Relational data and knowledge

Semantic similarity

- We want to use *background knowledge* to
  - determine similarity between classes,
  - instances,
  - and entities associated with classes

How to measure similarity?

- semantic similarity measures similarity between classes
- semantic similarity measures similarity between instances of classes
- semantic similarity measures similarity between entities *associated* with classes
- $\Rightarrow$ reduce all of this to similarity between classes

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- sim is a *normalized* similarity measure if it has values in $[0, 1]$

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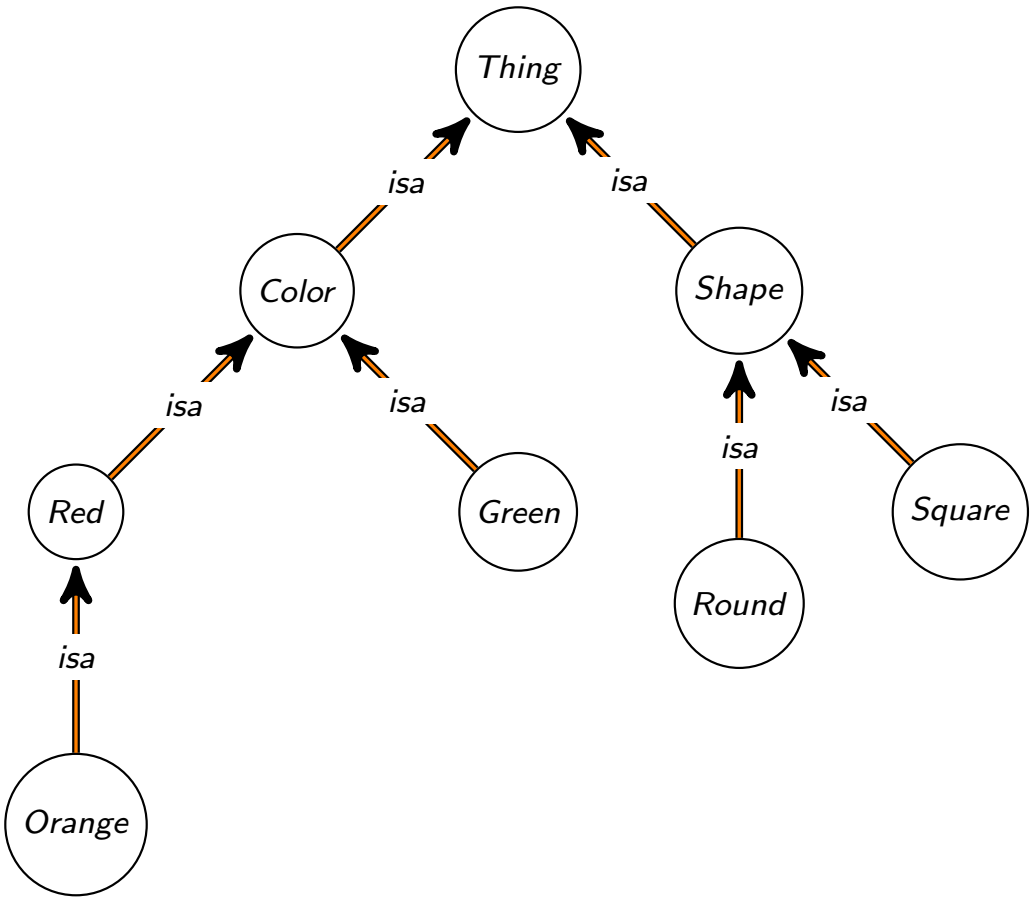

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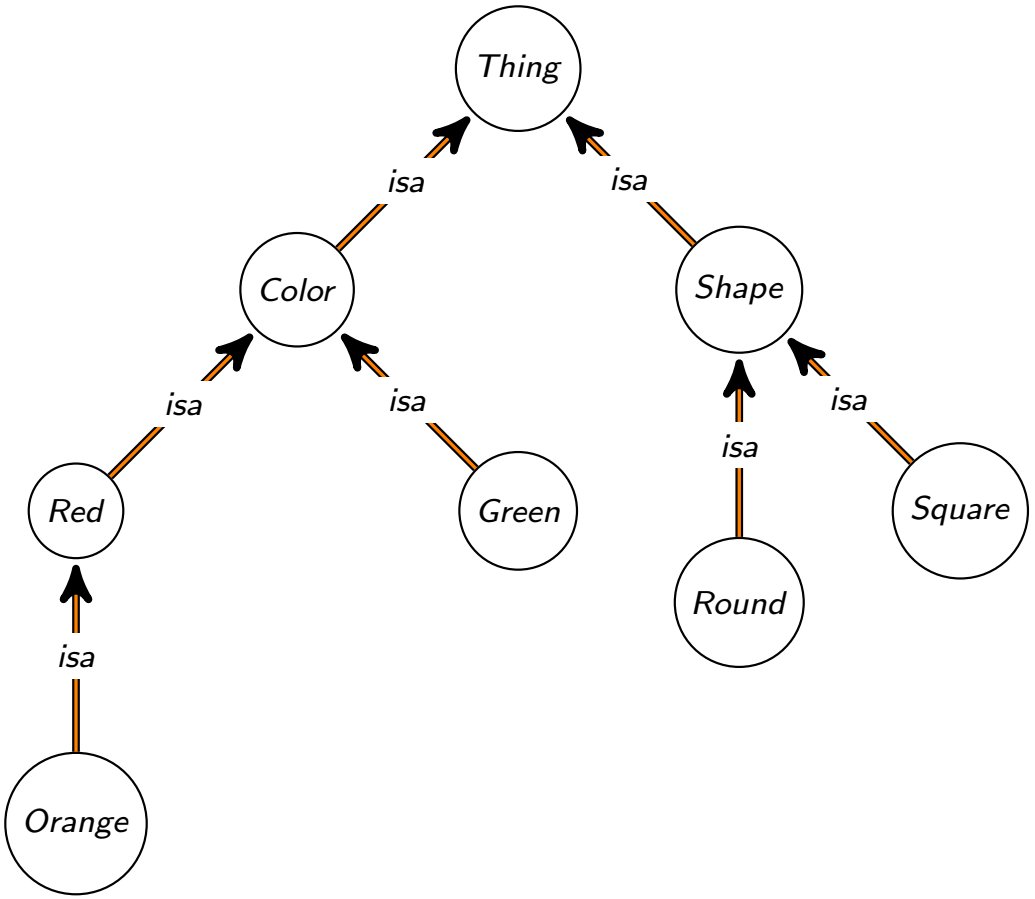

- distance on shortest path (Rada *et al.*, 1989)

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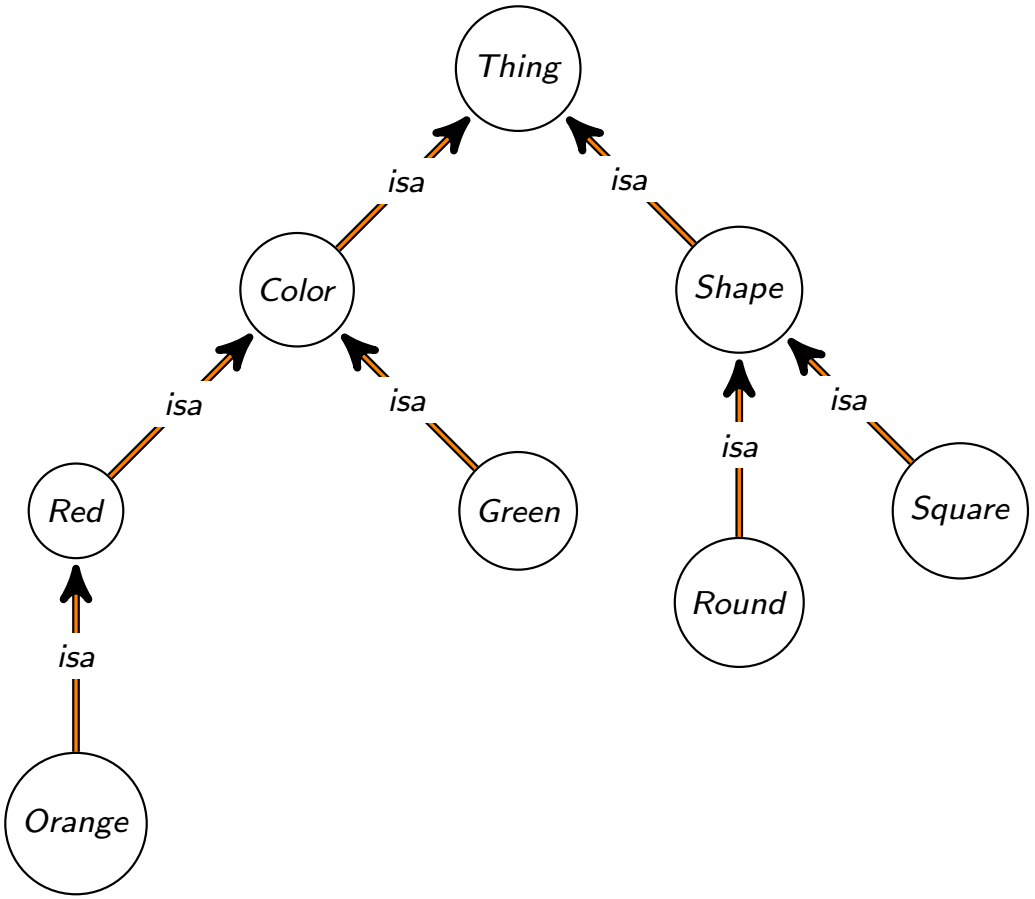

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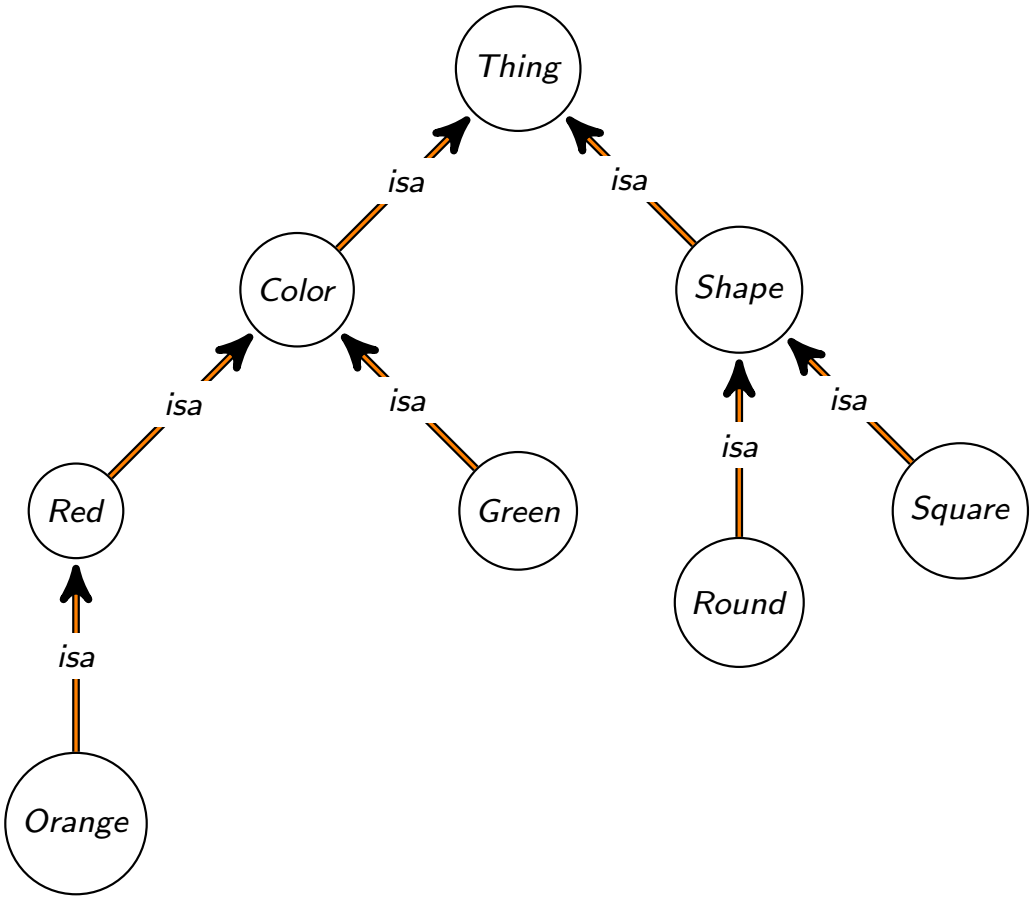

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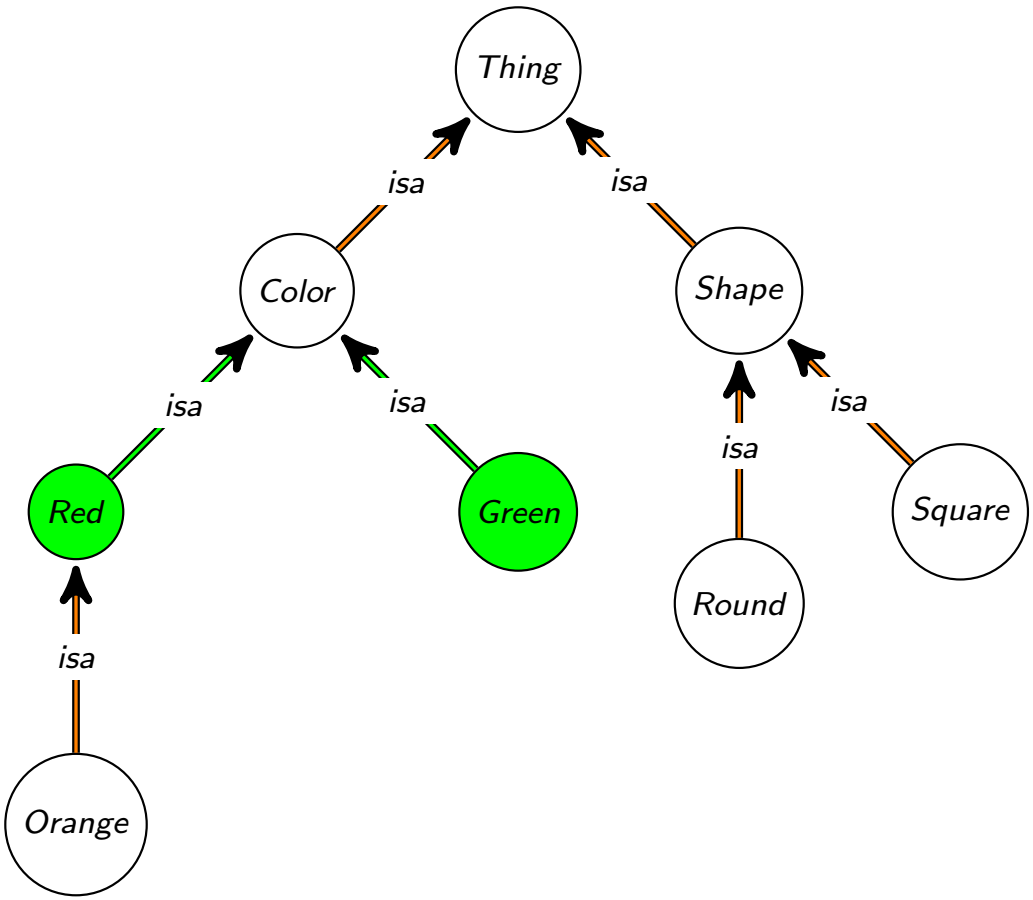

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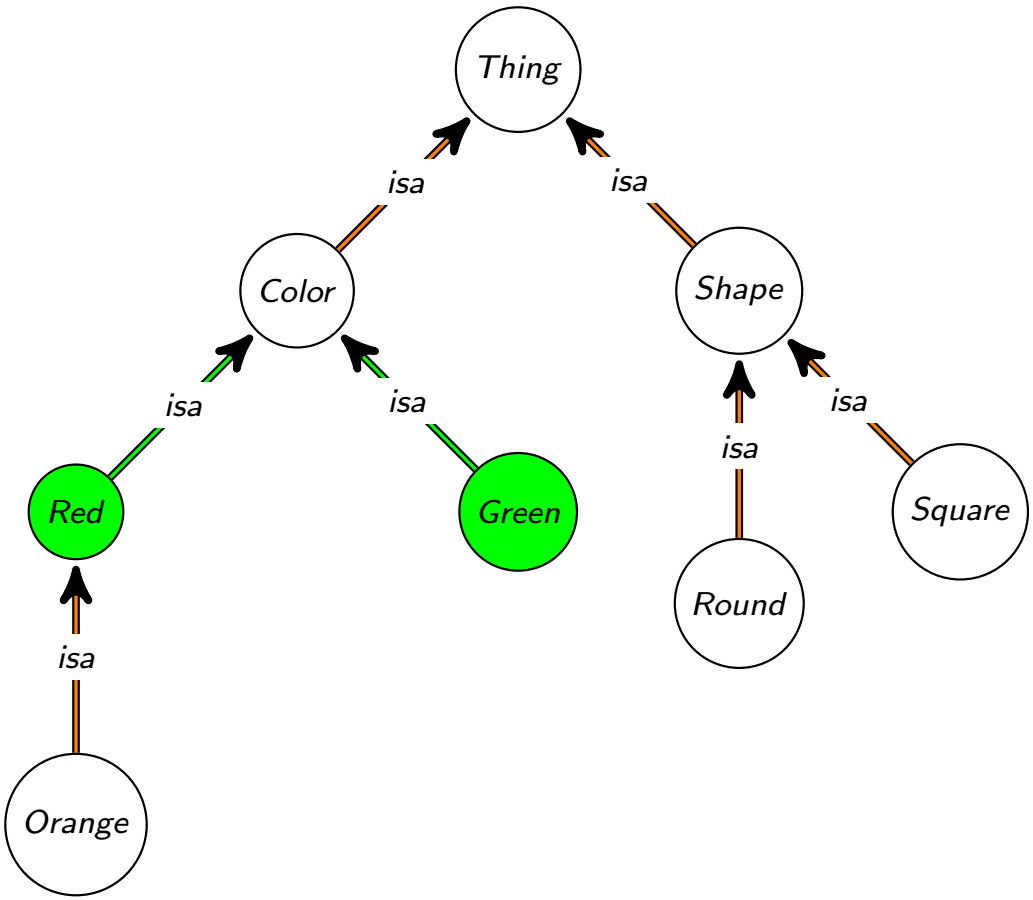

- distance on shortest path
- distance(green, red) $= 2$
- $sim_{Rada}(green, red) = \frac{1}{3}$

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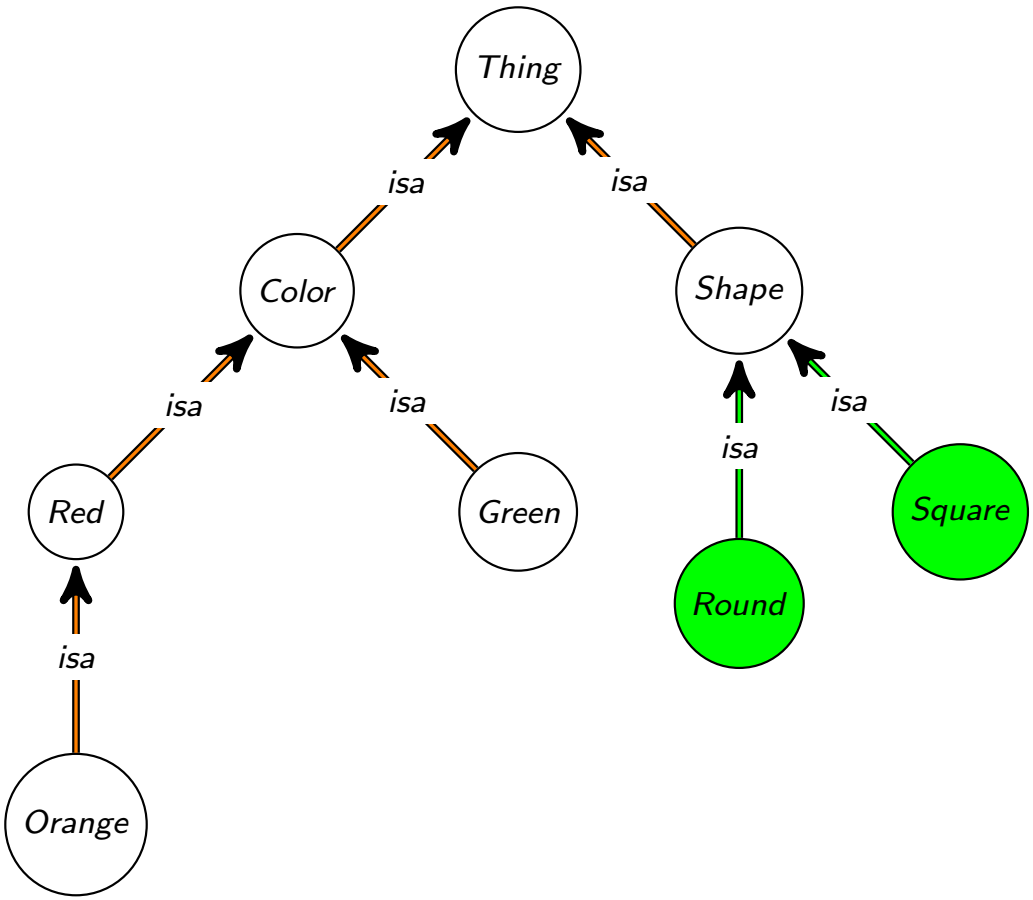

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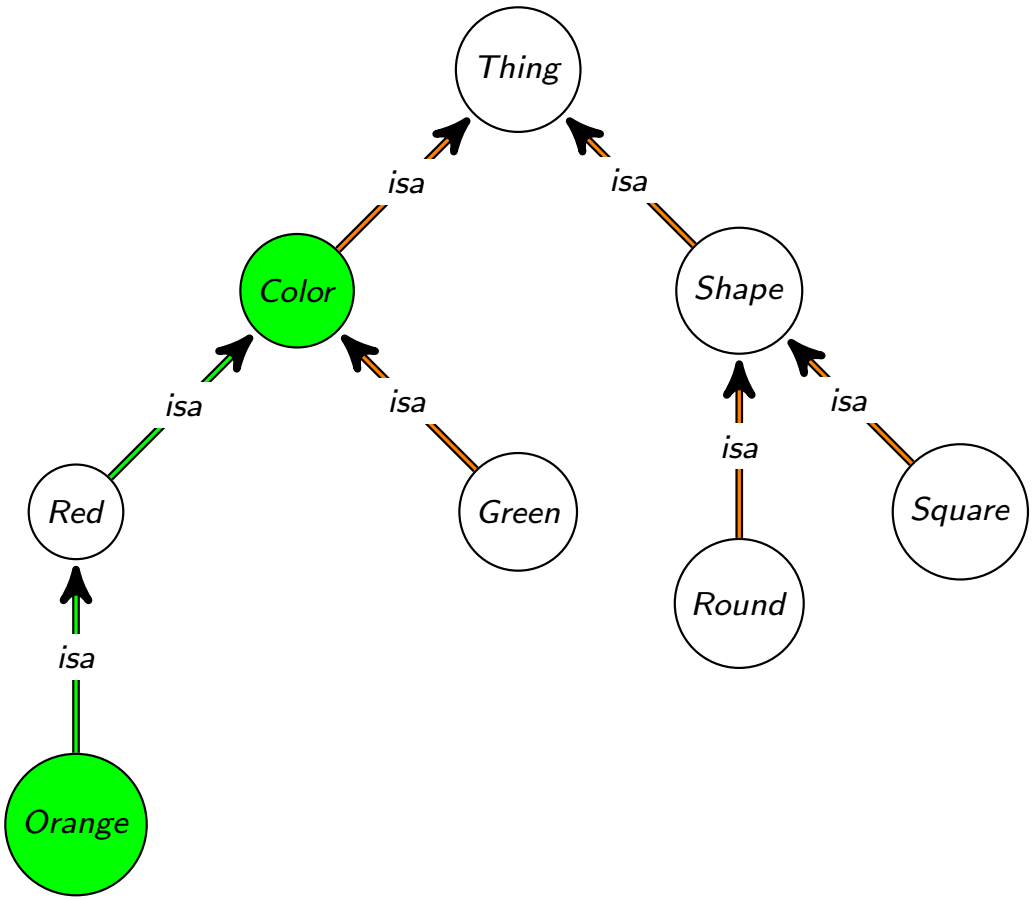

- distance on shortest path
- distance(orange, color) $= 2$
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- account for different edge types
  - non-uniform edge weighting

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  - many more, e.g., Zhou et al.:
    $\sigma(x) = k \cdot \left(1 - \frac{\log |D(x)|}{\log |C|}\right) + (1 - k)\frac{\log depth(x)}{\log depth(G_T)}$

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- extrinsic:
  - $\sigma(x)$ defined as a function of instances (or annotations) I
    - note: the number of instances monotonically decreases with increasing depth in taxonomies
  - Resnik 1995: $eIC_{Resnik}(x) = -\log p(x)$ (with $p(x) = \frac{|I(x)|}{|I|}$)
    - in biology, one of the most popular specificity measure when annotations are present

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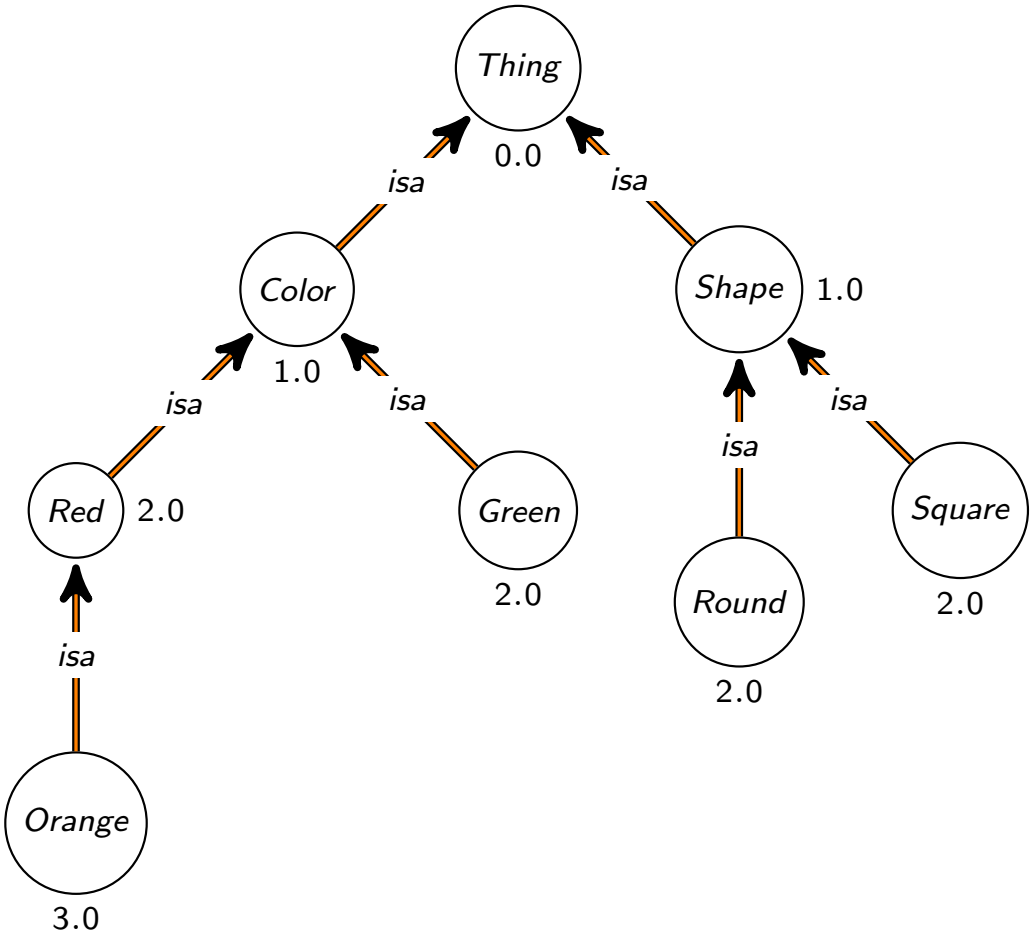

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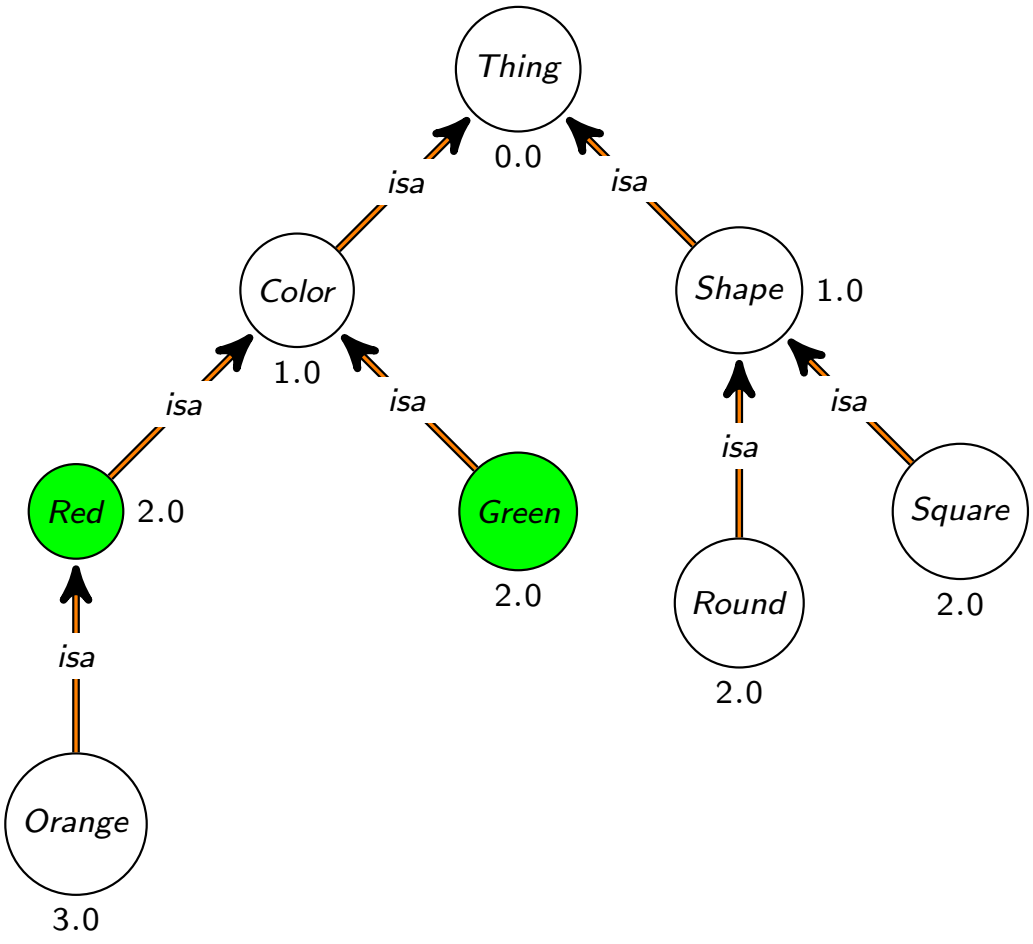

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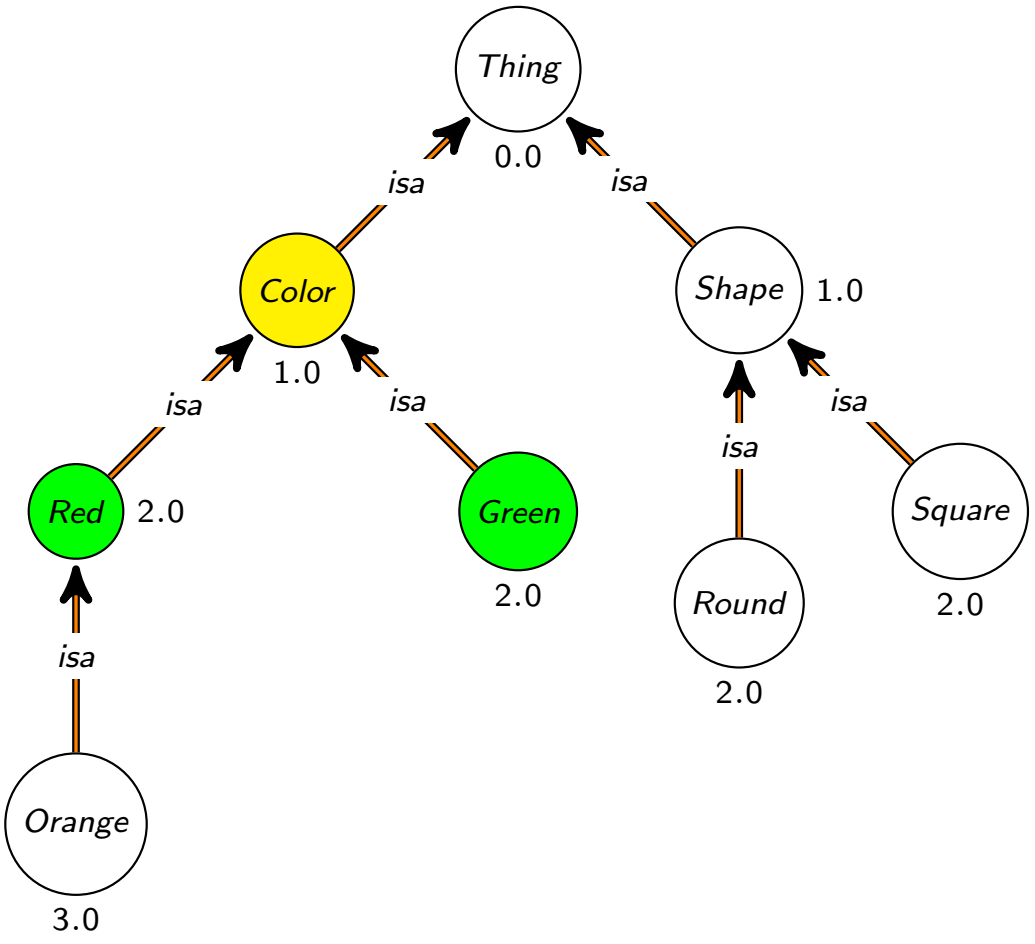

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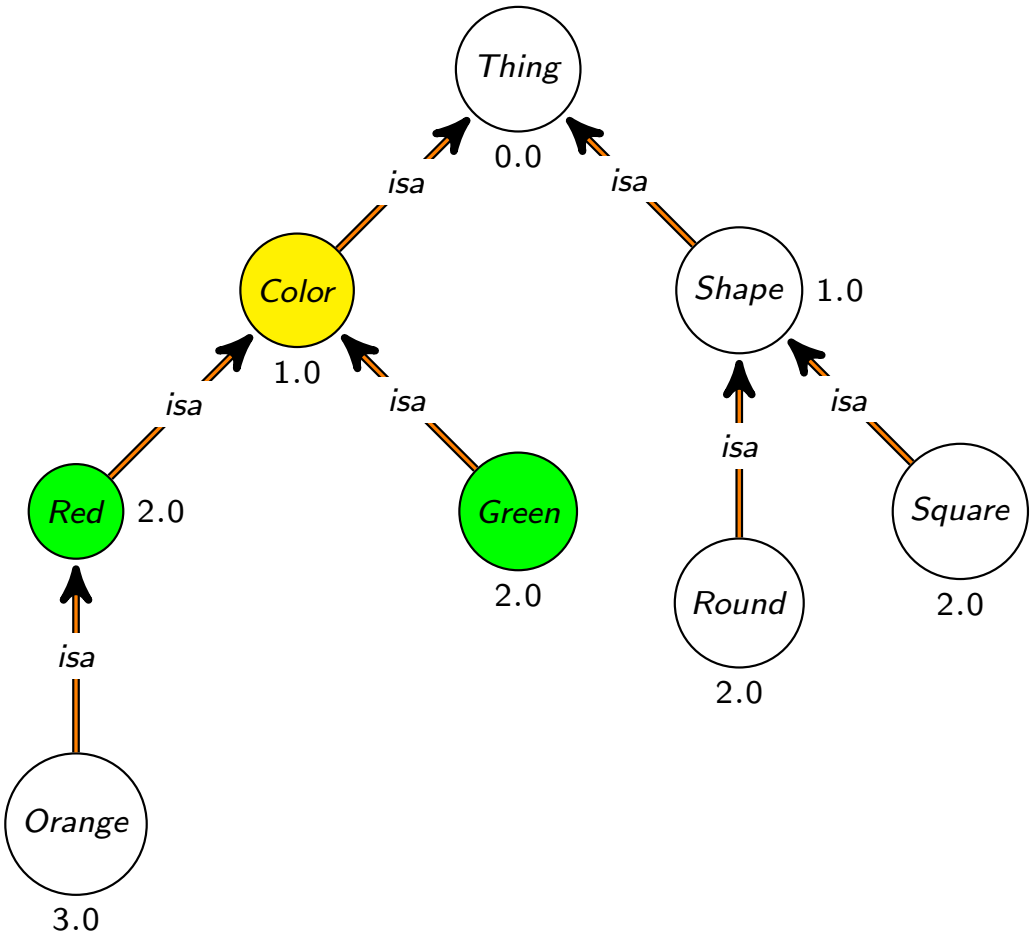

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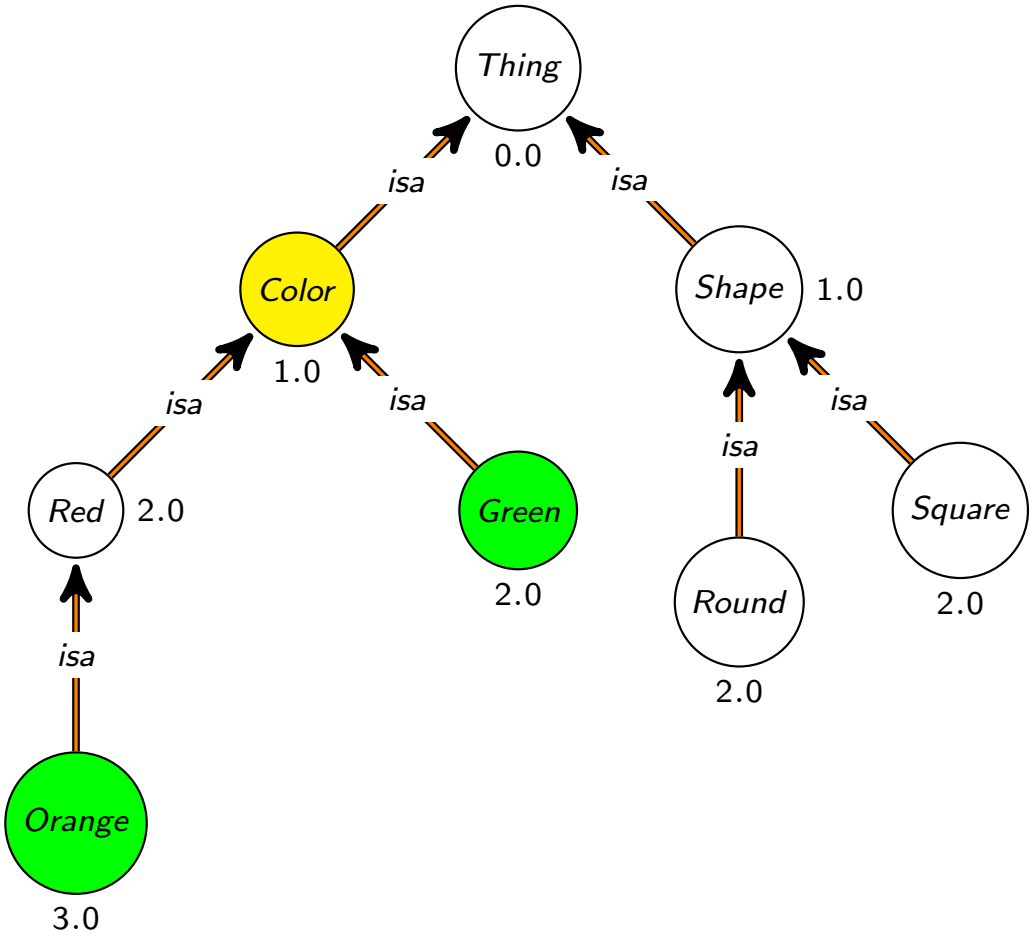

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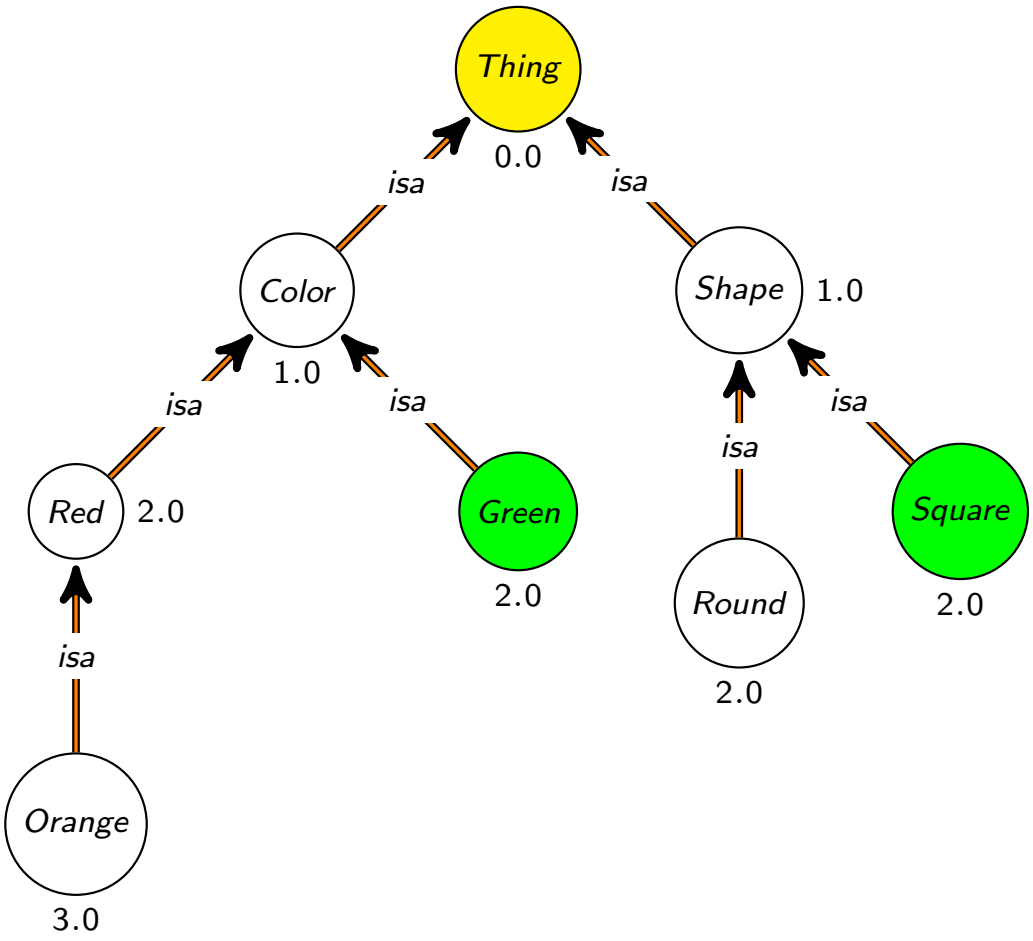

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- $sim_{Resnik}(Square, Orange)$ 0.0

How to measure similarity?

- (Red, Green) and (Orange, Green) have the same similarity
- need to incorporate the specificity of the compared classes

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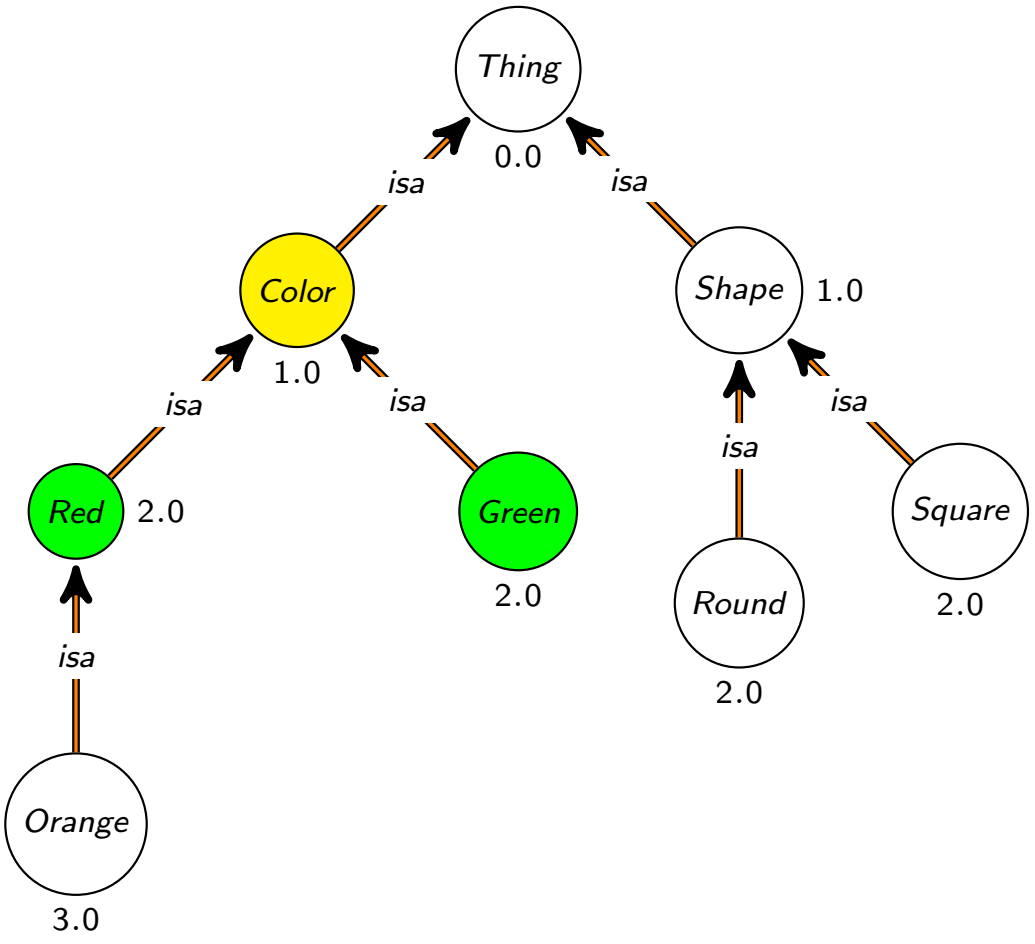

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  $sim_{Lin}(x, y) = \frac{2 \cdot IC(MICA(x,y))}{IC(x)+IC(y)}$

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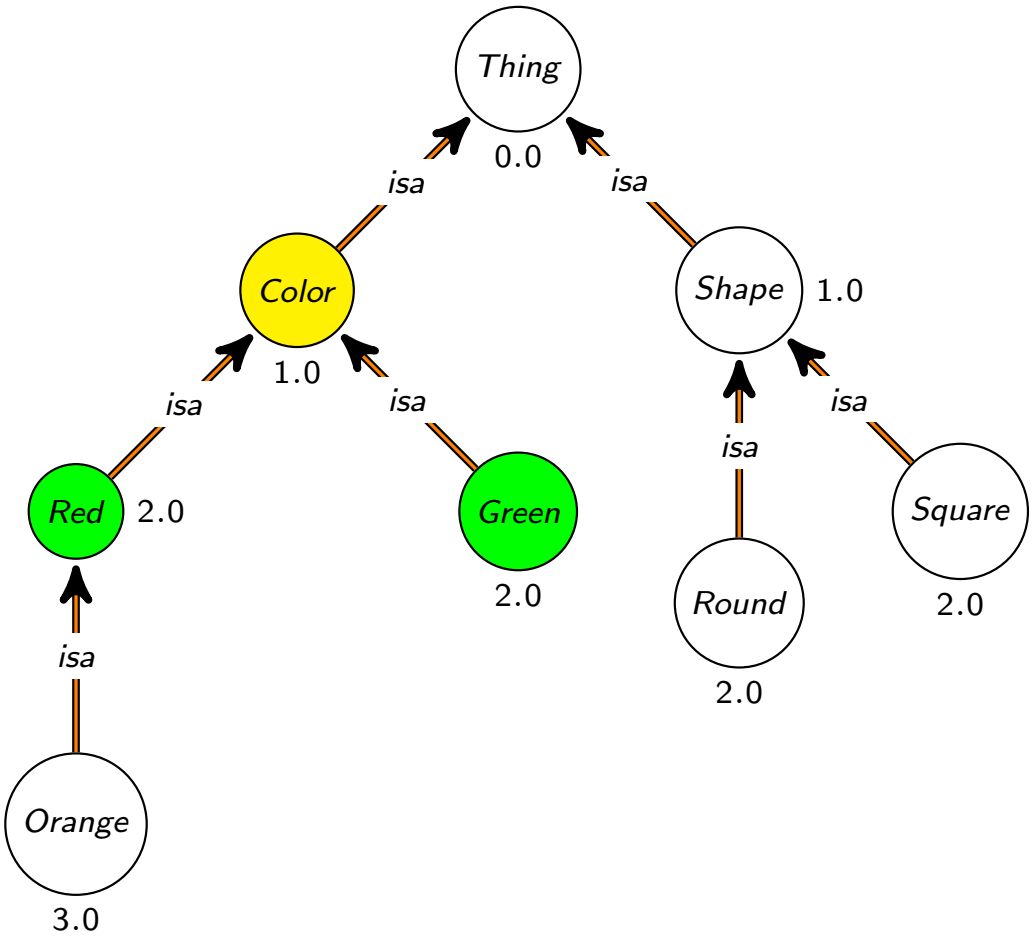

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- $sim_{Lin}(Green, Red) = 0.5$

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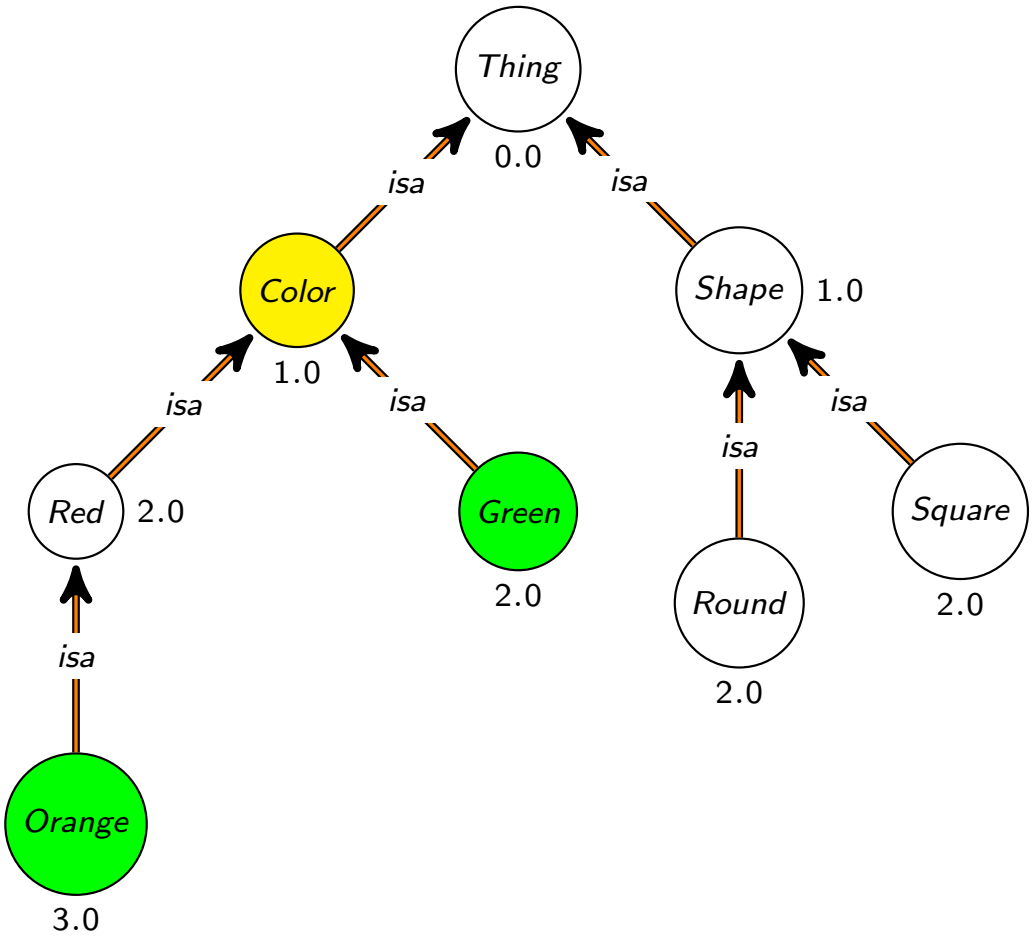

- Lin 1998:
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- $sim_{Lin}(Green, Orange) = 0.4$

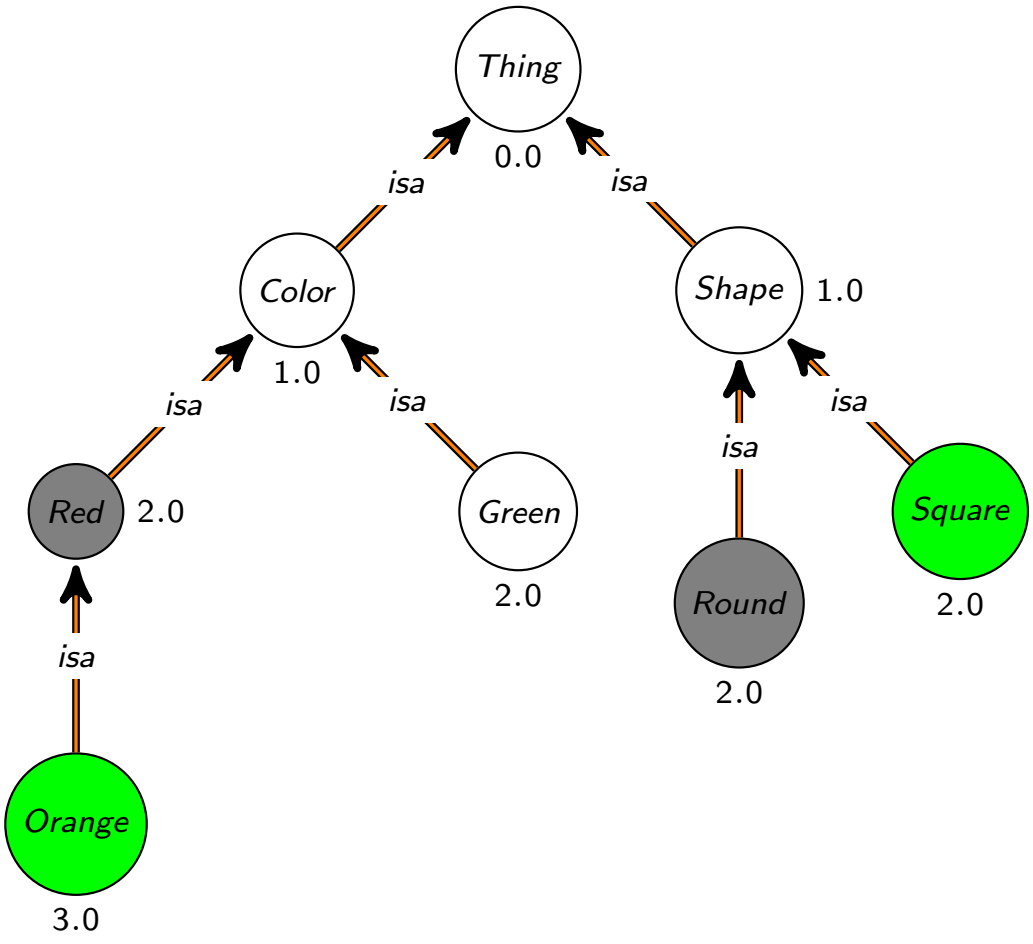
How to measure similarity?

- many(!) others:
  - Jiang & Conrath 1997
  - Mazandu & Mulder 2013
  - Schlicker et al. 2009
  - ...

How to measure similarity?

- we only looked at comparing pairs of classes
- mostly, we want to compare *sets* of classes
  - set of GO annotations
  - set of signs and symptoms
  - set of phenotypes
- two approaches:
  - compare each class individually, then merge
  - directly set-based similarity measures

How to measure similarity?



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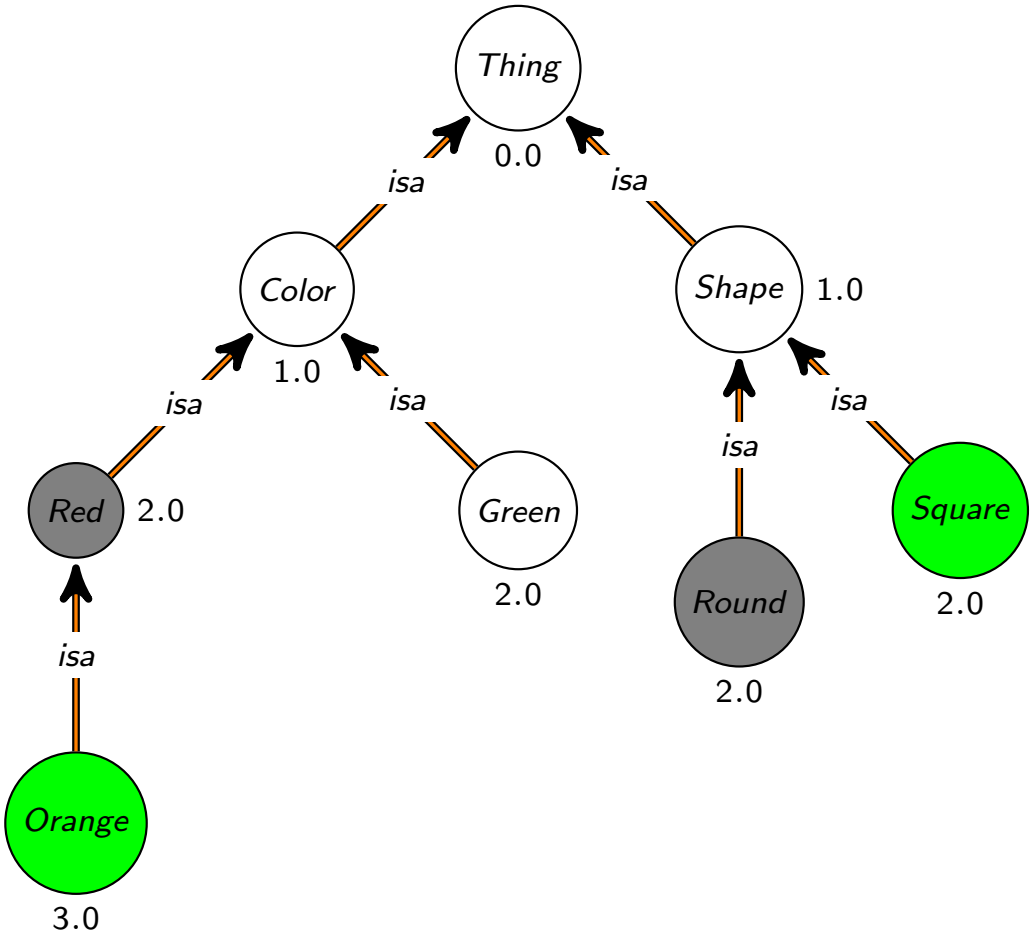

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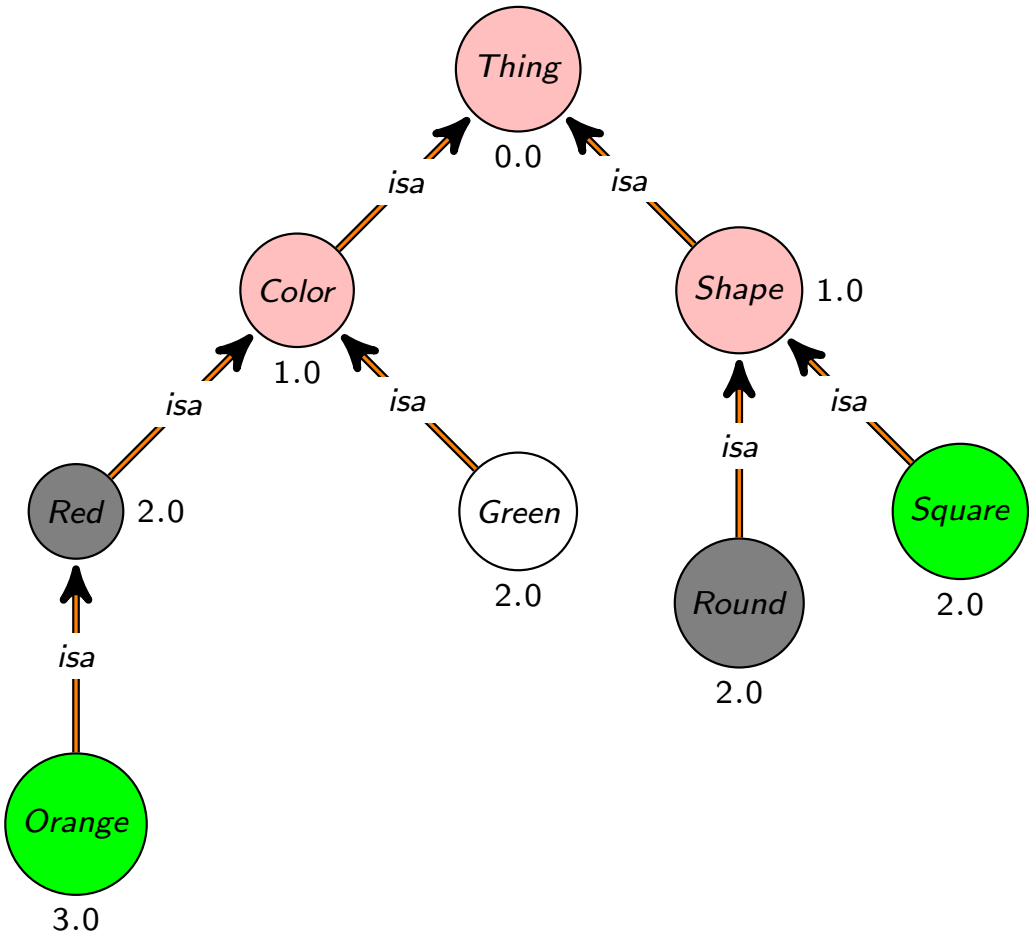

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- $simGIC(so, rr) = \frac{2}{11}$

How to measure similarity?

- alternatively: use different merging strategies
- common: average, maximum, **best-matching average**
  - Average: $sim_A(X, Y) = \frac{\sum_{x \in X} \sum_{y \in Y} sim(x,y)}{|X| \times |Y|}$
  - Max average: $sim_{MA}(X, Y) = \frac{1}{|X|} \sum_{x \in X} \max_{y \in Y} sim(x, y)$
  - Best match average: $sim_{BMA}(X, Y) = \frac{sim_{MA}(X,Y) + sim_{MA}(Y,X)}{2}$

How to measure similarity?

- Semantic Measures Library:
  - comprehensive Java library
  - `http://www.semantic-measures-library.org/`
- R packages: GOSim, GOSemSim, HPOSim, LSAfun, ontologySimilarity,...
- Python: sematch, fastsemsim (GO only)

Applications of semantic similarity

- no obvious choice of similarity measure
- depends on application
  - e.g., predicting PPIs in different organisms through similarity may benefit from a different similarity measure!
- different similarity measures may react differently to biases in data
- needs some testing and experience

Applications of semantic similarity

Recommendations:

- use Resnik's information content measure
- use Resnik's similarity
- use Best Match Average
- use all background knowledge
- classify knowledge using an automated reasoner before applying semantic similarity

Quiz: Semantic Similarity

What defines a semantic similarity measure?

1. Number of classes, OWL profile
2. Graph structure, term specificity, pairwise similarity, aggregation operation
3. Graph structure, term specificity, groupwise similarity

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LaTeX was unable to guess the total number of pages correctly. A
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the final page this extra page has been added to receive it.
If you rerun the document (without altering it) this surplus page
will go away, because LaTeX now knows how many pages to expe
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