Algorithmic exploration of axiom spaces for efficient similarity search at large scale

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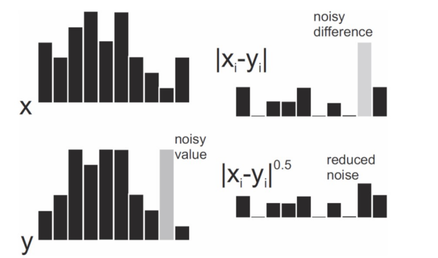
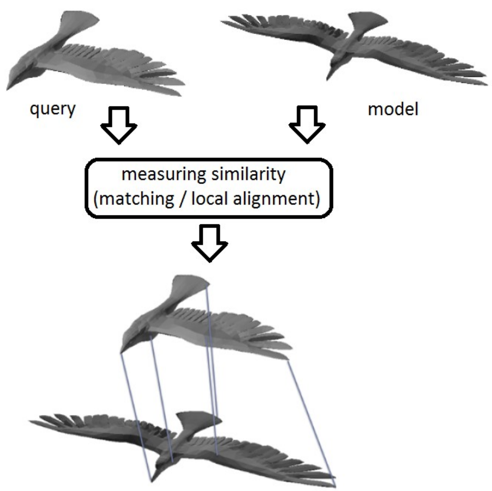
Outline

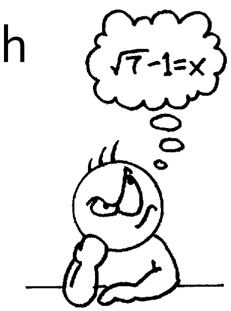
- nonmetric similarities
- indexing nonmetric similarities – related work
- motivation
  - ptolemaic indexing
- SIMDEX overview
  - main goals
  - framework stages
- preliminary experiments

Nonmetric similarities

- assuming nonmetric (unconstrained) similarity for complex measures
  - robustness (e.g., noise suppressed)
  - locality (partial matching)
  - comfort of modeling
    - domain expert not stressed by math
    - complex/algorithmic similarities undecidable







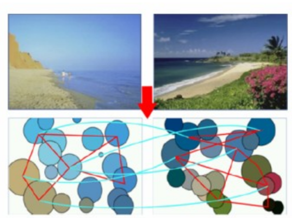
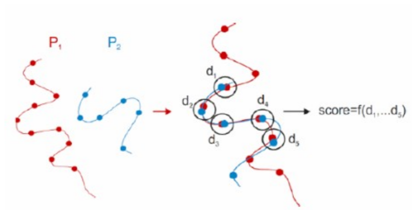


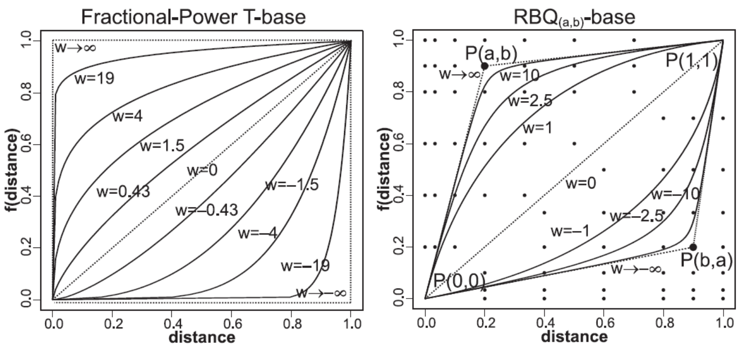
Image similarity



Protein similarity

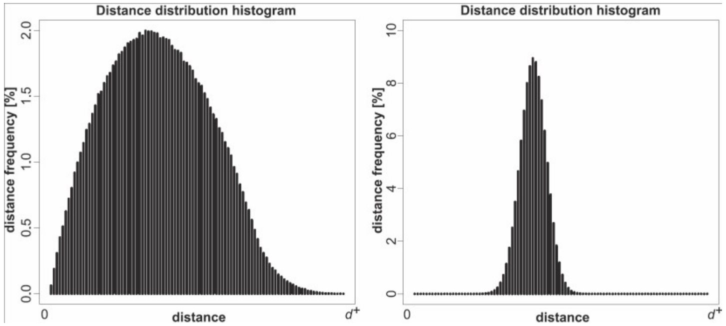
Indexing nonmetric similarities

- specific indexing (e.g., inverted index)
- general indexing
  - usually transformation into "simpler" space + indexing
  - Euclidean space + spatial access methods
    - NMDS, FastMap, MetricMap, SparseMap, BoostMap, …
    - mapping = altering the universe + distance function
  - metric space + MAMs
    - TriGen algorithm
    - mapping = universe is the same, just the distance function altered



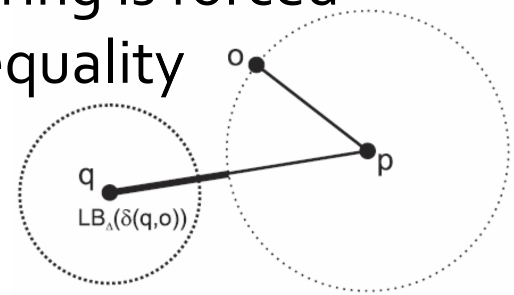
Any problem so far?

- is "metrization" of a nonmetric problem the best solution?
  - it is quite elegant solution, but the "devil lives in detail" – the target metric space is usually "overinflated" (high intrinsic dimensionality)



- why?
  - complex behavior of a similarity measuring is forced to comply with the "stupid" triangle inequality and simple filtering

$$LB_{\triangle}(\delta(q,o_i)) = |\delta(q,p) - \delta(p,o_i)|$$



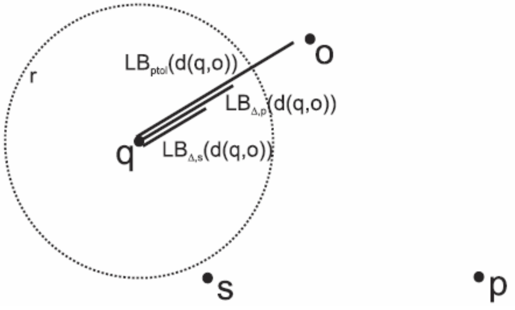
Motivation: Ptolemaic Indexing

- previous approaches
  - “rape data” to comply with an indexing formalism (metric space model)
- opposite approach
  - find an indexing formalism that comply with “data” the best
  - fuzzy similarity indexing [SISAP 2009 & 2011] – didn’t work ☹
  - **ptolemaic indexing** [SISAP 2011] – worked! ☺
    - ptolemaic inequality instead of (together with) the triangle one

$$\delta(x,v)\cdot\delta(y,u) \le \delta(x,y)\cdot\delta(u,v) + \delta(x,u)\cdot\delta(y,v)$$

    - works with for (signature) quadratic form distances (other practical distances? open problem)

$$\mathrm{LB}_{\mathrm{ptol}}(\delta(q,o)) = \frac{|\delta(q,p)\cdot\delta(o,s) - \delta(q,s)\cdot\delta(o,p)|}{\delta(p,s)}$$



SIMDEX idea

- so, we have metric indexing and ptolemaic indexing
  - we have a different way to construct the lower bounds to the original distance (or upper bound to similarity)

$$LB_{\triangle}(\delta(q,o_i)) = |\delta(q,p) - \delta(p,o_i)|$$

$$\mathrm{LB}_{\mathrm{ptol}}(\delta(q,o)) = \frac{|\delta(q,p)\cdot\delta(o,s) - \delta(q,s)\cdot\delta(o,p)|}{\delta(p,s)}$$

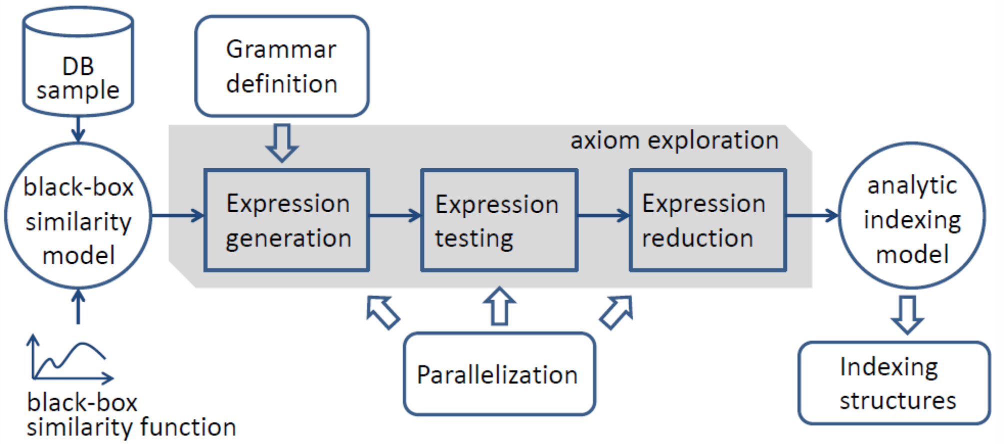
- how about to develop a framework that will discover (for a particular similarity model) an unknown **axiom**

$$\mathrm{LB}\left(\delta(q,o)\right) = \ ?$$

  such that the generated axiom will be computationally cheap and will perform better than any of the known (and named) axioms

SIMDEX framework

- no parameterized canonical forms but syntactically generated expressions
  - most general solution but very complex to handle
- stages
  - S1 – grammar definition
  - S2 – expression generation
  - S3 – expr. testing
  - S4 – expr. reduction
  - S5 – indexing
  - S6 – parallelization



SIMDEX framework

- S1 – Grammar definition
  - used to generate right-side lowerbound expressions
    - generally L3/Type-3 in Chomsky hierarchy
    - however, restriction specifics turn it into context-dependent language! (next slide)
  - terminals (combined)
    - descriptor variables ($q, o, p_1, \ldots, p_i$) and descriptor constants c_i used in the distance $\delta(\cdot, \cdot)$
    - functions f_i
    - standard arithmetic operators +,-,*,/, numeric constants
  - using the grammar a universe of expressions can be generated

SIMDEX framework

- S2 – Expression generation
  - exponential even when the grammar and recursion are limited
  - exploration of the expression universe
    - FIFO, LIFO, random, heuristic traversal
    - interleaved
  - restrictions complicating the language (context-dependent)
    - require $\delta(q,p_i)$, $\delta(p_i,o)$
    - avoid $\delta(q,o)$
    - avoid duplicates (lexical but also semantics, e.g., p_i, p_j the same)
    - avoid useless arithmetic operations (e.g., $\delta(p_i,o) - \delta(p_i,o)$)

SIMDEX framework

- S3 – Expression testing
  - testing each generated expression as an axiom candidate
  - application on the input distance/similarity matrix
  - either full axiom (all tests pass), or a partial
- S4 – Expression reduction
  - discarding weaker expressions
    (producing larger lowerbounds)
  - merging a set of expressions into a compound tighter form

SIMDEX framework

- S5 – Indexing
  - verifying the real usefulness of the passed expressions
  - Pivot table-like index can be always used (direct LB filter)
  - some expressions might be interpreted as “nestable” regions in the similarity space and so applicable to hierarchical indexing
    - such as the ball-regions for triangle inequality are
- S6 – Parallelization
  - the axiom space is huge even after all the optimization stages, so massive parallelization is critical
    - multicore CPU, manycore GPU, Map-Reduce on CPU farm

SIMDEX initial implementation

- covering stages S1-S3
- expressions generated by heuristics (fingerprints optimization)

Algorithm 1 SIMDEX (G, C, T, S, δ)

Require: Grammar definition G, validation conditions C, threshold probability value T, database sample S, distance function δ

$M_{\delta,S} \leftarrow$ new distance matrix (δ, S)
$expressions \leftarrow$ ExpressionGeneration(G, C)
for all E_i in $expressions$ **do**
  if $validate_C(E_i)$ equals **false then**
    $expressions$.Remove(E_i) {validity check fails}
    continue {skip further testing of the expression E_i}
  end if
  if $E\_test(E_i, M_{\delta,S}) < T$ **then**
    $expressions$.Remove(E_i) {probability test fails}
  end if
end for
return $expressions$ {remaining expressions compose the result set}

Preliminary experiments

Dataset	Expression	Success Ratio	MIN	MAX	AVG
Corel	triangle inequality	99 %	0.0034	0.9983	0.3764
	$\lvert\delta(q,p)\cdot\delta(o,p)\cdot(\delta(o,p)-\delta(q,p))\rvert$	100 %	0.1059	0.9991	0.5020
	$(\delta(q,p)-\delta(o,p))^2$	100 %	0.1352	0.9999	0.5054
	$\lvert(\delta(q,p_1)-\delta(o,p_1))(\delta(q,p_1)-\delta(o,p_2))\rvert$	100 %	0.0420	0.9999	0.5161
CoPhIR	triangle inequality	97.5 %	0.0021	0.9736	0.2696
	$(\delta(q,p)-\delta(o,p))^2$	100 %	0.0718	0.9979	0.3808
	$\lvert(\delta(q,p_1)-\delta(o,p_1))(\delta(q,p_2)-\delta(o,p_2))\rvert$	100 %	0.0845	0.9969	0.3935
Ratings	triangle inequality	100 %	0.6067	1.0	0.9037
	$\frac{1}{2\cdot\delta(o,p)}$	100 %	0.0119	0.5	0.4254
	$(\delta(q,p_1)+\delta(o,p_1))\cdot\frac{\delta(q,p_1)}{\delta(p_1,p_2)}$	100 %	0.0103	0.5845	0.4254
Listeria	triangle inequality	99 %	0	0.9559	0.1388
	$\delta(p_1,p_2)\cdot\frac{1}{\delta(p_1,p_2)+\delta(o,p_2)}$	100 %	0.0075	0.9994	0.2393
	$\delta(q,p_1)^2\cdot\frac{1}{\delta(o,p_2)\cdot\delta(q,p_2)}$	100 %	0.0008	0.9985	0.2401
	$(\delta(q,p_1)+\delta(o,p_1))\frac{\delta(q,p_1)}{\delta(p_1,p_2)}$	100 %	0.0032	0.9970	0.2555
Spectometry	triangle inequality	100 %	0.1823	0.93	0.7329
	$\delta(o,p)-\delta(o,p)^2$	100 %	0.0009	0.8758	0.6638
	$\lvert(\delta(q,p_1)\cdot\delta(o,p_2))-\delta(q,p_2)^2\rvert$	100 %	0.0148	0.9399	0.7054

Conclusions and future work

- SIMDEX sketched
  - universal algorithmical framework for discovering axioms suitable for indexing specific similarity models
  - breaking the metric space paradigm

- a lot of future work ahead!
  - all the stages need to be optimized

Challenges

- two challenges for the SISAP community
  - join us for developing the SIMDEX stages!
    (the axiom space is really huge to search by the current unoptimized implementation)
  - answer/prove the holy grail "SIMDEX spoiler" problem:

    Is the metric space model the "killer model" for general indexing, so that anything else (found by SIMDEX) is worse?

    (including a transformation step, like TriGen)

Thank you…

… for your attention!

questions?