Towards a theory of interactive learning

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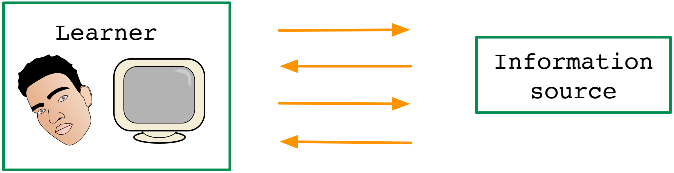
University of California, San Diego

Interactive learning

Adaptive engagement between a learning agent and information source(s).



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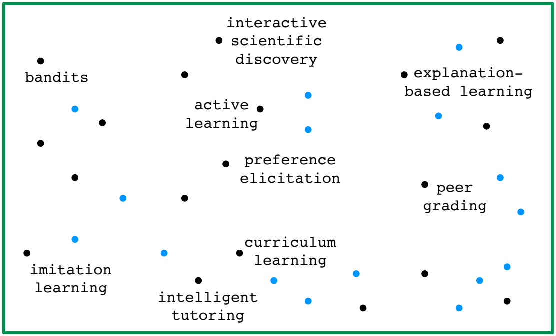

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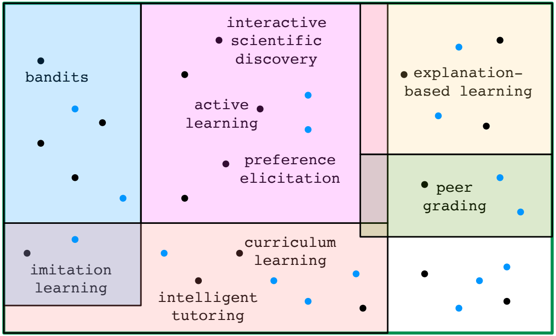

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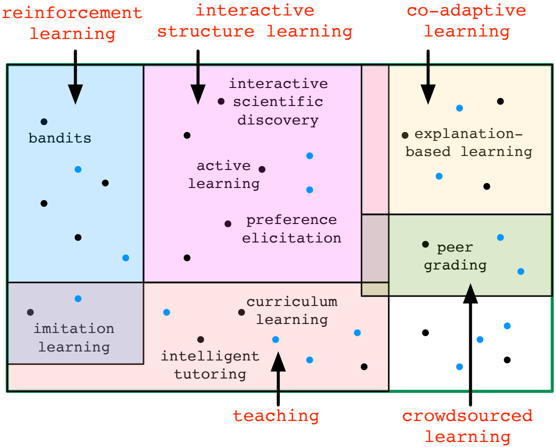


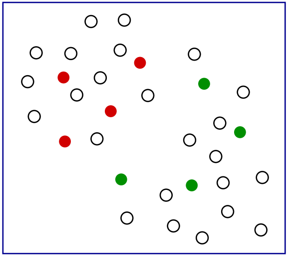
Outline

1. Interactive structure learning
2. Learning from partial correction
3. Structural query-by-committee
4. Interactive hierarchical clustering

Example: active learning of classifiers

Unlabeled data is often plentiful and cheap: documents off the web, speech samples, images, video. *But labeling can be expensive.*

Active learning: Machine queries just a few labels, choosing wisely and adaptively.



- Good querying schemes?
- Tradeoff between # labels and error rate of final classifier?

Example: interaction for unsupervised learning

Lots of progress on algorithms for unsupervised learning tasks, like

- Clustering
- Embedding
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But these could all benefit from interaction!

- What kind of feedback?
- How to incorporate?

Other examples

- Interactive learning of structured-output predictors
- Interactive knowledge graph construction
- Interactive scientific discovery
- $\vdots$

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Plan: Fit all these into a general framework.

Desirable outcomes:

- Generic interactive learning algorithms
- Bounds on "interaction complexity"
- Formal relationship with existing models of learning

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- Space of instances $\mathcal{X}$.
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  Examples:
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  - knowledge graphs on $\mathcal{X}$
- There is some target $g^* \in \mathcal{G}$ that meets the user's needs.
  In fact, there may be many. Call them $\mathcal{G}^* \subseteq \mathcal{G}$.

Loss function on structures

Which structure would be chosen in the absence of interaction?

1. Loss function $L(g)$ over structures $g \in \mathcal{G}$

   $\min L(g)$ *subject to expert-supplied constraints*

   Examples:

   - $L(g) =$ cost function for clusterings g
   - $L(g) =$ regularization term for classifier g
   - $L(g) =$ smoothness of metric g wrt default distance

2. Prior distribution $\pi(g)$ over $\mathcal{G}$

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   E.g. $\pi(g) \propto e^{-L(g)}$.

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What kind of interaction is allowed?

Example: feedback for clustering

$\mathcal{X}$: points to be clustered; $\mathcal{G}$: space of possible clusterings

Machine has chosen some clustering $g \in \mathcal{G}$ and wants feedback.

- Look at protocols for which interaction time is constant.
- Show expert the restriction of g to $O(1)$ points from $\mathcal{X}$.

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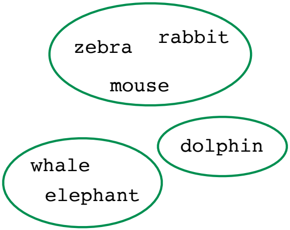

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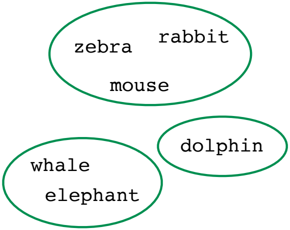

E.g. must-link `dolphin-whale`

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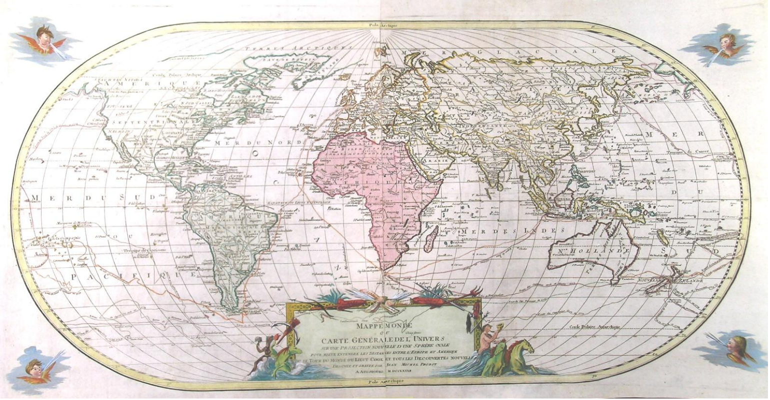

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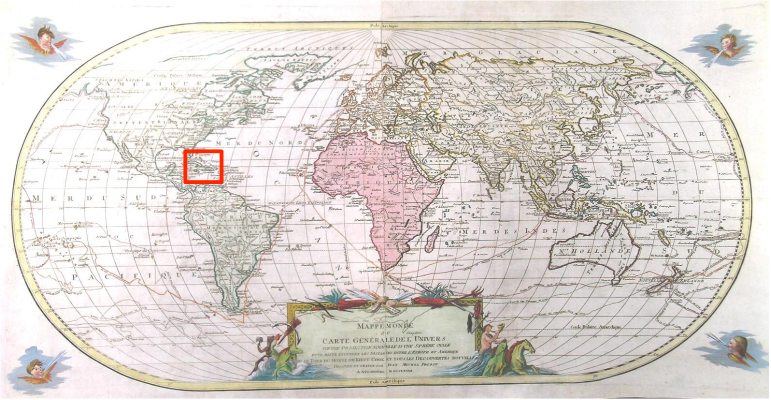

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Constant-time rounds of interaction:

- Learner displays a *snapshot* of g.
  For instance: the restriction of g to a small subset $S \subseteq \mathcal{X}$.
- Expert either accepts this snapshot or fixes part of it.
  These corrections serve as *constraints*.

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Requirement on snapshots:

$g \in \mathcal{G}^*$ iff expert accepts all snapshots

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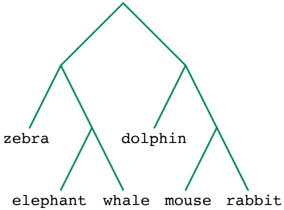

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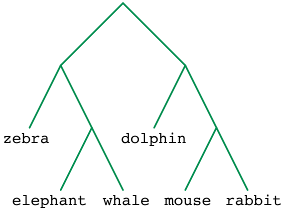

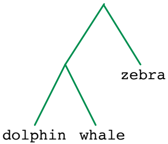

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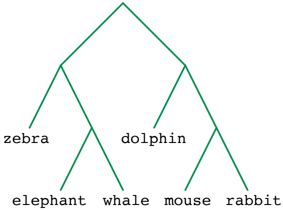

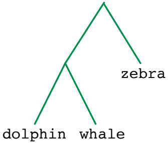

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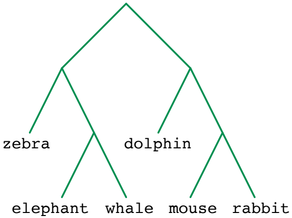
Key property: $g = g^*$ iff they agree on all triplets

Questions and atomic subquestions

Learner's current model: g



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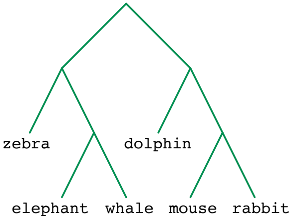

Snapshot: $g(\{$`dolphin, elephant, mouse, rabbit, whale, zebra`$\})$.

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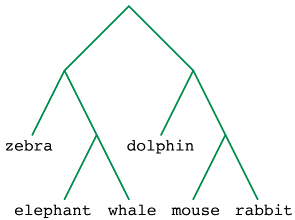

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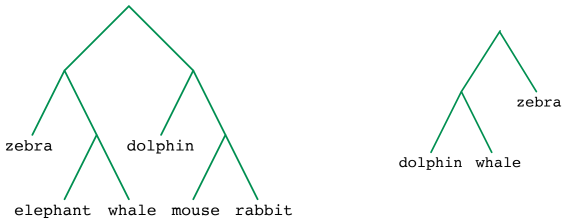

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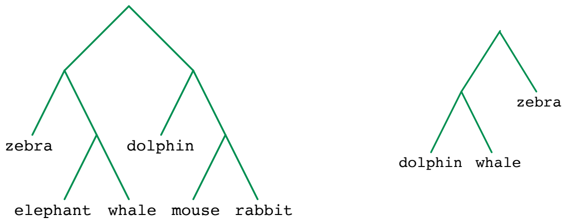

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- There are also smaller *atomic* questions, $\mathcal{A} = \binom{\mathcal{X}}{3}$.
- And g is also a function $g : \mathcal{A} \to \{\text{trees on 3 leaves}\}$.

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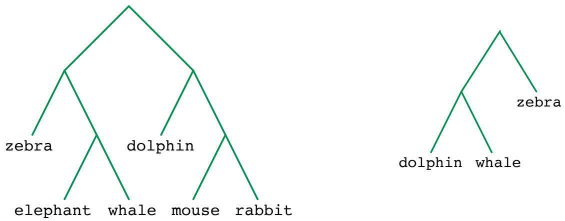

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- And g is also a function $g : \mathcal{A} \rightarrow \{\text{trees on 3 leaves}\}$.
- Each $q \in \mathcal{Q}$ contains atomic subquestions $A(q) \subseteq \mathcal{A}$.
- Expert provides feedback on one of these subquestions, $a \in A(q)$, for which $g(a) \neq g^*(a)$.

Summary of protocol

Learning problem:

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- Target structures: $\mathcal{G}^* \subseteq \mathcal{G}$

Protocol for learning:

Initial set of candidate structures: $\mathcal{G}_0 = \mathcal{G}$

For $t = 0, 1, 2, \ldots$:

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- $\mathcal{G}_{t+1}$ = structures in $\mathcal{G}_t$ that meet the new constraints

1. Reduction to multiclass classification

E.g. Think of any hierarchical clustering as a function from (subsets of s points) to (trees with s leaves):

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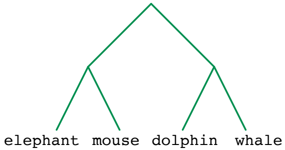

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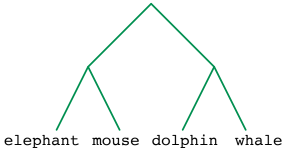
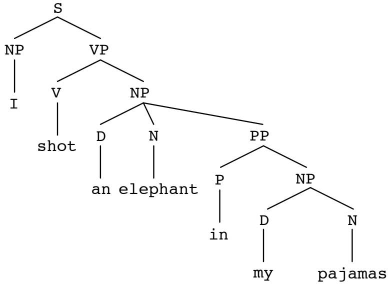
$\{$`dolphin, elephant, mouse, whale`$\} \longrightarrow$ 

Suggests many algorithms for interactive structure learning.

2. Partial correction



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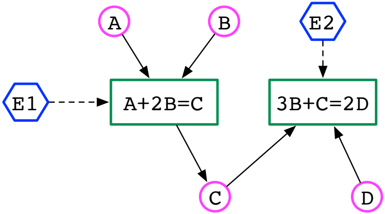

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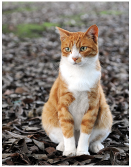

mammal
cat

arachnid
scorpion

bird
canary

amphibian
salamander

Benefits over the usual question-answer paradigm:

- Natural and intuitive interface that provides more context
- Gives the expert a chance to provide a teaching signal: identify key errors rather than minor ones
- More likely to contain an error than a single atomic subquestion
- More choice $\Rightarrow$ more reliable feedback?

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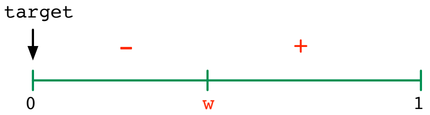
Structures to learn: threshold classifiers on $\mathcal{X} = [0, 1]$.

$$\mathcal{G} = \{g_w : w \in [0, 1]\}, \quad g_w(x) = 1(x \geq w).$$

Target $g^* = g_0$, i.e. everywhere 1.



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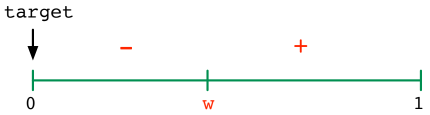

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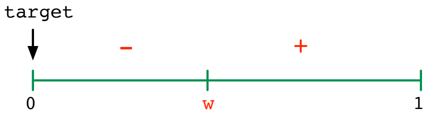

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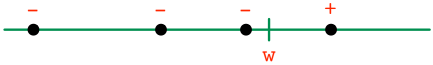
Expert sees c points chosen at random from $[0, 1]$, labeled by current w_t.



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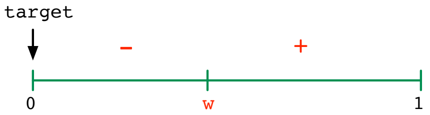

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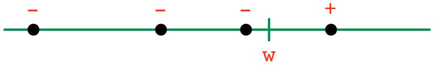
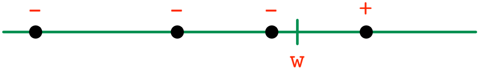


Which error will the expert point out?

Toy example, cont'd



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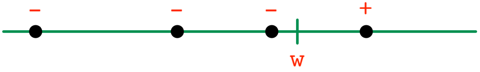

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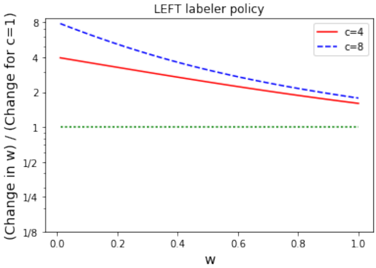
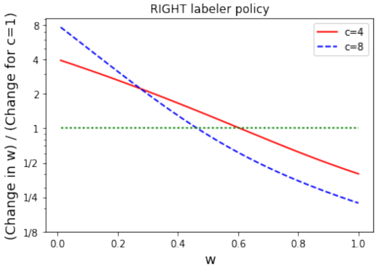
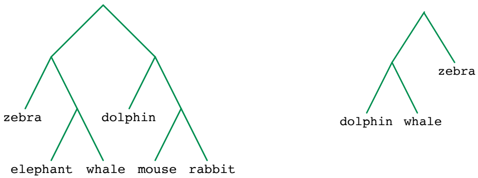




Convergence rates for partial correction



Here $\mathcal{Q} = \binom{\mathcal{X}}{6}$ and $\mathcal{A} = \binom{\mathcal{X}}{3}$

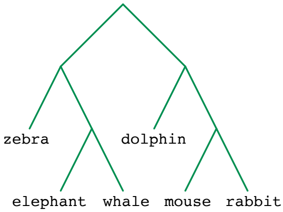
- Each query q contains $c = \binom{6}{3} = 20$ atomic subquestions $A(q)$
- Pick a distribution μ over $\mathcal{Q}$, e.g. uniform
- This induces a distribution ν over $\mathcal{A}$ (also uniform)
- Error rate of any hierarchy g: fraction of incorrect triples,

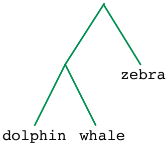
$$\mathrm{err}(g) = \Pr_{a \sim \nu}(g(a) \neq g^*(a)).$$

  Goal: want $\mathrm{err}(g) \leq \epsilon$.
- Random (i.i.d.) labeled triples: $O(\frac{1}{\epsilon} \ln |\mathcal{G}|)$ suffice.

But what if the triples are generated by partial correction?

Convergence rates for partial correction





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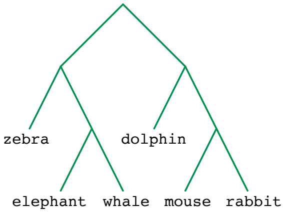

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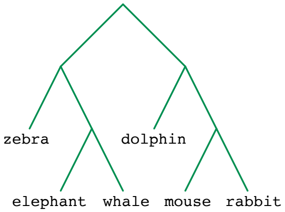

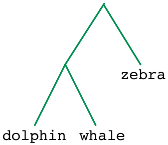

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But: even if snapshots are chosen at random, the feedback triples are not i.i.d.!

Sanity check: no matter what subquestions the expert chooses, sample complexity is $\widetilde{O}(\frac{1}{\epsilon} \ln |\mathcal{G}|)$.

Statistical analysis

Let ν be the desired distribution over atomic subquestions $\mathcal{A}$.
Let c be the maximum number of atomic questions in each query.

1. The distribution induced by partial correction on round t is some Γ_t such that:
$$\Gamma_t(a) \leq c \cdot \nu(a).$$
Therefore, at least $(1/c)$ fraction of the space $\mathcal{A}$ gets sampled.
2. Structures that have high error in the sampled region will be eliminated.
3. The sampling region keeps moving.
Once a region has been thoroughly sampled, structures that are bad in that region are removed. Subsequently-chosen structures g_t are bad elsewhere.

Outline

1. Interactive structure learning
2. Learning from partial correction
3. Structural query-by-committee (with Chris Tosh)
4. Interactive hierarchical clustering

Intelligent querying, by committee

QBC (Freund, Seung, Sompolinsky, Tishby)

$\mathcal{H}_0$: family of binary classifiers
π: prior on $\mathcal{H}_0$
μ: distribution on $\mathcal{X}$
At time $t = 0, 1, 2, \ldots$:
  Get a new data point $x_t \sim \mu$
  Pick $h, h' \sim \pi|_{\mathcal{H}_t}$
  If $h(x_t) \neq h'(x_t)$:
    Query the label y_t
    $\mathcal{H}_{t+1} = \{h \in \mathcal{H}_t : h(x_t) = y_t\}$
  Else: $\mathcal{H}_{t+1} = \mathcal{H}_t$

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  With probability $d(g, g'; q_t)$:
    Present $q_t, g(q_t)$ to expert
    Receive atomic constraints C_t
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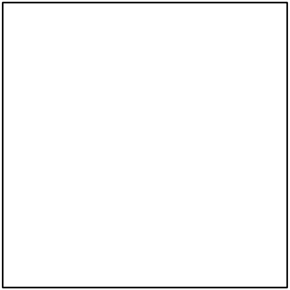
$\boxed{d(g, g'; q) = \text{fraction of atomic subquestions of } q \text{ on which } g, g' \text{ disagree.}}$

Statistical guarantees – convergence, rates – continue to hold.

Volume versus diameter

QBC (and many other schemes) pick queries to quickly shrink the volume of the version space: its probability mass under the prior π.

$\mathcal{G}$:



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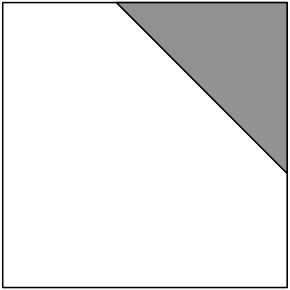

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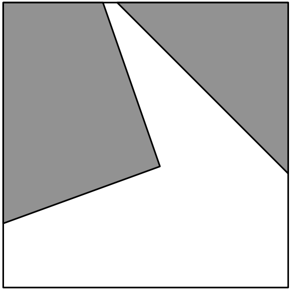

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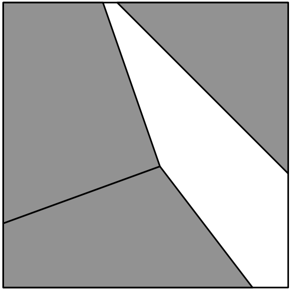

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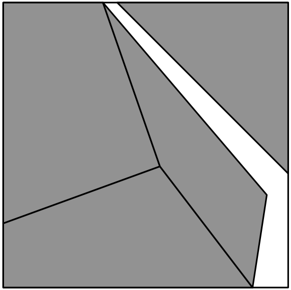

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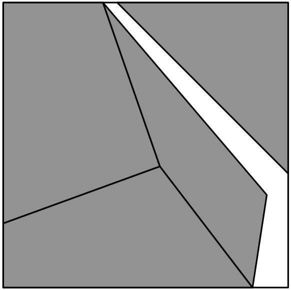

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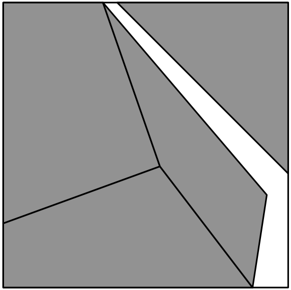

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Work in progress: extending this from active learning of binary classifiers to the general structure learning model.

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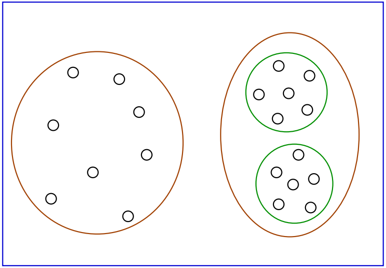
Hierarchical clustering



Useful tool for exploratory data analysis:

- Capture structure at all scales
- Well-established algorithms like average linkage.

As usual, the trees returned by these algorithms aren't necessarily aligned with the user's needs.

Hierarchical clustering with interaction

X = a set of points, $\mathcal{G}$ = all hierarchies on these points.

Three ingredients needed:

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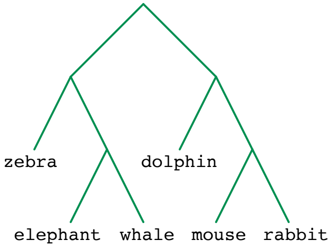

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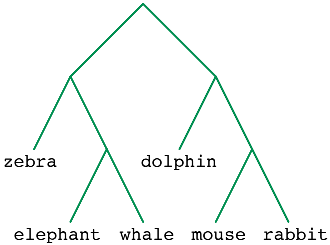

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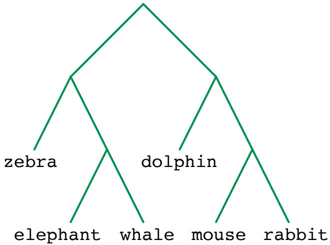

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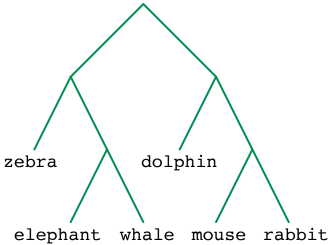

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3. An algorithm for $\min\{L(T) : T \in \mathcal{G} \text{ satisfies constraints}\}$

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Input: a similarity function on $X = \{x_1, \ldots, x_n\}$

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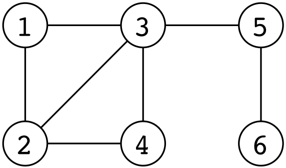
Can represent as an undirected graph with weights w_{ij}. Here's an example with unit weights:



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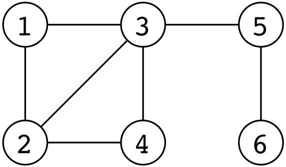

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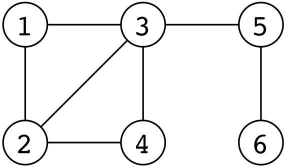

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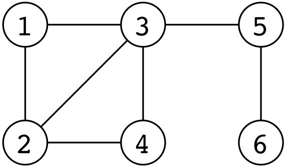
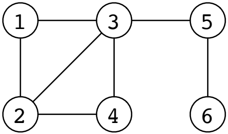
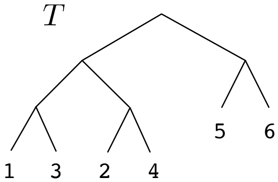


Idea for a cost function:

- Charge for edges that are cut.
  But: in a hierarchical clustering, all edges are cut.
- **Charge more the "higher up" an edge is cut.**

Cost function, cont'd





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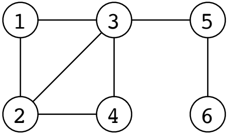

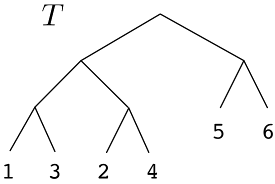

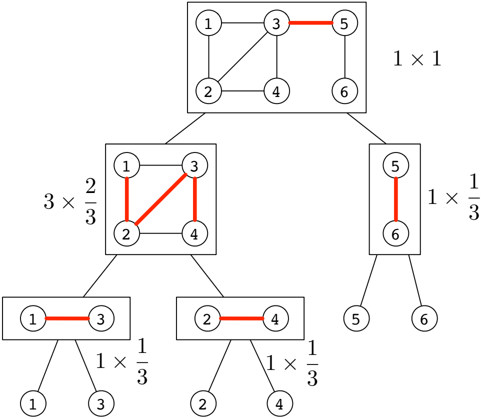

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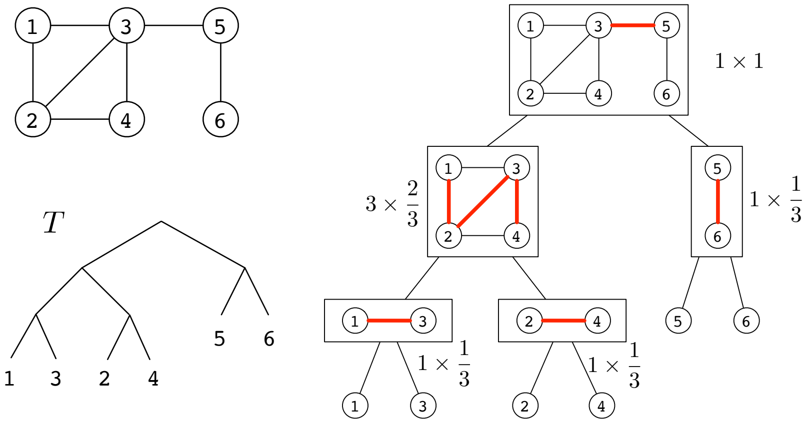

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Properties of cost function

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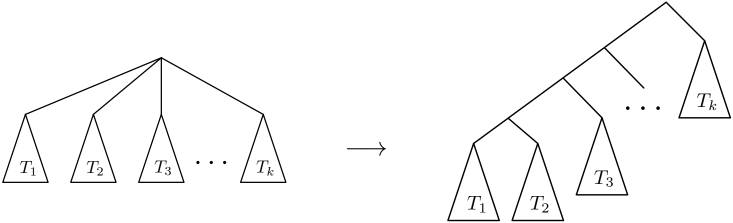
- There is always an optimal tree that is binary.



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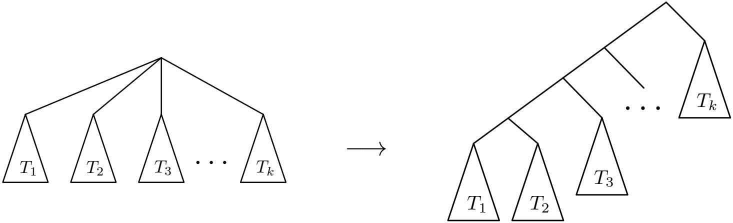
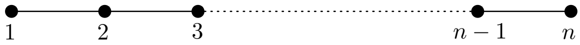


- If the similarity graph is disconnected, the top split of the optimal tree must cut no edges.

Three canonical examples

$$L(T) = \sum_{i,j} w_{ij} \cdot \#(\text{descendants of lowest common ancestor of } i, j)$$

1. Line graph on n nodes.



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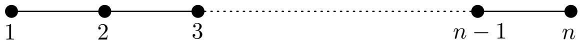

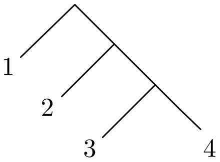

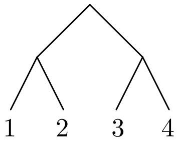

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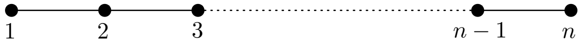

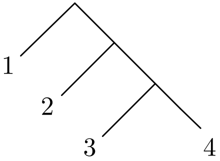

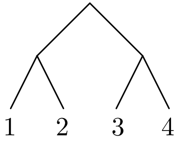

Unbalanced tree: cost $\Omega(n)$. Balanced tree: $O(\log n)$.

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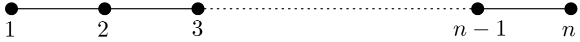

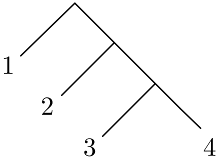

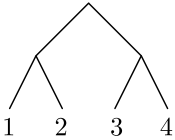

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2. Complete graph. All trees have the same cost.

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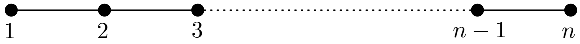

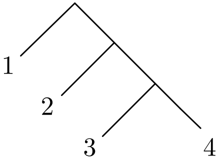

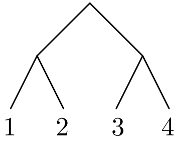

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3. Planted partition model. Correct clustering in expectation.

Algorithm for hierarchical clustering

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```
function MakeTree(V)
If |V| = 1: return leaf containing the singleton element in V
Let (S, V \ S) be an α-approximation to the sparsest cut of V
LeftTree = MakeTree(S)
RightTree = MakeTree(V \ S)
Return [LeftTree, RightTree]
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Let $(S, V \setminus S)$ be an α-approximation to the sparsest cut of V
LeftTree = MakeTree(S)
RightTree = MakeTree($V \setminus S$)
Return [LeftTree, RightTree]

This is an $(\alpha \log n)$-approximation to the optimal cost.

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This is an $(\alpha \log n)$-approximation to the optimal cost.

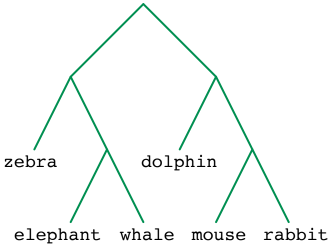
Actually [Charikar-Chatziafratis, Cohen-Kanade-Mathieu]: just $O(\alpha)$.

Hierarchical clustering with interaction

X = a set of points, $\mathcal{G}$ = all hierarchies on these points.

Three ingredients needed:

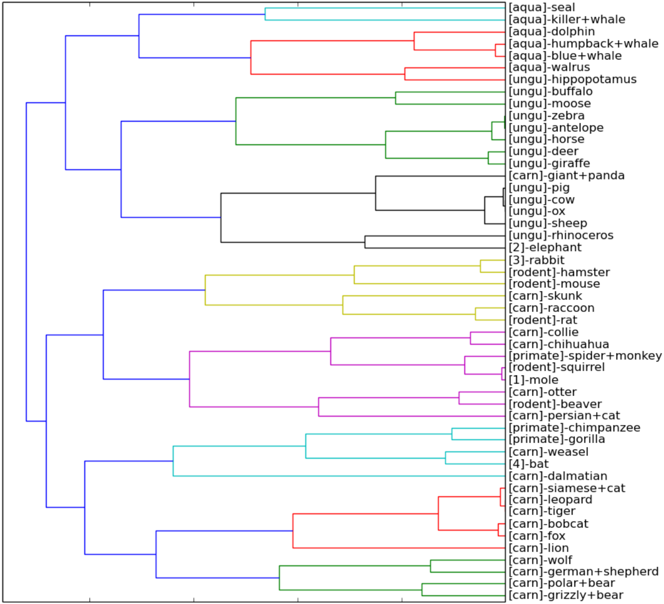
1. A method of interaction.



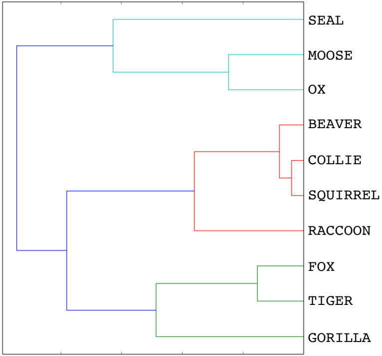
   Feedback: triplet constraint like $(\{\texttt{dolphin}, \texttt{whale}\}, \texttt{zebra})$

2. A cost function $L : \mathcal{G} \to \mathbb{R}$ over hierarchies.
   We have this now.
3. An algorithm for $\min\{L(T) : T \in \mathcal{G} \text{ satisfies constraints}\}$

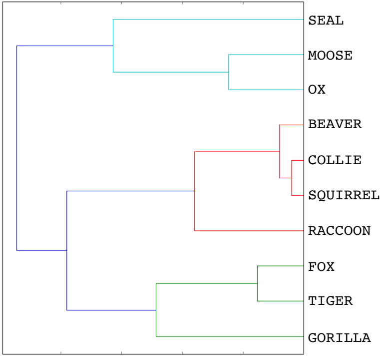
Animals with attributes, before interaction



Interaction example

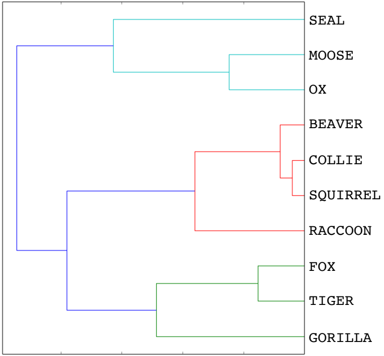


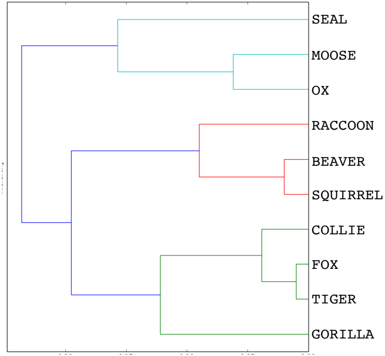
Interaction example



Constraint: $(\{\text{tiger}, \text{collie}\}, \text{gorilla})$

Interaction example





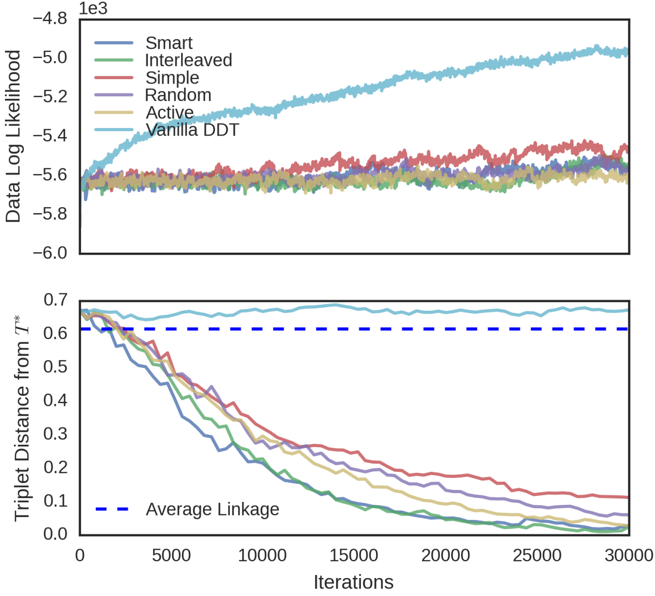
Constraint: $(\{\text{tiger}, \text{collie}\}, \text{gorilla})$

Intelligent querying

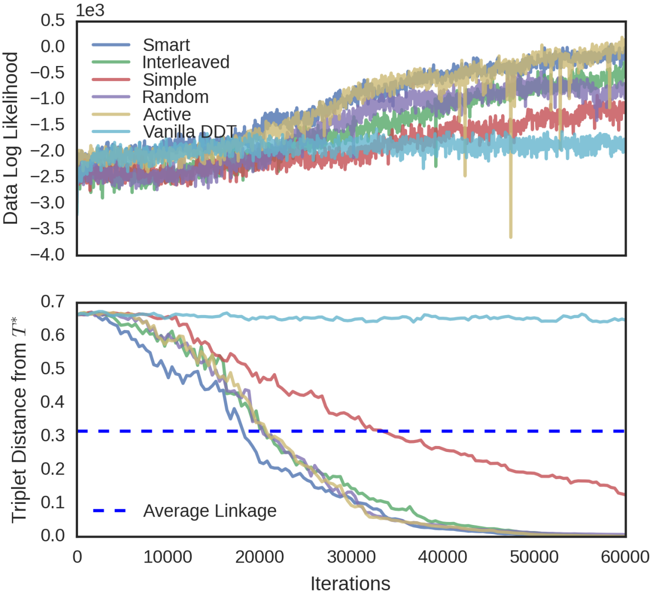
Structural QBC:

- Prior on trees: Dirichlet diffusion tree.
- Sample using Metropolis-Hastings walk with subtree-prune-and-regraft moves.
- Easy to incorporate constraints (and maintains strong connectedness of state space)
- Query every 100 iterations of the sampler.

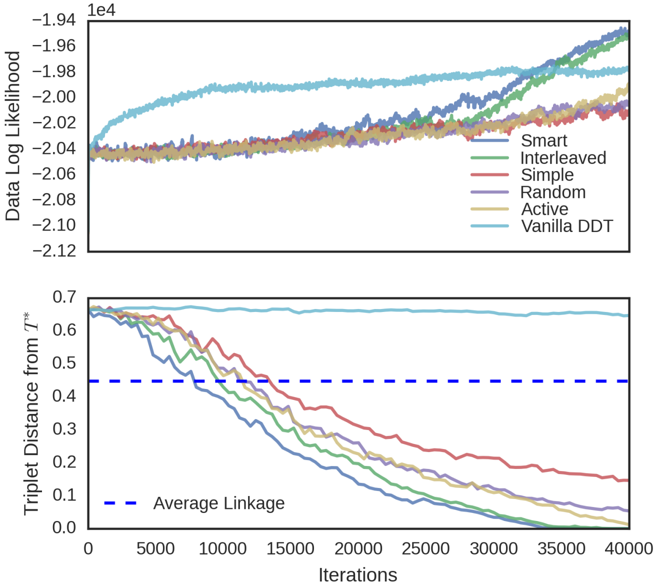
20 Newsgroups



Zoo


1e3
Data Log Likelihood
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
−3.5
−4.0
Smart
Interleaved
Simple
Random
Active
Vanilla DDT
Triplet Distance from T^*
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Average Linkage
0
10000
20000
30000
40000
50000
60000
Iterations

MNIST

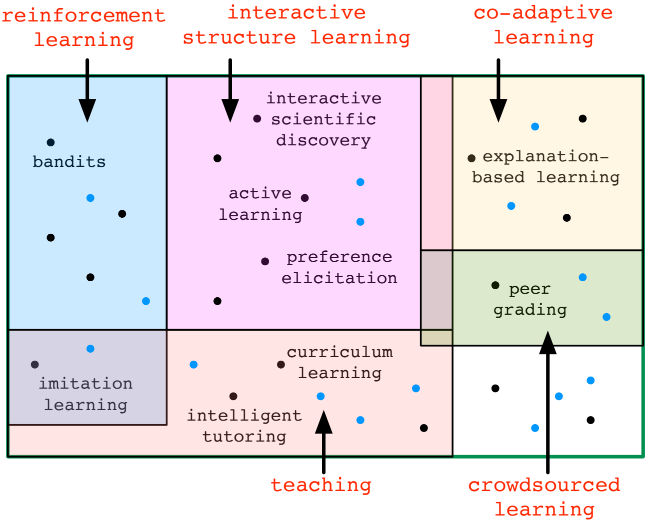


1e4
−1.94
−1.96
−1.98
−2.00
−2.02
−2.04
−2.06
−2.08
−2.10
−2.12
Data Log Likelihood
Smart
Interleaved
Simple
Random
Active
Vanilla DDT
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Triplet Distance from T^*
Average Linkage
0
5000
10000
15000
20000
25000
30000
35000
40000
Iterations

Outline

1. Interactive structure learning
2. Learning from partial correction
3. Structural query-by-committee
4. Interactive hierarchical clustering

Interesting directions



Bibliography

- A similarity-based cost function for hierarchical clustering. STOC 2016.
- With Sharad Vikram
  Interactive Bayesian hierarchical clustering. ICML 2016.
- With Mike Luby
  Learning from partial corrections. 2017.
- With Chris Tosh
  Diameter-based active learning. arXiv:1702.08553.
  Structural Query-by-Committee. 2017.