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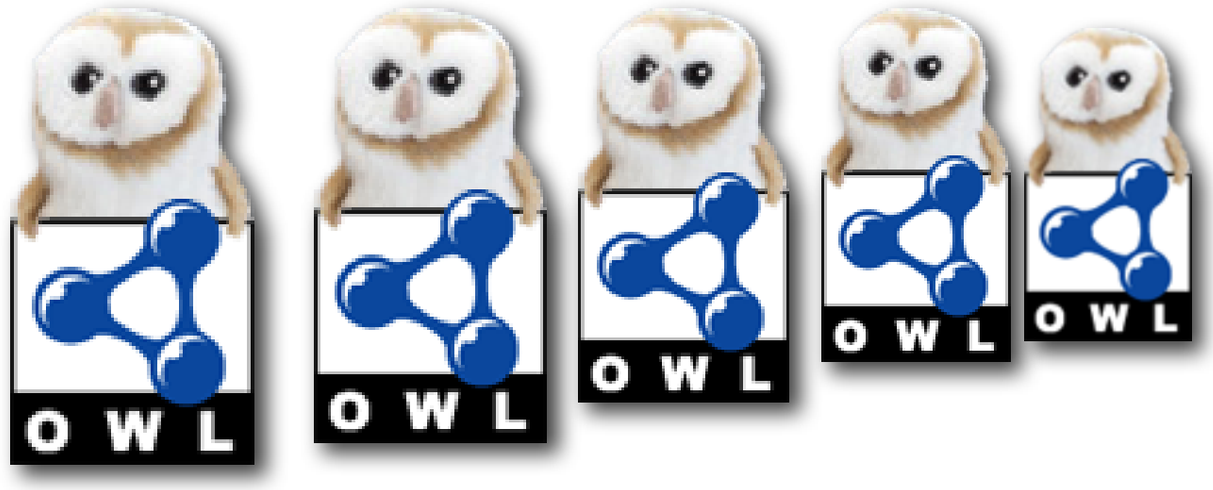
Sequences in OWL

Nick Drummond, A. Rector, G. Moulton, Robert Stevens, M. Horridge, H. Wang, J Seidenberg



JISC

CO ODE cooperative ontologies programme

protégé

NIBHI

BHIG

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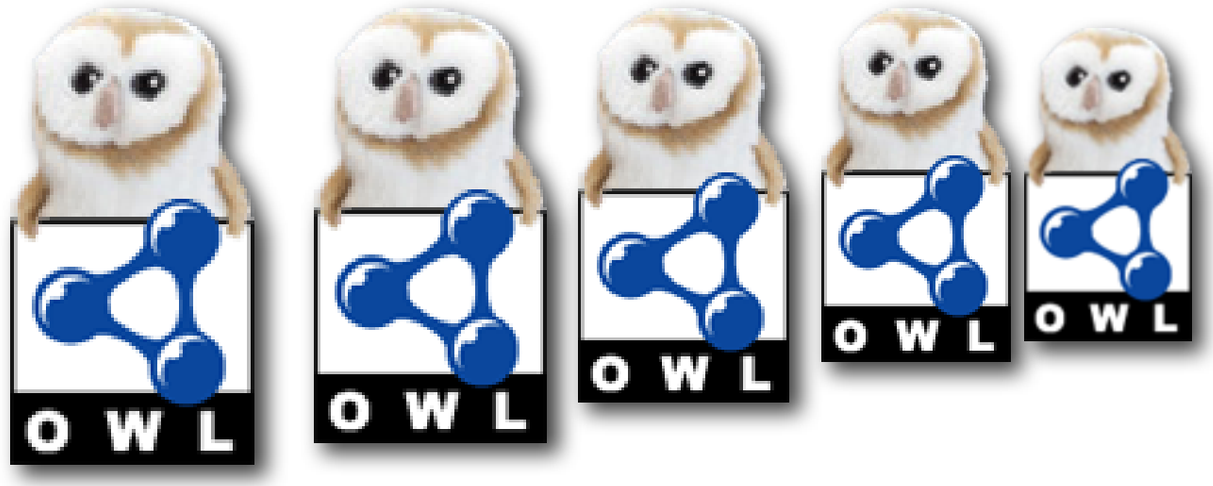

Or “Making reasoners work hard”

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Overview

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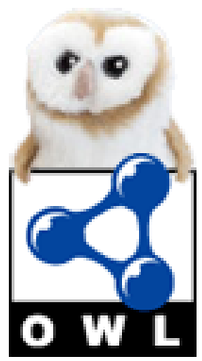

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Overview

- Presentation AND (hasContents SOME **UseCases**) AND
- (hasNext SOME (Presentation AND (hasContents SOME **ListTheory**) AND
- (hasNext SOME (Presentation AND (hasContents SOME **RDFLists**) AND
- (hasNext SOME (Presentation AND (hasContents SOME **OWLLists**) AND
- (hasNext SOME (Presentation AND (hasContents SOME **ProteinSequences**) AND
- (hasNext SOME (Presentation AND (hasContents SOME **AdvantagesAndDisadvantages**) AND
- (hasNext SOME (Presentation AND (hasContents SOME **Conclusion**) AND
- (hasNext SOME EmptyList)))))))))))))

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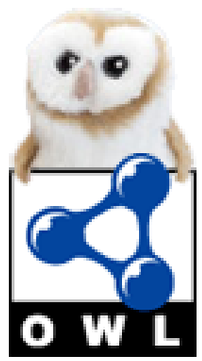

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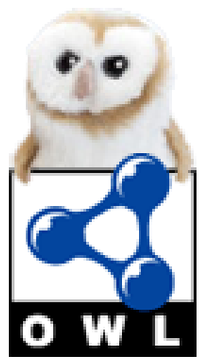
Lists: Use Cases



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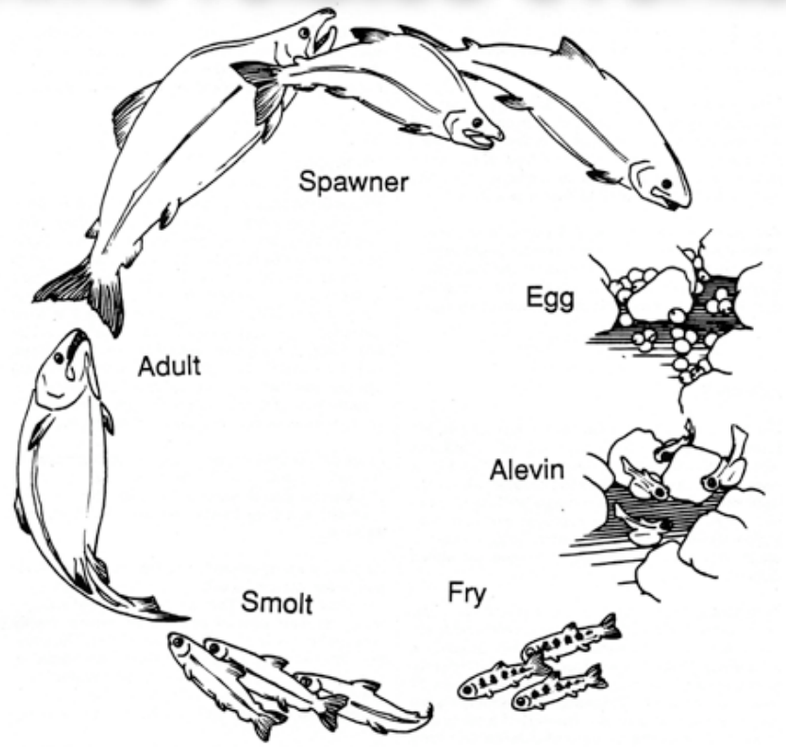
Lists: Use Cases

Time related events



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Lists: Use Cases

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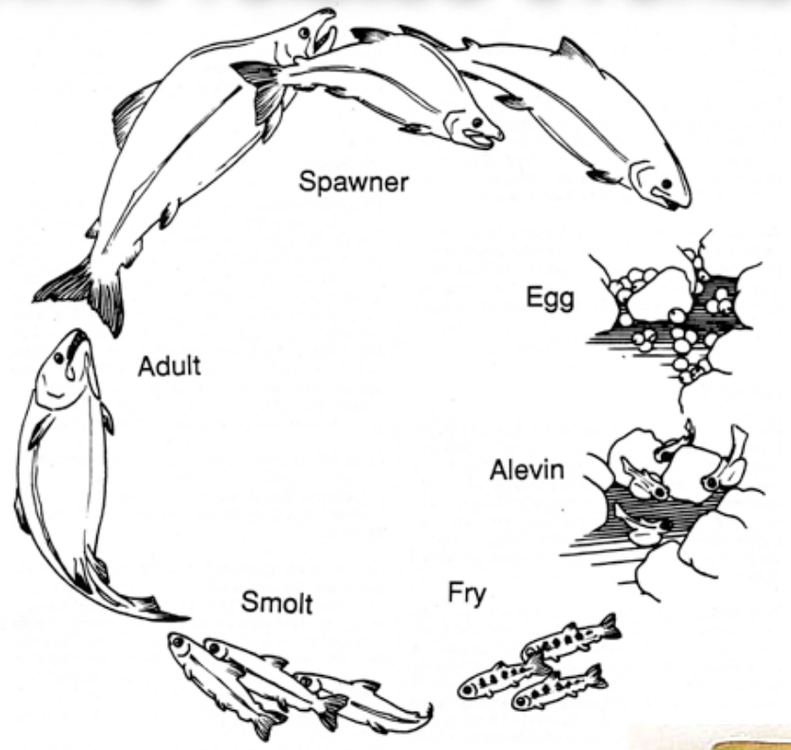
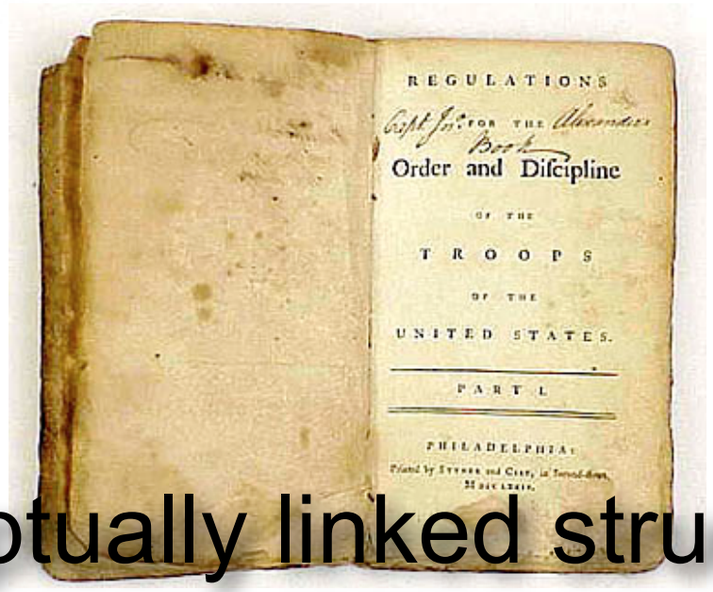


Conceptually linked structures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Lists: Use Cases

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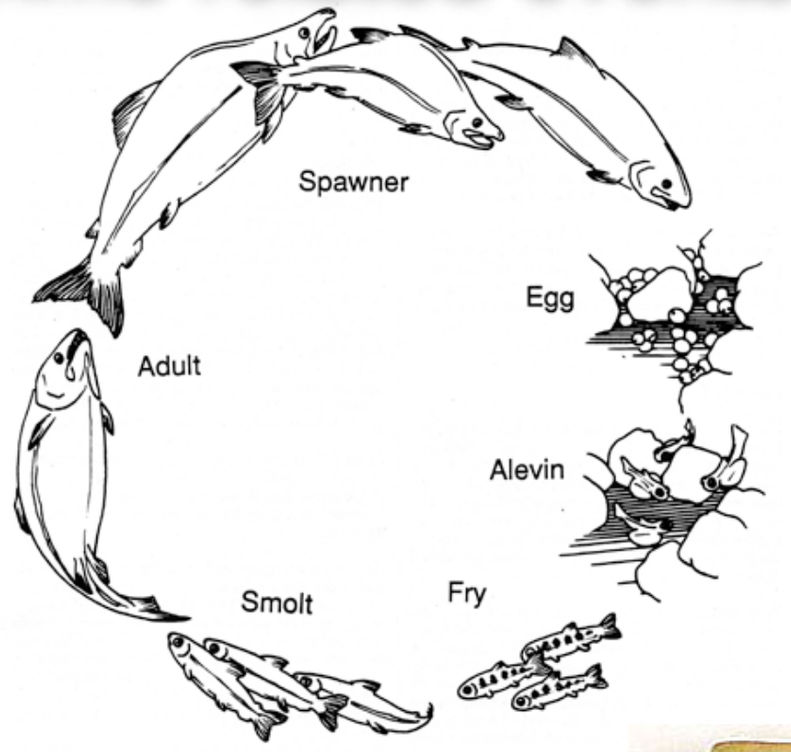
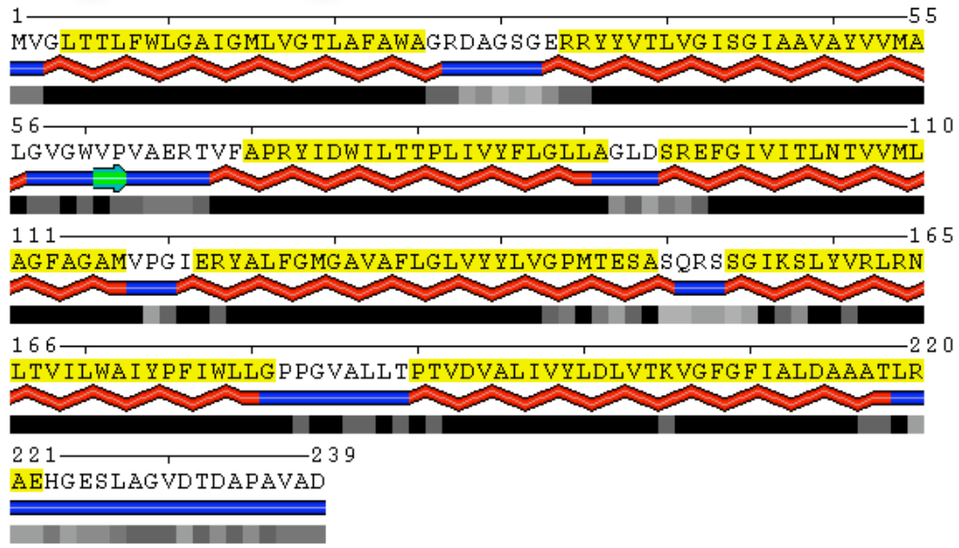
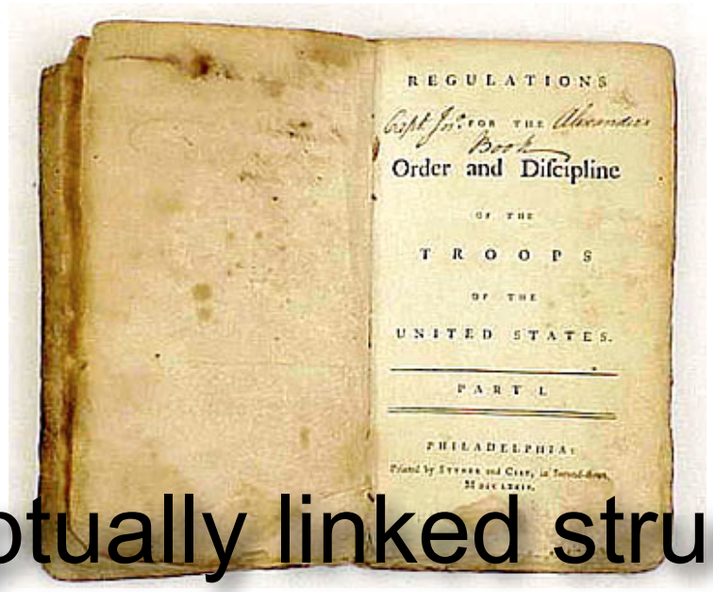


Physically linked structures



Conceptually linked structures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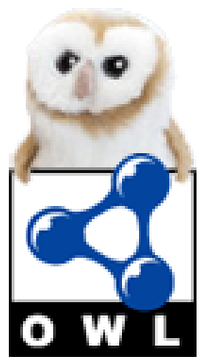
Lists Theory



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Lists Theory

- OWL & RDF Lists use the same idea

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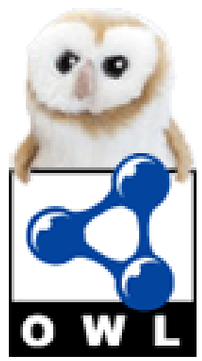

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Lists Theory

- OWL & RDF Lists use the same idea
- A head, followed by by a tail (sublist)

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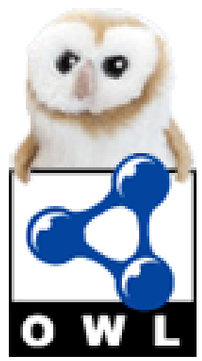

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A B C nothing

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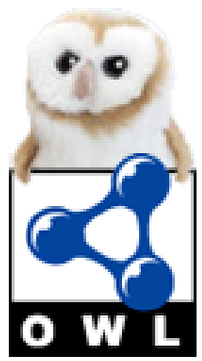

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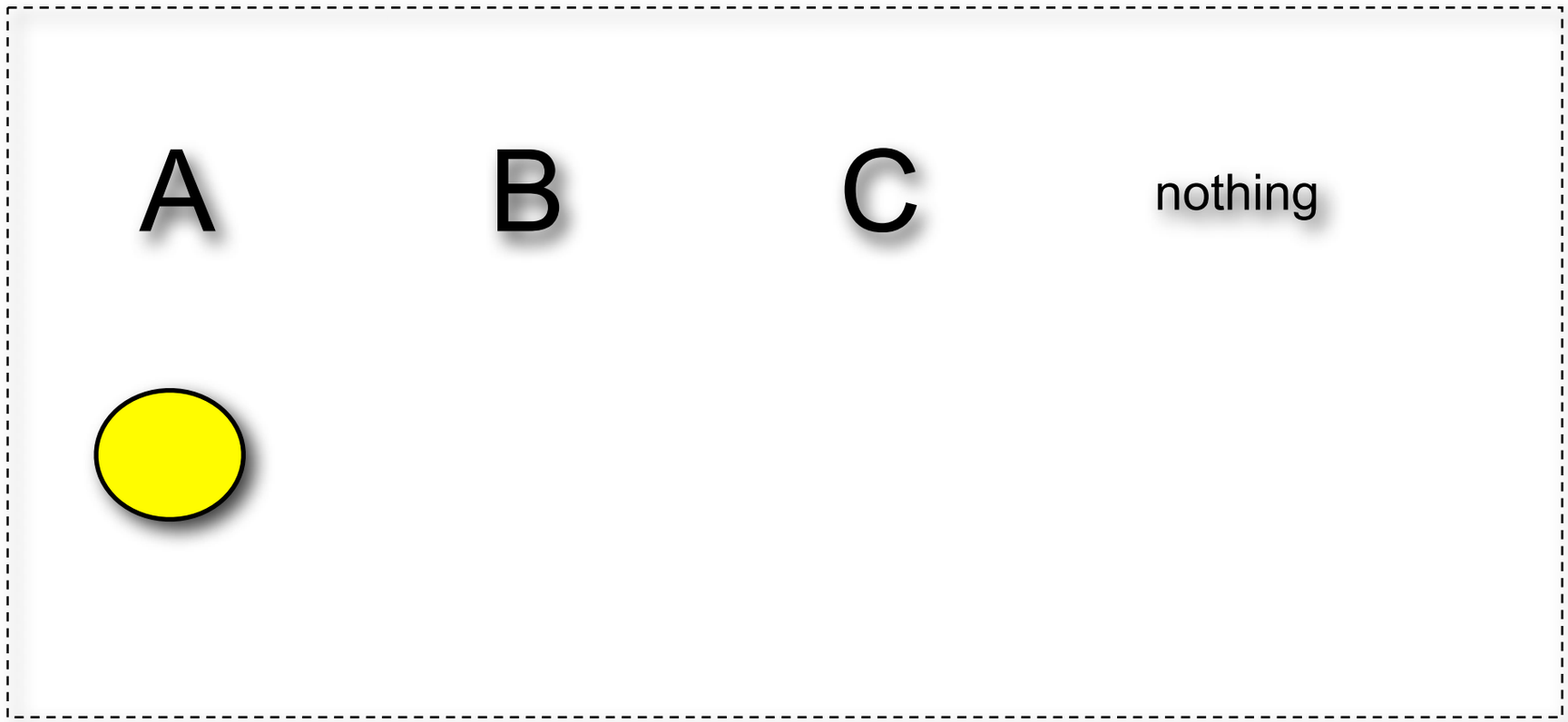

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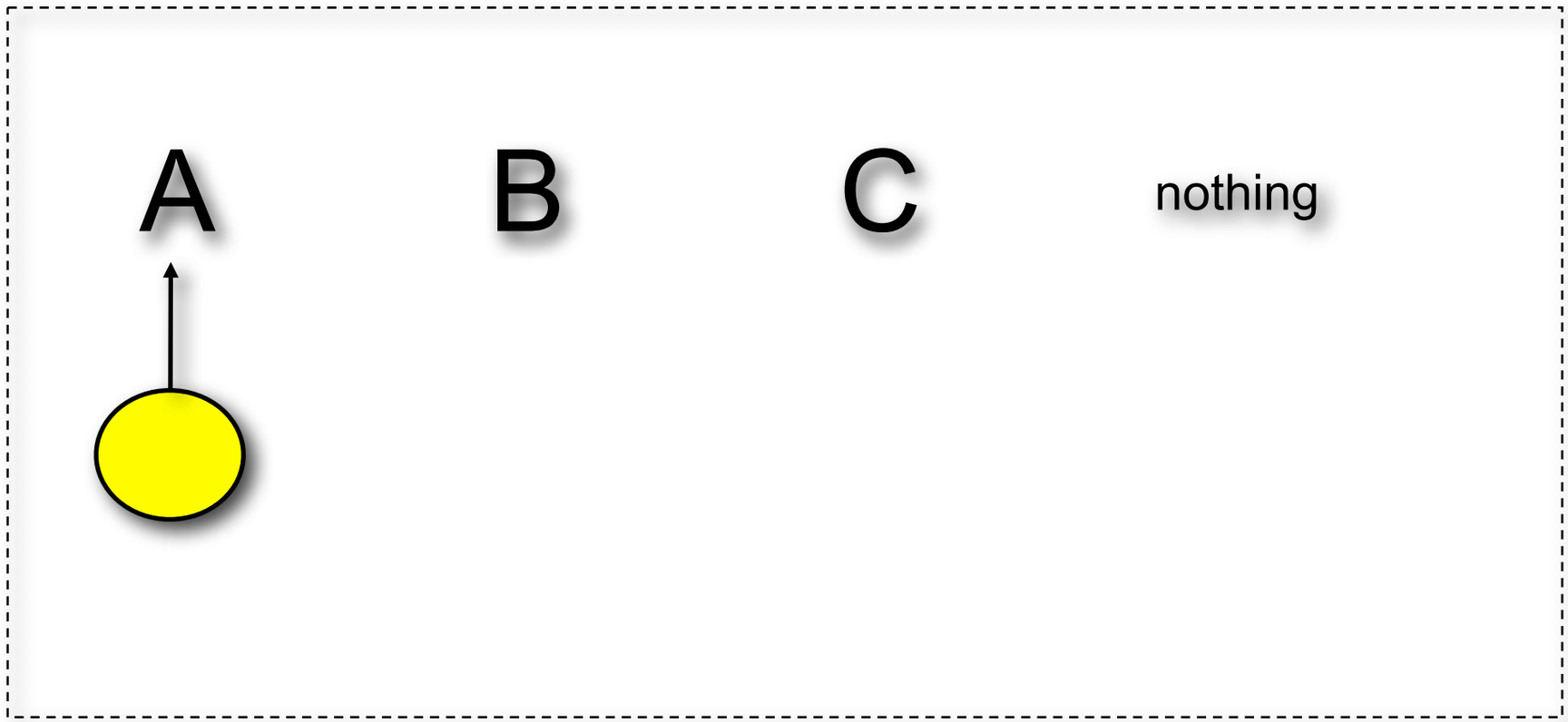

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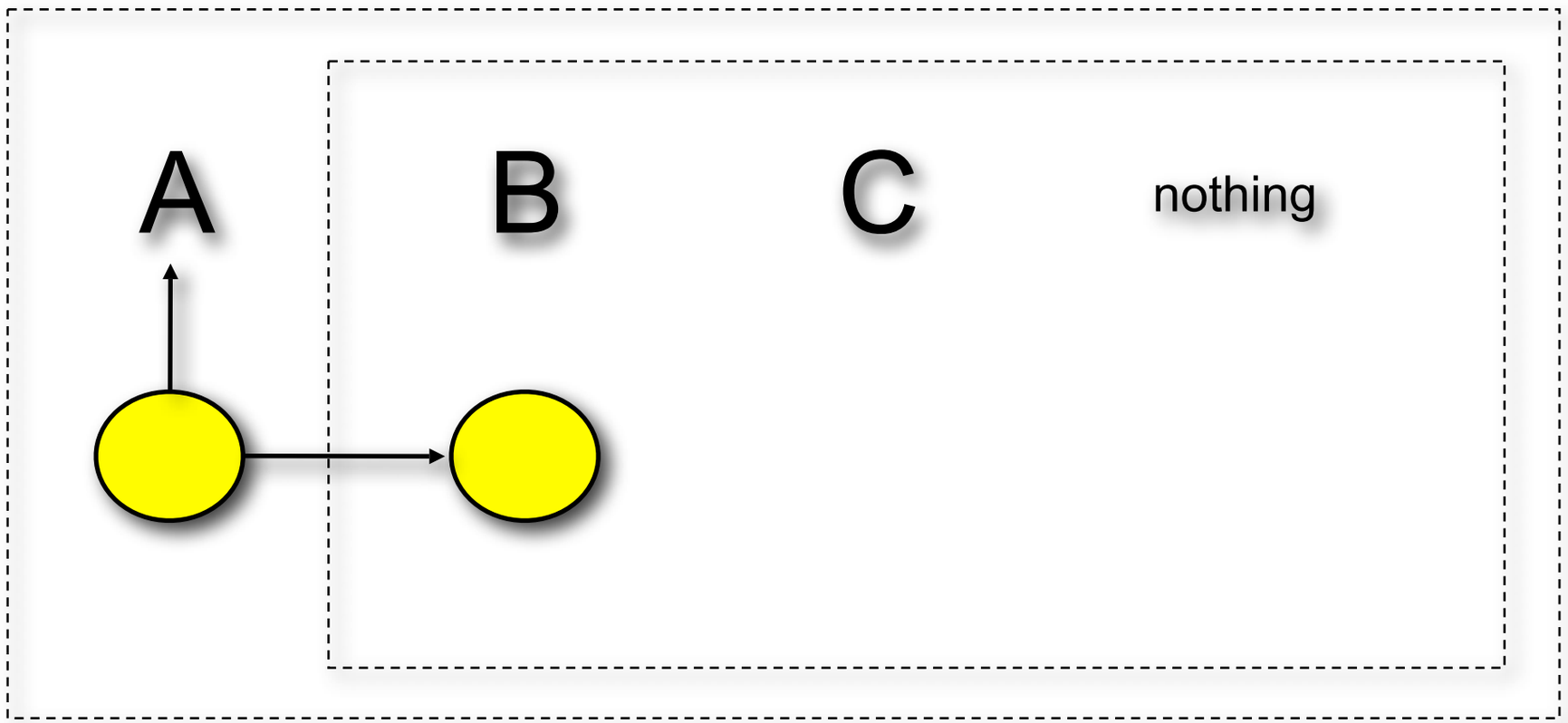

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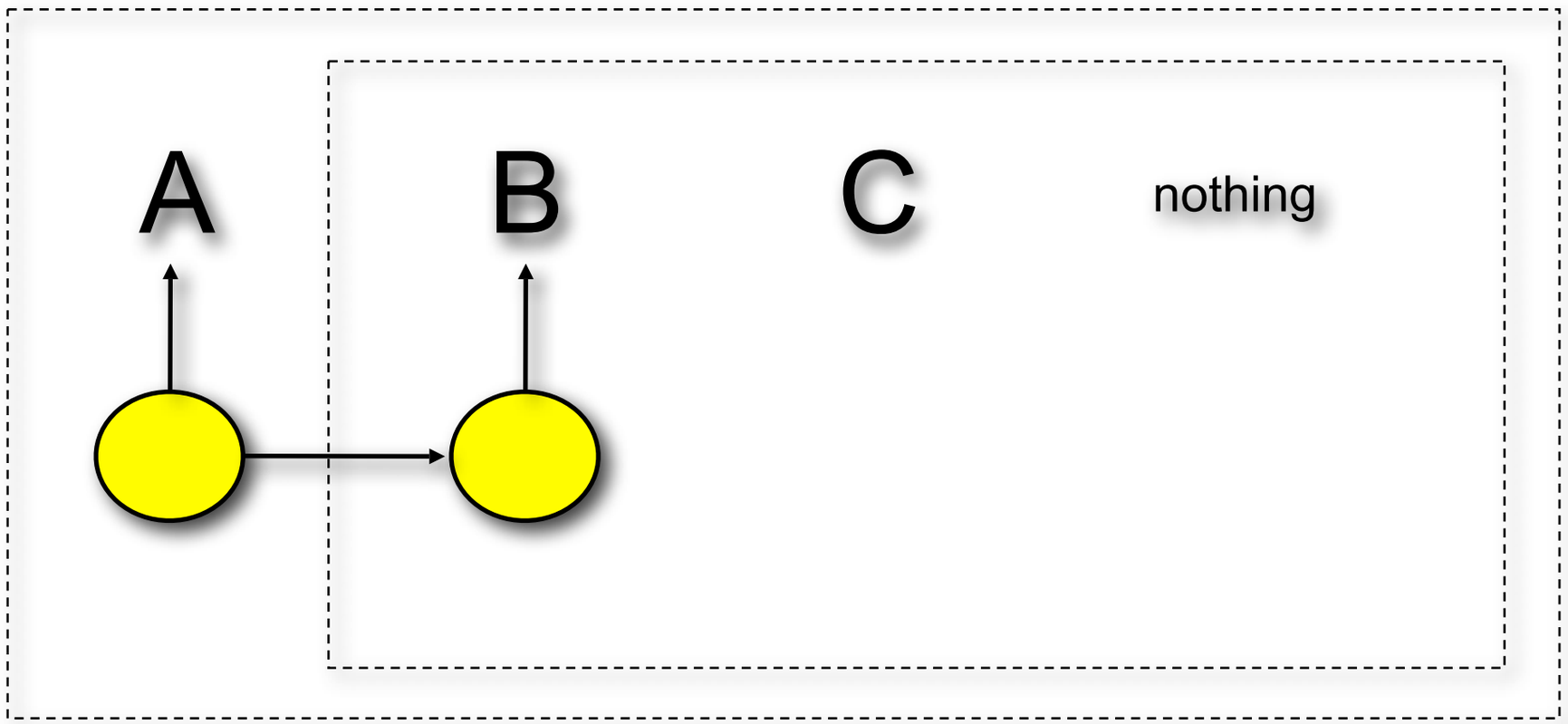

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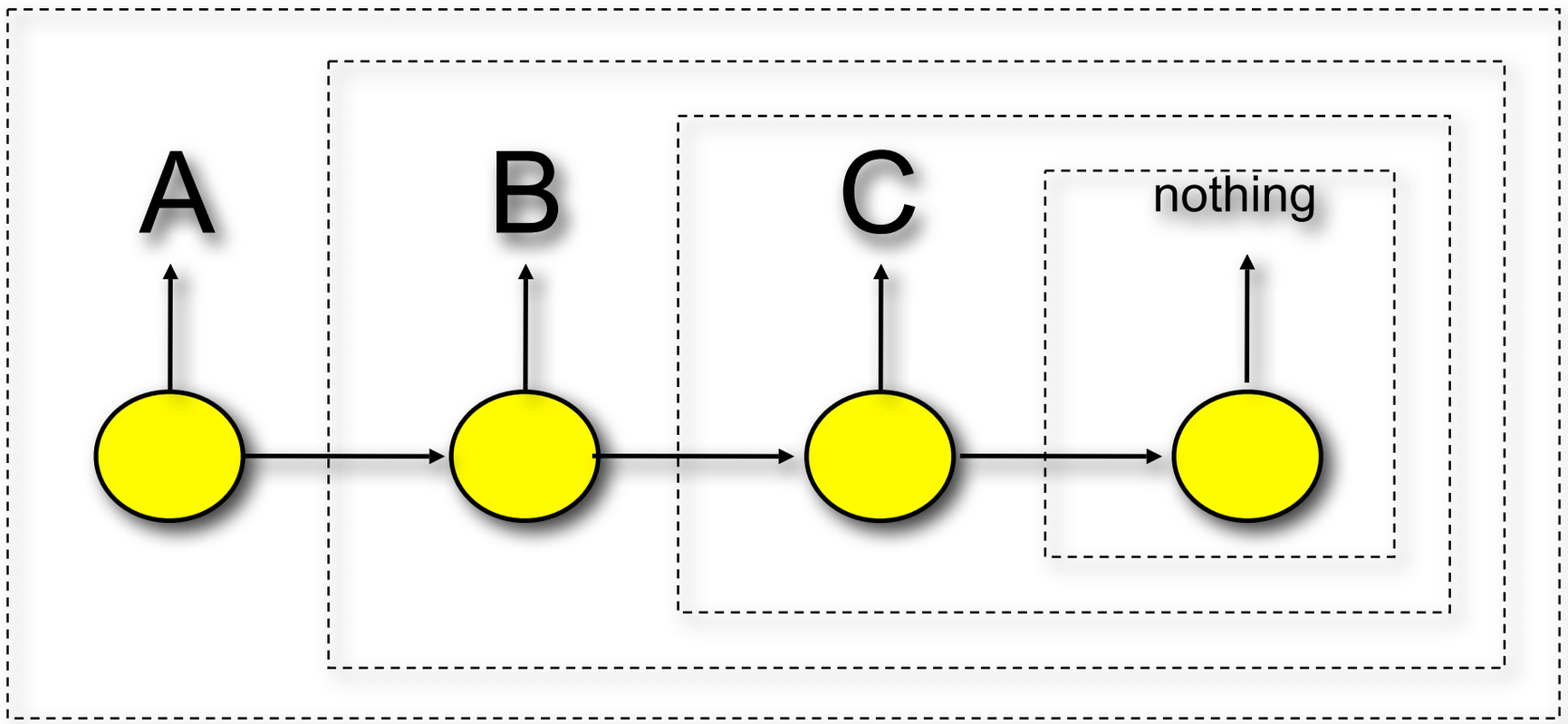

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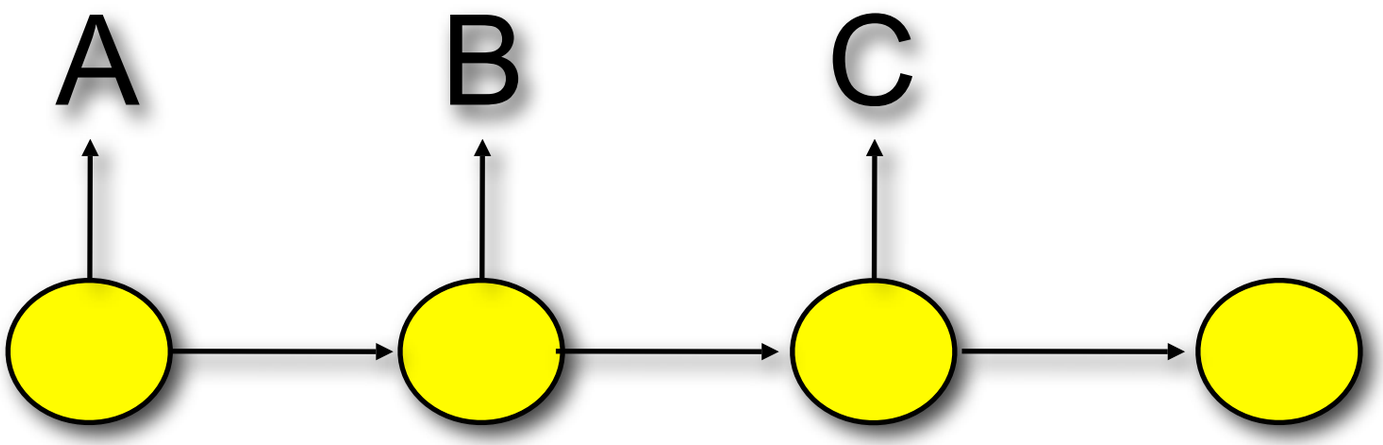
RDF Lists



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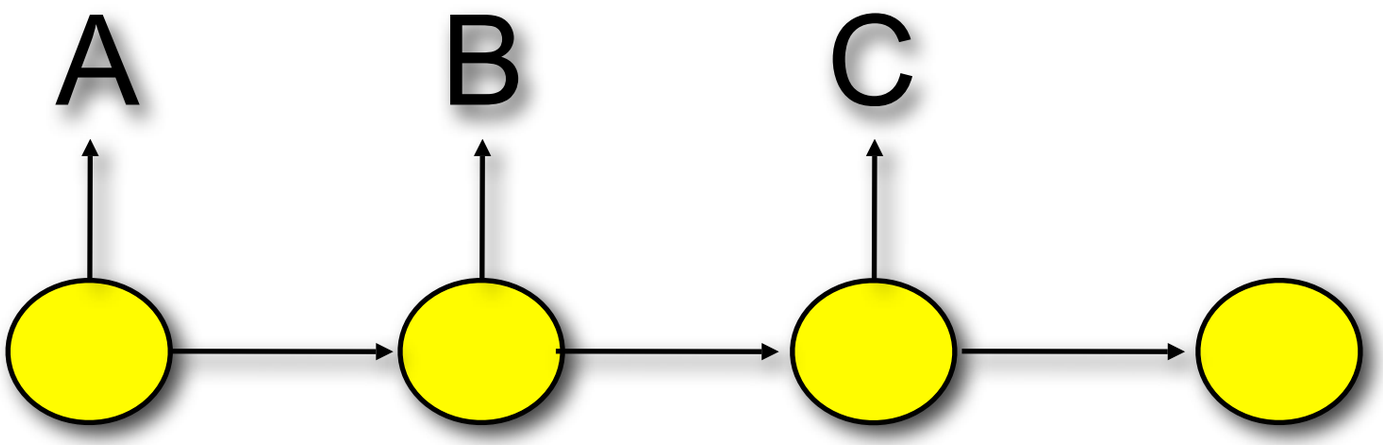
RDF Lists

Constructs are:



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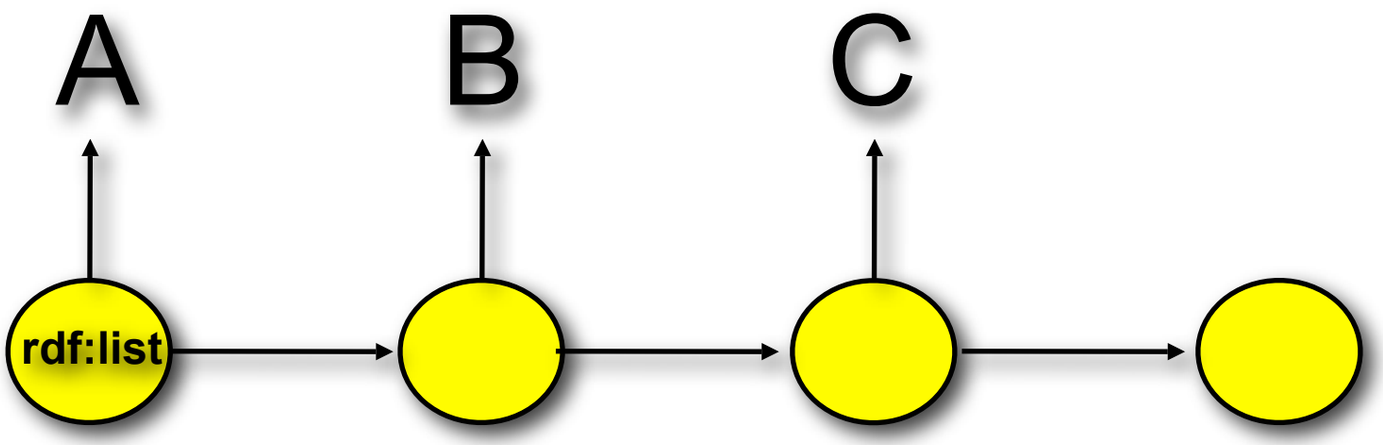
RDF Lists

Constructs are:

- **rdf:list** – the list itself (can be thought of as the list element)



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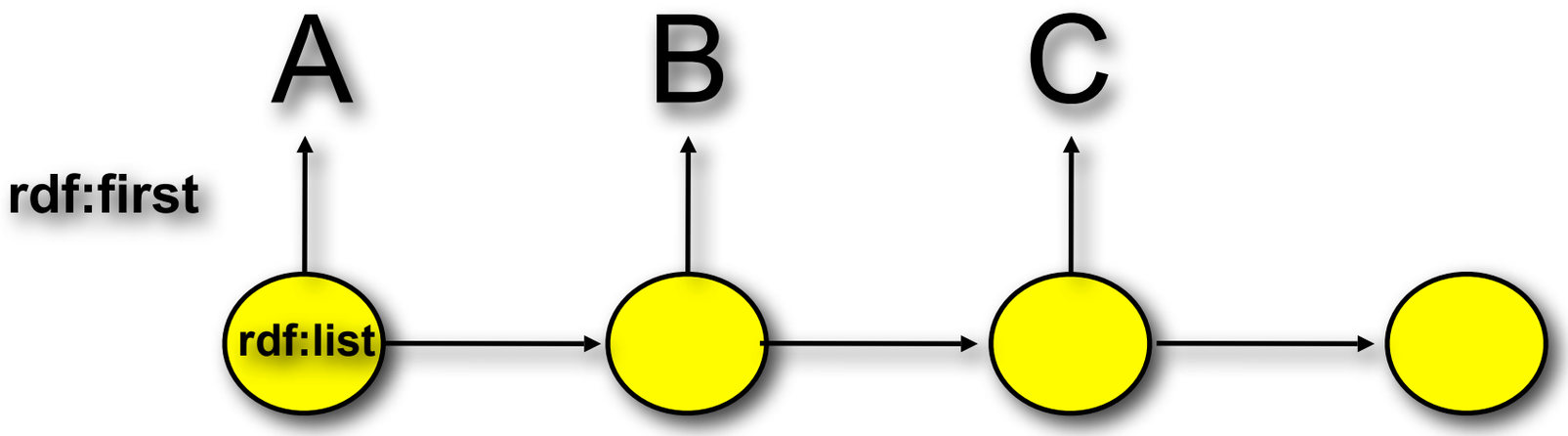
RDF Lists

Constructs are:

- **rdf:list** – the list itself (can be thought of as the list element)
- **rdf:first** – a pointer to the head of the list



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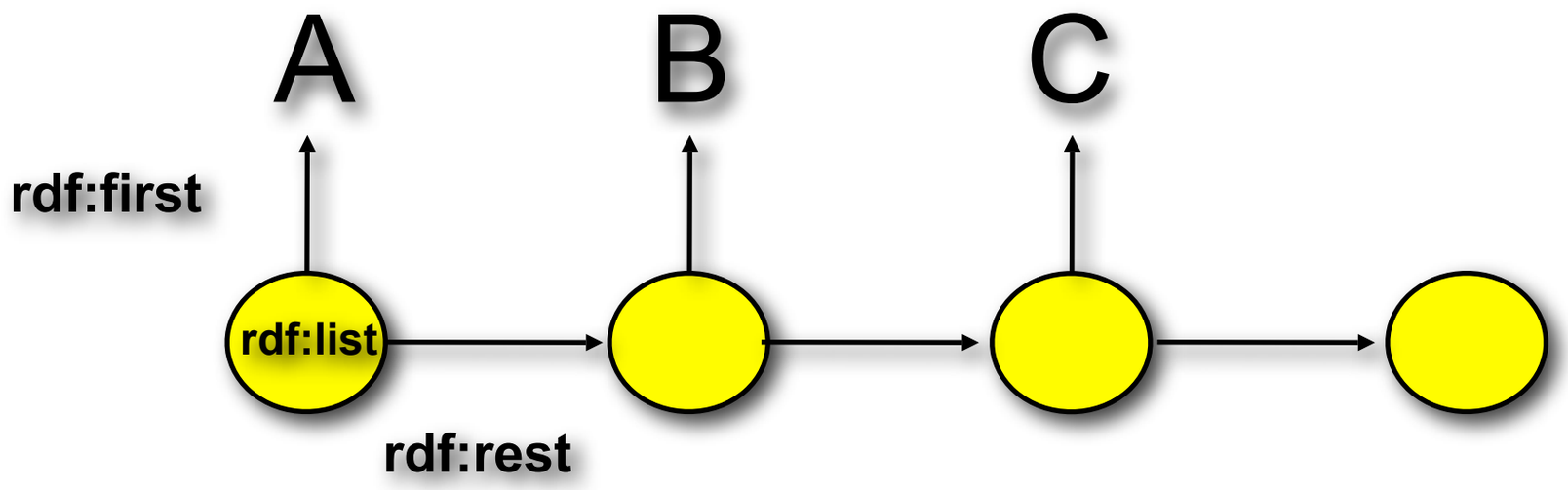

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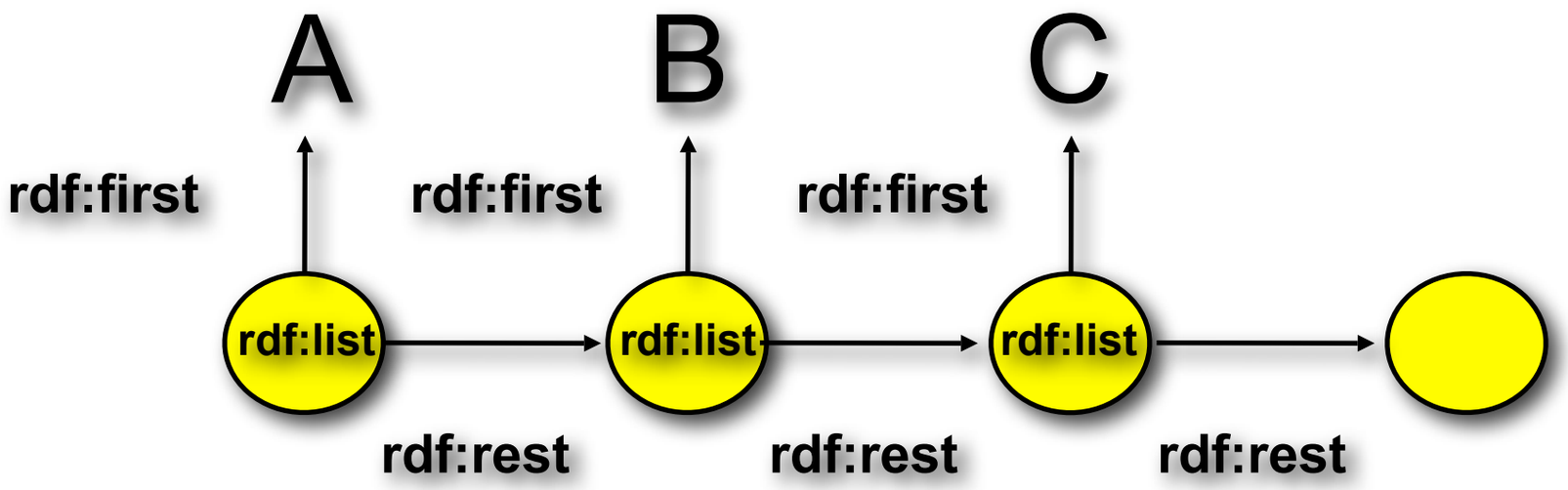

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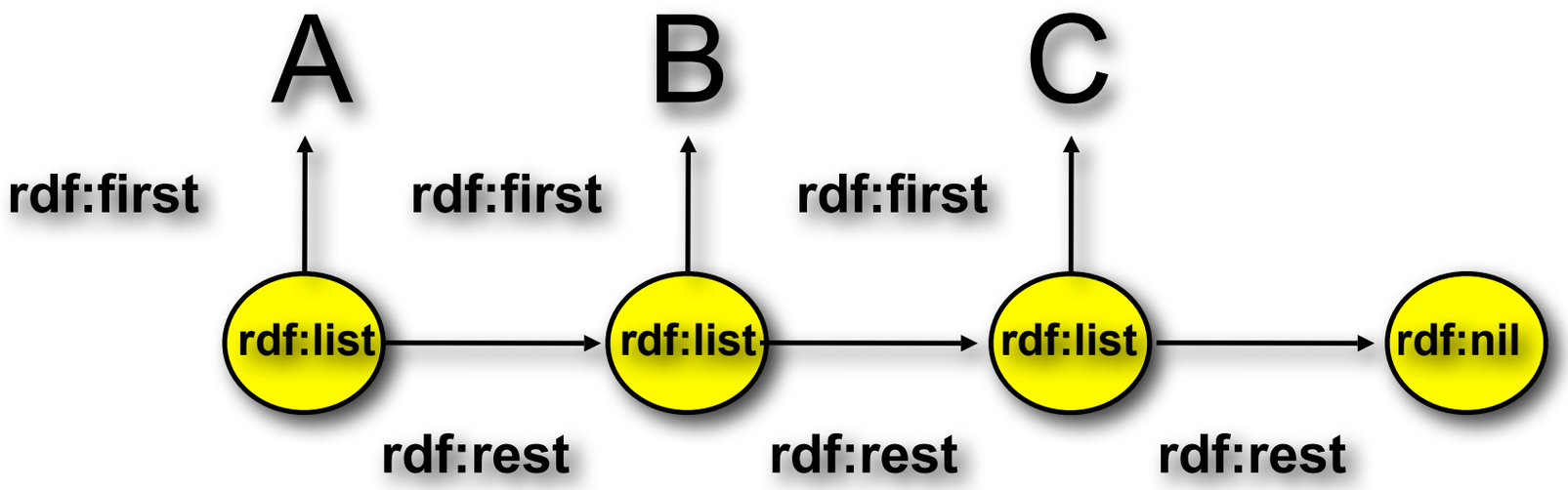
- **rdf:nil** – an rdf:list containing no other elements (terminator)



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RDF Lists: Example

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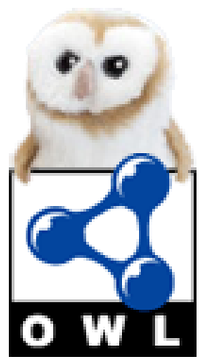

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RDF Lists: Example

- The closed list ABC:

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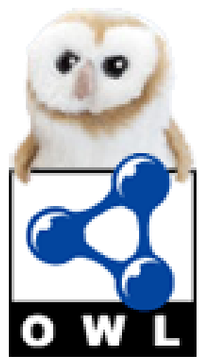

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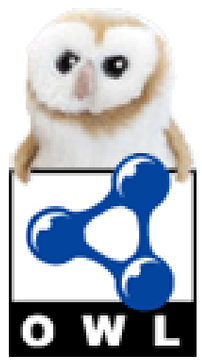

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RDF Lists: Example

- The closed list ABC:

rdf:list (rdf:first A

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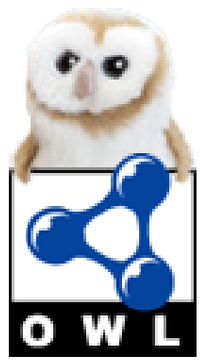

RDF Lists: Example

- The closed list ABC:

```
rdf:list (    rdf:first A
              rdf:rest rdf:list (        rdf:first B
```

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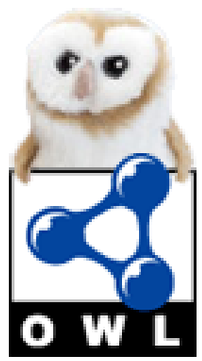

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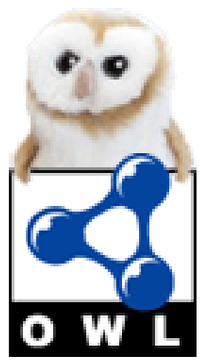

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RDF Lists: Example

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rdf:list (    rdf:first A
              rdf:rest rdf:list (      rdf:first B
                                       rdf:rest rdf:list (      rdf:first C
                                                                rdf:rest rdf:nil)))
```

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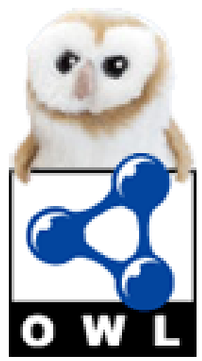

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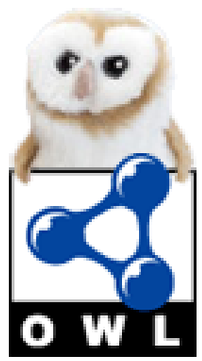

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                                       rdf:rest rdf:list (      rdf:first C
                                                                rdf:rest rdf:nil)))
```

- Without the nil, this would be an open list ie one that starts with ABC

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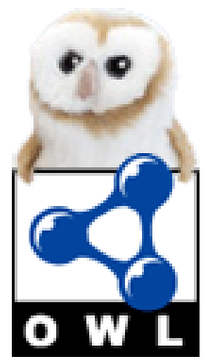

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OWL Ordering Support

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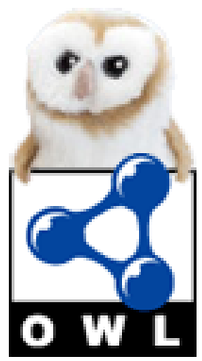

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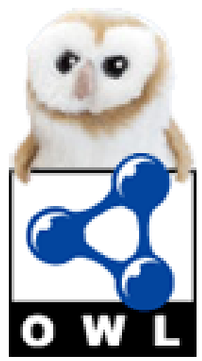
OWL Ordering Support

- There is no inbuilt ordering in OWL



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OWL Ordering Support

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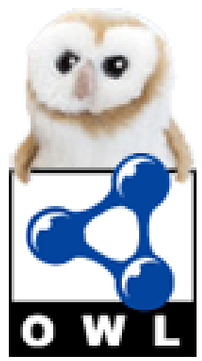

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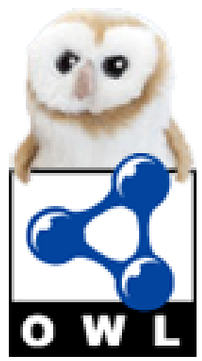

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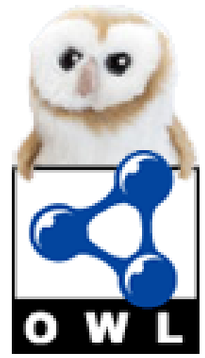

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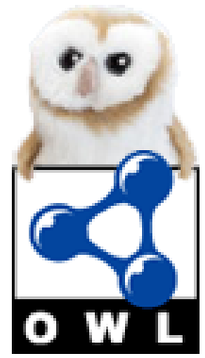

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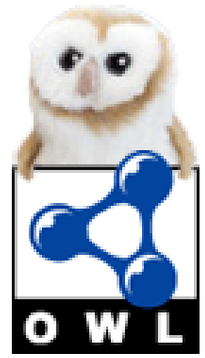

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OWL Lists: Constructs

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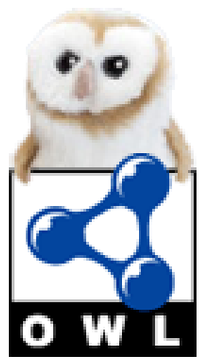

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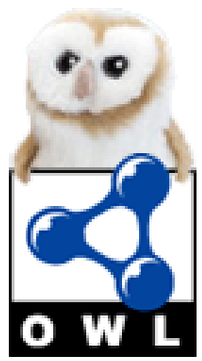

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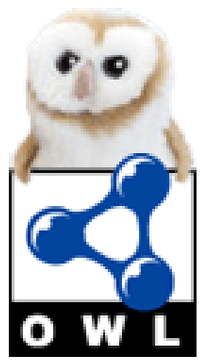

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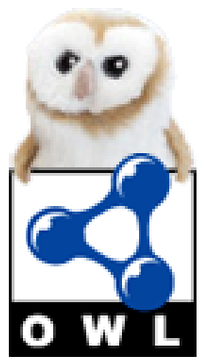

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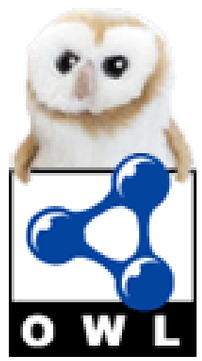

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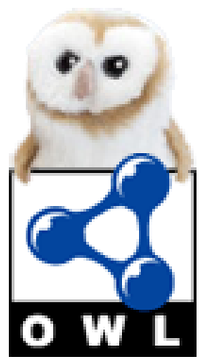

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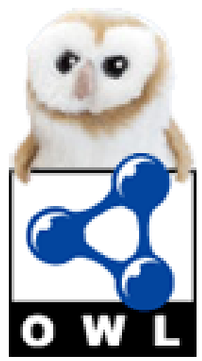

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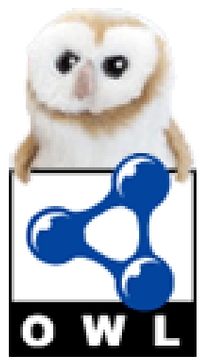

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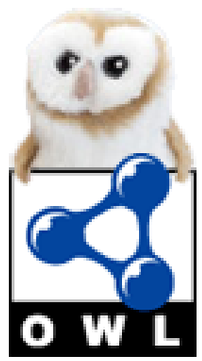

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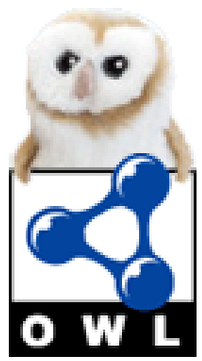
- NB domain of properties is OWLList



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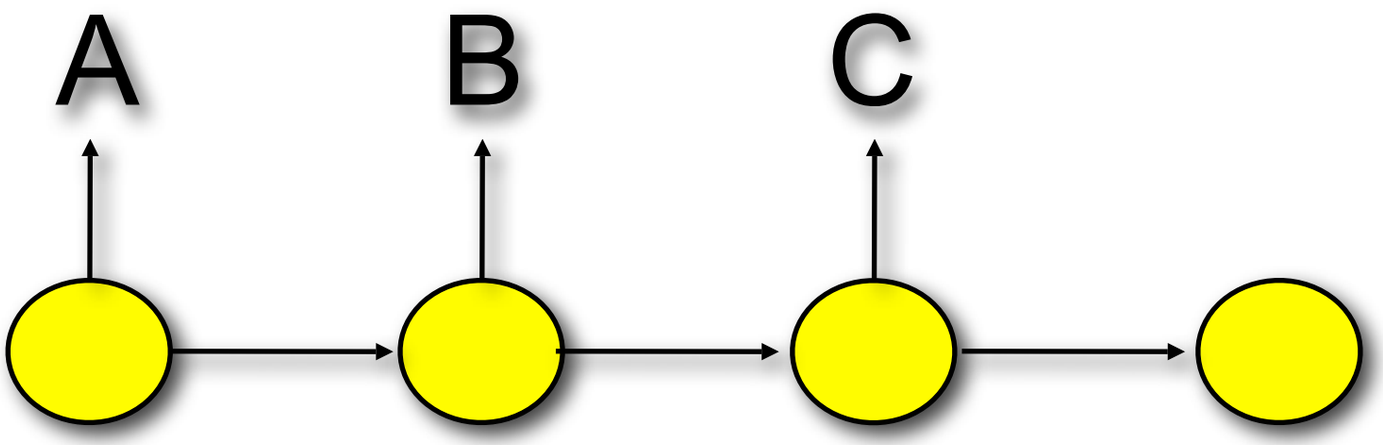

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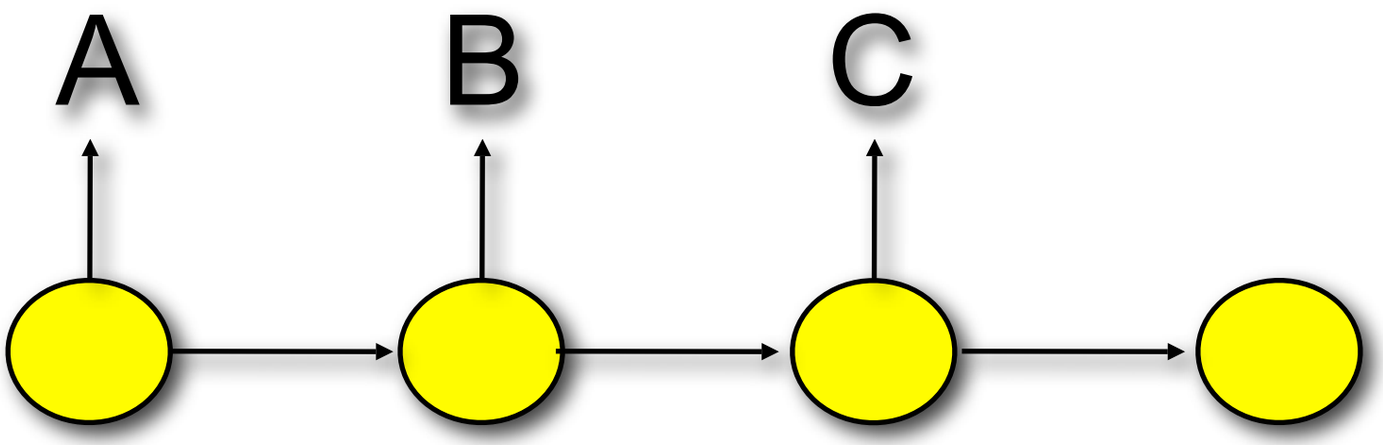

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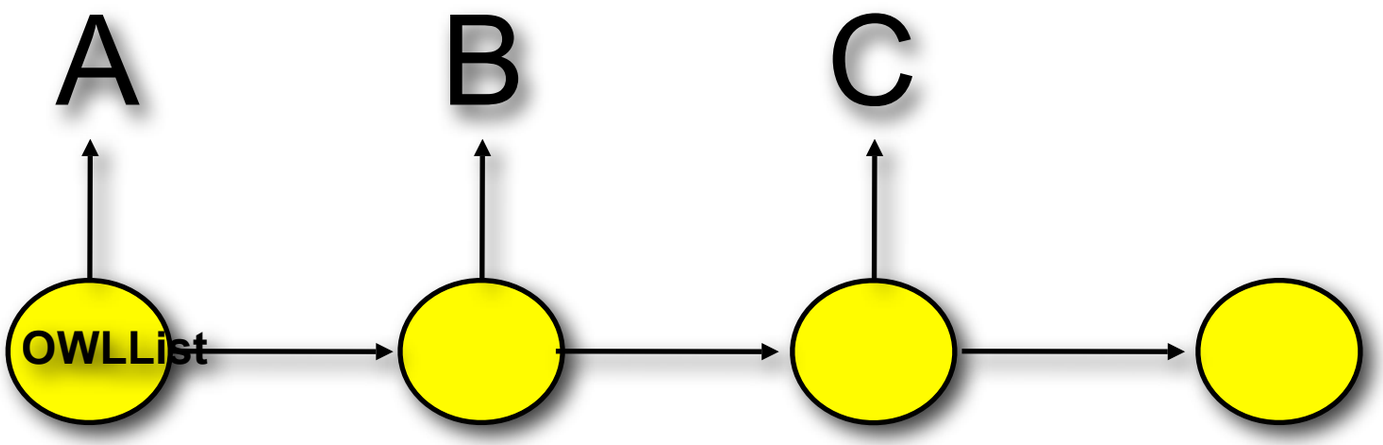

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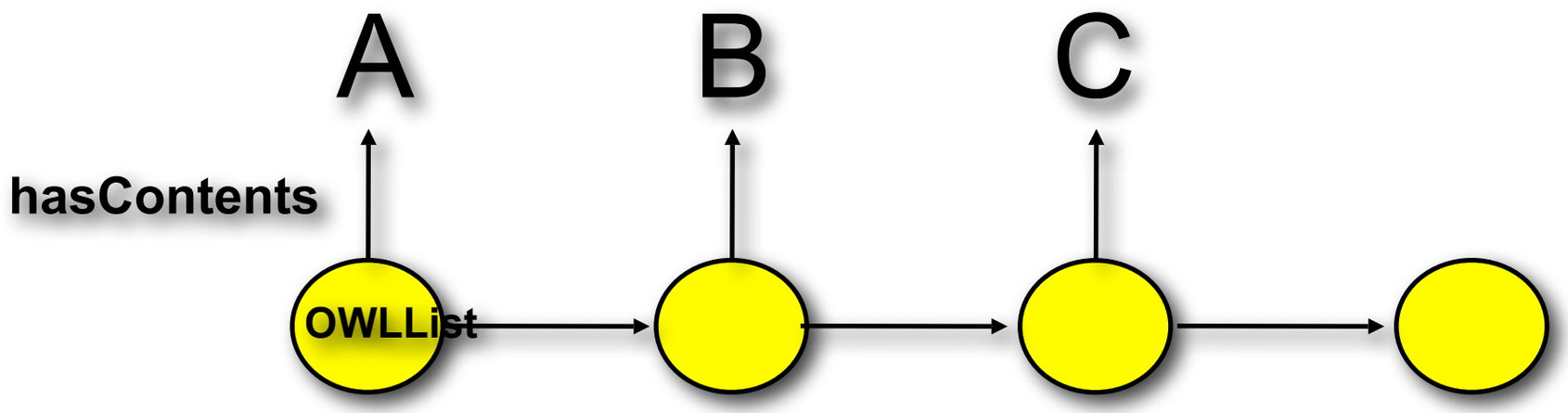

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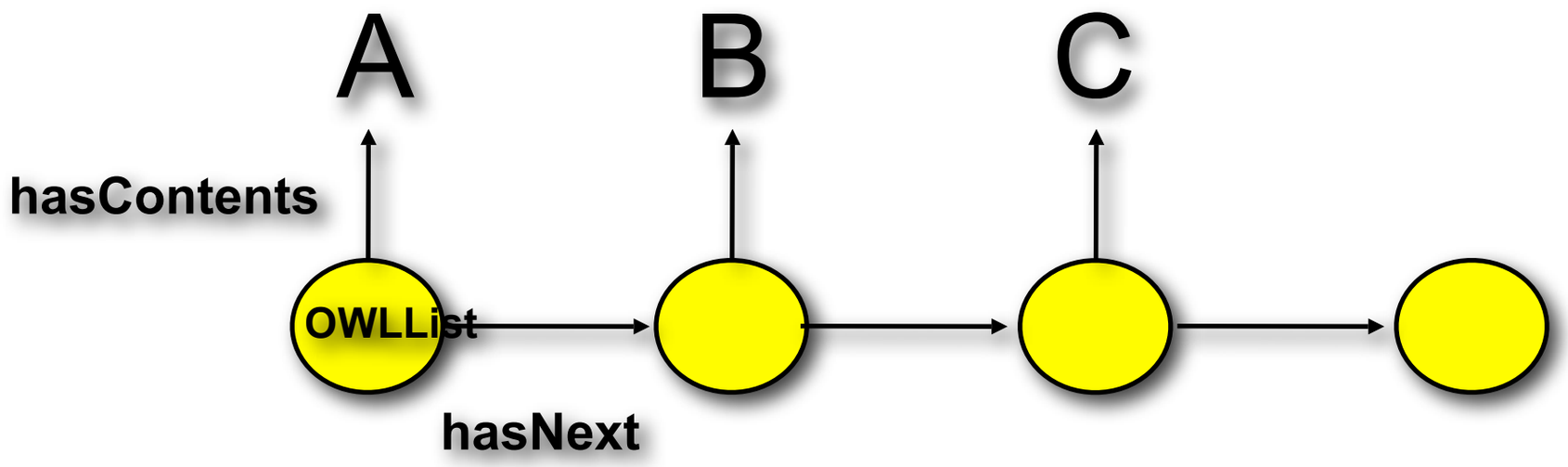

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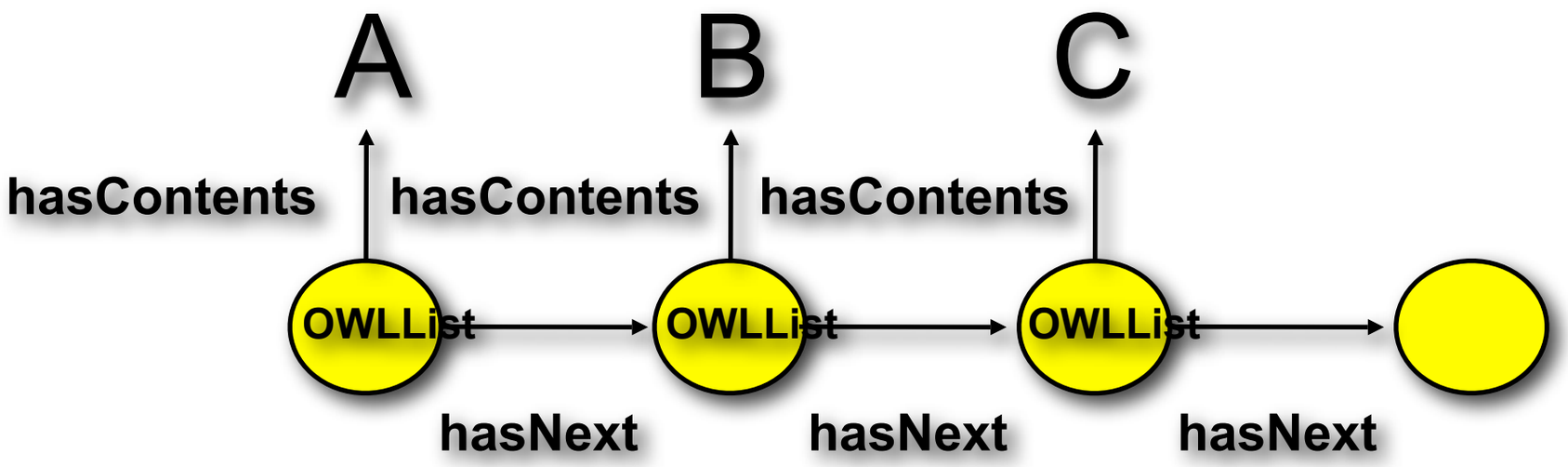

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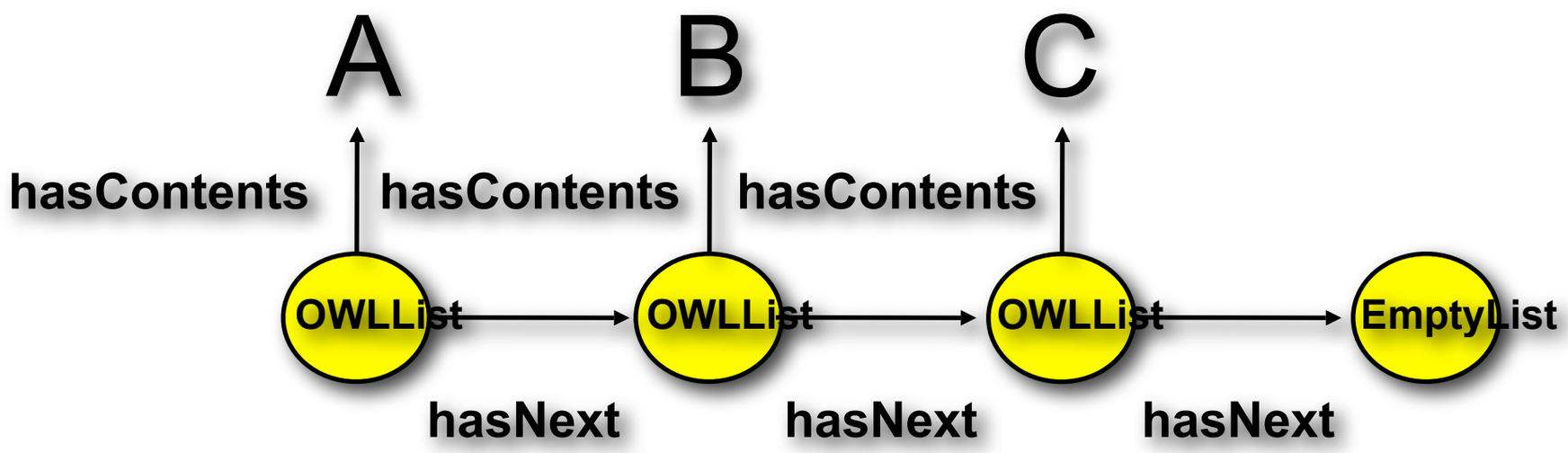

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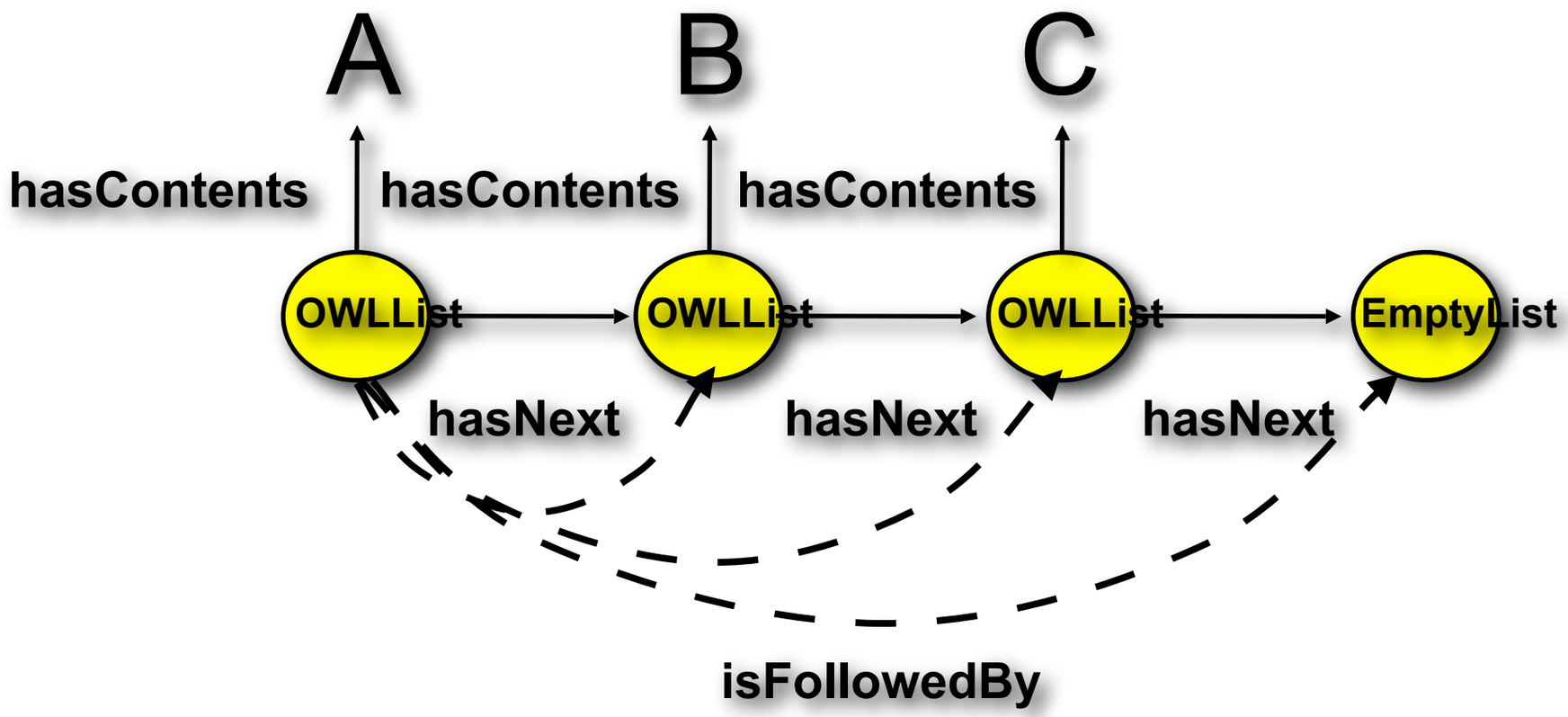
- **isFollowedBy** - transitive hasNext - for inferring indirect following elements



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OWL Lists: Example

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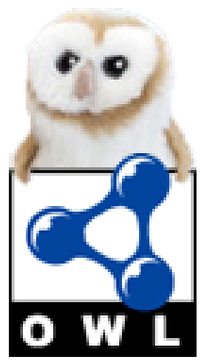

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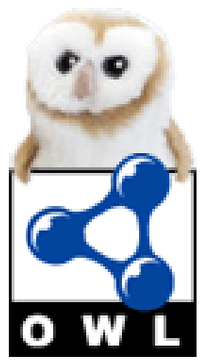

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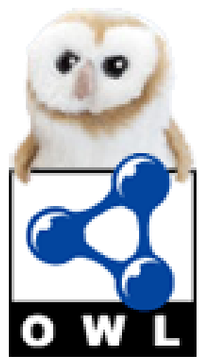

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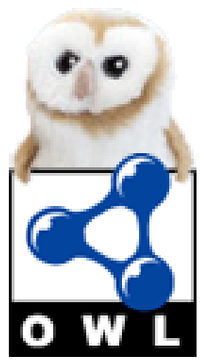

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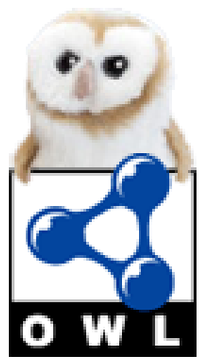

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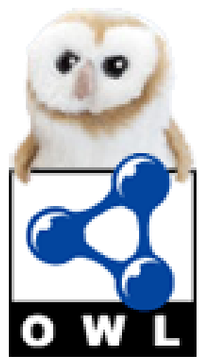

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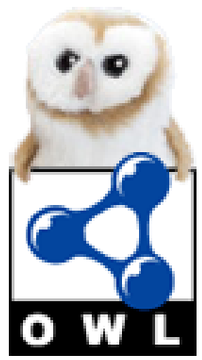

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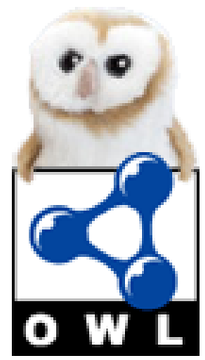

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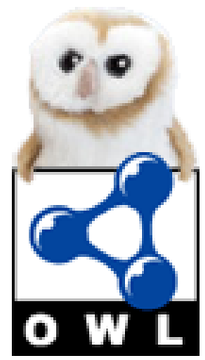
Eg ABC - isFollowedBy some (List and hasContents some C)



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OWL Lists: Expressivity

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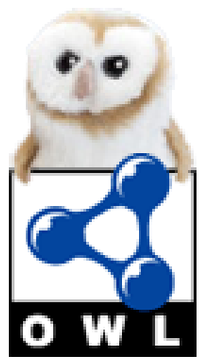

OWL Lists: Expressivity

- What can we express?

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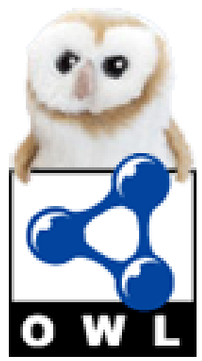

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- What can we express?
  - seqA exactly matches seqB

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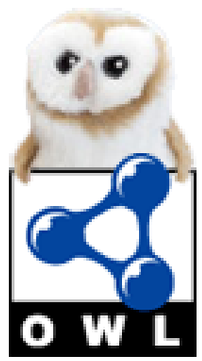

OWL Lists: Expressivity

- What can we express?
  - seqA exactly matches seqB
  - seqA contains seqB

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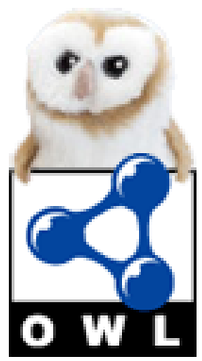

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OWL Lists: Expressivity

- What can we express?
  - seqA exactly matches seqB
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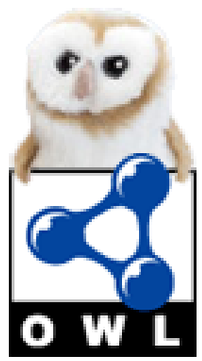

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- What can we express?
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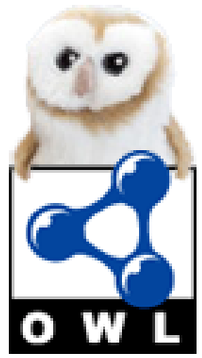

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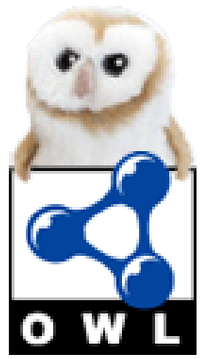

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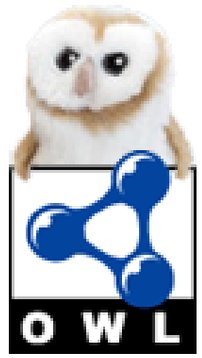

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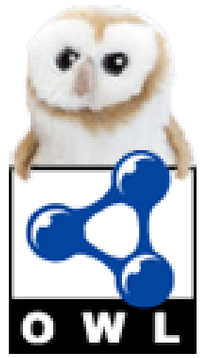

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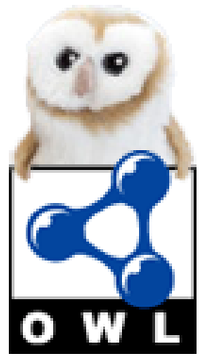

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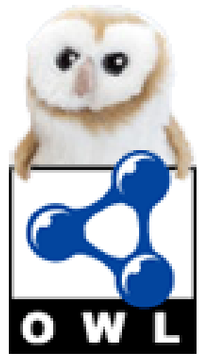

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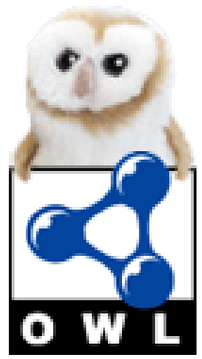

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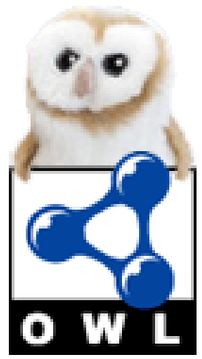
    - eg seqA starts with seqB and ends with seqC
  - Elements can be any arbitrary OWL expression
    - unions, restrictions etc



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Motivating case: Protein Seqs

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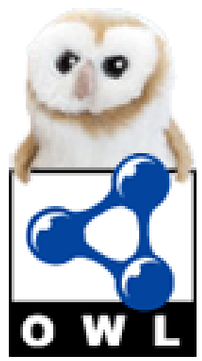

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F26_YEAST Fructose-2,6-bisphosphatase:

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LKDICEKNNIQPMFLESWSNDHELIINNAKDIGSTSPDY
ENSEPHVAEADFLERIRQYERFYEPLDPQKDKDMTFIKL
VNIIEEVVINKIRTYLESRIVFYVMNIRPKPKYIWLSRHGE
SIYNVEKKIGGDSSLSERGFQYAKKLEQLVKESAGEINL
TVWTSTLKRTQQTANYLPYKKLQWKALDELDAGVCDG
MTYEEIEKEYPEDFKARDNDKYEYRYRGGESYRDVVIR
LEPVIMELERQENVLIITHQAVLRCIYAYFMNVPQEESP
WMSIPLHTLIKLEPRAYGTKVTKIKANIPAVSTYKEKGTS
QVGELSQSSTKLHQLLNDSPLEDKF

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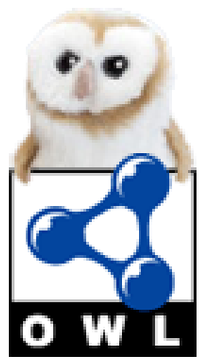

Motivating case: Protein Seqs

- Biologists want to classify proteins by recognising parts of the sequence that are similar to parts of other sequences

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Motivating case: Protein Seqs

- Biologists want to classify proteins by recognising parts of the sequence that are similar to parts of other sequences
- Identifiable parts of the sequence are **motifs**

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Motifs (Pattern Matching)

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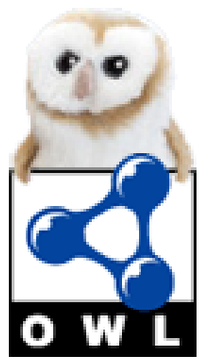

Motifs (Pattern Matching)

- An identifiable part of a protein sequence

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Motifs (Pattern Matching)

- An identifiable part of a protein sequence
- A simple example:
  [IV]-A-[VI]-F-D-A-T-N-[TS]-T-[RK]-[EDK]-R-R-[HSDARK]
  that is:
  [Isoleucine or Valine], then Alanine, then [Isoleucine or Valine], then Phenylalanine ...etc

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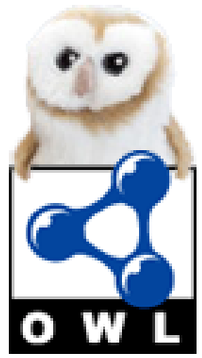

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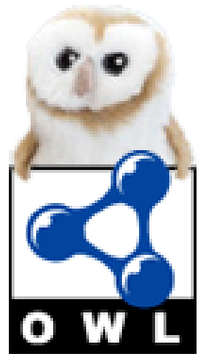
  that is:
  [Isoleucine or Valine], then Alanine, then [Isoleucine or Valine], then Phenylalanine ...etc
- It is simple to model the [XY] elements as OWL unions
- But there are other things also worth investigating...



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Underspecification of Patterns

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- Motifs reflect the current level of knowledge and may, in cases, be over-constrained

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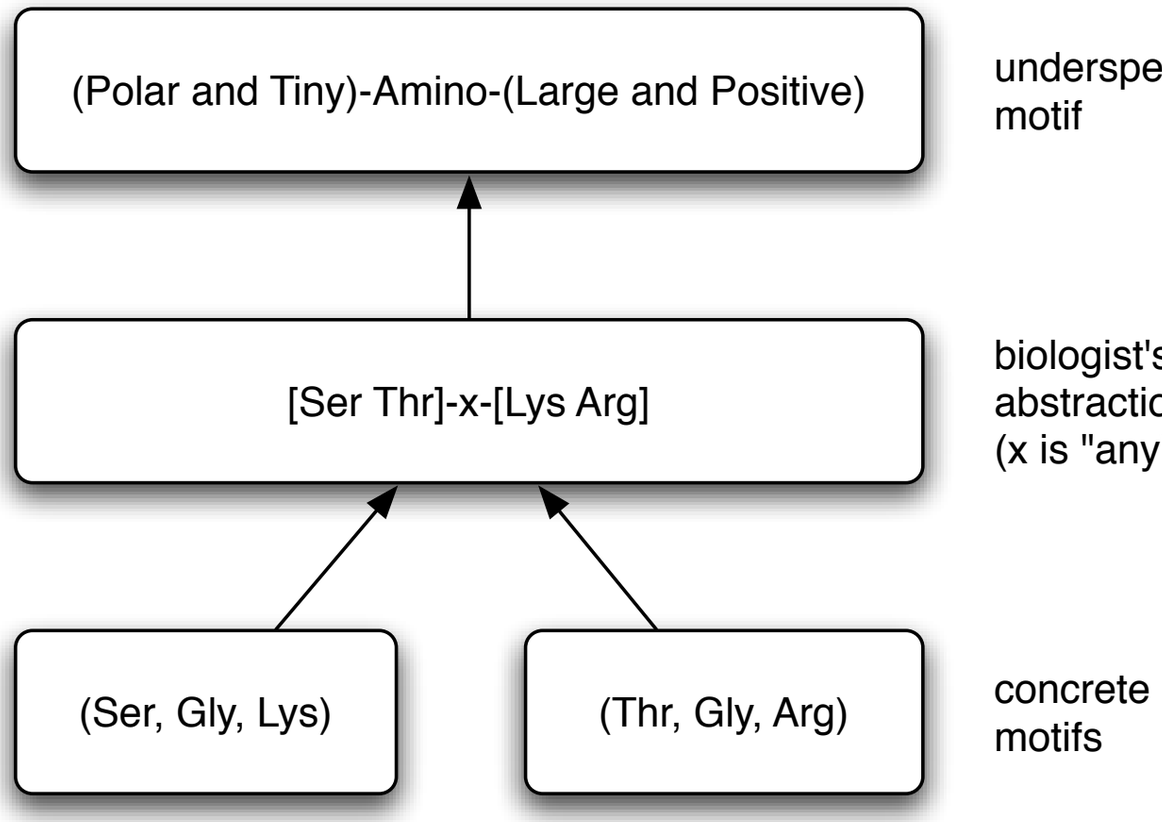

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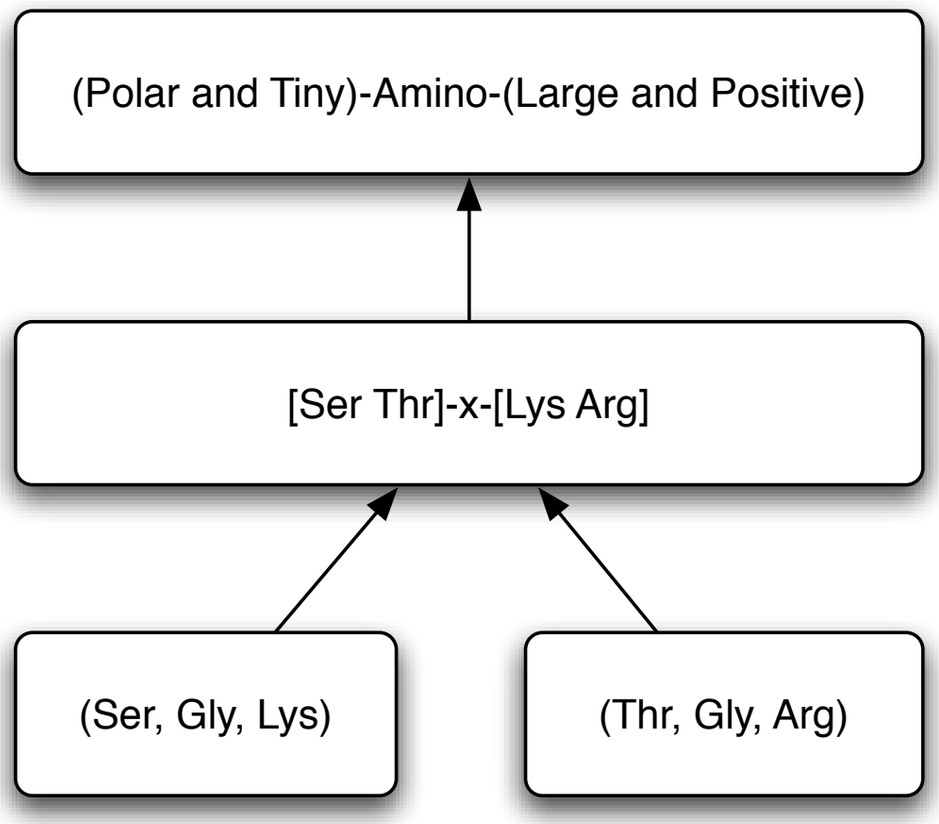
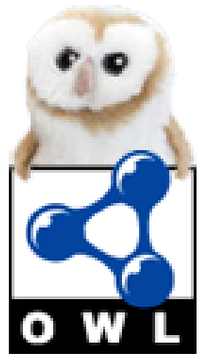


- By relaxing the description, we might find additional potential matches that could be investigated



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Fingerprints (sets of motifs)

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Fingerprints (sets of motifs)

Match a set of motifs (in order) in a sequence:

6PFRUCTKNASE fingerprint:

Motif 1 = [IV]-A-[VI]-F-D-A-T-N-[TS]-T-[RK]-[EDK]-R-R-[HSDARK]

Motif 2 = [KRQ]-[TVCPA]-[FLM]-F-[IVL]-E-S-[IVW]-[CS]-[DVN]-D-[PH]-[GDEAT]-[IVL]-[IV]

Motif 3 = P-D-Y-[KEVIPT]-[GNDE]-[CRLSK]-[NDHME]-[PTSQR]-[AEDGH]-[VSEKN]-[AVQS]-[AELTM]-[AKED]-[DE]-[FD]

Motif 4 = [VI]-[QR]-[DGT]-[HYF]-[IVL]-[QEA]-S-[RQK]-[ITAV]-[VA]-[YF]-[YF]-[LV]-[ML]-N-[ITF]-[HRN]-[VPL]-[QTHLKA]-[PD]-[RK]-[TSAYQ]

Motif 5 = I-[YW]-[LI]-[CST]-R-[HS]-G-[EQ]-[NS]-[IEQ]-[HYLFD]-N-[VLAI]-[QRLKMES]-[GK]-[RK]-[IL]-G-G-[DN]-[SPA]-[GPSH]-L

Motif 6 = A-G-[VID]-[CY]-[ED]-[EG]-[LM]-T-Y-[EA]-[ED]-I-[RQEK]-[DKEQN]-[THRQEN]-[YF]-P

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Matching

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LVNIIEEVVINKIRTYLESRIVFYVMNIRPKPKYIWLSRHG
ESIYNVEKKIGGDSSLSERGFQYAKKLEQLVKESAGEIN
LTVWTSTLKRTQQTANYLPYKKLQWKALDELDAGVCD
GMTYEEIEKEYPEDFKARDNDKYEYRYRGGESYRDVVI
RLEPVIMELERQENVLIITHQAVLRCIYAYFMNVPQEESP
WMSIPLHTLIKLEPRAYGTKVTKIKANIPAVSTYKEKGTS
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QVGELSQSSTKLHQLLNDSPLEDKF

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OWL Lists: Advantages

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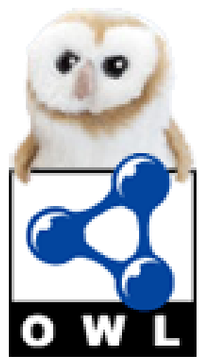

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OWL Lists: Advantages

- More expressive than rdf:list

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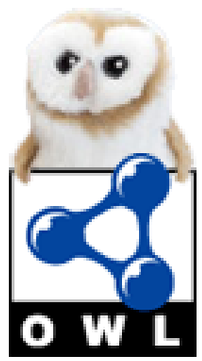

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    eg transitivity of isFollowedBy allows statements to be made about (indirectly) following elements

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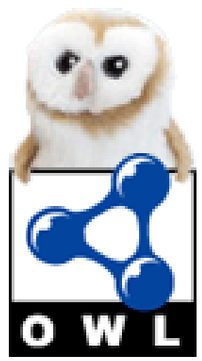

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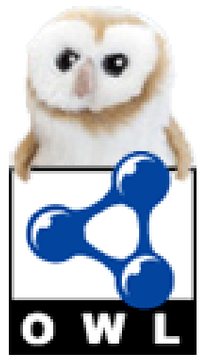

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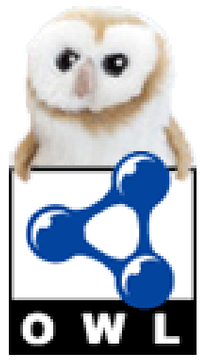

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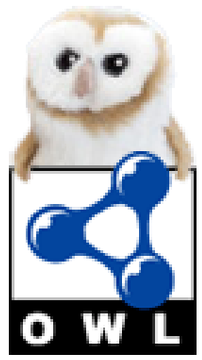
    eg transitivity of isFollowedBy allows statements to be made about (indirectly) following elements
  - Logical statements can be made to represent many different patterns and many different elements
- Knowledge can all be kept in one place (in the ontology)
- Some (very basic) tool support



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OWL Lists: Disadvantages

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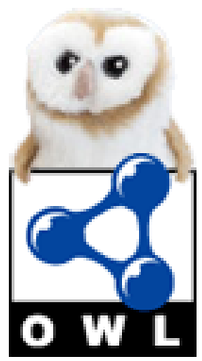

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OWL Lists: Disadvantages

- Computationally expensive compared to alternatives (reg exp deterministic finite automata)

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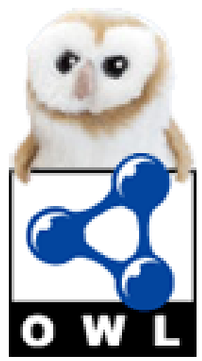

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OWL Lists: Disadvantages

- Computationally expensive compared to alternatives (reg exp deterministic finite automata)
- Difficult to maintain without specialist tools

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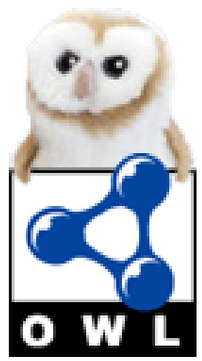

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OWL Lists: Disadvantages

- Computationally expensive compared to alternatives (reg exp deterministic finite automata)
- Difficult to maintain without specialist tools
  - Current tool support is basic

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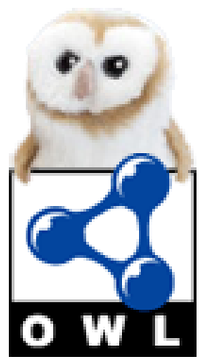

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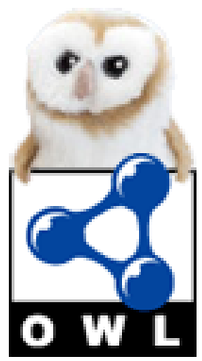

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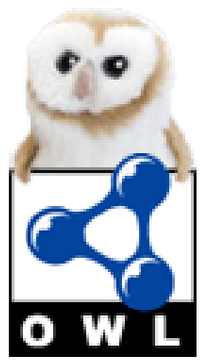

OWL Lists: Disadvantages

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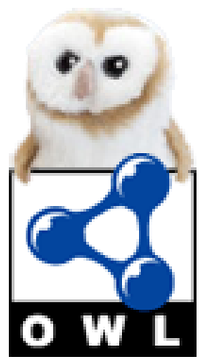
    - Classes, not Individuals (at this point)
    - Only some of the simple patterns are currently supported
- Memory intensive (expressions are very large and heavily nested)



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OWL Lists: Example (100 elements)

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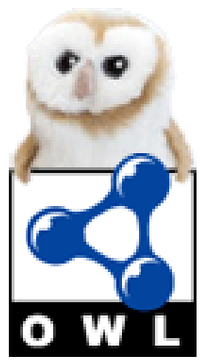

OWL Lists: Example (100 elements)

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    amino:N) and (meta:hasNext some (SequenceOfAminoAcids and (meta:hasContents some amino:S) and (meta:hasNext some (SequenceOfAminoAcids and (meta:hasContents some amino:T) and (meta:hasNext
    some (SequenceOfAminoAcids and (meta:hasContents some amino:R) and (meta:hasNext some (SequenceOfAminoAcids and (meta:hasContents some amino:K) and (meta:hasNext some (SequenceOfAminoAcids
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Basic Tools

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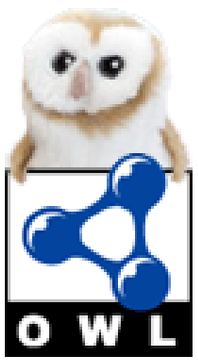
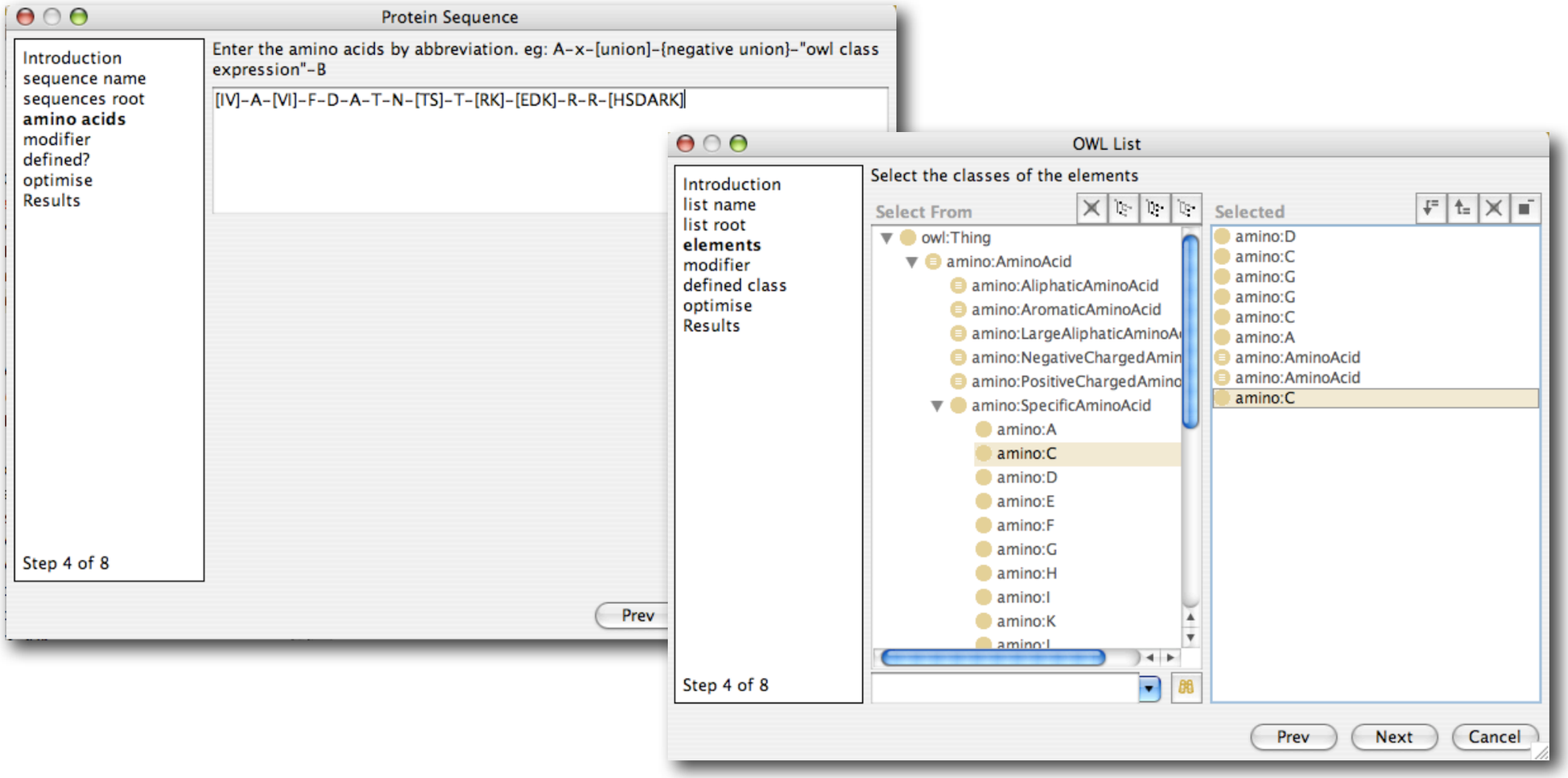


Basic Tools

- Wizard for basic patterns



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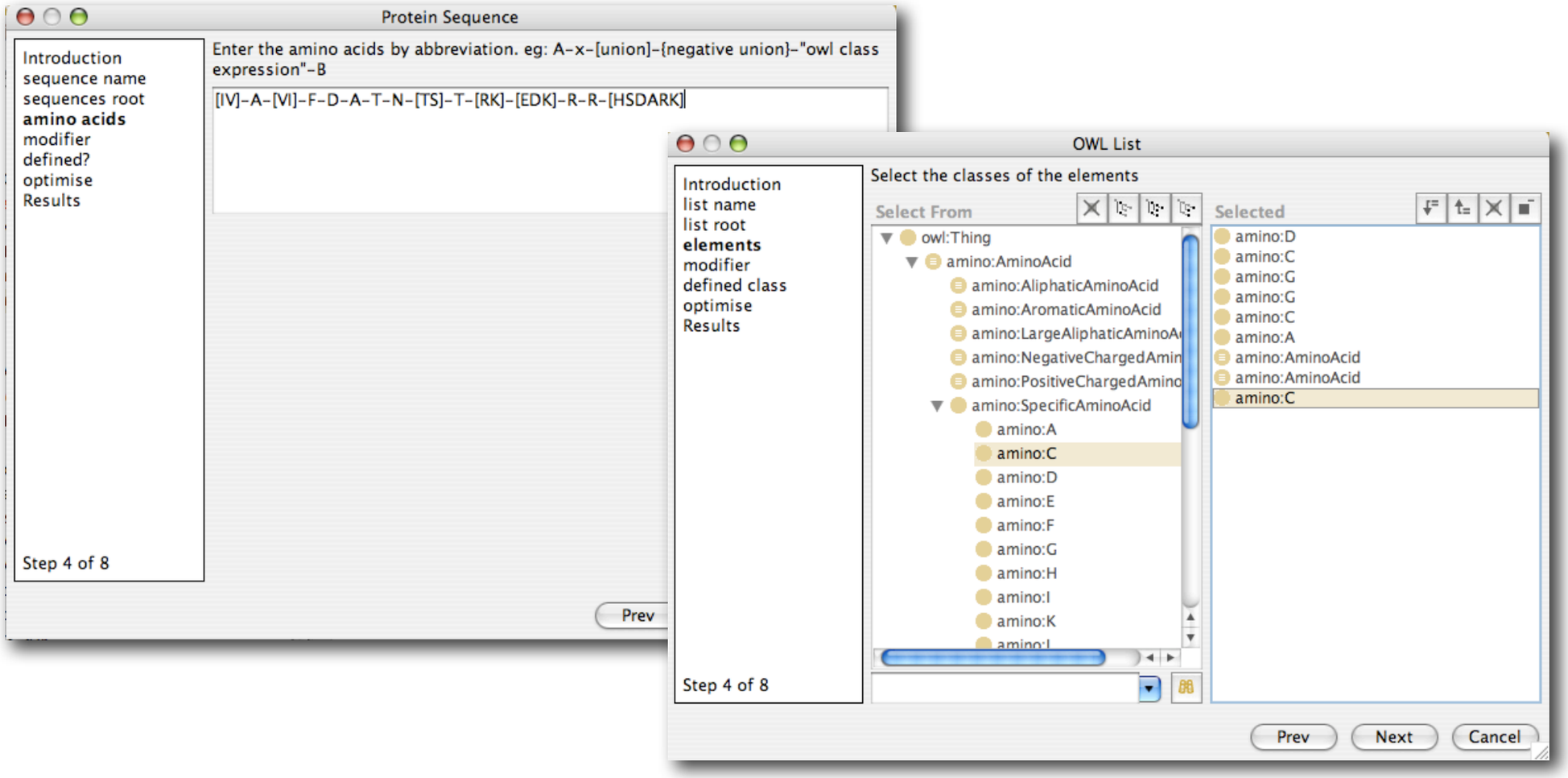
Basic Tools

- Wizard for basic patterns
- exact match, starts/ends with, contains



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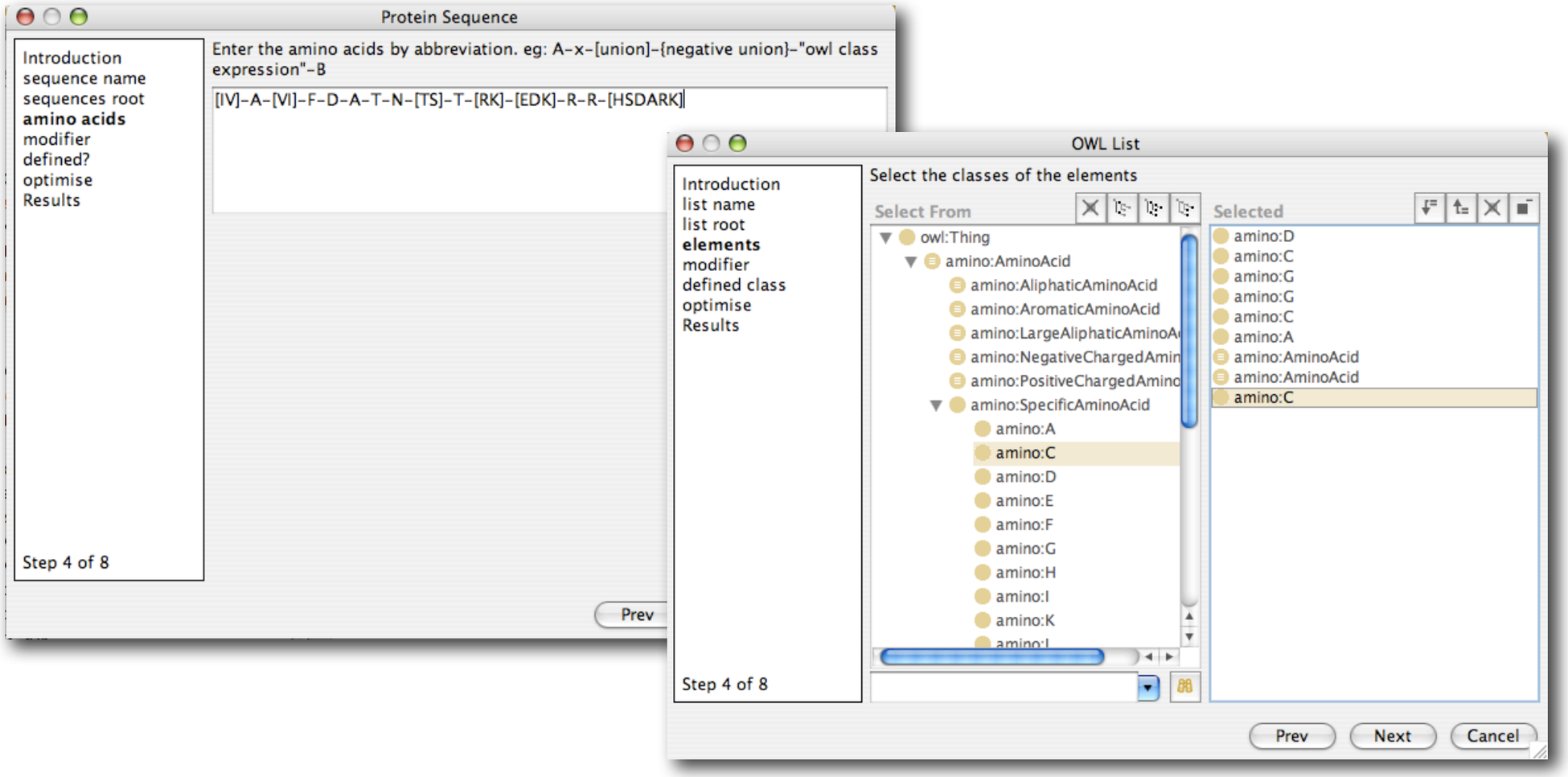
Basic Tools

- Wizard for basic patterns
- exact match, starts/ends with, contains
- Bio-specific for sequences/motifs/fingerprints



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Conclusion

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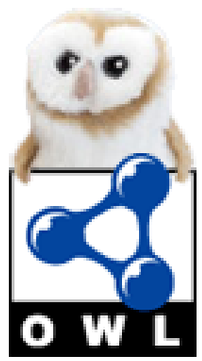

Conclusion

- Useful for pattern matching with similar expressivity to regular expressions

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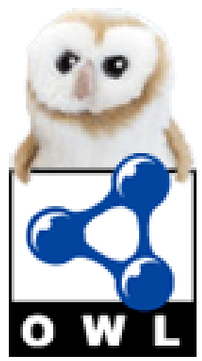

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Conclusion

- Useful for pattern matching with similar expressivity to regular expressions
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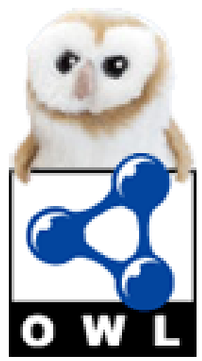

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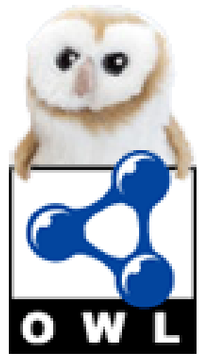

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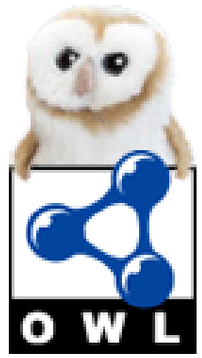

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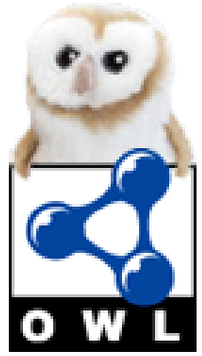

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Conclusion

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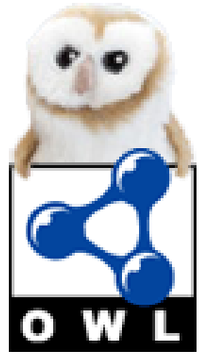
- Pattern matching surprisingly fast using reasoners
- Tools exist for doing the basics
- Possible, in theory, to create other structures by reifying the elements
  - Trees or Tables?



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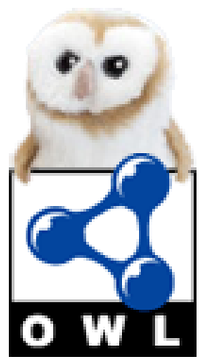
2nd to last slide

Demo ontologies at
http://www.co-ode.org/ontologies/lists/

Basic OWLLists supported by OWL Wizards
http://www.co-ode.org/downloads/wizard/

Thanks to Uli Sattler and Bijan Parsia for comments on the hard stuff



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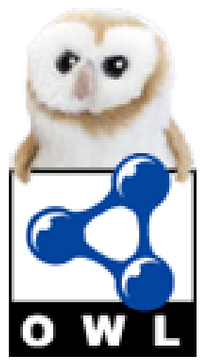
EmptyList (The End)

(Thankyou)



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