A Factorized Version Space Algorithm for "Human-in-the-Loop" Data Exploration

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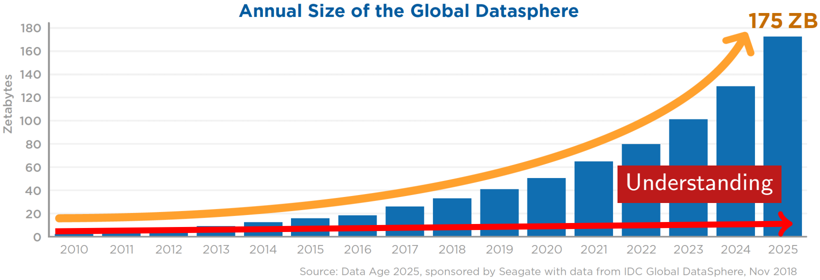
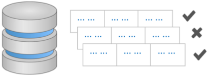
Motivation

- Data is growing extremely fast
- Human ability to comprehend data remains limited



Active Learning-based Interactive Data Exploration (IDE)

– in an **"explore-by-example"** framework



Database

$x_1, x_2, x_3, \ldots$

User

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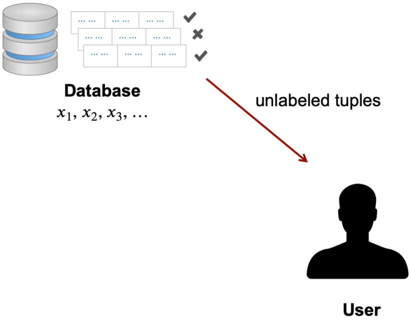

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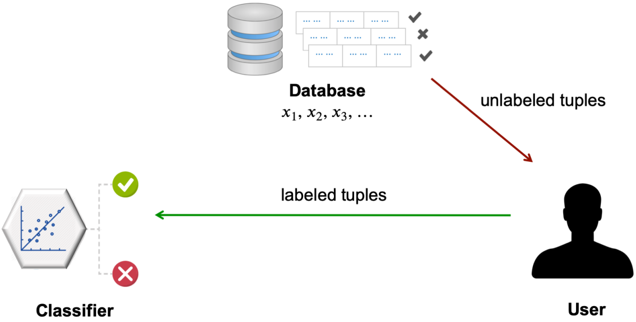

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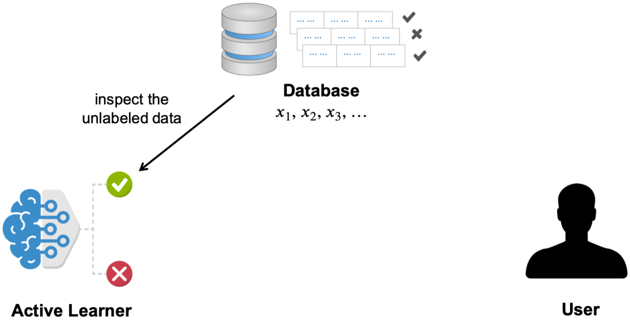

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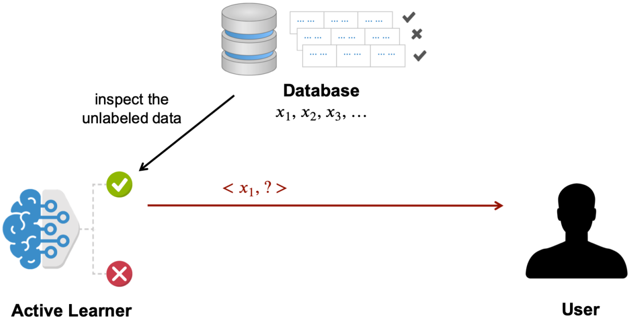

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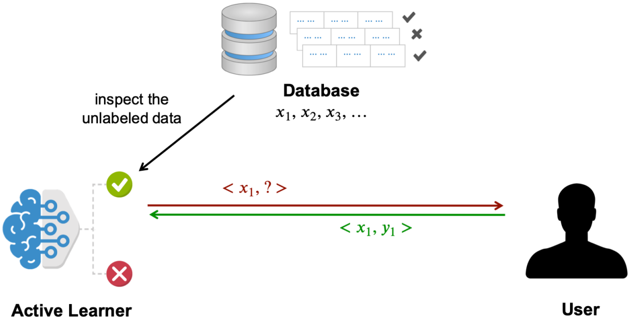

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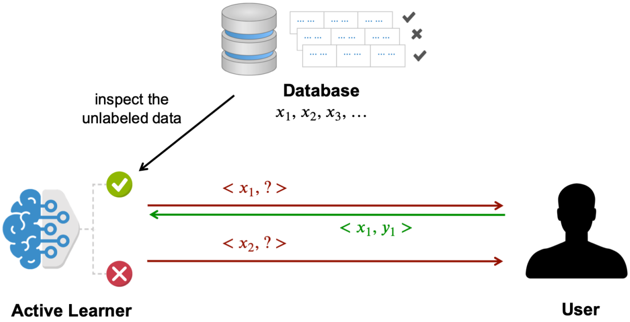

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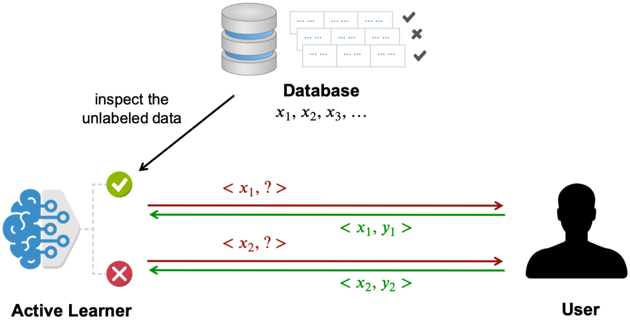

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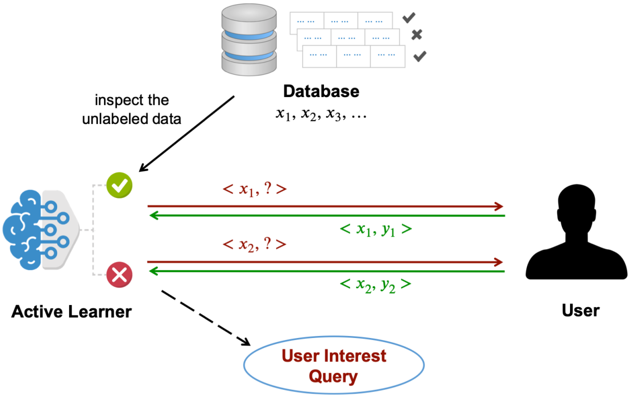


Active learning-based framework requires fewer labeled examples than a traditional learner

Focus of our work

Slow convergence problem

Existing AL algorithms and state-of-the-art IDE systems may require hundreds of labeled examples to reach high accuracy.

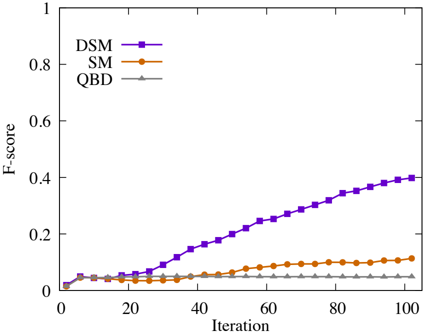


Figure: Comparison of explore-by-example IDE methods (SDSS 6D, 0.01%)

Idea #1: Explore Version Space algorithms

- **Main feature**: strong theoretical guarantees on performance.[1]
- **Main drawbacks**:
  - Usually too expensive for the IDE scenario.
  - In practice, still suffers from slow convergence in high-dimensional settings.

Question

Can we leverage their strong theoretical results, while still running under interactive performance?

Our solution

We propose an **optimized** version space algorithm meeting the interactive performance requirements.

More details in our paper!

[1] D. Golovin, A. Krause, *Adaptive Submodularity: A New Approach to Active Learning and Stochastic Optimization*, JMLR, 2007

The bisection rule

- $\mathcal{H}$: set of classifiers $h : \mathcal{X} \to \mathcal{Y}$ (e.g. linear, svm, ...)
- **Version Space**: subset of $h \in \mathcal{H}$ consistent with the labeled data $\mathcal{L}$:

$$\mathcal{V} = \{h \in \mathcal{H} : h(x) = y \text{ for all } (x, y) \in \mathcal{L}\}$$

- **Main idea**: shrink $\mathcal{V}$ as quickly as possible.

Bisection Rule[2]

Let $\mathcal{V}_{x,y} = \{h \in \mathcal{V} : h(x) = y\}$. The bisection rule selects x^* satisfying:

$$x^* \in \arg\max_x 1 - \sum_{y \in \mathcal{Y}} p_{x,y}^2$$

where $p_{x,y} = vol(\mathcal{V}_{x,y})/vol(\mathcal{V})$.

[2] Gonen and al., *Efficient Active Learning of Halfspaces: an Aggressive Approach*, JMLR, 2013

Idea #2: add factorization information

- The user decision-making process can usually be broken into a set of simple yes or no questions.
- **Example**: consider a user who wishes to buy a car. The user may have the following questions in mind:
  1. Is gas mileage good enough?
  2. Is the vehicle spacious enough?
  3. Is the color a preferred one?

Question

Can we leverage this decomposition information to help us expedite our algorithm's convergence?

Factorization: formalism

- Q: user's unknown interest query, involving attributes $\{A_1, \dots, A_d\}$
- Based on intuition, Q is broken down into sub-queries $Q_1, \dots, Q_K$, with each Q_k involving a subset of attributes $\mathbf{A^k} = \{A_{k1}, \dots, A_{kd_k}\}$.
- $(\mathbf{A^1}, \dots, \mathbf{A^K})$ is called the **factorization structure**.
- The final query Q is related to Q_k by a **boolean function** F:

$$Q(x) = F(Q_1(x^1), \dots, Q_K(x^K))$$

- For each x, the user must provide the **partial labels** $Q_1(x^1), \dots, Q_K(x^K)$ in a consistent and independent fashion.

This decomposition lets us model each sub-query Q_k directly, breaking down the original classification task into several, simpler classification tasks.

Factorized Version Space: formalism

Given a factorization structure $(A^1, \ldots, A^K)$, we define:

- **Factorized hypothesis space**: we model one classifier per subspace:

$$\tilde{\mathcal{H}} = \mathcal{H}^1 \times \ldots \times \mathcal{H}^K$$

  where each tuple $H = (h_1, \ldots, h_K)$ is treated as a multi-label classifier:

$$x \to \big(h_1(x^1), \ldots, h_K(x^K)\big) \in \{-, +\}^K$$

- **Factorized version space**: by applying the usual definition, we can show the version space to be:

$$\tilde{\mathcal{V}} = \mathcal{V}^1 \times \ldots \times \mathcal{V}^K$$

  where $\mathcal{V}^k = \{h \in \mathcal{H}^k : h(x^k) = y^k, \text{ for } (x, y) \in \mathcal{L}\}$.

A Factorized Bisection Rule

Applying the bisection rule over $\tilde{\mathcal{V}}$ translates to:

$$x^* \in \arg\max_x 1 - \sum_{y \in \{-,+\}^K} p_{x,y}^2$$

where $p_{x,y} = vol(\tilde{\mathcal{V}}_{x,y})/vol(\tilde{\mathcal{V}})$

Theorem

The above computation can be simplified to:

$$x^* \in \arg\max_x 1 - \prod_k \big(1 - 2p_{x^k,+}(1 - p_{x^k,+})\big)$$

where $p_{x^k,+} = vol(\mathcal{V}^k_{x^k,+})/vol(\mathcal{V}^k)$.

In other words, we simply have to repeat the usual version space computations for each subspace.

Theoretical results

- $\mathcal{A}_f$: any Active Learner making use of the partial labels information.
- $H = (h_1, \ldots, h_K)$: classifiers matching the user preference in each subspace.
- $cost(\mathcal{A}_f, H)$: # of queries that $\mathcal{A}_f$ takes to identify h_k in every subspace.
- $cost(\mathcal{A}_f)$: average cost of $\mathcal{A}_f$ across all possible labeling H.

Theoretical guarantees on performance

The Factorized Version Space algorithm satisfies:

$$cost(Fact\,VS) \leq OPT_f \cdot \left(1 + \sum_k \ln\left(\frac{1}{\min_{h_k} \pi_k(h_k)}\right)\right)^2$$

where $OPT_f = \min_{\mathcal{A}_f} cost(\mathcal{A}_f)$.

Experimental Evaluation

- Datasets
  - Sloan Digital Sky Survey (SDSS)
    – a large sky survey database
    – 1% sample: 1.9 million tuples, 4.9GB
    – user interest queries from the SDSS query release[3]
- Algorithms for comparison
  - Factorized VS
  - DSM (w/ factorization)
  - AL algorithms: ALuMa[4], Simple Margin[5], Query-by-Disagreement[6]
- Total number of queries: 11

3 Sloan digital sky survey: Dr8 sample sql queries. `http://skyserver.sdss.org/dr8/en/help/docs/realquery.asp`

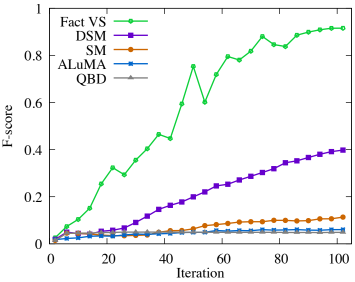
4 *Efficient Active Learning of Halfspaces: an Aggressive Approach*, JMLR, 2013

5 *Support Vector Machine Active Learning with Applications to Text Classification*, JMLR, 2001

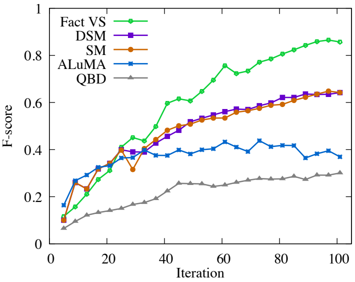
6 *Active Learning*, Morgan & Claypool Publishers, 2012

Experimental results: classification accuracy

- **Q6** (**6D**, 0.01%): $(a_1 - 682.5)^2 + (a_2 - 1022.5)^2 < 280^2$ AND $b_1 \in (150, 240)$ AND $b_2 \in (40, 70)$ AND $c_1^2 + c_2^2 > 0.2^2$
- **Q10** (**5D**, 0.5%): $g \leq 22$ AND $u - g \in (-0.27, 0.71)$ AND $g - r \in (-0.24, 0.35)$ AND $r - i \in (-0.27, 0.57)$ AND $i - z \in (-0.35, 0.70)$



(a) **Q6** (**6D**, 0.01%)



(b) **Q10** (**5D**, 0.5%)

The Factorized VS algorithm outperforms both DSM and AL algorithms for high-dimensional exploration.

Experimental results: running time

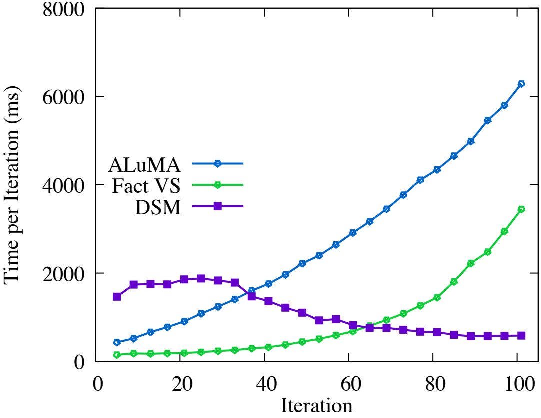


Figure: Time per iteration for Q10

Conclusion and Future Work

Our main take-aways are:

- We successfully extended version space algorithms to the IDE scenario, including several optimizations and extension to factorization.
- Our algorithms significantly outperform the existing state-of-the-art AL algorithms and IDE systems in accuracy and convergence speed, while maintaining the per-iteration time within a couple seconds.

Future work:

- Address **inconsistent labeling** by extending our models to a probabilistic one.
- Relax the assumption that a factorization structure is provided before the exploration beginning.
- Learn the factorization structure on-the-fly.

Thank you! Questions?

Code: `https://gitlab.inria.fr/ldipalma/aideme`

Bisection rule: theoretical guarantees

- Let $\mathcal{A}$ be an AL algorithm, and h a classifier matching the user interest. We define $cost(\mathcal{A}, h)$ as the number of queries that $\mathcal{A}$ takes to identify h. Additionally, we set:

$$cost(\mathcal{A}) = \sum_h cost(\mathcal{A}, h)\pi(h)$$

- **Theorem**[7]: the VS bisection rule satisfies:

$$cost(\text{VS bisection}) \leq OPT \cdot \left(1 + \ln \frac{1}{\min_h \pi(h)}\right)^2$$

where $OPT = \min_{\mathcal{A}} cost(\mathcal{A})$.

[7] D. Golovin, A. Krause, *Adaptive Submodularity: A New Approach to Active Learning and Stochastic Optimization*, Journal of Machine Learning Research, 2007

Bisection rule: implementation

- Every point x splits $\mathcal{V}$ into two sets:

$$\mathcal{V}_{x,\pm} = \{h \in \mathcal{V} : h(x) = \pm\}$$

- The bisection rule looks for x^* satisfying:

$$x^* \in \arg\min_x \left| \frac{vol(\mathcal{V}_{x,+})}{vol(\mathcal{V})} - 0.5 \right|$$

- Since computing volumes is hard, we fall back to sampling:

$$p(x) = \frac{vol(\mathcal{V}_{x,+})}{vol(\mathcal{V})} \approx \frac{1}{M} \sum_{i=1}^{M} \mathbb{1}(H_i(x) = +)$$

where $\{H_i\}_{i=1}^{M}$ is a random sample from $\mathcal{V}$.

Sampling the version space: linear case

- Let's consider the case of homogeneous linear classifiers:

$$\mathcal{H}_{hom} = \{h_w(x) = \text{sign}(w^T x), \text{ where } \|w\| \leq 1\}$$

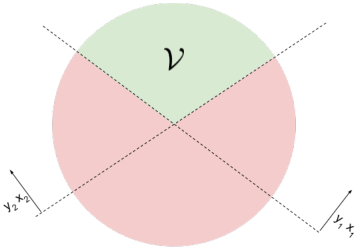
- Given a labeled set $\mathcal{L} = \{(x_i, y_i)\}$, the version space is:

$$\mathcal{V}_{hom} = \{h_w \in \mathcal{H}_{hom} : y_i x_i^T w \geq 0, \text{ for all } (x_i, y_i) \in \mathcal{L}\}$$

- Sampling from $\mathcal{V}_{hom}$ amounts to sample w from:

$$W = \{w \in \mathbb{R}^d : \|w\| \leq 1 \wedge Aw \geq 0\}$$

where $A_i = y_i x_i$ is the i-th row of A.



Sampling from W: the Hit-and-Run algorithm

- **Hit-and-Run**: algorithm for sampling from a convex body
- It generates a Markov Chain converging to the **uniform distribution** over the convex body

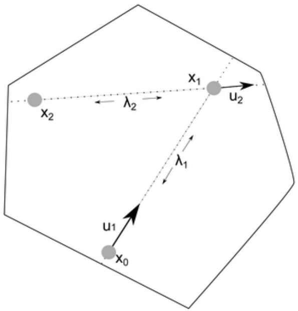


Figure: Hit-and-Run algorithm illustration

Optimizing Hit-and-Run: rounding

Problem: mixing time can be very large when convex set is elongated.

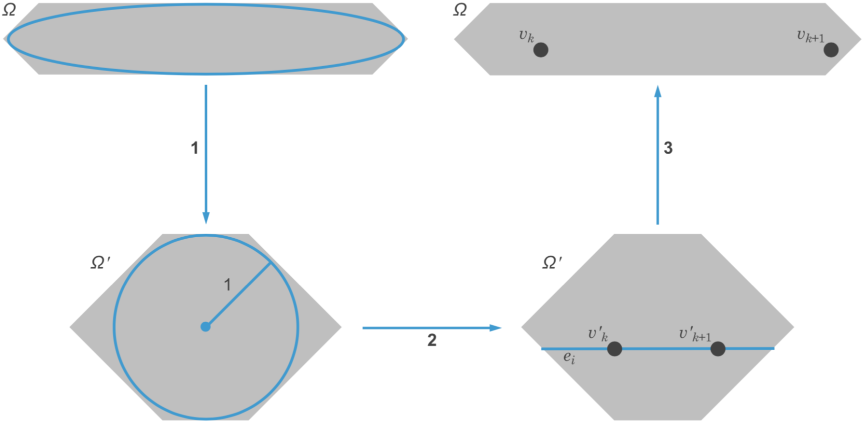


Figure: Rounding illustration

Effect of version space optimizations

- **Q2** (**2D**, 0.1%): $(rowc - 682.5)^2 + (colc - 1022.5)^2 < 29^2$
- **Q3** (**2D**, 0.1%): $ra \in (190, 200)$ AND $dec \in (53, 57)$

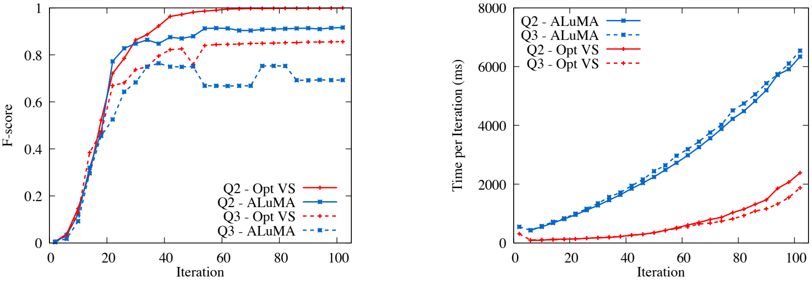
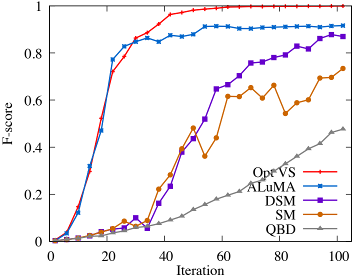


Figure: Effect of sampling optimizations on f-score and time

The proposed optimizations improve accuracy and reduce computation time.

State-of-the-art comparison: no factorization

- **Q2 (2D**, 0.1%): $(rowc - 682.5)^2 + (colc - 1022.5)^2 < 29^2$
- **Q3 (2D**, 0.1%): $ra \in (190, 200)$ AND $dec \in (53, 57)$



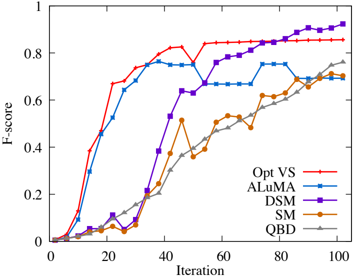


Figure: Comparison of AL methods for 2 selected queries

Our optimized VS algorithm is effective against the cold-start problem.