uses vertex labels, but no edge labels.
editing to include cost of edge label substitution.

Comparing Stars: On Approximating Graph Edit Distance
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we exploit the upper and lower bounds of edit distance to improve the search performance by filtering out graphs that definitely will not be in the answer set and thus avoid the expensive graph edit distance computation.

AppFull: efficient for performing approximate full graph over graph databases using graph edit distance as the similarity measure

Given a query graph q and the edit distance threshold ω,
for each graph g in graph database D,
L_m(g, q) is first used to filter g if L_m is greater than ω (lines 2-4), because λ > ω must hold in the case of L_m > ω. Subsequently, if τ(g, q) ≤ ω, we know that the edit distance between g and q must be no greater than ω, and q can therefore be reported as a result(lines 5-8). If g passes the above two tests, then ρ is exploited further. Like in the case of τ, if ρ(g,q) ≤ ω, λ(g,q) must be no greater than ω and g can be output as a result (lines 9-12). Finally, if g passes all the above three tests, then λ(g,q) must be computed(lines 13-15). The order of the above three tests is quite significant because the costs of their computation are different. Among three of them, the computation of L_m is the most efficient, while the computation of ρ is the most expensive. Therefore, if g does not pass an earlier test, the rest of the expensive tests are avoided.

Distance	Complexity	Distance	Complexity
L_m	$\Theta(n^3)$	τ	$\Theta(n^3)$
ρ	$O(n^6)$	λ	NP-Hard

Algorithm 3 APPFULL - Approximate Full Graph Search

Input: A query graph q and a graph database $\mathcal{D}$
Input: Distance threshold ω
Output: All graphs g in $\mathcal{D}$ s.t. $\lambda(g,q) \leq \omega$

1. **for** each graph $g \in \mathcal{D}$ **do**
2. **if** $L_m(g,q) > \omega$ **then**
3. **continue;**
4. **end if**
5. **if** $\tau(g,q) \leq \omega$ **then**
6. report g as a result;
7. **continue;**
8. **end if**
9. **if** $\rho(g,q) \leq \omega$ **then**
10. report g as a result;
11. **continue;**
12. **end if**
13. **if** $\lambda(g,q) \leq \omega$ **then**
14. report g as a result;
15. **end if**
16. **end for**

$$L_m \leq \lambda \leq \rho \leq \tau$$

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class diagram for the AppFull and AppSub algorithms

StarStructure
==========
w/ node and edge labels, both >= 0

// index of root; label of root
rootIdx : int ; rootLabel : int;
// the adjacent vertexes of root in V[i] treated as leaves. values are labels.
// vLabels is sorted by value.
vLabels : int[]
// root -> V[i] edge labels, sorted by the vLabel sorting
eLabels : int[]
// the original indexes in V[i] of vLabels before sorting
origVIndexes : int[]

-StarStructure()
+StarStructure(int root, int[] vLabels, int[] eLabels)
// protected. node and edge labelling functions which can be overridden with
// specialization. default is to use graph values
labels(Graph g, int rootIndex) : int[]
// —- static methods —-
// Lemma 4.1
+calculateEditDistance(StarStructure s1, StarStructure s2) : double
+calculateEditDistanceNoRelabelling(StarStructure s1, StarStructure s2) : double

//create edit distance matrix for S(g_1) to S(g_2) from
//StarStructure.calculateEditDistance
createDistanceMatrix(StarStructure[] sg1, StarStructure[] sg2) : double[][]

//create multiset of |V| star structures from graph g with |V| vertices
createStarStructureMultiset(Graph g) : StarStructure[]

createStarStructure(Graph g, int rootIndex) : StarStructure

// sort array a in place, and return an array of the original indexes also sorted
sort(int[] a) : int[]

LEMMA 4.1. **(Star Edit Distance)** *Given two star structures s_1 and s_2,*

$$\lambda(s_1, s_2) = T(r_1, r_2) + d(L_1, L_2)$$

+ a term for edge labels

where

$$T(r_1, r_2) = \begin{cases} 0 & \text{if } l(r_1) = l(r_2), \\ 1 & \text{otherwise.} \end{cases}$$

$$d(L_1, L_2) = ||L_1| - |L_2|| + M(L_1, L_2)$$

$$M(L_1, L_2) = \max\{|\Psi_{L_1}|, |\Psi_{L_2}|\} - |\Psi_{L_1} \cap \Psi_{L_2}|$$

Ψ_L is the multiset of vertex labels in L.

modifying Star Edit Distance to include edge labels:
lambda(s1, s2) = T(r1, t2) + d(L1, L2)
where T(r1, r2) = 0 if label(r1)==label(r2), else = 1
d(L1, L2) = ||L1|-|L2|| + M(L1, L2)
where psi(L) is the multiset of vertex labels on L
where M(L1,L2) = max(|psi(L1)|, |psi(L2)|) - | intersection of psi(L1) with psi(L2) |
edge labels: node labelling difference does not use distance, so edge will not either.
will compare edge label values after they have been sorted by the vertex label sorting. a cost of 1 when edge labels are not equal, else the cost is 0.
call this function d(L1E, L2E) and modified Star Edit Distance:
lambda(s1, s2) = T(r1, t2) + d(L1, L2) + d(L1E, L2E)

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Symbols	Description
$deg(v)$	$\lvert\{u\lvert(u,v) \in E\}\rvert$, the degree of v
$\delta(g)$	$\max_{v \in V(g)} deg(v)$
$\lambda(g_1, g_2)$	the edit distance between graphs g_1 and g_2
$L_m(g_1, g_2)$	the lower bound of $\lambda(g_1, g_2)$
$\tau(g_1, g_2)$	the suboptimal value of $\lambda(g_1, g_2)$
$\rho(g_1, g_2)$	the refined suboptimal value $\lambda(g_1, g_2)$

class diagram for the AppFull and AppSub algorithms

ApproxGraphSearchZeng
==========
———————————————-
//AppFull for performing approximate full graph search.
// implements Algorithm 3
// q is the query, db is the graph to search, w is the edit distance threshold
+approxFullGraphSearch(Graph q, List<Graph> db, double w) : List<Graph>

//AppSub for performing approx subgraph search.
//the subgraph isomorphism problem is a computational task in which
//two graphs G and H are given as input, and one must determine
//whether G contains a subgraph that is isomorphic to H
+approxSubGraphSearch(Graph g, Graph h) : Graph

//pg5, col1 and col2. presumably, the best assignments of s_1_i to s_2_j
// have a best approach: greedy ordered by distMatrix?
calculateMappingDistance(StarStructure[] sg1, StarStructure[] sg2) : double

refine(Graph g,Graph h, int[][] permutation) : int[][], double

during normalization of S(g1) to S(g2), k vertices with the label ε are inserted into g2. this is considered vertex relabelling so it does not change the edit distance between g1 and g2. normalization is performed before the balanced weighted bipartite matching.

Given two multisets of star structures S1 and S2 with the same cardinality, and assume P :S1 →S2 is a bijection. The distance ζ between S_1 and S_2 is

$$\zeta(S_1, S_2) = \min_P \sum_{s_i \in S_1} \lambda(s_i, P(s_i))$$

equivalent to solving the assignment problem

where P is an n×n permutation matrix that is an orthogonal matrix having the property P*P^T = P^T*P = I where I is the identity matrix.

NOTE: S_1 originally has the same number or more vertexes than S2 and if the later, then normalization is S_2 gets added vertexes with labels ε (graph notation ε→u is insertion of u, and u→ε is deletion of u)

DEFINITION 4.3. **(Mapping Distance)** *The mapping distance $\mu(g_1, g_2)$ between g_1 and g_2 is defined as:*

$$\mu(g_1, g_2) = \zeta(S(g_1), S(g_2))$$

Comparing Stars: On Approximating Graph Edit Distance
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needed for AppFull (the approx full graph search)

Lower Bound of Graph Edit Distance

Based on Lemma 4.2, μ provides a lower bound L_m of λ, i.e.,

$$\lambda(g_1, g_2) \geq L_m(g_1, g_2) = \frac{\mu(g_1, g_2)}{\max\{4, [\max\{\delta(g_1), \delta(g_2)\} + 1]\}}$$

Refine is guaranteed to be terminated in $2n + n^2$ steps

Algorithm 2 REFINE(g,h,P)

Input: two graph structures g and h
Input: a permutation matrix P of g and h
Output: refined suboptimal distance of g and h

```
1.  dist ← C(g, h, P);
2.  min ← dist;
3.  for any pair (u_i, u_j) ∈ V(g) do
4.     get P' based on u_i and u_j;
5.     if min > C(g, h, P') then
6.        min ← C(g, h, P');
7.        P_min ← P';
8.     end if
9.  end for
10. if min < dist then
11.    min ← REFINE(g, h, P_min)
12. end if
13. return min;
```

τ(g,h) : the suboptimal value of λ(g, h)
Assuming that the output from the Hungarian algorithm in Section 4.2.1

$$\zeta(S_1, S_2) = \min_P \sum_{s_i \in S_1} \lambda(s_i, P(s_i))$$

equivalent to solving the assignment problem

leads to a mapping P^- from V(g) to V(h), we can simply use Equation 1 from Section 3.1

$$C(g, h, P) = \sum_{i=1}^{n} \sum_{j=1}^{n} C_{i,j} P_{i,j} + \frac{1}{2} ||A^g - P A^h P^T||_1 \qquad (1)$$

to compute C(g,h,P^-), denoted as τ(g,h).

ρ(g,h) : the refined suboptimal value λ(g, h)
P^- is calculated using REFINE(g, h, P).
Refine will only find a local optimal solution
ρ(g,h) =

$$\lambda(g, h) = \min_P C(g, h, P) \qquad (2)$$

λ(g,h) : the edit distance between graphs g and h

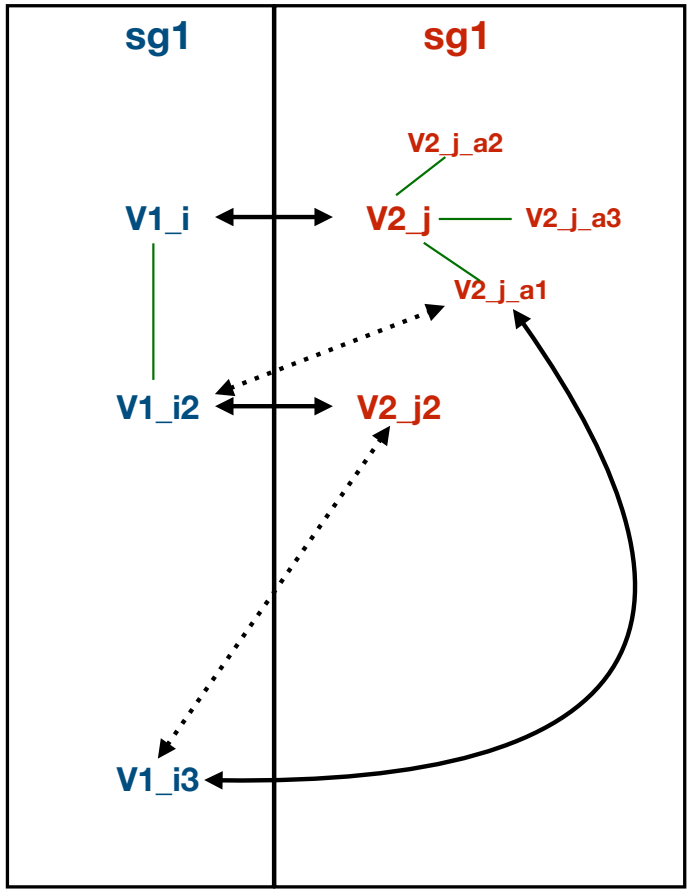
$$\lambda(g, h) = \min_P C(g, h, P) \qquad (2)$$

in REFINE, one way to select the assignments to swap

V1_i maps to V2_j

V1_i2 maps to V2_j2

V1_i is adj to V1_i2
in sg1, but V2_j is not
adj to V2_j2 in sg2



choose a vertex adj to V2_j
as a member of the swap.

new assignments:
V1_i2 <—> V2_j_adj
V1_i3 <—> V2_j2

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$\rho(g_1, g_2)$	the refined suboptimal value $\lambda(g_1, g_2)$

needed for AppSub (the approx sub graph search)

hold. Accordingly, we devise a filtering algorithm AppSub to perform θ-subgraph search, in which L'_m is used as a filter: if $L'_m(q_1, g_2) > \mathcal{L} + 2\theta$, g_2 can be safely filtered.

if g1 is subgraph isomorphic to g2, no vertex relabelling will exists in the optimal alignment that make g2 reach g1, so the edit distance between two star structures is therefore redefined as:

$$\lambda'(s_1, s_2) = T'(s_1, s_2) + d(L_1, L_2) \quad \text{where}$$

$$T'(s_1, s_2) = \begin{cases} 2 + |L_1| + |L_2| & \text{if } l(r_1) \neq l(r_2), \\ 0 & \text{otherwise.} \end{cases}$$

In [35], Yan et al. introduced Grafil for performing approximate subgraph search by allowing edge relaxations(no vertex relabelling).

Assuming that g3 is the maximal common subgraph between a query graph g1 and a data graph g2 ,
the number of edge relaxations in Grafil is defined as |E1 |−|E3 |.
*Note that, the definition of edge relaxation implicitly implies that no vertex relabelling is allowed.
This similarity measure, however, does not take the vertex mismatches into account.
We therefore introduce the following similarity measure based on the graph edit distance to overcome this weakness of edge relaxation.

A graph g1 is said to be θ-subgraph isomorphic to g2 if there exists a graph g3 s.t.
g3 ⊑ g2 (i.e. ***g3 is a subset of g2***) and ***λ'(g1, g3) ≤ θ***.

Given a query g1 and a graph database D, the problem of θ-subgraph search is to find out all graphs g2 in D of which g1 is a θ-subgraph.

if g1 is a θ-subgraph of g2, λ'(g1, g2) ≤ L + 2θ must hold
AppSub inherently supports both of two kinds of subgraph search, i.e., traditional subgraph search[37] and containment search[9

A Coding Method for Efficient Subgraph Querying on Vertex- and Edge-Labeled Graphs

- May 2014PLoS ONE 9(5):e97178

DOI:10.1371/journal.pone.0097178

Zhu et al.

The subgraph query problem is to retrieve all the supergraphs of a given graph from a graph database. It can be defined as follows: for a large graph database D = {D_1, D_2, …, D_n} and a query graph Q, subgraph query is to find all the graphs D_i (i=1,2,…,m<n) such that Q is a subgraph of D_i.

Fig. 1 shows an example of subgraph query, where the graph database consists of graphs D1,D2,D3 and D4, and Q is the query graph. Obviously, only graph D3 contains Q

example for tests

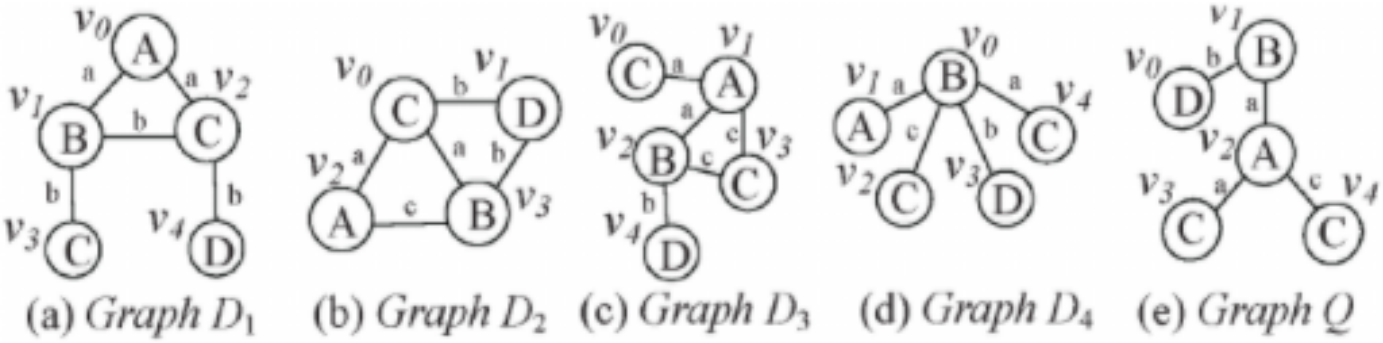


Figure 1. An Example of Subgraph Query. Four labeled graphs (a) *Graph* D_1, (b) *Graph* D_2, (c) *Graph* D_3, and (d) *Graph* D_4 compose the database, and (e) *Graph* Q is a query graph.
doi:10.1371/journal.pone.0097178.g001

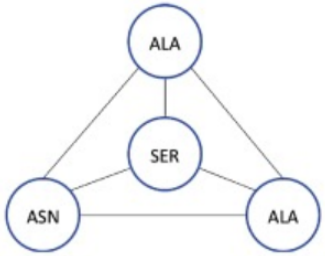
Fast processing of graph queries on a large database of small and medium-sized data graphs,

Dipali Pal, Praveen Rao, Vasil Slavov, Anas Katib,
Journal of Computer and System Sciences, Volume 82, Issue 6, 2016, Pages 1112-1143,
https://doi.org/10.1016/j.jcss.2016.04.002.

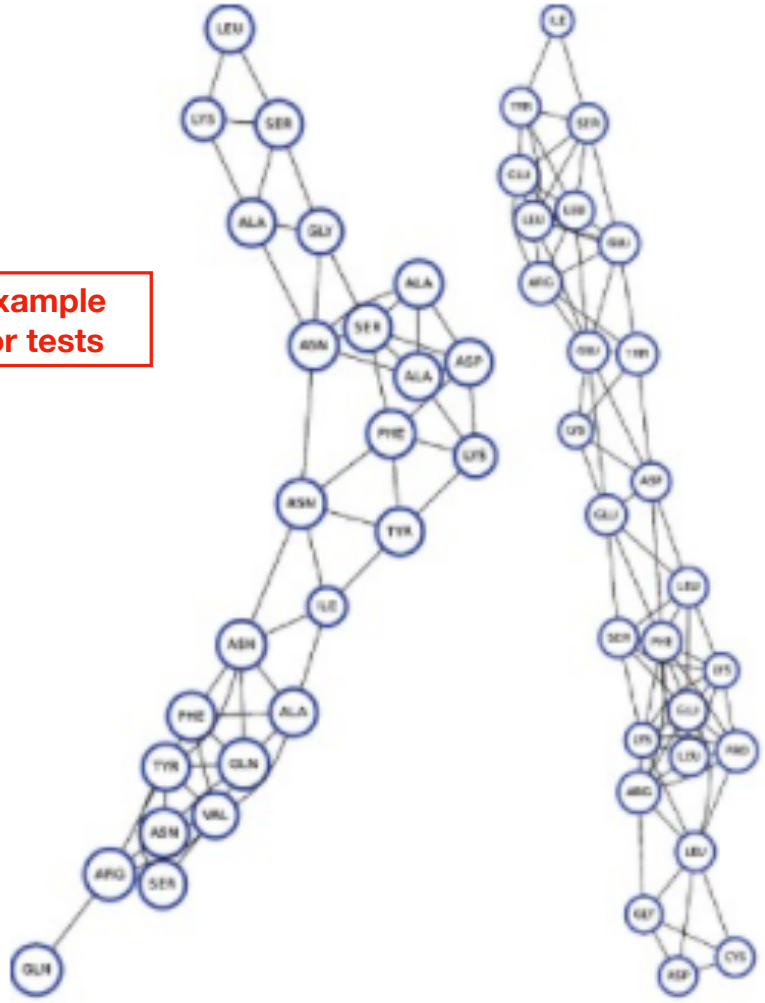
Exact subgraph matching:
Given a query graph Q, an exact subgraph matching query finds all graphs in D that contain a subgraph that is isomorphic to Q.
(This query is also referred to as a subgraph containment query in prior work.)
Approximate (full) graph matching:
Given a query graph Q and a distance threshold d, an approximate graph matching query finds all graphs in D whose edit distance with Q is at most d.

Fig. 1(a), which are ***undirected graphs without edge labels***
and are called contact map graphs [14]. A contact map graph is used to represent the 3D structure of a protein,
where the amino acid residues in the protein are represented by vertices.
An edge exists between two residues if the distance between their c_α atoms is below a particular threshold [14].

an exact subgraph matching queryon the protein contact map graphs in Fig. 1(a) by ALA, SER, ASN, and ALA: only the data graph on the left-hand side of Fig. 1(a) contains a subgraph isomorphic to the query.



example for tests



(a) Protein contact map graphs

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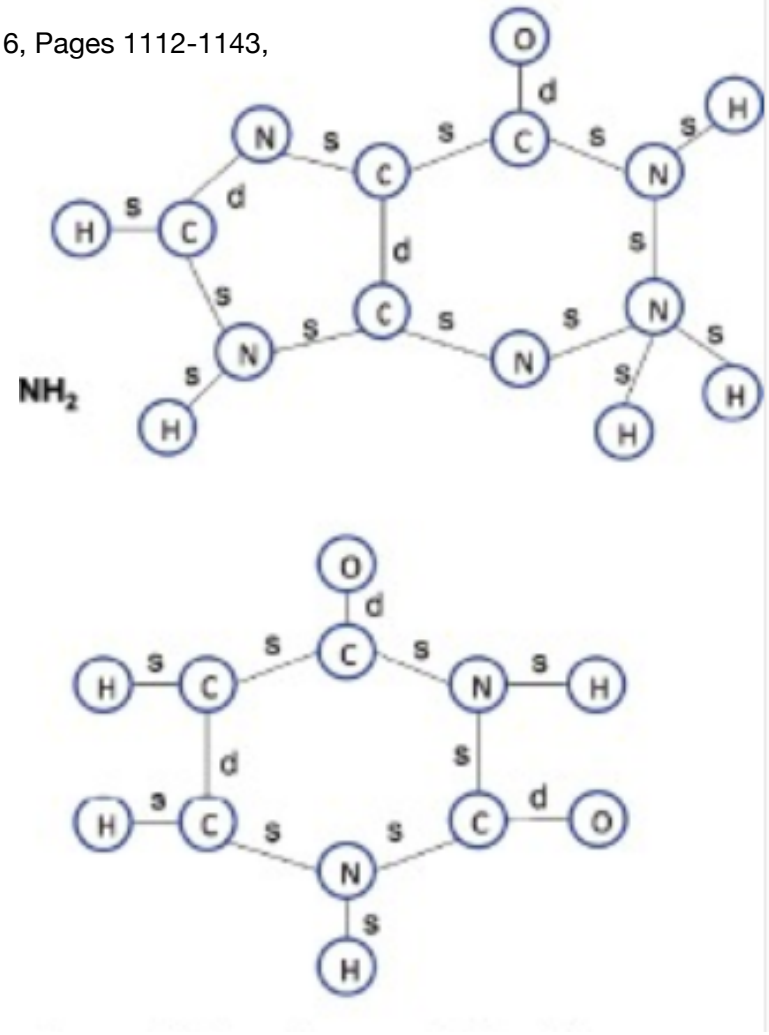
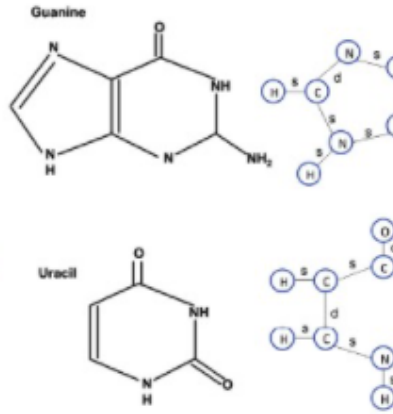
Fig. 1(b), ***undirected graphs with edge labels***
to model chemical compounds such as Guanine and Uracil.
The vertices of each graph denote the atoms in the compound, and the edge labels denote the type of bond between two atoms.

example for tests





(b) Graph representation of Guanine

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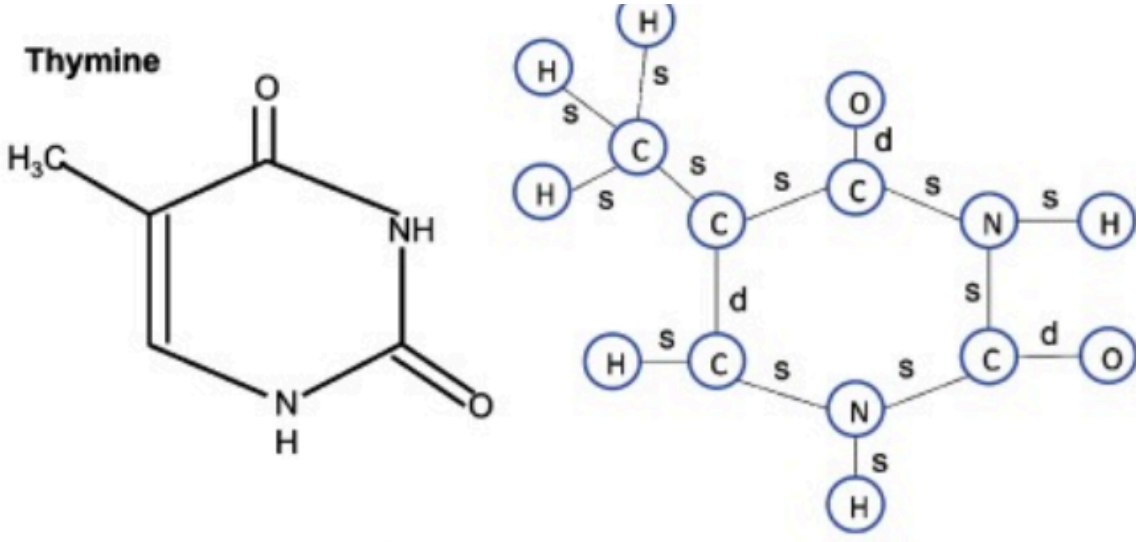
Consider the query in ***Fig. 3(b) for approximate (full) graph matching on the chemical compounds in Fig. 1(b).***
Suppose we want to find the compounds that are similar to Thymine within an edit distance of 7 (assuming unit cost for each edit operation). Uracil shown in Fig. 1(b) is a match for the query as one vertex relabel, three vertex additions, and three edge insertions are needed to transform Uracil to Thymine. Note that Uracil and Thymine belong to a particular family of compounds called Pyrimidine.

example for tests

NOTE: can compare results with Riesen's Graph Matching Toolkit, but the algorithm choices are A-star, A*-beam search, and A*-path length. The later can be used on graphs with |V| > 12.



(b) Approximate (full) graph matching query (chemical compounds)

Fig. 3. Examples of query graphs on real datasets.