Towards the discovery of exceptional local models: descriptive rules relating molecules and their odors

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Definition and challenges of olfaction

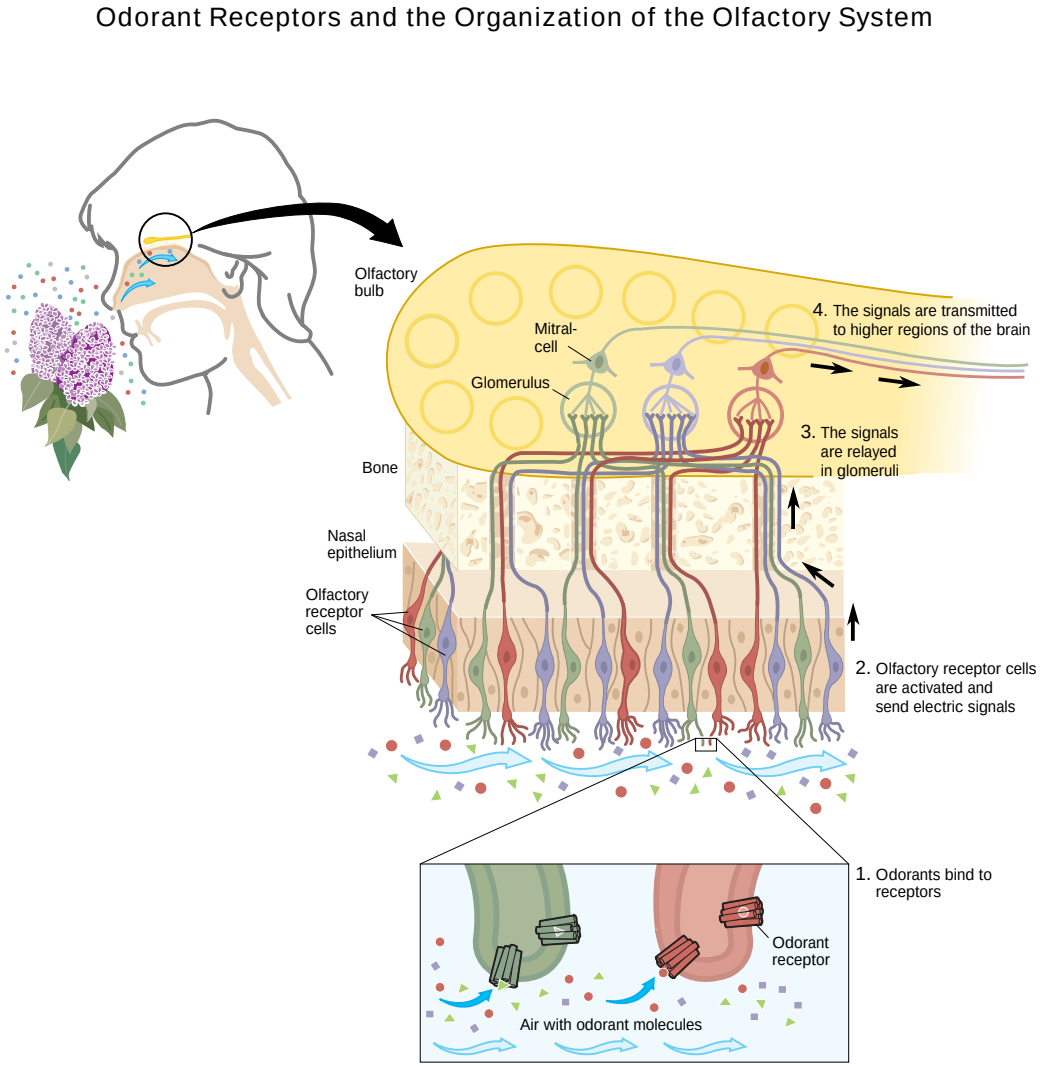
Olfaction, ...

- Ability to perceive odors
- Complex phenomenon from molecule to perception

C. Sezille et M. Bensafi

De la molécule au percept.
In *Biofutur*, 2013.

Definition and challenges of olfaction



http://www.nobelprize.org/nobel_prizes/medicine/laureates/2004/press.html

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Interest, ...

- Fundamental neuroscience research
- Industry (agri-food industry , perfume industry, ...)
- Health (anosmia, ...)

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Problem setting

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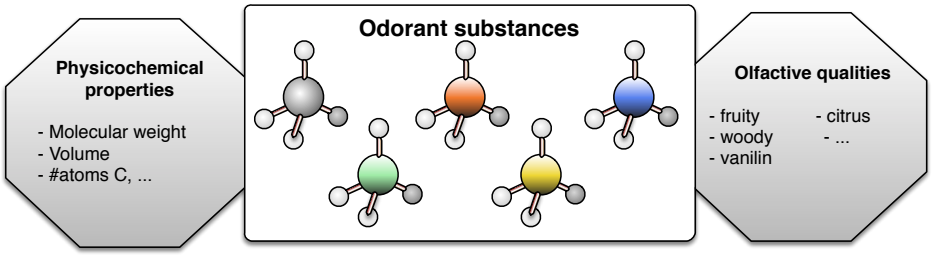

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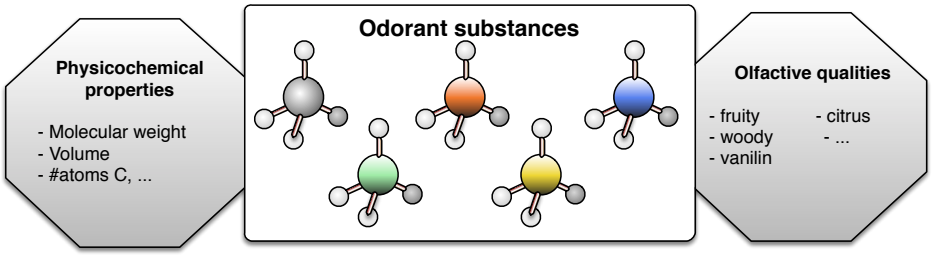

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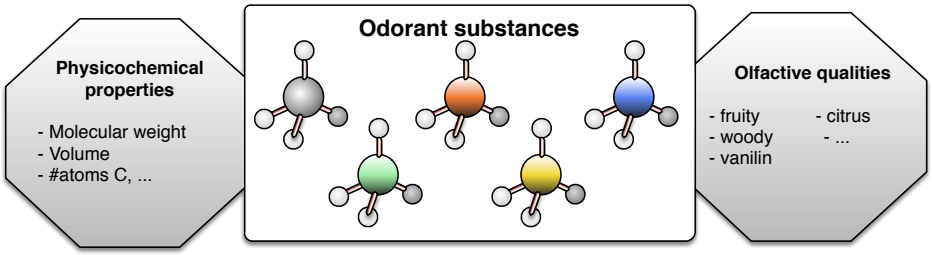

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$\rightsquigarrow$ How to **characterize** and **describe** the relationship between the **physicochemical properties** of a molecule and its **olfactory qualities** ?

Find (e.g.):

- $\langle MW \leq 151.28, 23 \leq nAT \rangle \longrightarrow Honey$, with a high quality measure

P.K. Novak, N. Lavrač, and G.I. Web

Supervised Descriptive Rule Discovery: A Unifying Survey of Contrast Set, Emerging Pattern and Subgroup Mining.
In *Journal of Machine Learning Research*, 2009.

Outline

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Subgroup discovery 1/2

Task: *Find and describe subgroups of odorant molecules significantly different for* ***a*** *[1] (or* ***all*** *[2]) olfactory quality(ies).*

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- **Algorithm:** heuristic approach (*beam-search*) to make search tractable

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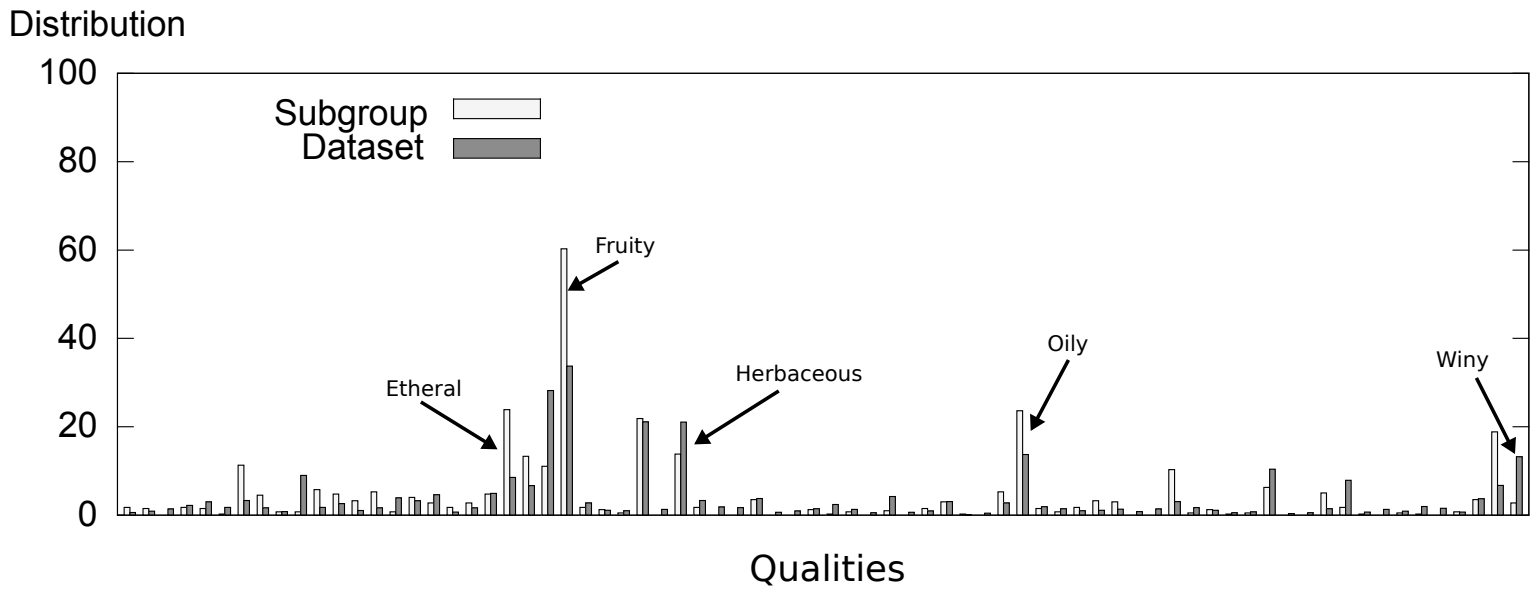

Outline

Exceptional local Model Mining 1/2

Principle: *Find and describe subgroups of objects (eg. odorants) significantly different for **a subset** of values of the class attribute (eg. olfactory qualities).*

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$$F_1(d, L) = \frac{2 \times (P(d, L) \times R(d, L))}{P(d, L) + R(d, L)}$$

where $P(d, L) = \frac{E11}{E11+E10}$ is the precision
$R(d, L) = \frac{E11}{E11+E01}$ is the recall

with $E10 = |\{o \in \mathcal{O} | o \in supp(d), class(o) \cap L \neq L\}$,
$E11 = |\{o \in \mathcal{O} | o \in supp(d), class(o) \cap L = L\}$,
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Objective: The task of EIMM is to extract the top-k local subgroups (d, L) *wrt* the quality measure such that:

- $|supp(d)| \geq minSupp$
- $|d| \leq maxDesc$
- $|L| \leq maxLab$

Exceptional local Model Mining 2/2

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High-level overview of ElMMut:

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- *Search space* based on a lattice structure of the local subgroups (partial order relation $\preceq$)

  eg. $\langle MW \leq 151.28, 23 \leq nAT, 10 \leq nC \rangle \preceq \langle MW \leq 151.28, 23 \leq nAT \rangle$

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- *Beam-search*: efficiently exploring search space top-down (from general to specific local subgroups)
- *Pruning step* realized thanks to constraints
- *On-the-fly bucketing* to handle numerical attributes and find best cut points (improve the quality measure of local subgroups)

U.M. Fayyad, and K.B. Irani
Multi-Interval Discretization of Continuous-Valued Attributes for Classification Learning.
In *IJCAI*, 1993.

ElMMut example

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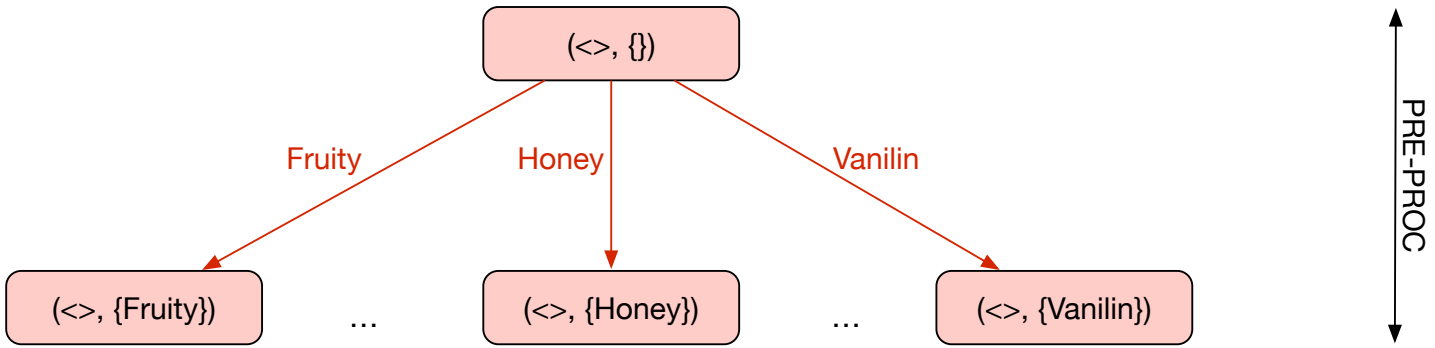

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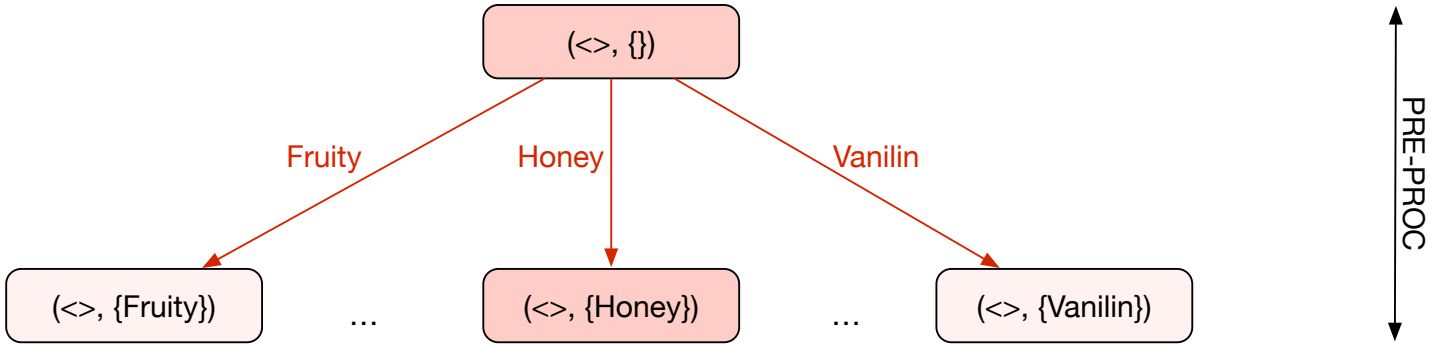

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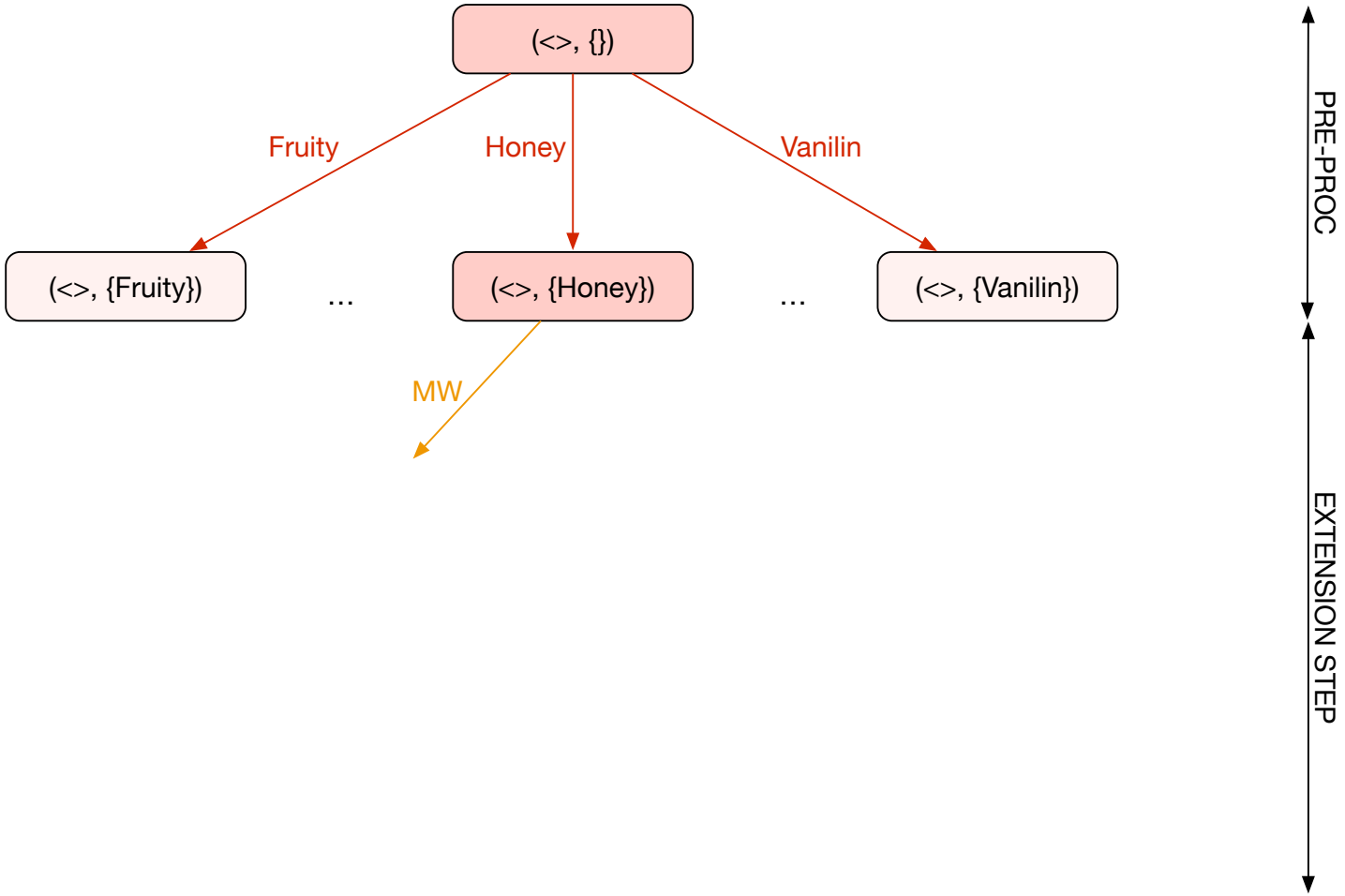

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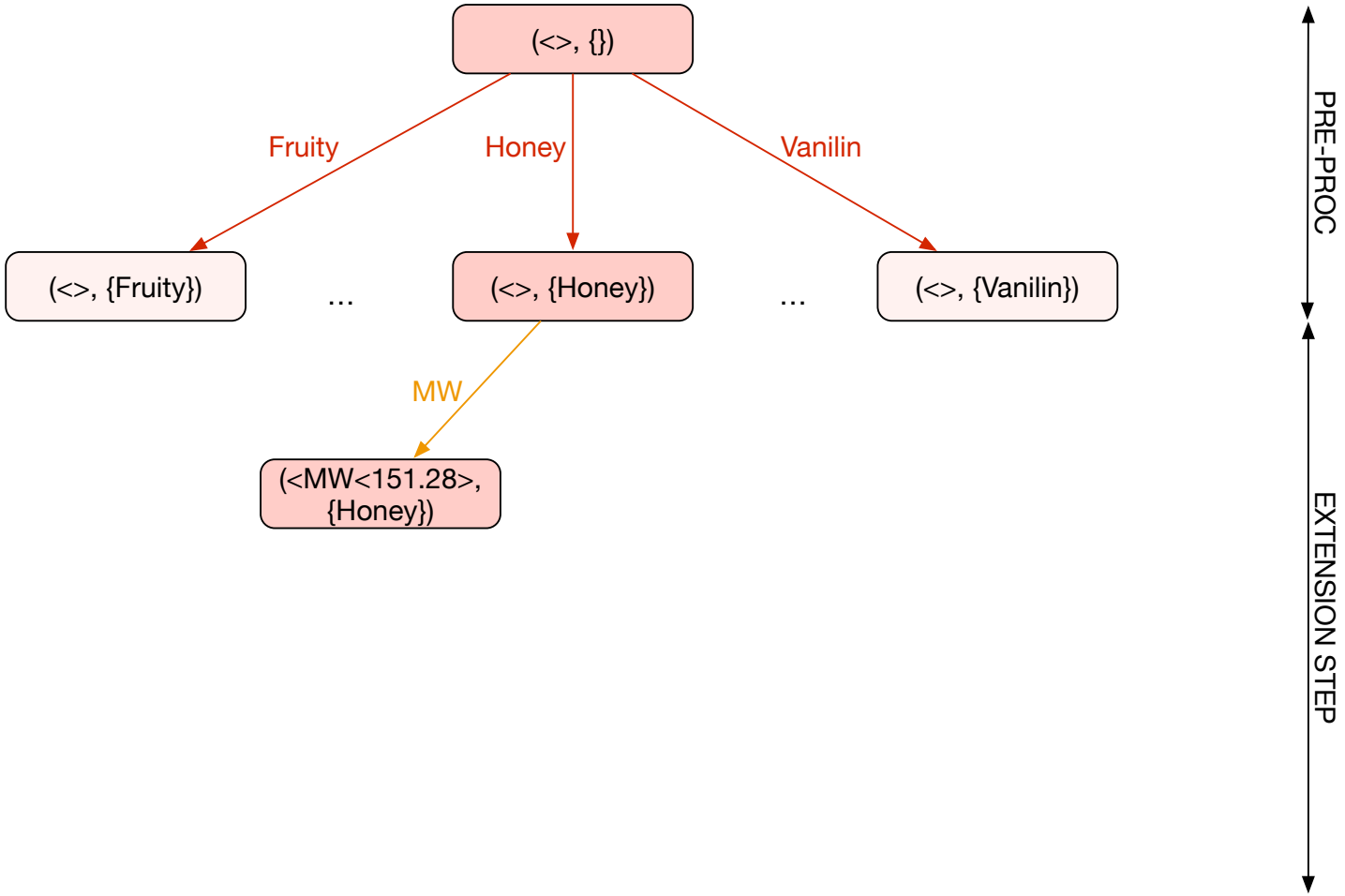

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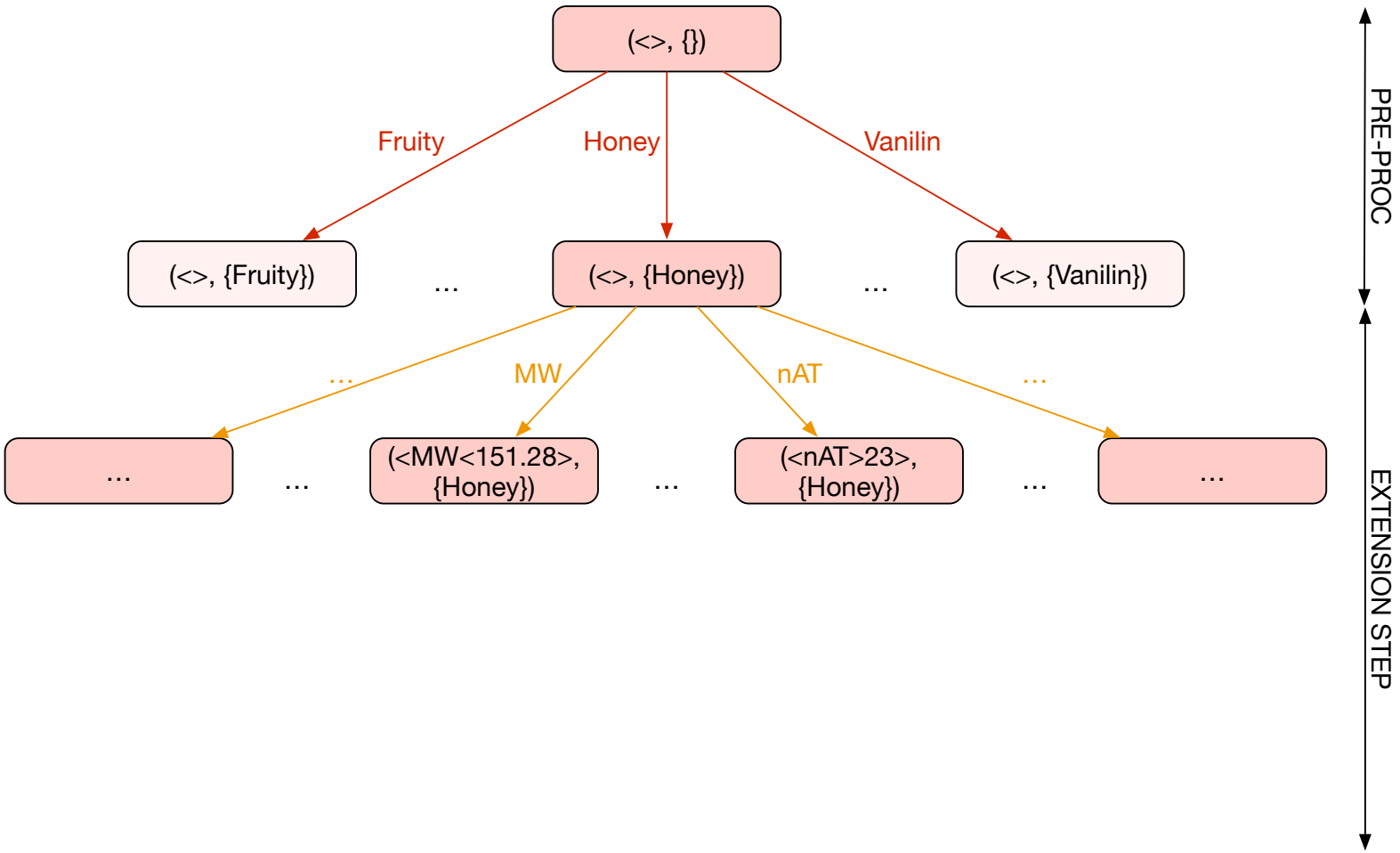

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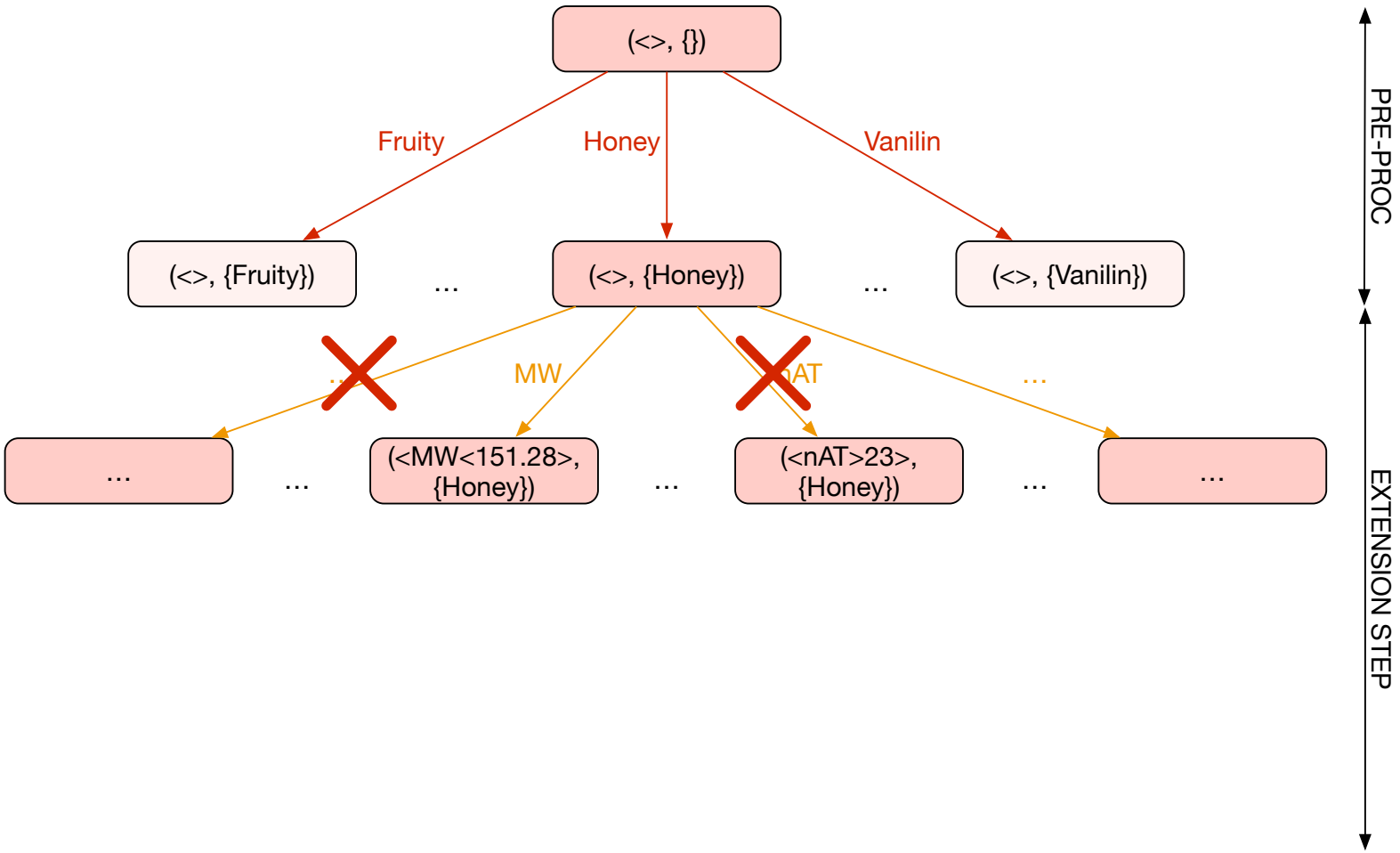

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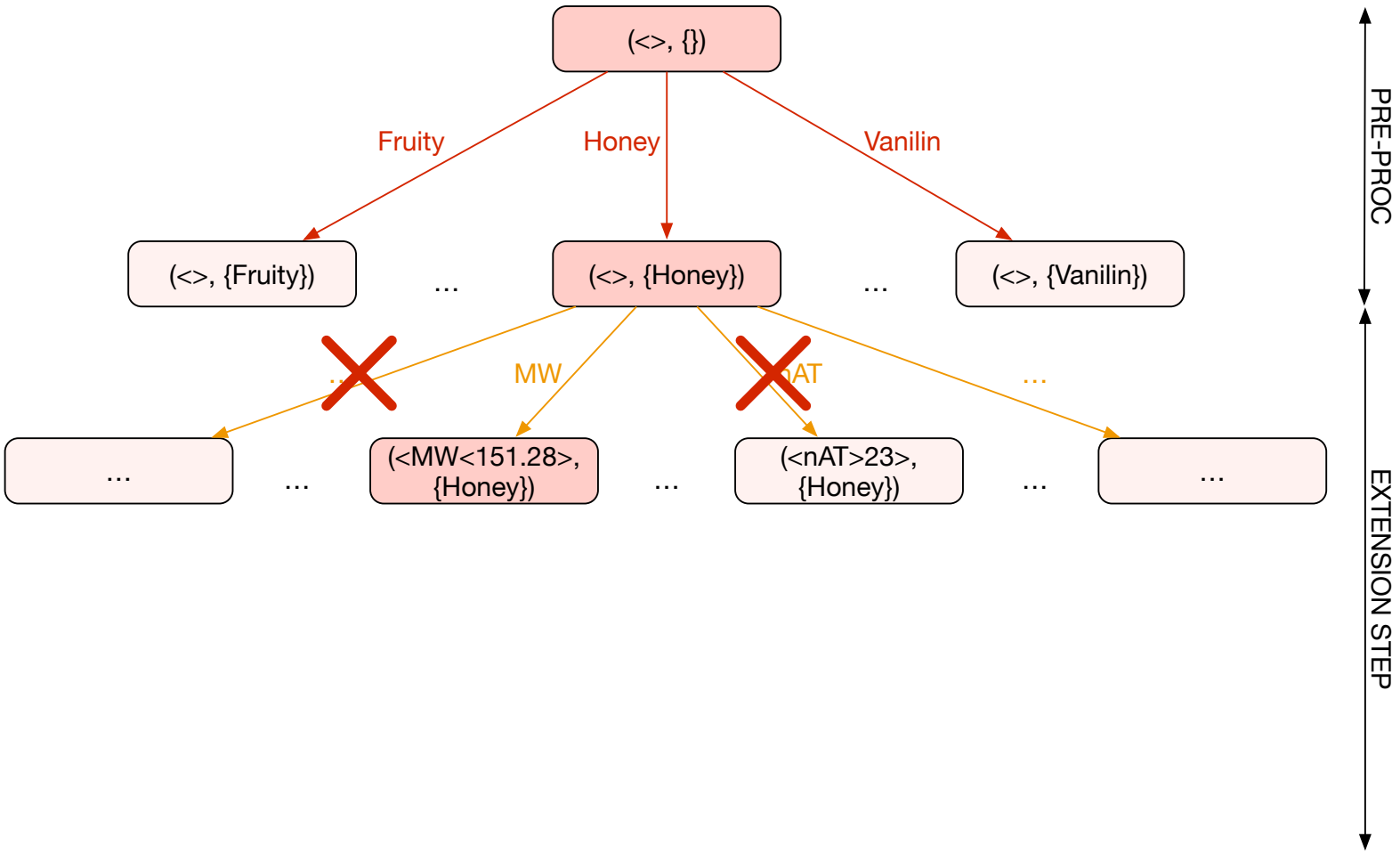

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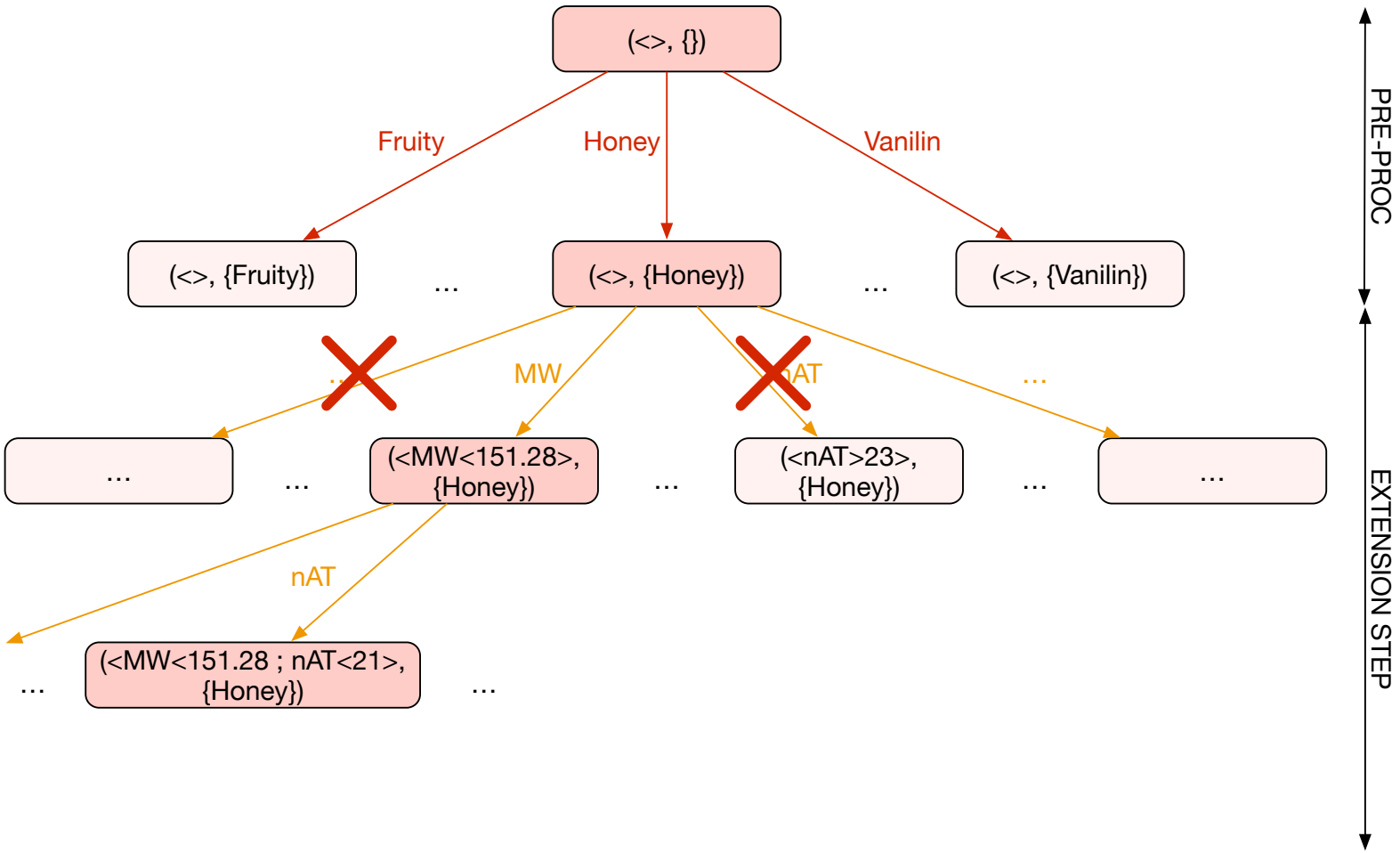

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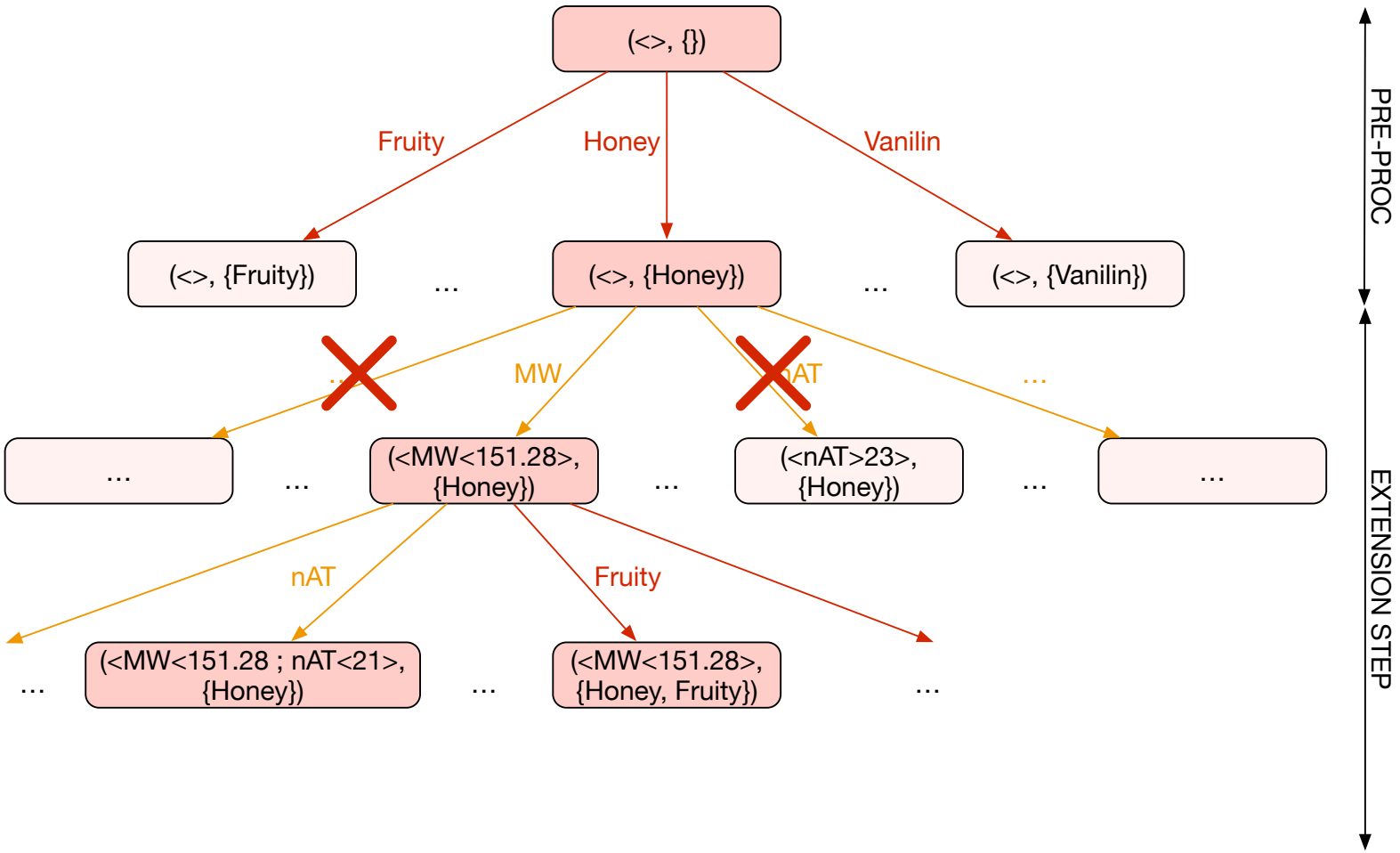

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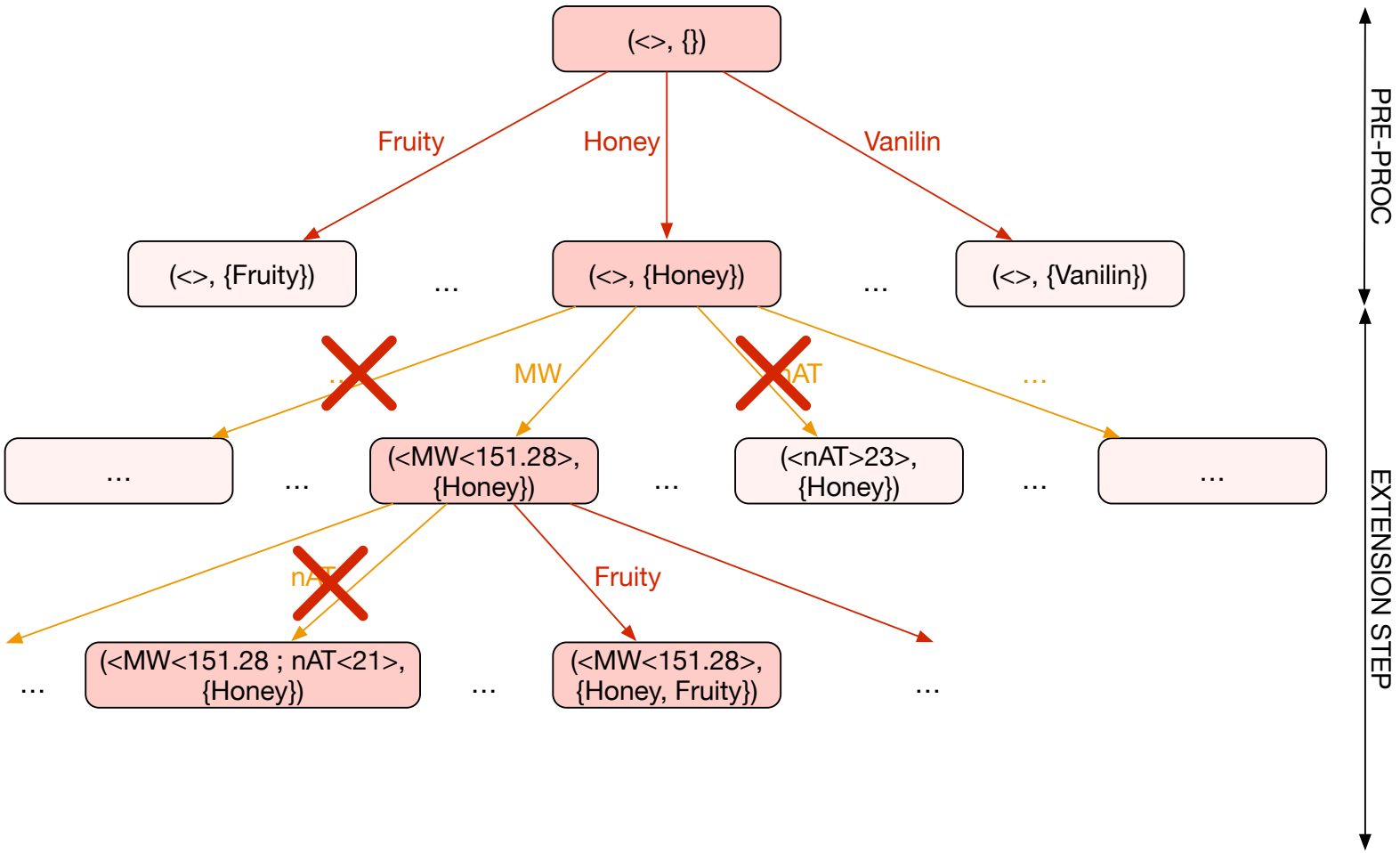

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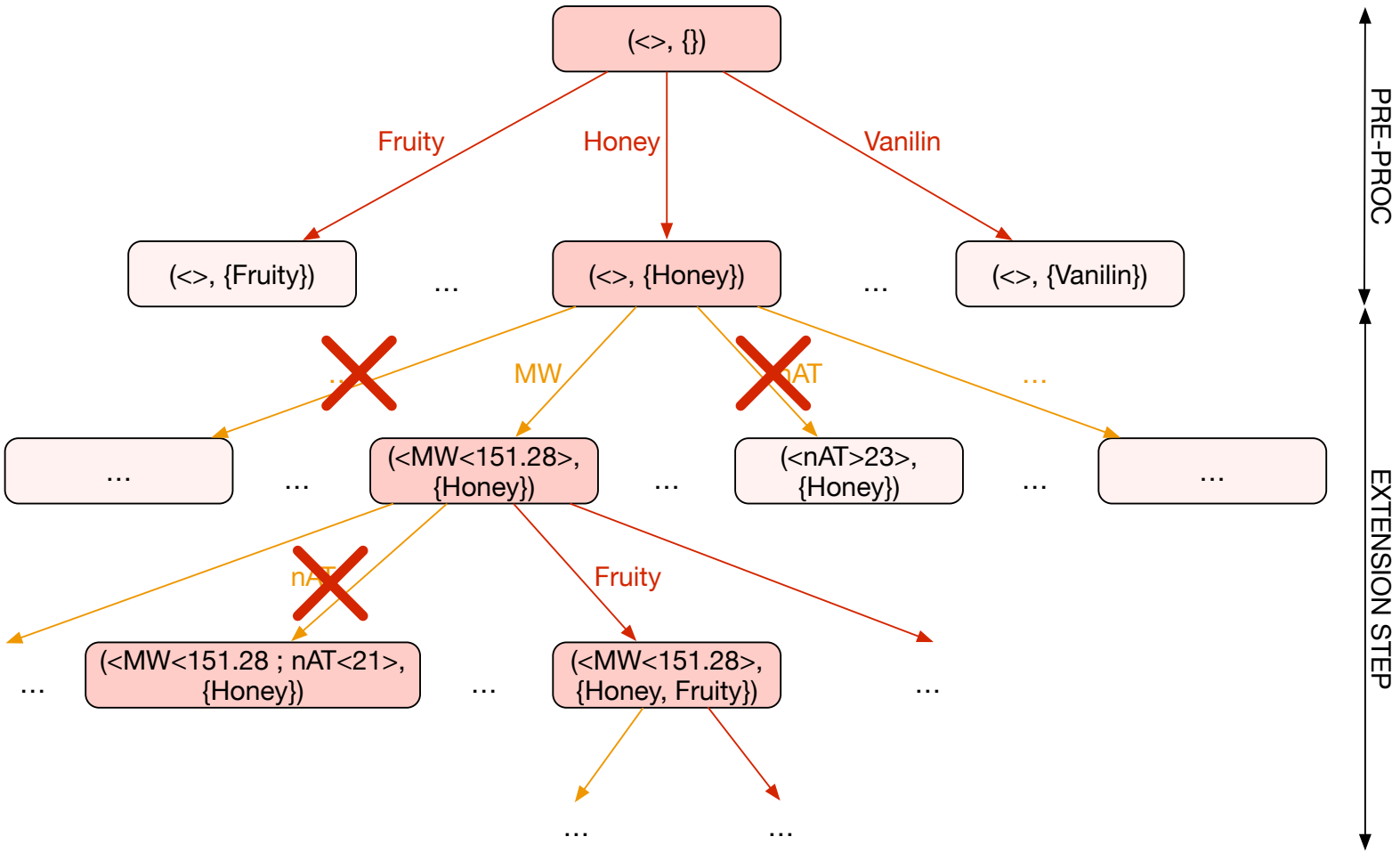

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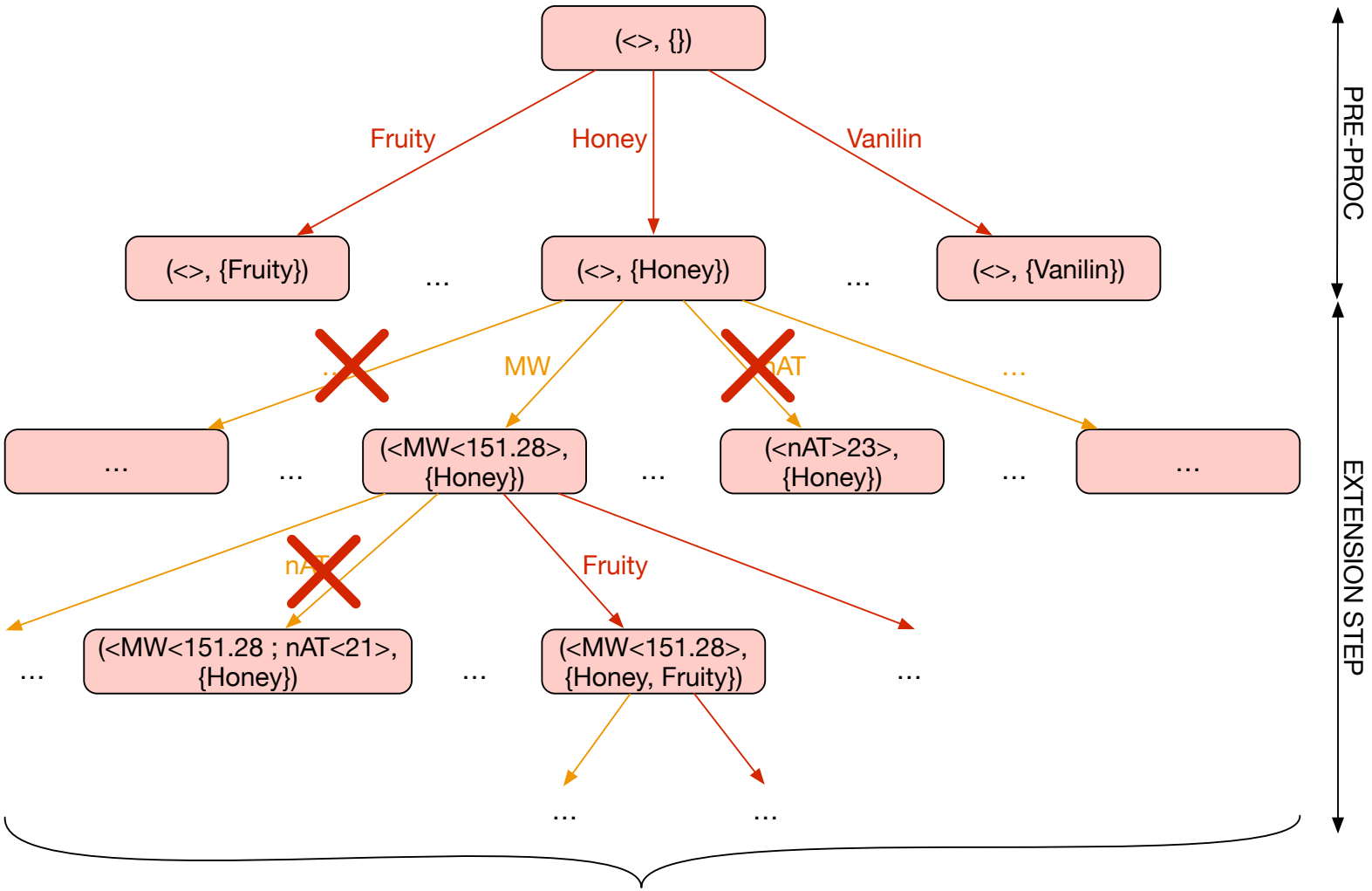


Extract the top-k of explored local subgroups

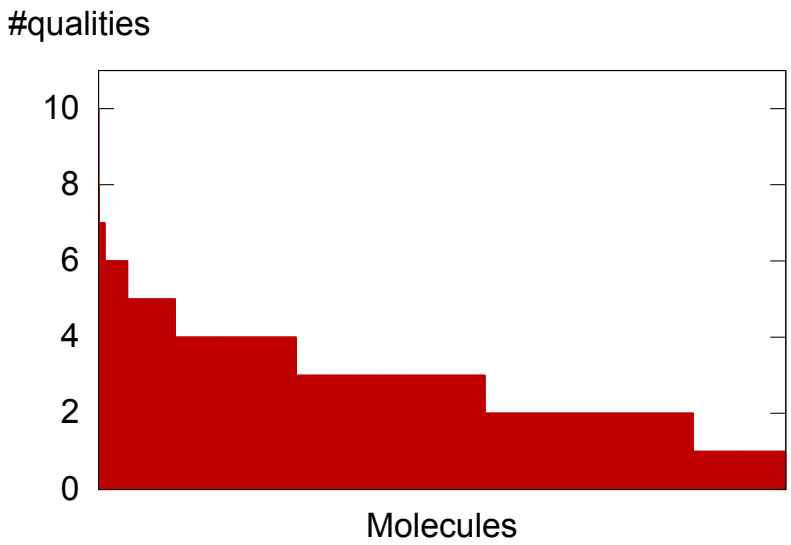
Outline

Establishment of datasets:

- 1 atlas (Arctander) provided by neuroscientists
- 2 datasets with different characteristics derived from atlas

	Dataset D1	Dataset D2
Atlas	Arctander	Arctander
Number of molecules	1689	1689
Number of physical properties	**43**	**243**
Number of olfactory qualities	74	74
Number of olfactory qualities per molecules	2.88	2.88

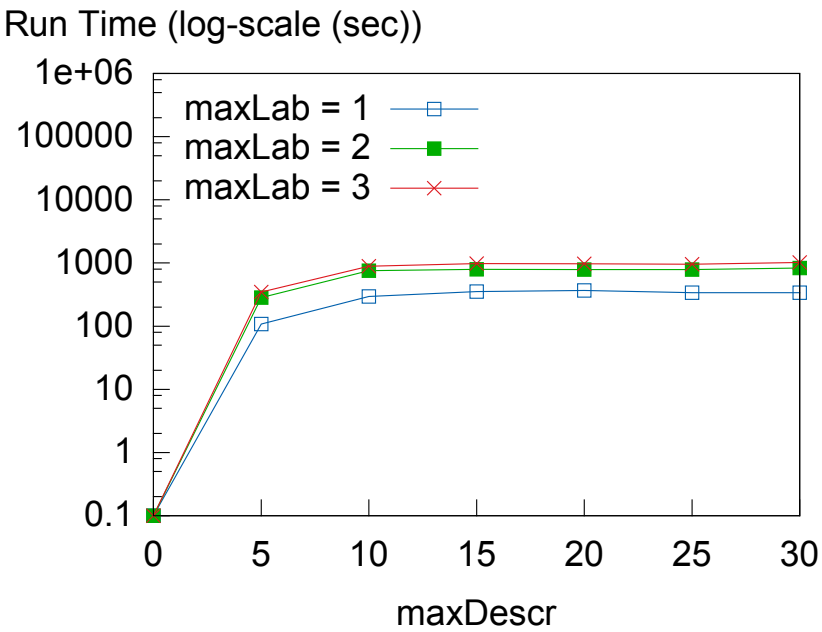
Characteristics of both datasets



S. Arctander
Perfume and flavor chemicals:(aroma chemicals).
In *Allured Publishing Corporation, Volume 2*, 1969.

Quantitative results

- Dataset D_1, no optimization bucketing
- Key factors: *maxDescr* and *maxLab*
- *maxDescr* = 15
  maxLab = 2 or 3



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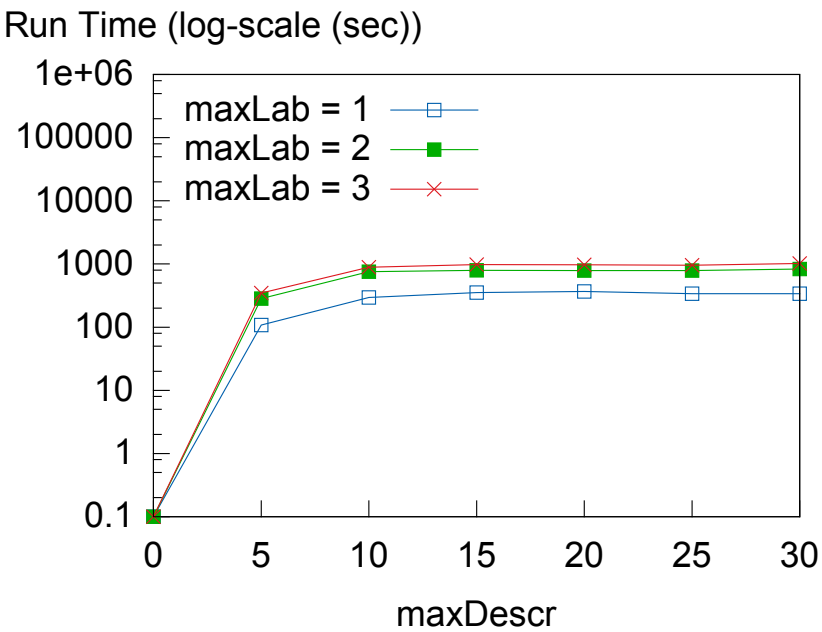
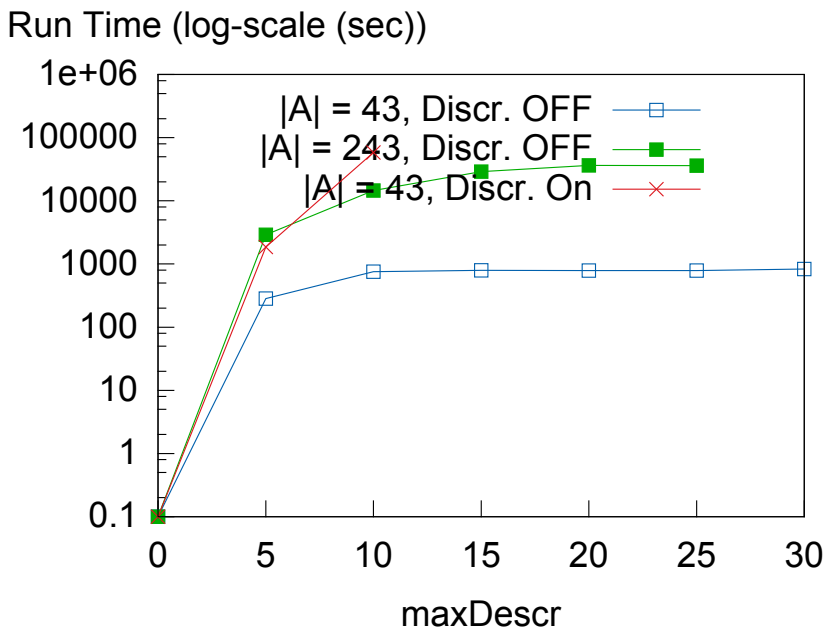
  maxLab = 2 or 3



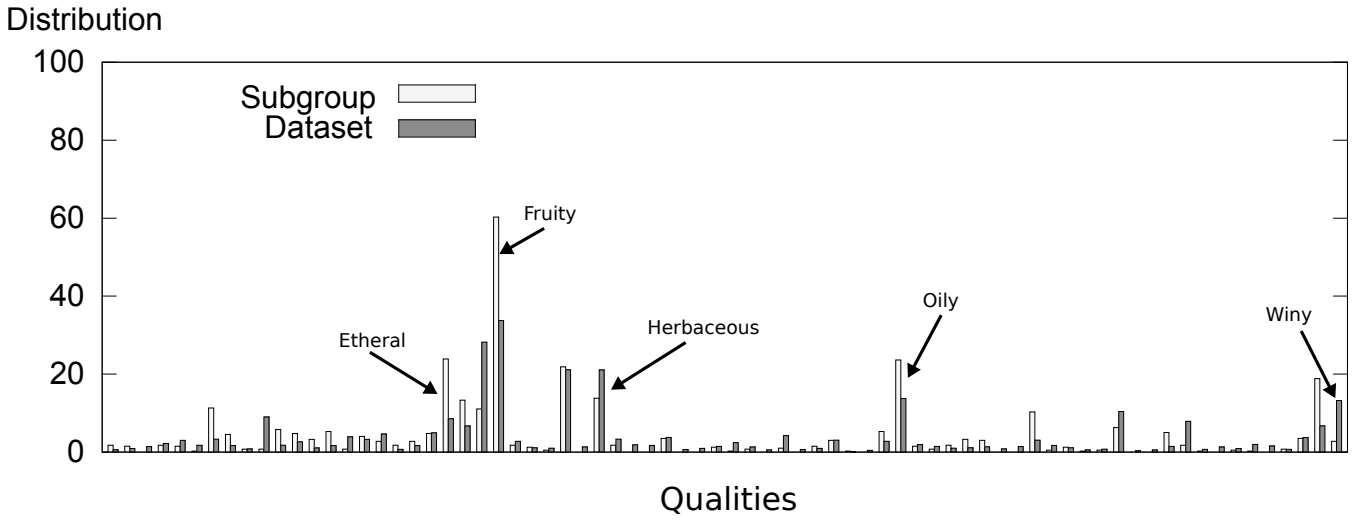
- Datasets D_1 and D_2
- Key factors: number of attributes and optimization bucketing



Qualitative results 1/2

Example of result existing method (EMM):

- Difficulties to interpret result
- Too many qualities are involved



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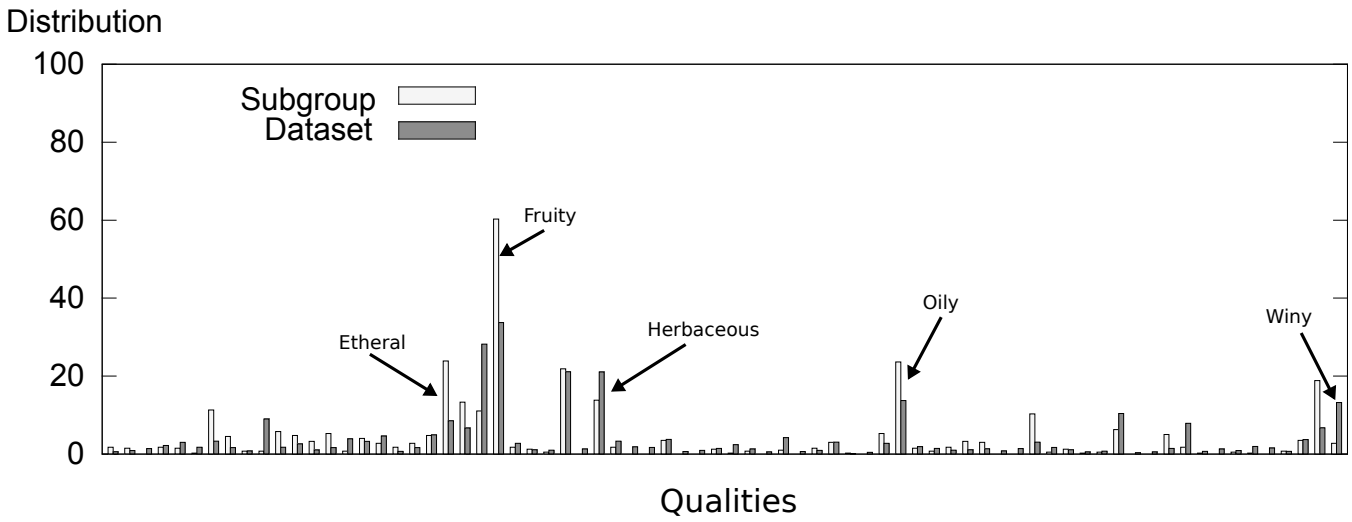

Example of result our method (EIMM):

- 74.6% of local subgroups involve 1 quality
- 22.9% of local subgroups involve 2 qualities
- 2.5% of local subgroups involve 3 qualities

Qualitative results 2/2

Top-5 local subgroups where:

- Dataset D_1
- Optimization bucketing
- $maxDescr = 10$, $maxLab = 2$, $minSupp = 30$

d	L	$\lvert supp(d) \rvert$	F_1
$\langle 0.116 < X\% < 0.314, 1.0 < nHet < 11.0, 5.159 < Sv < 8.792, 0.0 < nCIC < 0.0, 2.0 < nR03 < 8.0, 0.416 < Ui < 3.551, 4.0 < nArOH < 5.0, 1.0 < nCsp2 < 3.0, 12.0 < nCs < 47.0, 8.0 < nArCOOR < 25.0 \rangle$	{Fruity}	654	0.66
$\langle 134.19 < MW < 349.51, 14.0 < nCconj < 100.0, 4.76 < Sv < 8.277, 0.048 < X\% < 0.212, 22.0 < nCs < 49.0, 1.077 < Ui < 3.85, 18.0 < nAB < 49.0 \rangle$	{Floral}	740	0.55
$\langle 3.462 < Ui < 3.719, 30.0 < nCconj < 56.0, 40.0 < nAT < 57.0, 35.0 < nO < 50.0 \rangle$	{Musk}	32	0.5
$\langle 2.442 < TPSA(Tot) < 4.028, 4.74 < Sv < 6.095, 2.777 < Ui < 3.921, 0.208 < X\% < 0.31 \rangle$	{Oily}	213	0.44
$\langle 9.0 < nHet < 15.0, 6.095 < Sv < 8.258, 0.0 < Nr05 < 0.0, 2.749 < Ui < 3.517, 25.0 < nAB < 45.0, 2.279 < TPSA(Tot) < 3.334, 24.0 < nRCOOH < 34.0, 21.0 < nCconj < 51.0, 0.074 < X\% < 0.171 \rangle$	{Floral, Balsamic}	38	0.33

Outline

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The goals

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- Study the relationship between physicochemical properties and olfactory qualities

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Promising results

- Experiment on datasets provided by CRNL
  - Results considered interesting by expert
  - Theoretical avenues of improvements identified
- We invite you to explore further: ($\rightarrow$ *http://liris.cnrs.fr/olfamining*)

Perspectives

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2D and 3D representation of molecules: how take into account these key parameters to improve the efficiency of our method ?

Thank you for your attention.

Any questions ?