP)
  - Soft matches are allowed

Soft matches

- Substructures will never exactly match if there are "hubs" or high-degree vertices

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- Example: the relation `has_word` between words and webpages

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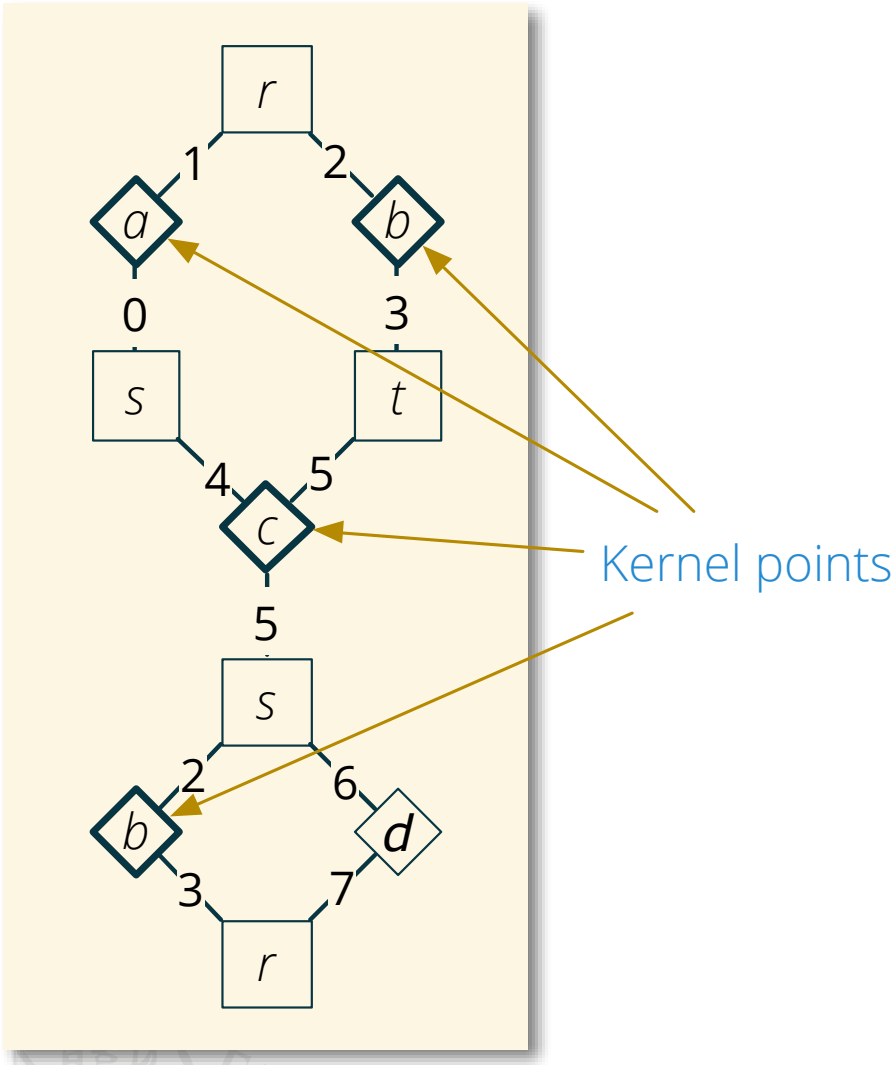
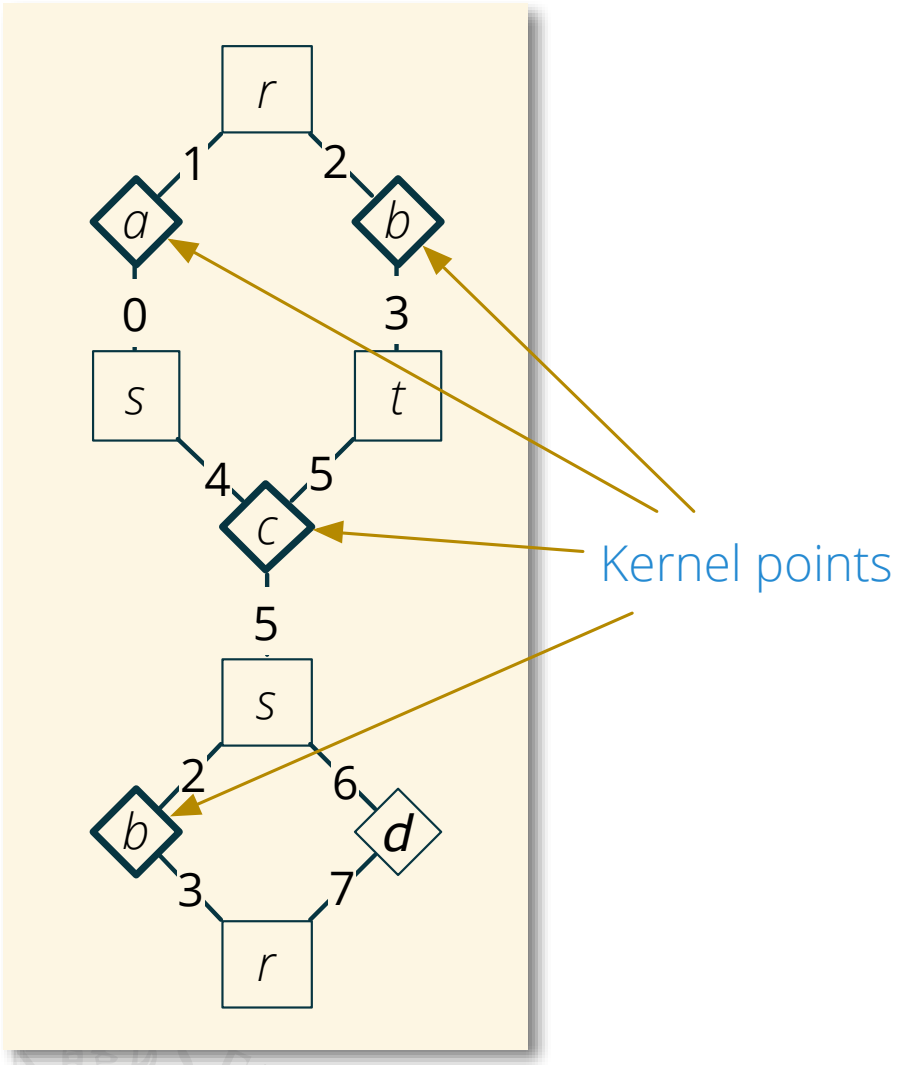
- Example: the relation `has_word` between words and webpages
- Soft match kernel:

$$\kappa_{r,d}(G, G') = \sum_{\substack{(A,B) \in R_{r,d}^{-1}(G) \\ (A',B') \in R_{r,d}^{-1}(G')}} \sum_{\substack{v \in V(A) \cup V(B) \\ v' \in V(A') \cup V(B')}} \mathbb{1}\{\ell(v) = \ell(v')\}$$

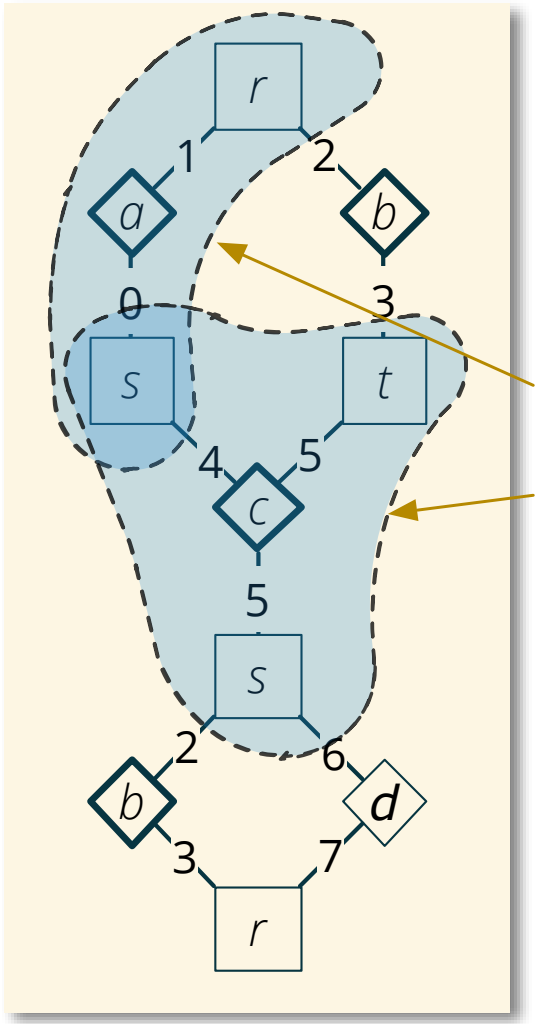
Kernel details



Kernel details

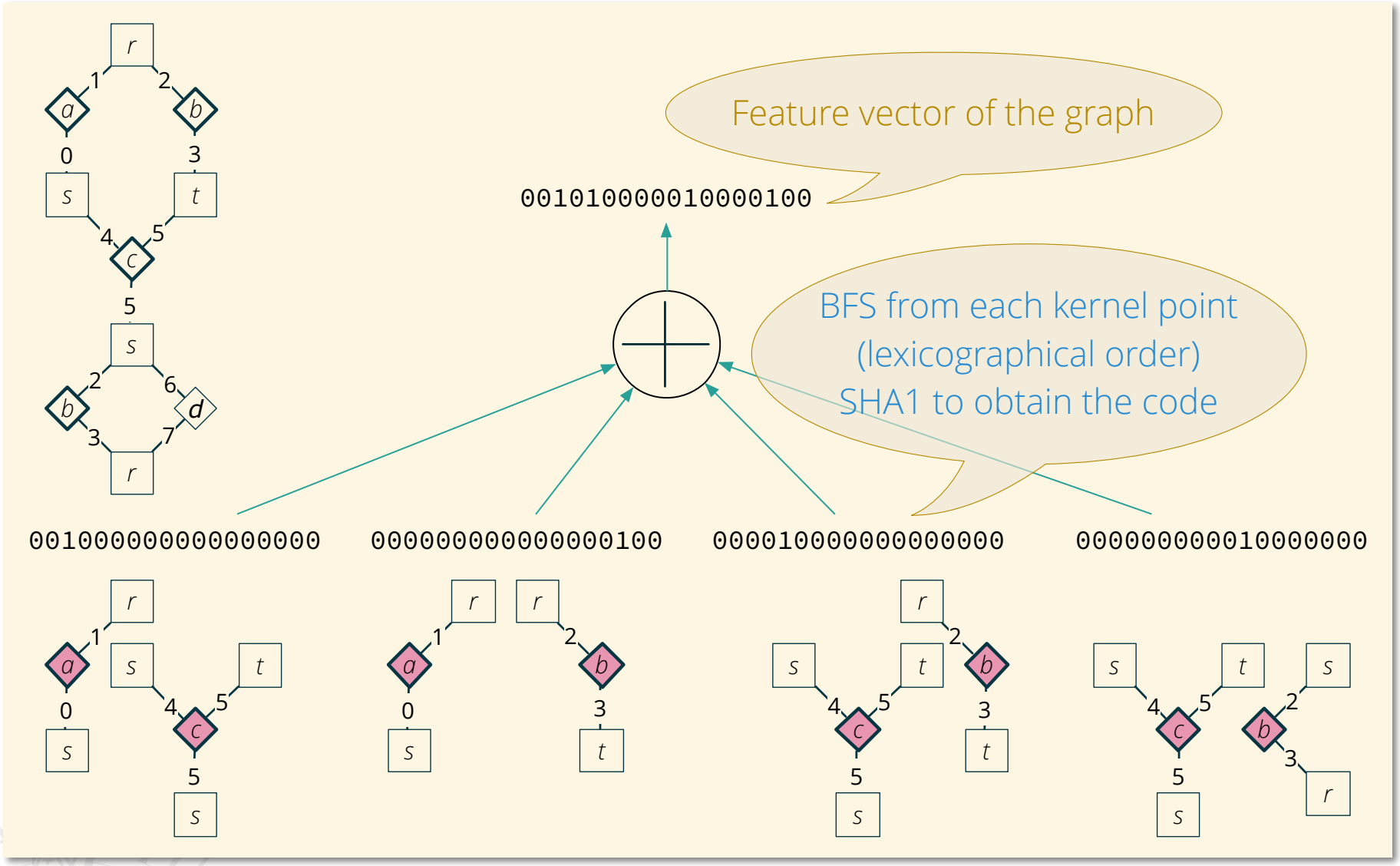


Kernel points



A neighborhood pair
radius=1
distance=2

Kernel details



- Let x and y denote the sets of input ground atoms (predictors) and output ground atoms (responses).

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- Fit a linear *potential* function:

$$F(x, y) = w^\top \phi(x, y)$$

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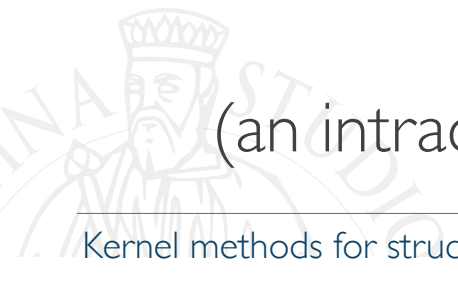
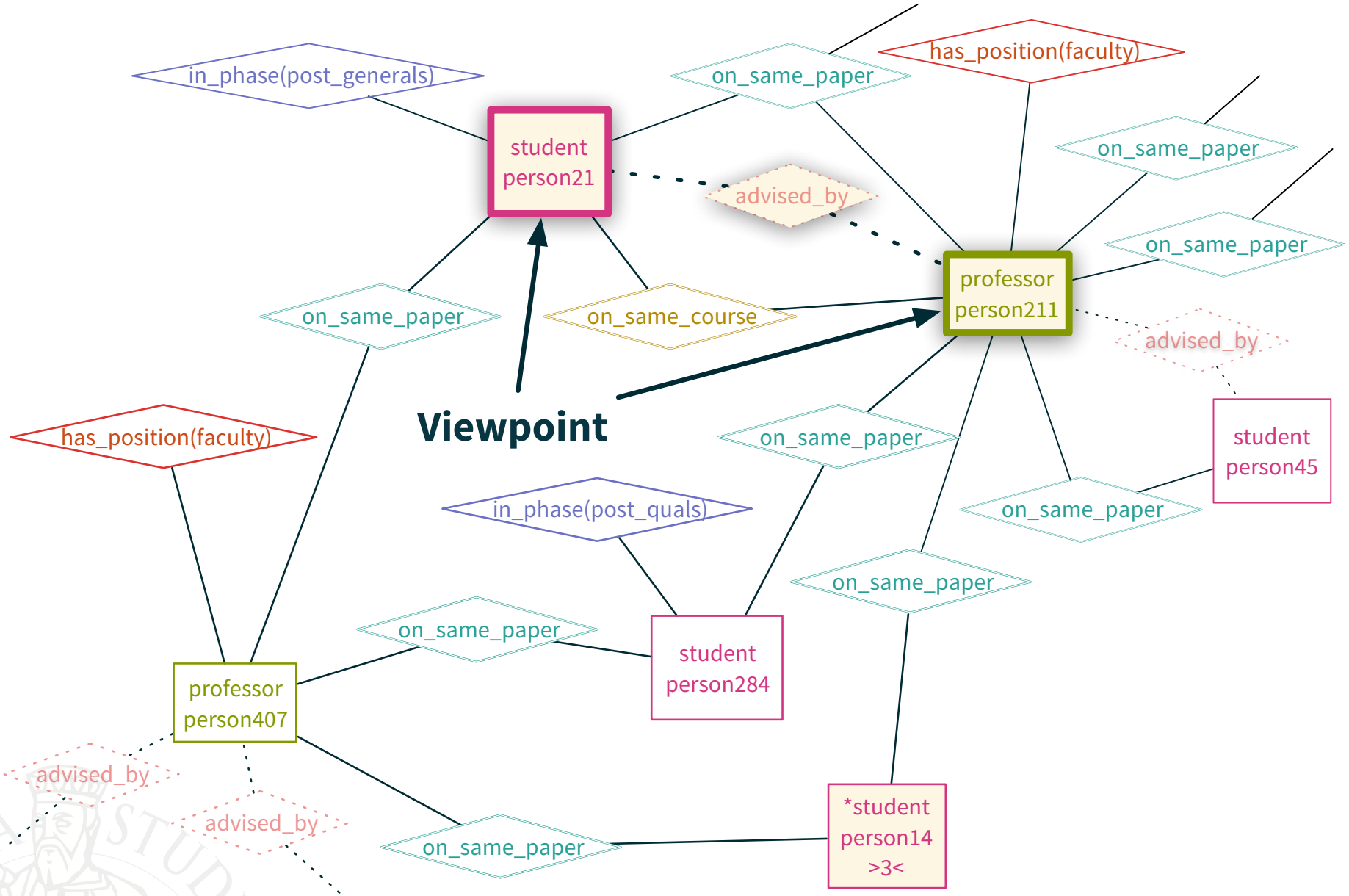
- Prediction: solve the "inference" problem

$$f(x) = \arg\max_y F(x, y)$$

(an intractable step, in general)



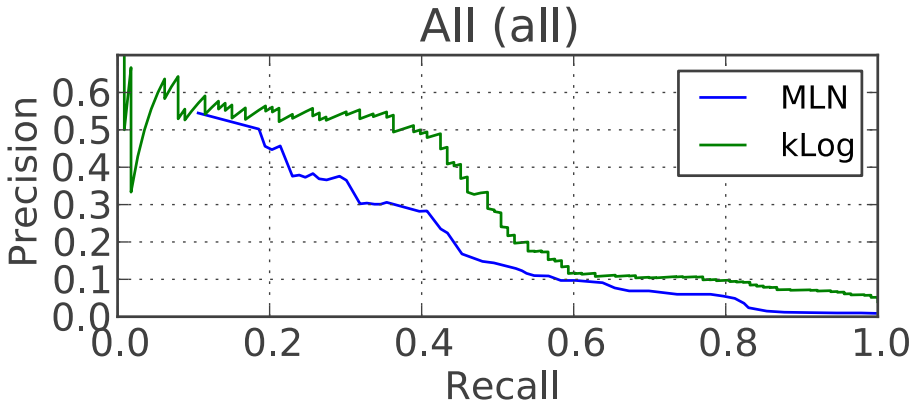
Viewpoints example

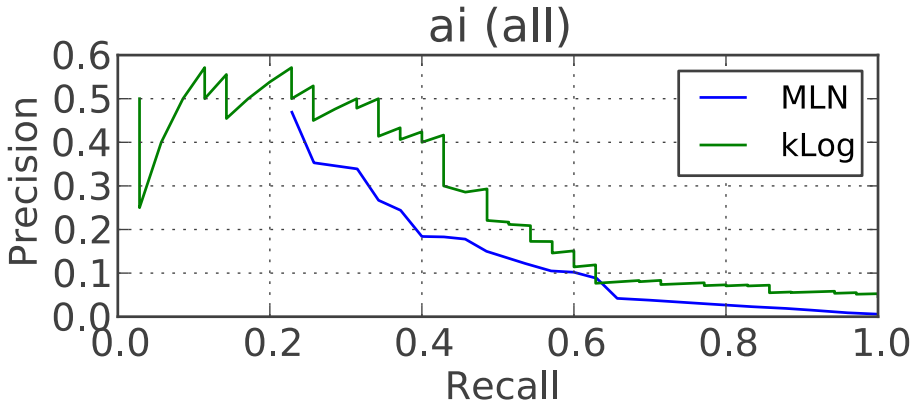


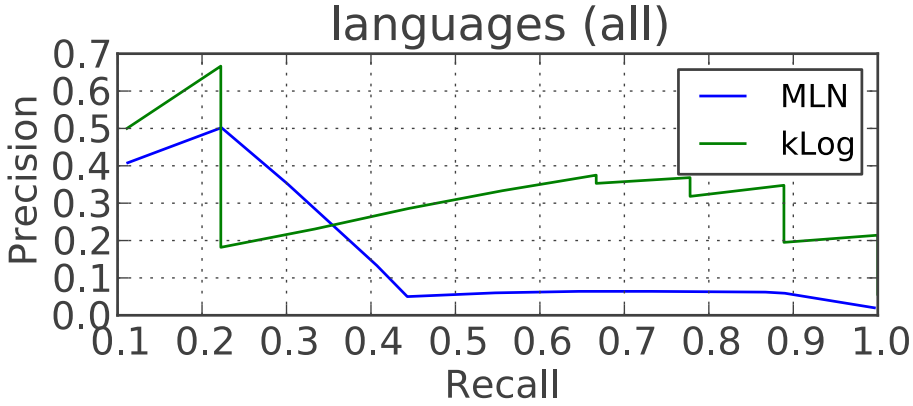
A whole kLog script

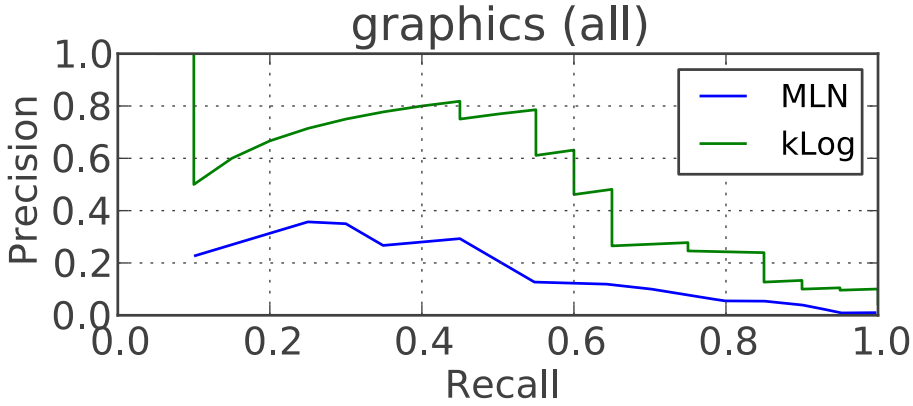
```
:- use_module('klog').
begin_domain.
  signature student(student_id::self)::extensional.
  signature professor(professor_id::self)::extensional.
  signature on_same_course(s::student,p::professor)::intensional.
  on_same_course(S,P) :-
      professor(P), student(S), ta(C,S,Term), taught_by(C,P,Term).
  signature on_same_paper(s::student,p::professor)::intensional.
  on_same_paper(S,P) :-
      student(S), professor(P), publication(Pub, S), publication(Pub,P).
  signature advised_by(s_id::student,p_id::professor)::extensional.
  kernel_points([student,professor,on_same_course,on_same_paper]).
end_domain.

experiment :-
   new_feature_generator(my_fg,nspdk),
   set_klog_flag(my_fg,radius,2),
   set_klog_flag(my_fg,distance,2),
   attach(uwcse_ext),
   new_model(my_model,svm_sgd),
   set_klog_flag(my_model,lambda,0.0001),
   set_klog_flag(my_model,epochs,5), %% ... etc
   kfold(advised_by,5,my_model,my_fg).
```

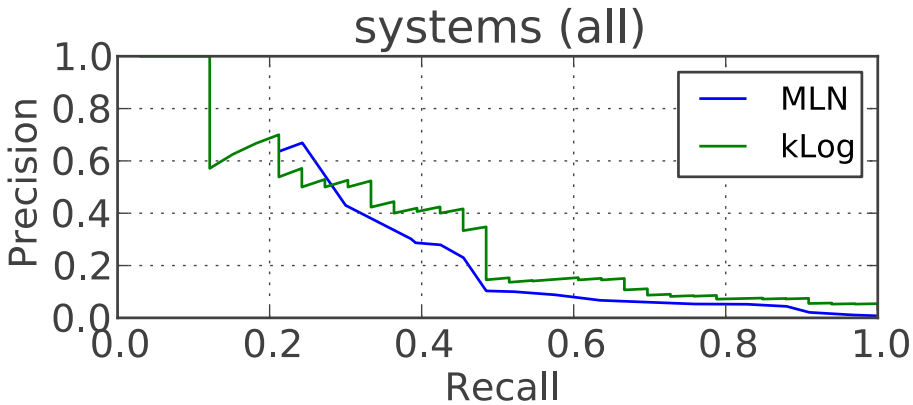
Example: UW-CSE (All information)

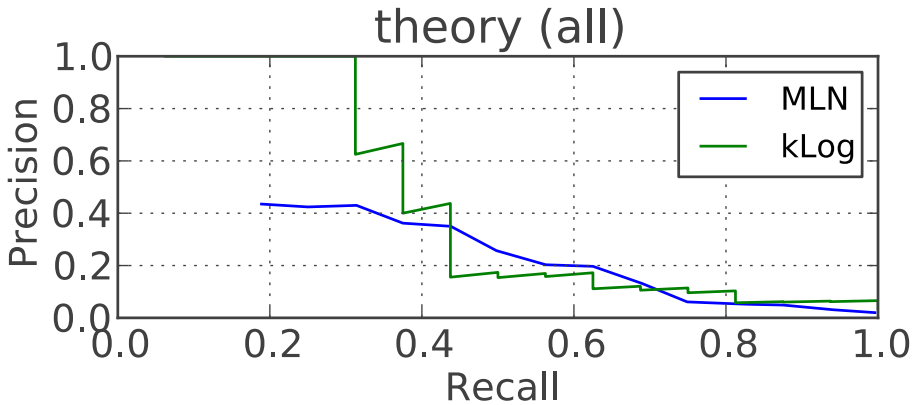












Alternative setting: partial information

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  - First, learn to discriminate between professors and students

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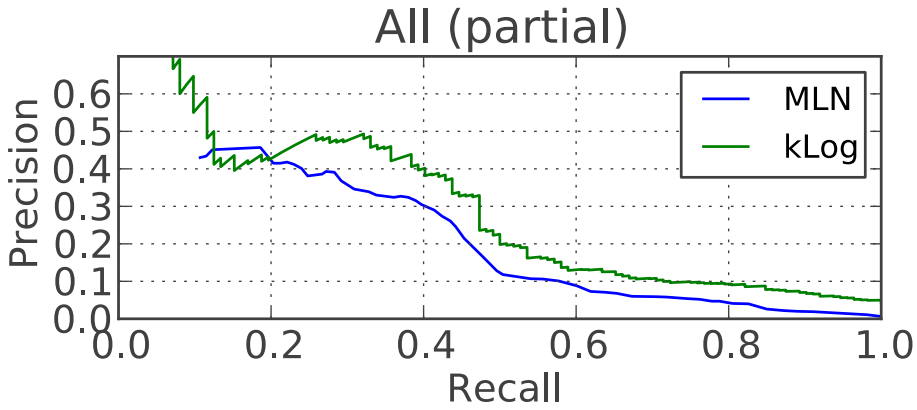
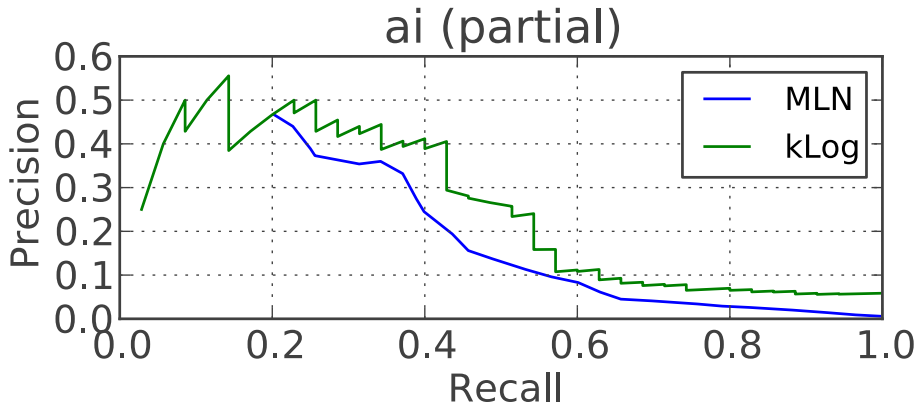
  - Assert *induced* groundings (predicted in cross-validation mode)

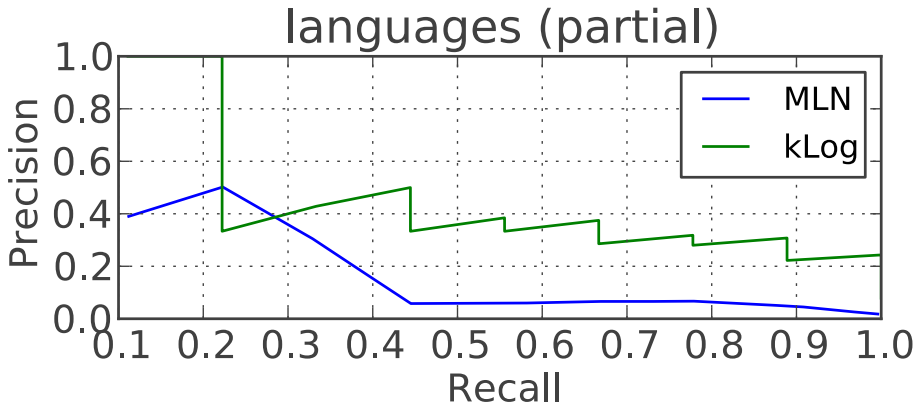
Alternative setting: partial information

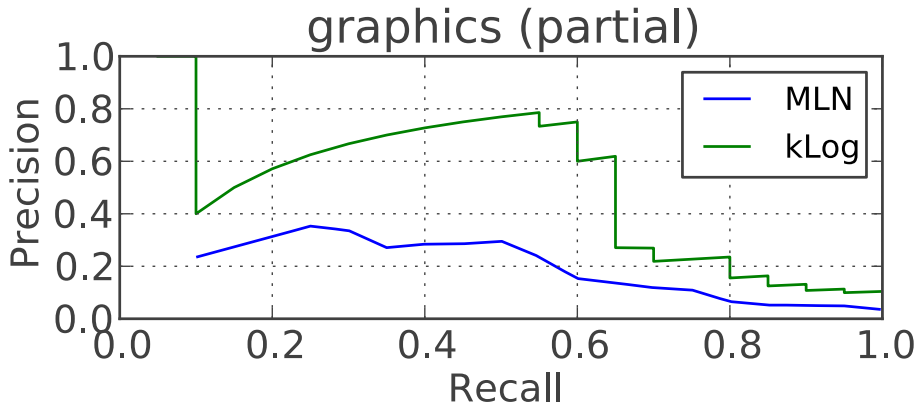
- We only know about *persons* without knowing whether they are professors or students
- Stacking in kLog
  - First, learn to discriminate between professors and students
  - Assert *induced* groundings (predicted in cross-validation mode)
  - Learn the binary relation taking saved groundings as additional data

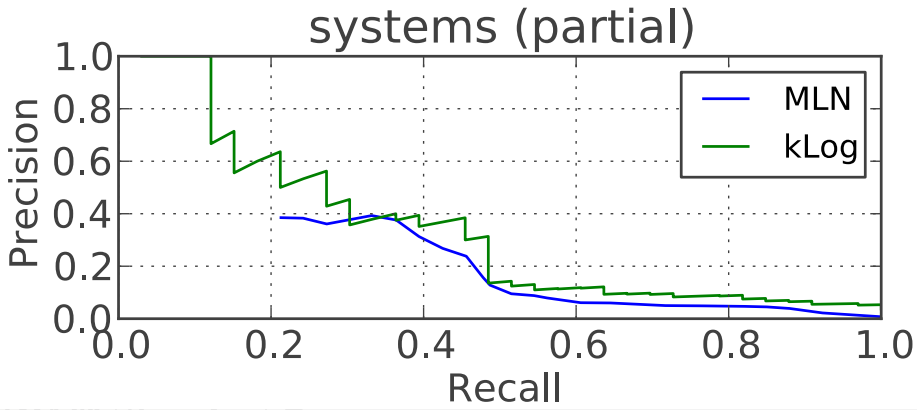
Example: UW-CSE (Partial information)

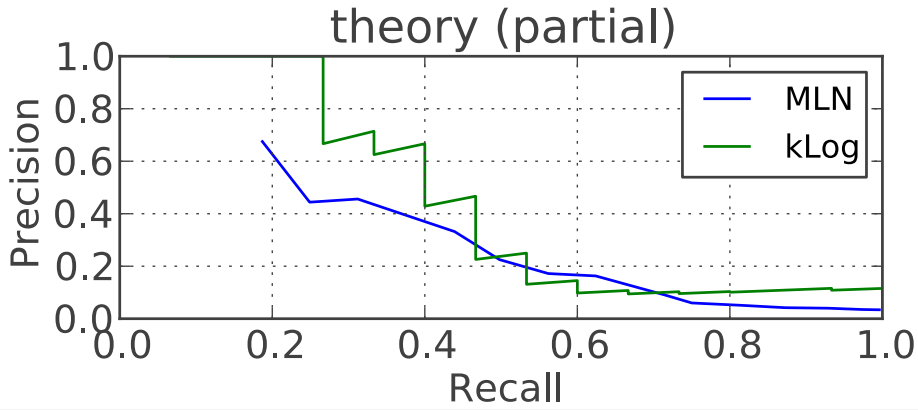












WebKB: results

	kLog		Markov Logic		Tilde	
	Acc	F_1	Acc	F_1	Acc	F_1
research	94%	0.68	95%	0.66	93%	0.54
faculty	91%	0.74	92%	0.71	91%	0.71
course	99%	0.98	98%	0.95	99%	0.98
student	90%	0.91	89%	0.90	88%	0.89
Average	88%	0.88	88%	0.81	86%	0.78
Time	< 1m		450m		87m	

IMDb: results

Year	# Movies	# Facts	kLog	MLN	Tilde
1997	311	8031	0.86	0.79	0.80
1998	332	7822	0.93	0.85	0.88
1999	348	7842	0.89	0.85	0.85
2000	381	8531	0.96	0.86	0.93
2001	363	8443	0.95	0.86	0.91
2002	370	8691	0.93	0.87	0.89
2003	343	7626	0.95	0.88	0.87
2004	371	8850	0.95	0.87	0.87
2005	388	9093	0.92	0.84	0.83
All			0.93 ± 0.03	0.85 ± 0.03	0.87 ± 0.04
Time			1,394s	220s	12,812s

- Natural language processing:
  - Hedge cue detection (Verbeke et al. 2011)
  - Evidence-based medicine (Verbeke et al. 2012)
- Vision:
  - Indoor scene classification (Antanas et al. 2013)

kLogNLP (Verbeke et al. 2014)

- Natural language module for kLog
- NLP-specific preprocessors, enabling the use of existing libraries, currently:
  - The Python Natural Language Toolkit (NLTK)
  - The Stanford CoreNLP
- `http://people.cs.kuleuven.be/~mathias.verbeke/klognlp/`

Hedge cue detection

- Hedge cues are linguistic devices that indicate whether information is being presented as uncertain or unreliable within a text
- Indicate caution or uncertainty towards content
- Task: discriminate between factual vs uncertain sentences, e.g.

Factual *"Among adolescents, the rate was found to be between 8 to 12 percent"*

Uncertain *"Some technologies are known to perform better than others in this regard"*

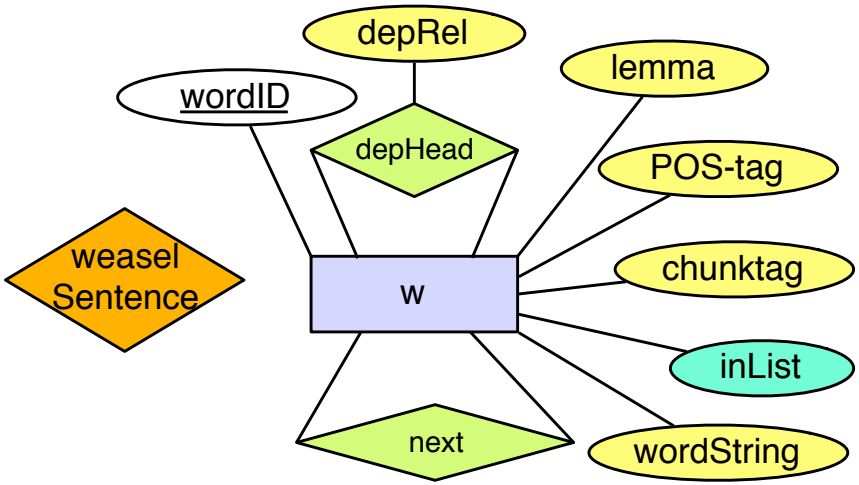
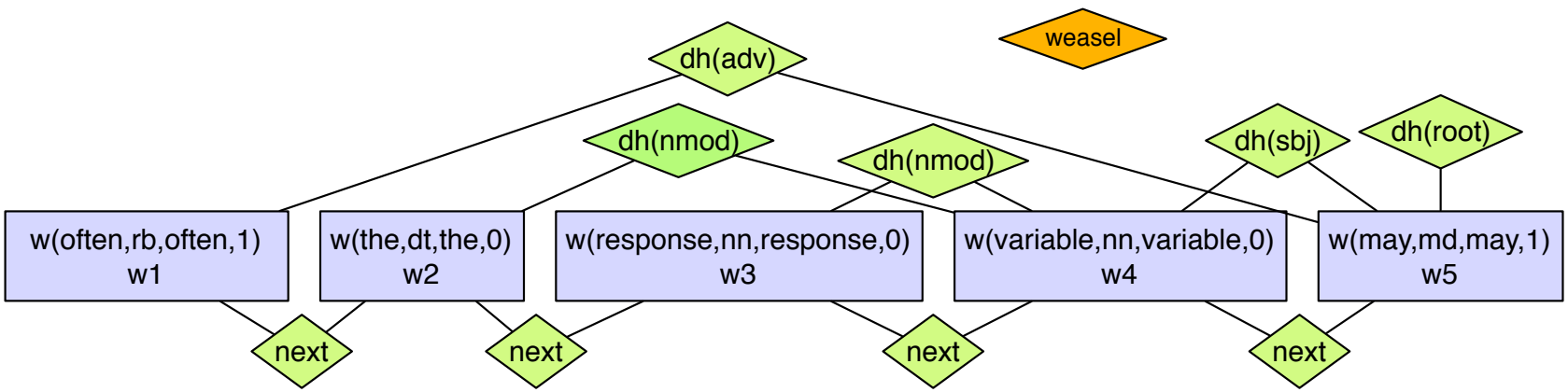


Fig. 2: E/R diagram modeling the hedge cue detection task



Results on CoNNL 2010 shared task (Verbeke et al. 2011)

Table 3: Evaluation performance in terms of precision, recall and F1 of the top 5 CoNLL 2010 systems and the kLog approach for the Wikipedia dataset

Official Rank	System	P	R	F
-	**kLog**	67.04	56.77	61.48
1	Georgescul	72.0	51.7	60.2
2	Ji[1]	62.7	55.3	58.7
3	Chen	68.0	49.7	57.4
4	Morante	80.6	44.5	57.3
5	Zhang	76.6	44.4	56.2

Part 5

Dealing with continuous/high dimensional attributes

Continuous and/or high-dimensional attributes

- Many kernels seen so far use hard-matching, which makes no sense in this setting

Continuous and/or high-dimensional attributes

- Many kernels seen so far use hard-matching, which makes no sense in this setting
- We will briefly review the following possible approaches:
  - Propagation kernels (Neumann et al. 2015, 2012)
  - GraphHopper (Feragen et al. 2013)
  - Graph invariant kernels (Orsini et al. 2015)

Propagation kernels

- Like in Weisfeiler-Lehman, define a sequence of graphs $G_0 = G, G_1, \ldots, G_T$ being T the number of propagation steps

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- As in W-L, the kernel between two graphs is

$$K(G, G') = \sum_{t=0}^{T} k(G_t, G'_t)$$

where

$$k(G_t, G'_t) = \sum_{v \in V_t} \sum_{v' \in V'_t} \kappa_{\text{node}}(v, v')$$

for some κ_{node} we will define later

- The propagation mechanism is based on the following diffusion process (Neumann et al. 2015):

$$P_{t+1} = TP_t$$

where

  - T is the row-normalized adjacency matrix
  - P_t contains a node distribution in each row

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where

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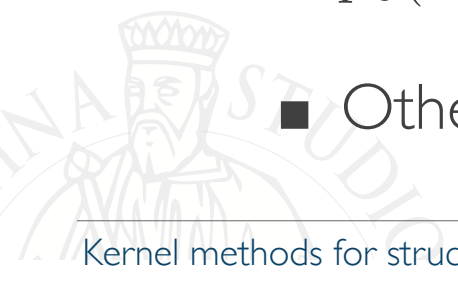
- Initialization:
  - $p_0(v) = \delta_{\ell(v)}$ if v is labeled
  - Otherwise put a uniform distribution



Propagation kernels

- Distinguish between node labels $\ell(u)$ (categorical symbols) and node attributes $x(u)$ (may be real vectors)

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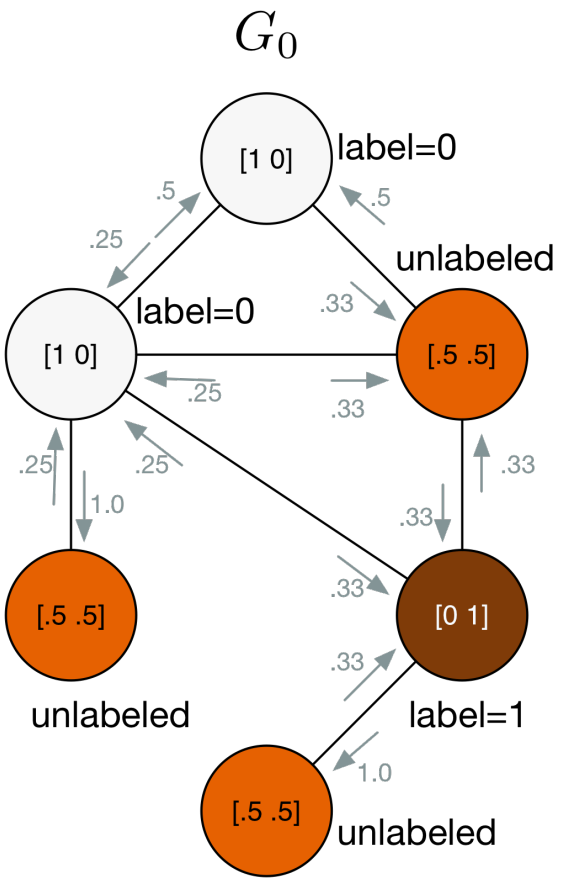
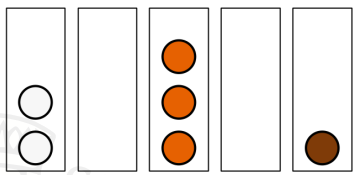
- κ_{label} and κ_{attr} are based on discretization (e.g. via locality-sensitive hashing):

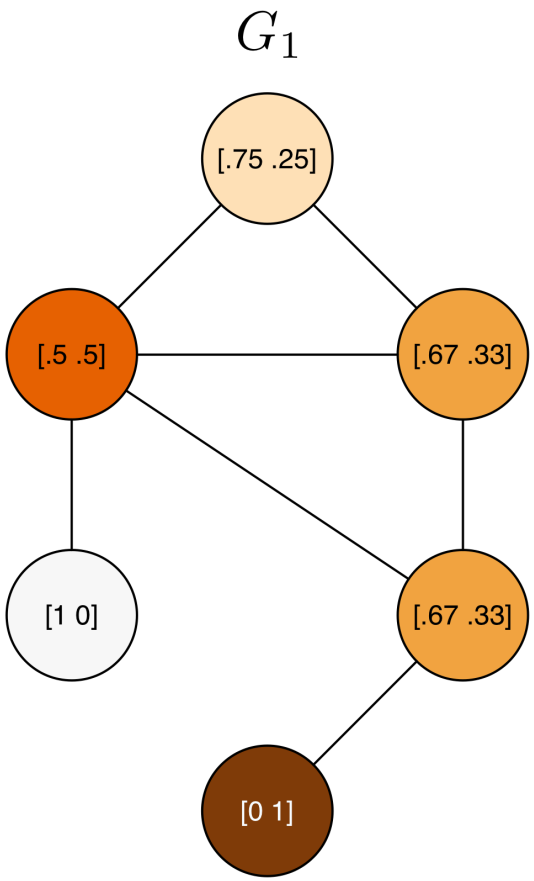
$$\kappa_{\text{label}}(\ell(v), \ell(v')) = \mathbb{1}\{h(p(v)) = h(p(v'))\}$$

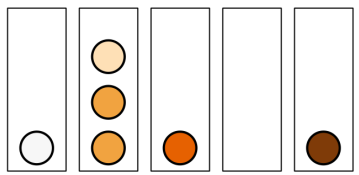
Propagation kernels — Example



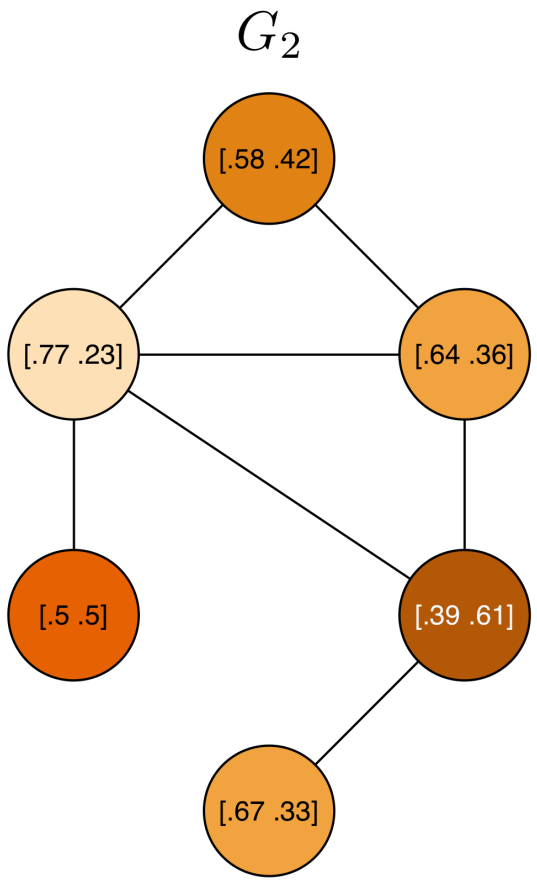


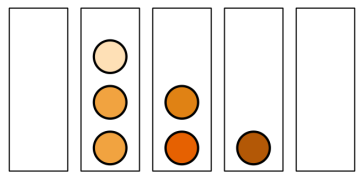
$\phi(G_0) = [2, 0, 3, 0, 1]$





$\phi(G_1) = [1, 3, 1, 0, 1]$





$\phi(G_2) = [0, 3, 2, 1, 0]$

- Start from a given kernel κ_{node} on node attributes (e.g. RBF)

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- Define a kernel on paths as follows:
  - Let π_j and π'_j be the vertices at position j in two paths π and π', respectively
  - Let $x(\pi_j)$ and $x(\pi'_j)$ be their (high-dimensional) labels
  - Path kernel:

$$\kappa_{\text{path}}(\pi, \pi') = \mathbb{1}\{|\pi| = |\pi'|\} \sum_{j=1}^{|\pi|} \kappa_{\text{node}}\left(x(\pi_j), x(\pi'_j)\right)$$

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- Finally define the graph kernel as

$$K(G, G') = \sum_{\pi \in R^{-1}(G)} \sum_{\pi' \in R^{-1}(G')} \kappa_{\text{path}}(\pi, \pi')$$

where $(\pi, G) \in R$ if π is a shortest-path in G

- To speed-up the computation, rewrite the kernel as

$$K(G, G') = \sum_{v \in V} \sum_{v' \in V'} w(v, v') \kappa_{\text{node}}(v, v')$$

where $w(v, v')$ counts the number of times v and v' appear at the same hop in a shortest-path

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- The kernel $w(v, v')$ can be computed as

$$w(v, v') = \langle M(v), M(v') \rangle$$

where $M(v)$ is a $\delta \times \delta$ matrix with entries

$m_{ij}(v) =$ # times v appears at hop i in a shortest-path of length j

and δ is the largest graph diameter

- All matrices $M(v)$ can be computed in $O(V^2(E + \log V + \delta^2))$ calling Dijkstra as a subroutine — see (Feragen et al. 2013) for details

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- The overall running time is therefore $O(V^2(d + E + \log V + \delta^2))$ where d is the dimension of the node attribute vector
- Additionally, $M(v)$ only need to computed once per graph on a given dataset, yielding an amortized running time of $O(dV^2)$
- Nice improvement compared to the running time $O(dV^4)$ of the naive implementation based on the shortest-path kernel

- An invariant is a function $\mathcal{I}$ such that

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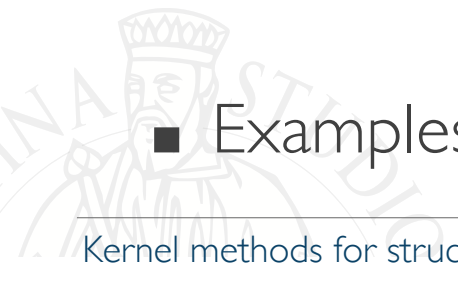
- Examples: $\mathrm{degree}(v)$, W-L color of v, etc.



Graph invariant kernels (Orsini et al. 2015)

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- Note that in this setting $x(v)$ may have any type

Graph invariant kernels

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- Then define the structural similarity between nodes as

$$w(v, v') \doteq \sum_{g \in R_v^{-1}(G)} \sum_{g' \in R_{v'}^{-1}(G')} \kappa_{\text{inv}}(v, v') \frac{\delta(g, g')}{|V_g||V_{g'}|}$$

where $\delta(g, g')$ is used to compare patterns g and g'

- Weisfeiler-Lehman coloring:

$$\kappa_{\text{inv}}(v, v') = \sum_{t=0}^{T} \mathbb{1}\{\mathcal{L}_t(v) = \mathcal{L}_t(v')\}$$

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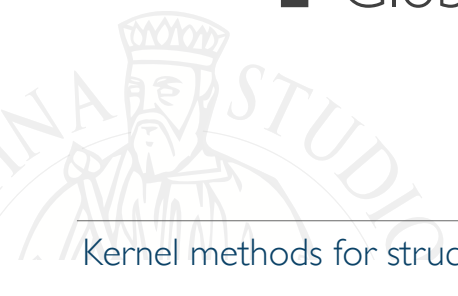
- Both a local version and a global version of the coloring are possible
  - Local version: run W-L on ech pattern g
  - Global version: run W-L on the whole graph G



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$$\mathcal{L}_i(v) = \begin{cases} |x_i(v)| & \text{if } \lambda_i \text{ has multiplicity } 1 \\ 0 & \text{if } \lambda_i \text{ has multiplicity } > 1 \end{cases}$$

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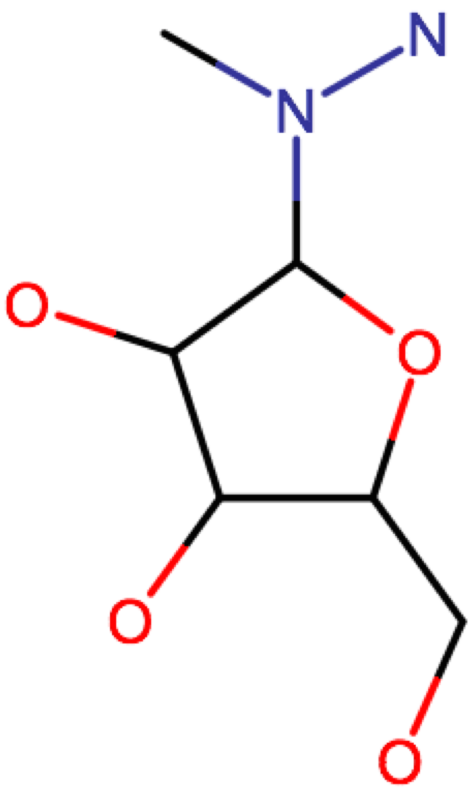
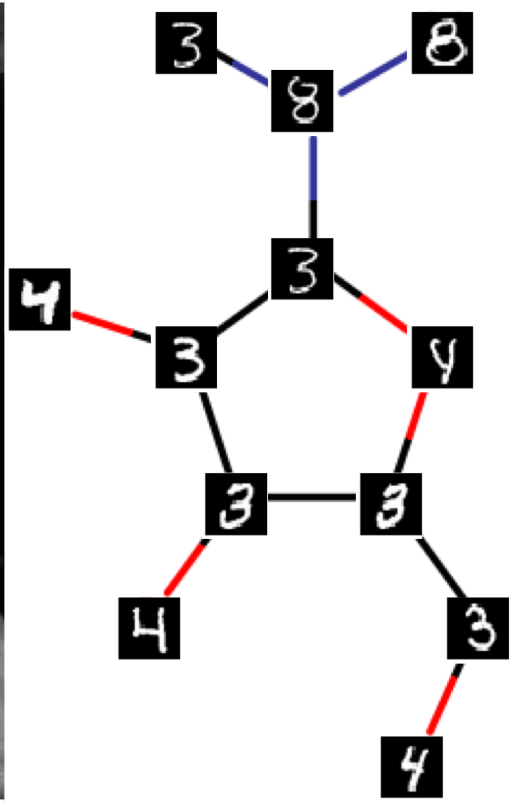
- Let

$$\kappa_{\text{inv}}(v, v') = \exp\left(-\gamma \|\mathcal{L}(v) - \mathcal{L}(v')\|^2\right)$$





- Start from mutagenicity data set of Bursi *et al.*
- Atoms masquerading as MNIST digits

GIK vs GraphHopper

	ENZYMES$_{SYM}$		PROTEIN		SYNTHETIC$_{NEW}$		FRANKENSTEIN		QC	
	WITHOUT CONT.	WITH CONT.	WITHOUT CONT.	WITH CONT.	WITHOUT CONT.	WITH CONT.	WITHOUT CONT.	WITH CONT.	WITHOUT CONT.	WITH CONT.
NSK$_V$	25.9 ± 1.1	71.8 ± 1.0	72.1 ± 0.4	74.2 ± 0.7	78.4 ± 1.9	81.9 ± 1.1	67.9 ± 0.2	72.9 ± 0.3	37.8	92.6
NSK$_{WL}$	56.5 ± 1.1	72.2 ± 0.8	71.7 ± 0.4	76.2 ± 0.4	50.0 ± 0.0	50.0 ± 0.0	74.2 ± 0.3	77.3 ± 0.1	47.8	91.0
GWL$_V$	55.7 ± 1.0	72.6 ± 0.8	**74.9 ± 0.6**	76.1 ± 0.8	**80.8 ± 1.2**	82.8 ± 1.0	73.5 ± 0.3	77.3 ± 0.2	49.8	93.6
GWL$_{WL}$	**58.6 ± 1.4**	71.3 ± 1.1	73.6 ± 0.5	75.8 ± 0.6	50.0 ± 0.0	50.0 ± 0.0	**75.1 ± 0.2**	**78.9 ± 0.3**	48.6	89.6
LWL$_V$	54.5 ± 1.1	**73.3 ± 0.9**	74.4 ± 0.4	**76.6 ± 0.6**	80.6 ± 1.5	**83.0 ± 1.0**	73.0 ± 0.2	77.6 ± 0.2	47.2	**94.6**
LWL$_{WL}$	57.0 ± 1.1	72.0 ± 0.9	71.9 ± 0.6	76.5 ± 0.5	50.0 ± 0.0	50.0 ± 0.0	74.1 ± 0.2	78.3 ± 0.3	47.4	91.8
GSGK$_V$	29.8 ± 0.6	71.8 ± 1.0	73.2 ± 0.3	74.7 ± 0.5	78.2 ± 2.1	82.4 ± 0.9	70.1 ± 0.3	74.0 ± 0.3	44.4	92.6
GSGK$_{WL}$	56.7 ± 1.2	72.2 ± 0.7	72.9 ± 0.5	76.4 ± 0.4	50.0 ± 0.0	50.0 ± 0.0	75.0 ± 0.3	77.6 ± 0.2	47.8	91.0
LSGK$_V$	31.9 ± 1.0	71.9 ± 1.0	72.3 ± 0.4	74.4 ± 0.6	78.7 ± 2.0	82.2 ± 1.1	72.1 ± 0.2	74.9 ± 0.2	42.4	92.2
LSGK$_{WL}$	56.6 ± 1.3	72.1 ± 0.8	71.7 ± 0.3	76.1 ± 0.5	50.0 ± 0.0	50.0 ± 0.0	74.2 ± 0.2	77.4 ± 0.2	**51.4**	91.0
GRAPHHOPPER		69.5 ± 0.7		72.7 ± 0.3		73.9 ± 1.7		68.7 ± 0.4		91.4

Final remarks

- Kernel methods may be effective in relational domains
- Large datasets require $\phi(G)$ but not all available graph kernels allow to compute it explicitly
- Limited by the "fixed-representation" approach: see e.g. (Narayanan et al. 2016; Niepert et al. 2016; Yanardag et al. 2015) for alternatives

References I

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