fast effective molecular feature mining by local optimization

Albrecht Zimmermann, Björn Bringmann, Ulrich Rückert

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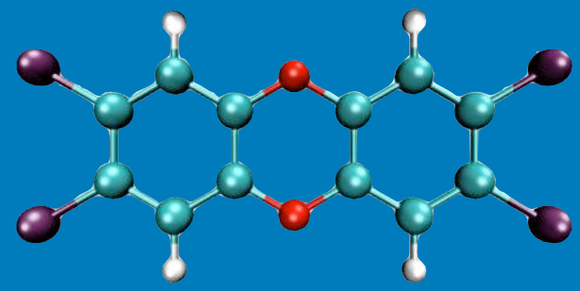
qsar



You are here

(1 1 0 ... 1 0)

?

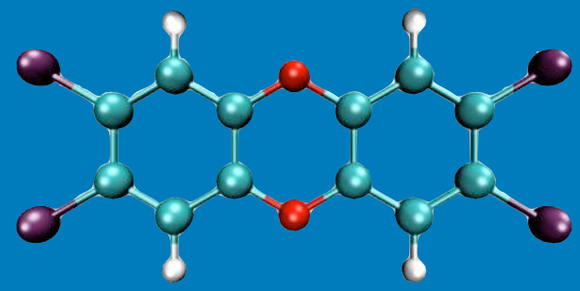
cancer

svm

model

simple approach: **qsar**

dump a load of patterns into svm



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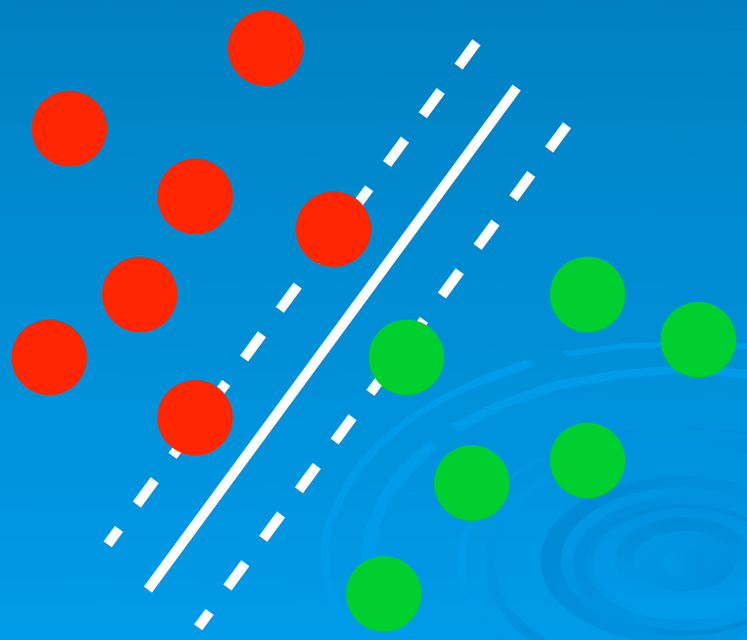

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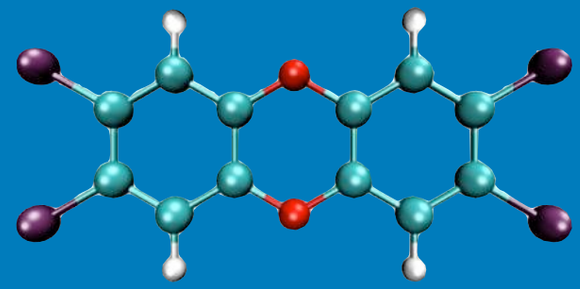


You are here

(1 1 0 ... 1 0)

?

cancer

svm

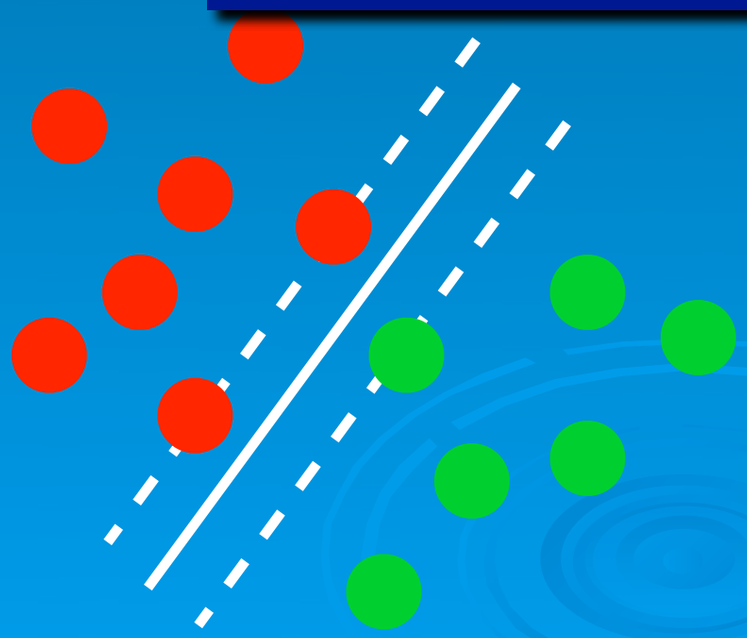
model

better

pattern set mining with

a) post-processing

b) iterative mining



a tale of two paradigms

Supervised

pattern set to
distinguishes classes

correspondences, ig, ...

Bringmann & Zimmermann ’05
Cheng et al. ’08 Thoma et al. ‘09

Unsupervised

pattern set to induce
fine, balanced partition

joint entropy

Knobbe & Ho ‘06
Bringmann & Zimmermann ‘07

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Knobbe & Ho ‘06
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Trade-off

Combined Scores

Trade-off

Cheng et al. ‘07
Rückert & Kramer ‘07

class-correlated dispersion score

how does this translate?

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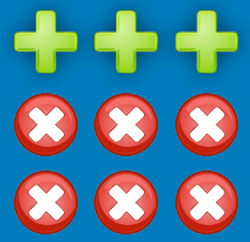

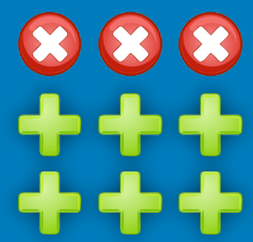

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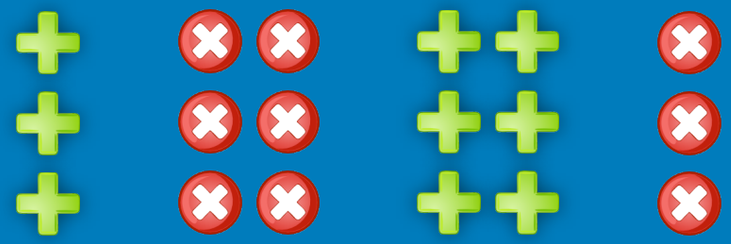

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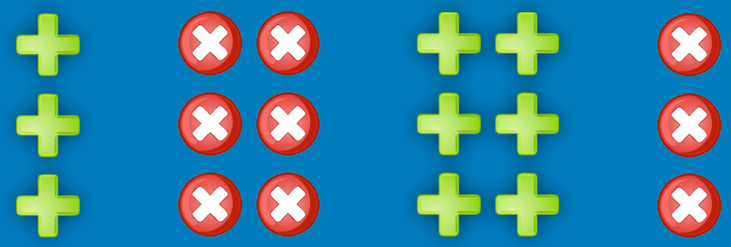

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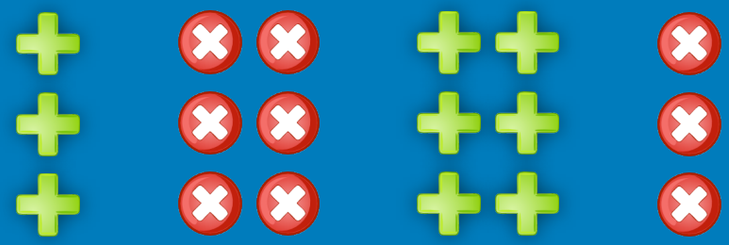
Unsupervised



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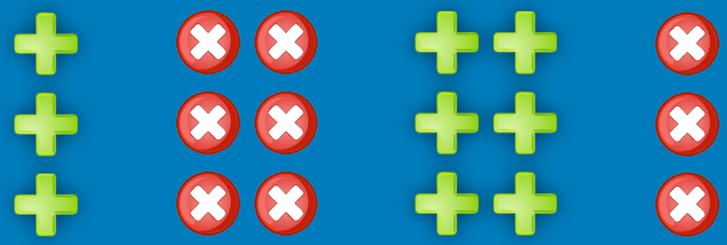

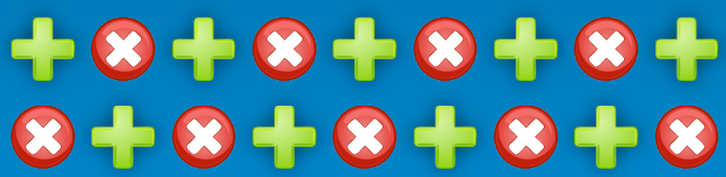

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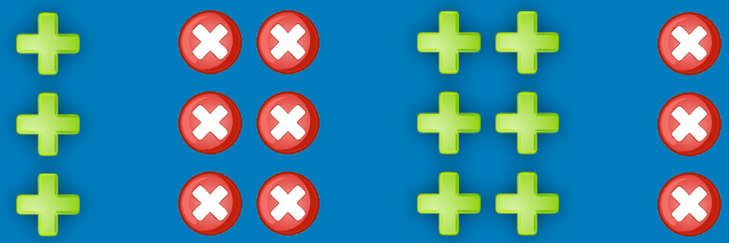

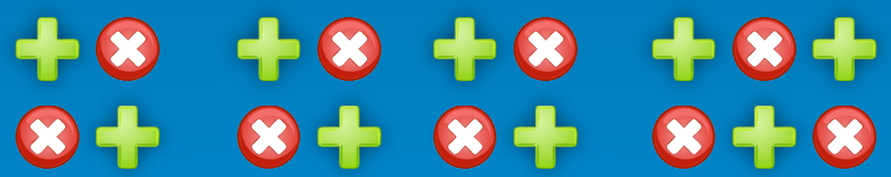

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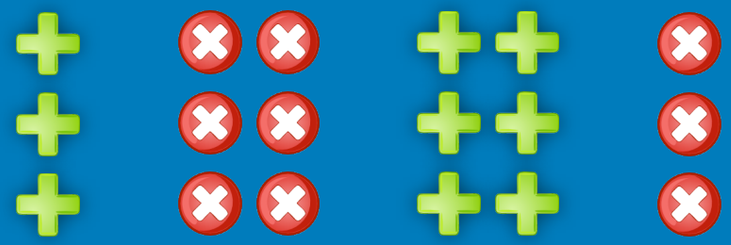

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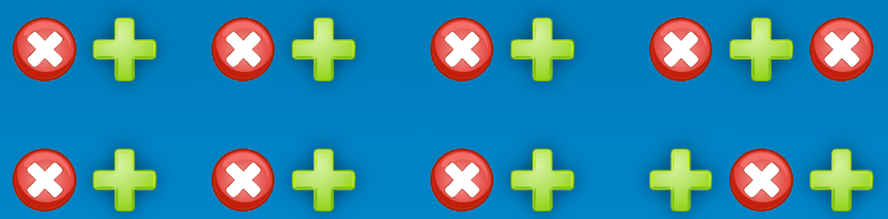

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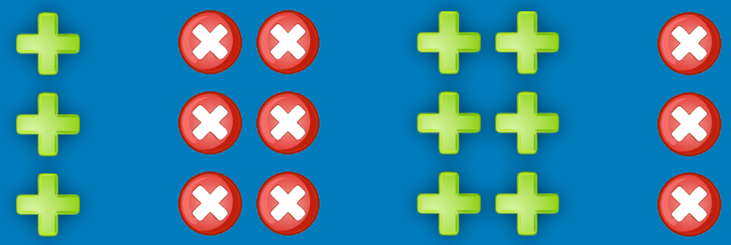

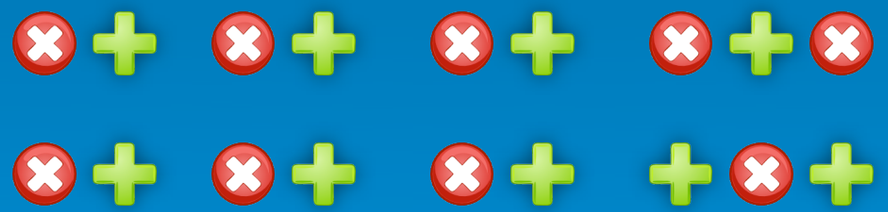

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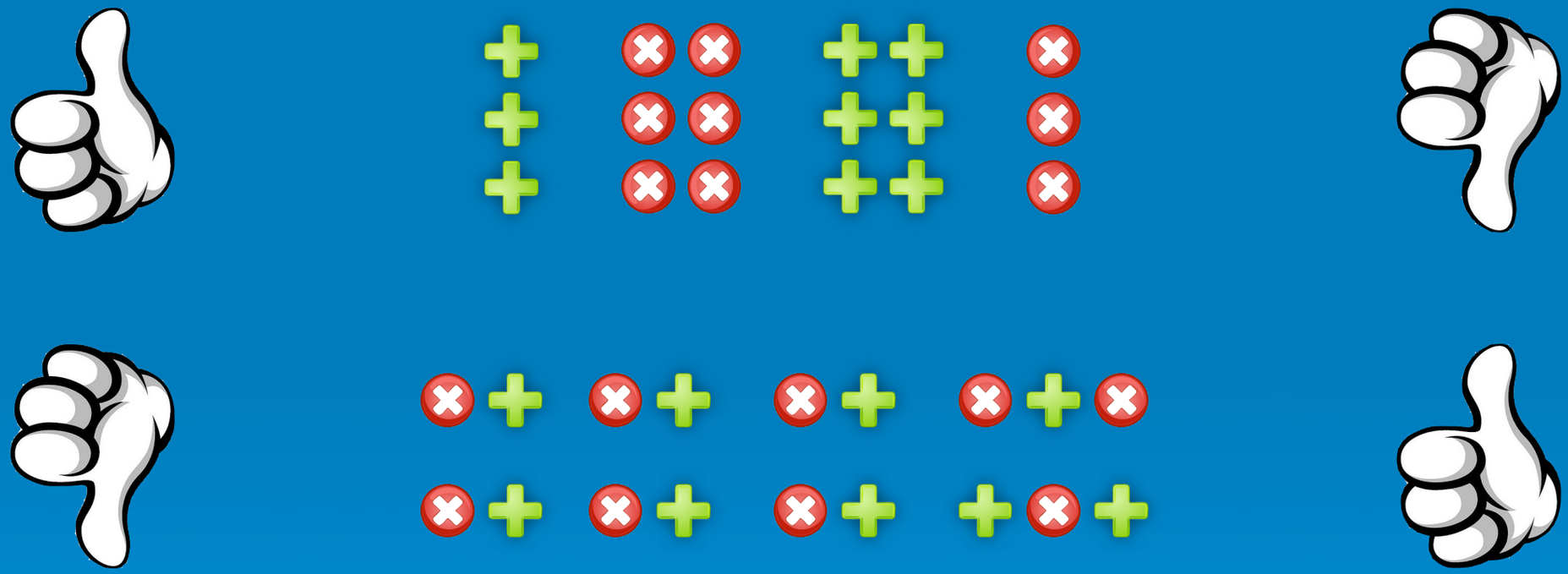

which paradigm is justified?

some empirical exploration

algorithm	properties	
baseline	500 most general frequent graphs	
*picker**	cond. pattern prob.	post processing
rückert '07	class-correlated disp-score	iterative
fcork	correspondence-based	iterative
dtm	information gain	iterative

relation to AUC?

some empirical exploration

algorithm	properties	
baseline	500 most general frequent graphs	
*picker**	cond. pattern prob.	**Unsupervised**
rückert '07	class-correlated disp-score	**Combined**
fcork	correspondence-based	**Supervised**
dtm	information gain	**Supervised**

relation to AUC?

what we found - correlations

characteristic	correlates w/auc	expected?
# features	✗	✓
joint entropy	+ + +	⚡
# equivalence classes	+ +	✓ / ⚡
high correspondence	− − −	✓
low correspondence	✗	⚠
dispersion score	+	
disp. score w/class	+ +	✓

what we found - correlations

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⊗ ⊗ ⊗ / ⊗ ⊗ ⊗ / ⊗ ⊗ ⊗	+ + + / + + + / + + +	overfitting?!
dispersion score	+	
disp. score w/class	+ +	✓

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what we found - algorithms

characteristic	result
auc	dtm >> fcork
# correspondences	dtm ~ fcork
# equivalence classes	dtm > fcork
# features	dtm >> fcork
running times	dtm >> fcork

what we found - algorithms

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auc	dtm >> fcork
# correspondences	dtm ~ fcork
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# features	dtm >> fcork
running times	dtm >> fcork

💡 it's in the way they work! 🙂

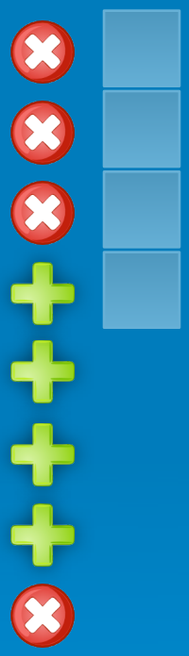
another tale of two paradigms

mine global,
use global

another tale of two paradigms

mine global,
use global

p_1



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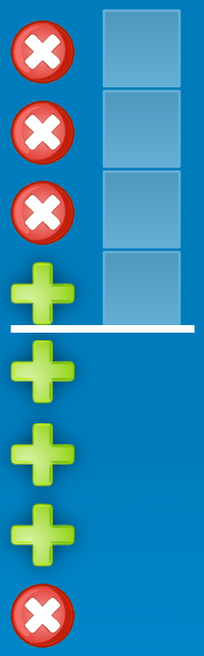

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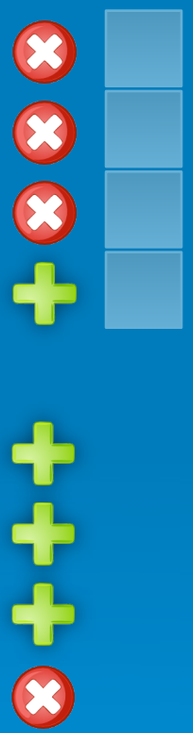

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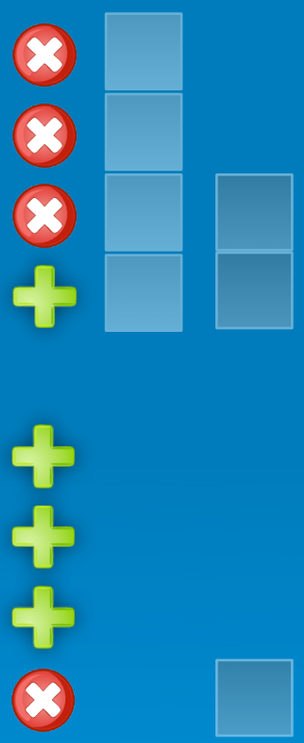
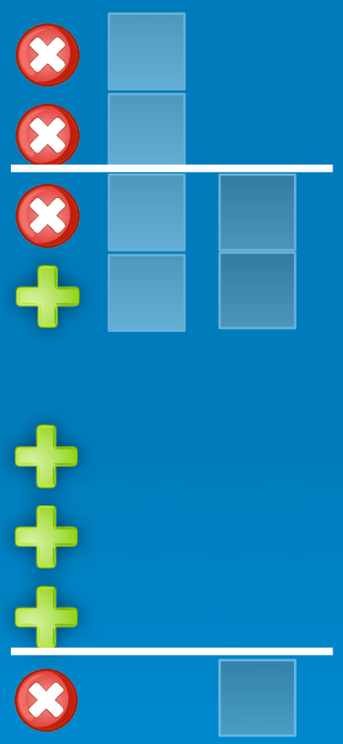


- patterns mined on **all** data

another tale of two paradigms

mine global, use global

p_1 p_2



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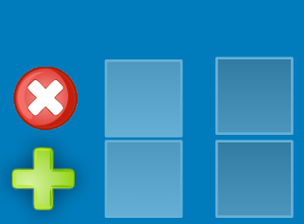

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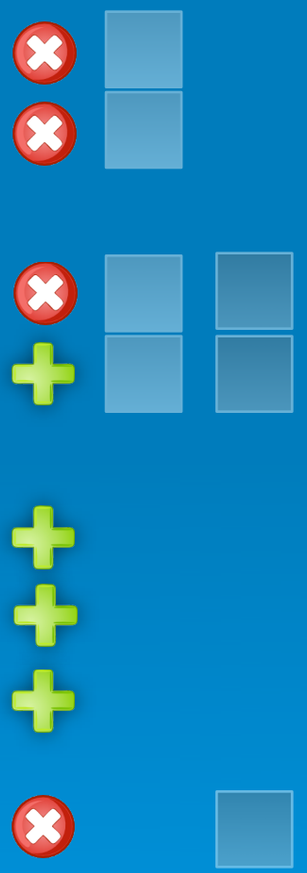

mine local, use local

- patterns mined on **all** data
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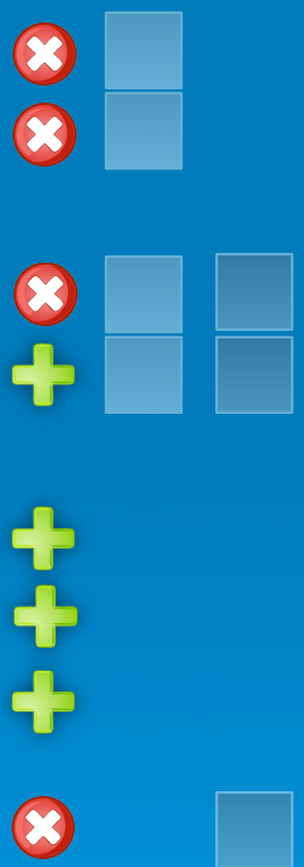

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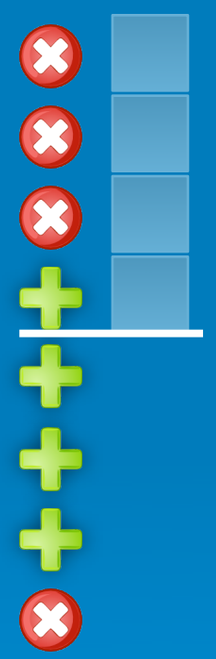

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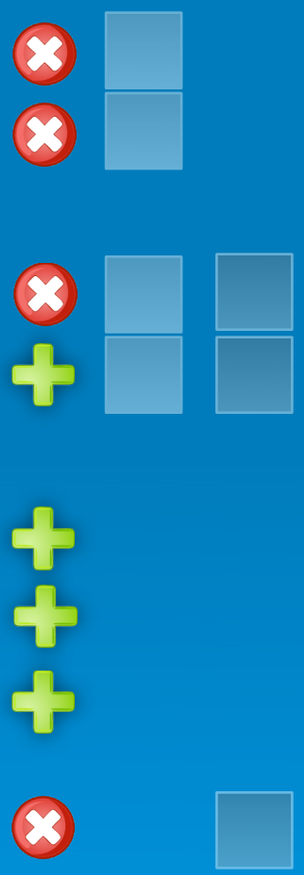

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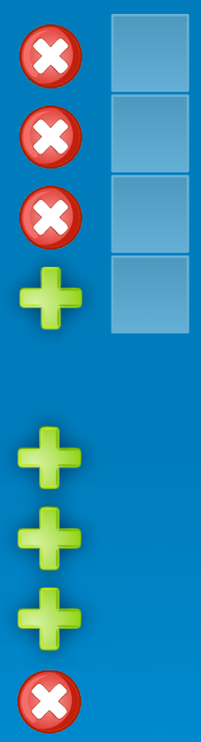

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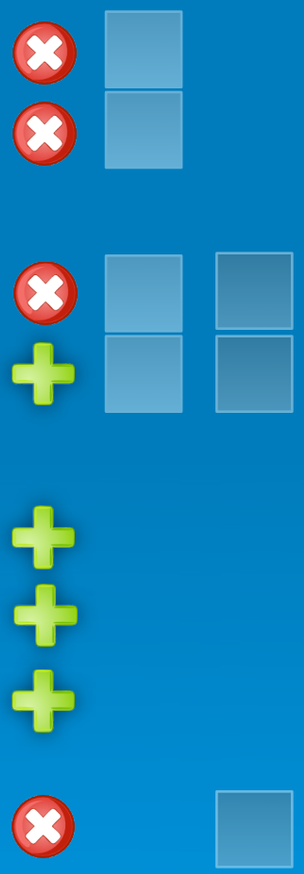

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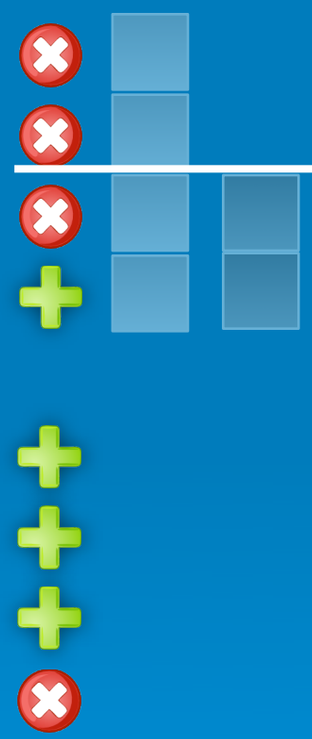
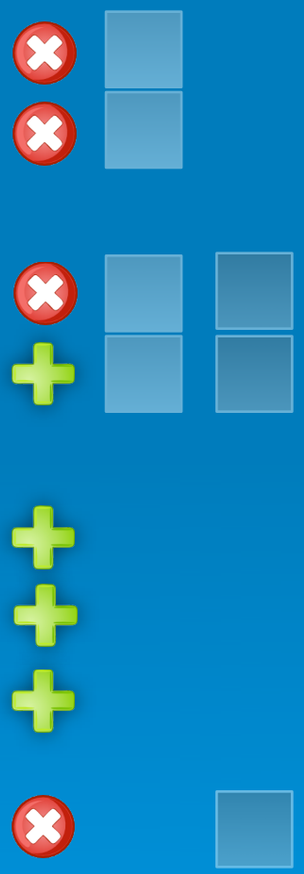


- patterns mined on **subset**

another tale of two paradigms

mine global, use global

p_1 p_2



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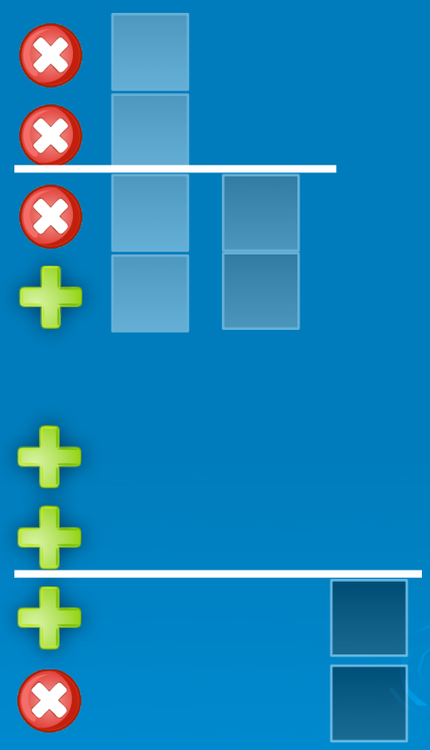
mine local, use local

p_1 p_2 p_3

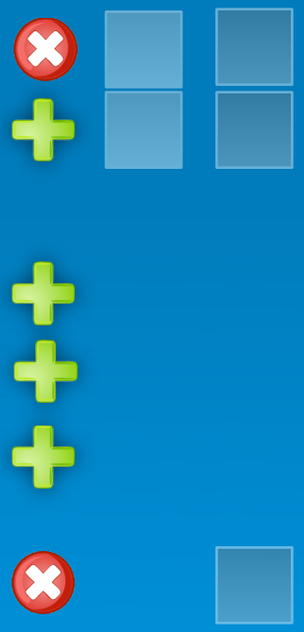


- patterns mined on **subset**
- patterns applied its **subset**

another tale of two paradigms

mine global, use global

p_1 p_2



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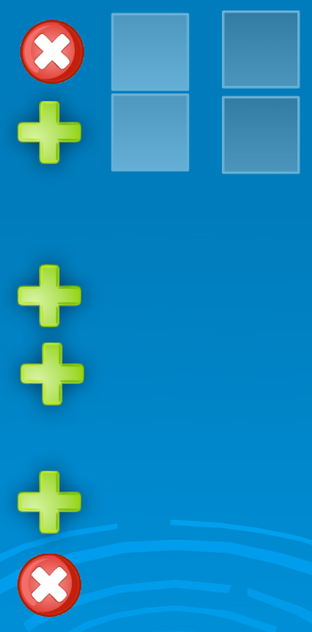

- patterns mined on **subset**
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another tale of two paradigms

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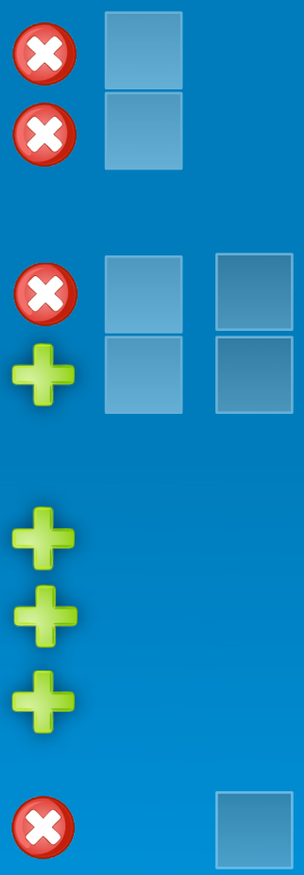
p_1 p_2



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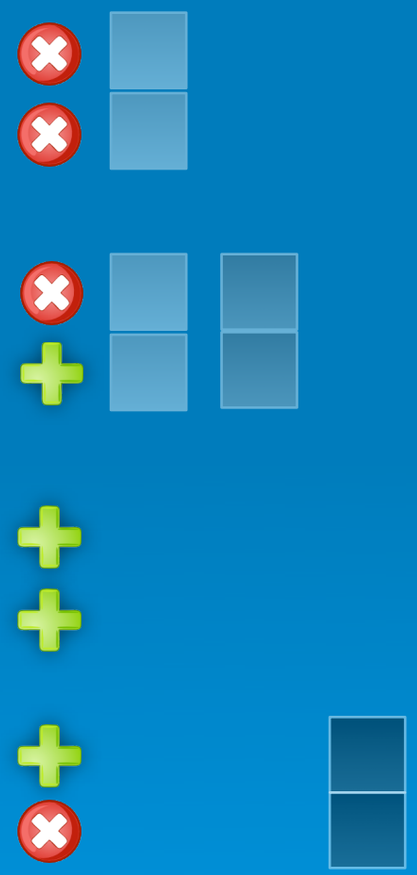
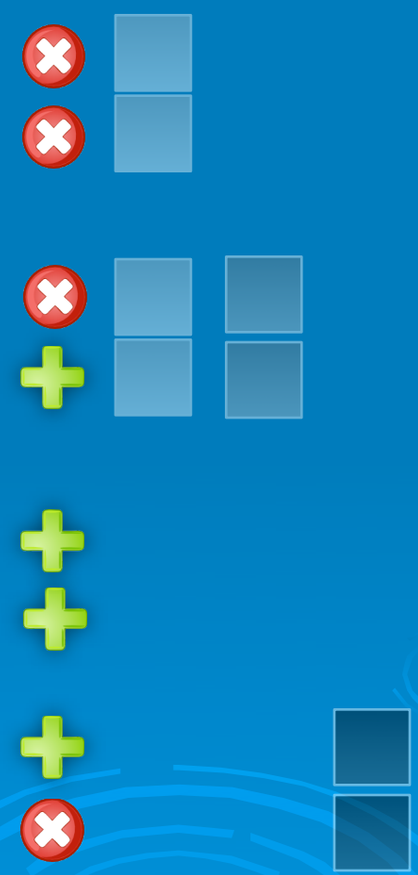
p_1 p_2 p_3



mine local, use local

p_1 p_2 p_3

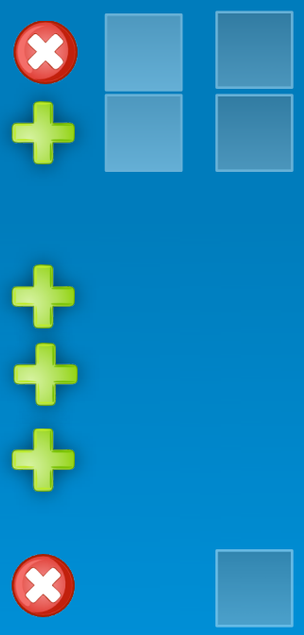


- patterns mined on **subset**

another tale of two paradigms

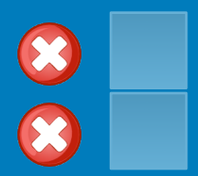
mine global, use global

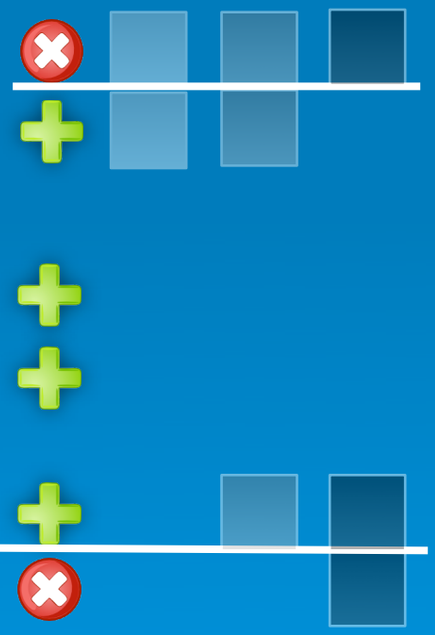
p_1 p_2



- patterns applied to **all** data

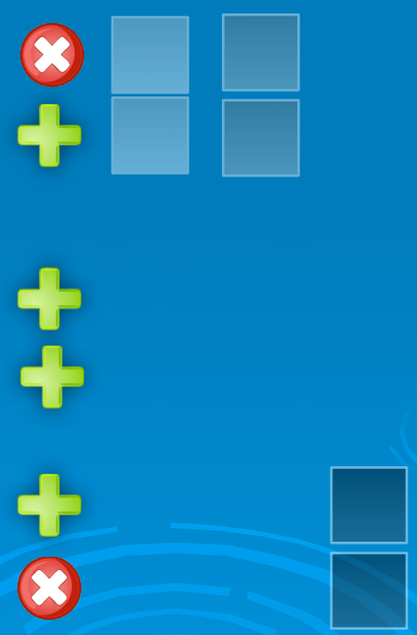
p_1 p_2 p_3





mine local, use local

p_1 p_2 p_3

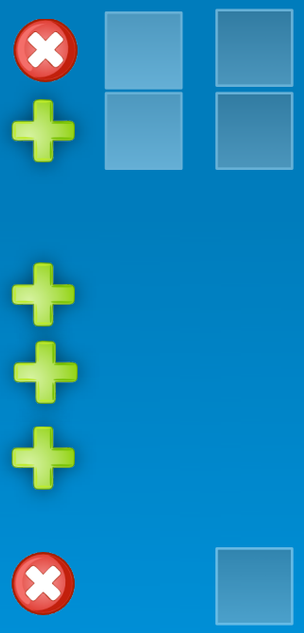


- patterns mined on **subset**

another tale of two paradigms

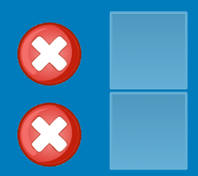
mine global, use global

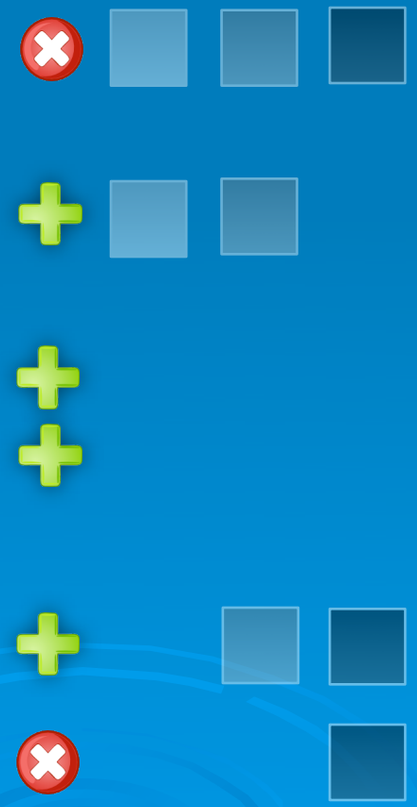
p_1 p_2



- patterns applied to **all** data

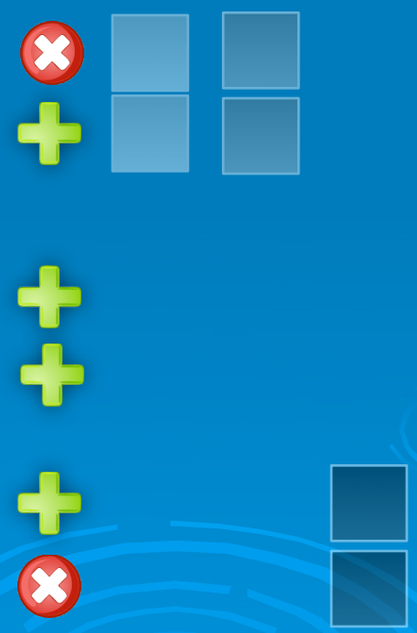
p_1 p_2 p_3





mine local, use local

p_1 p_2 p_3

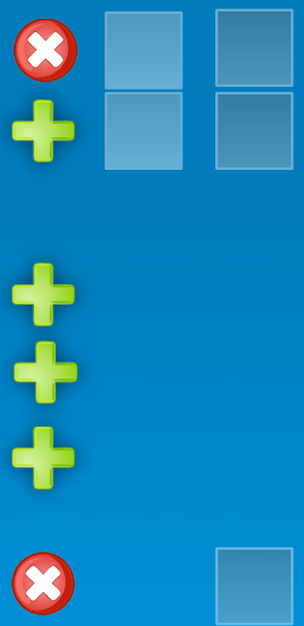


- patterns mined on **subset**

another tale of two paradigms

mine global, use global

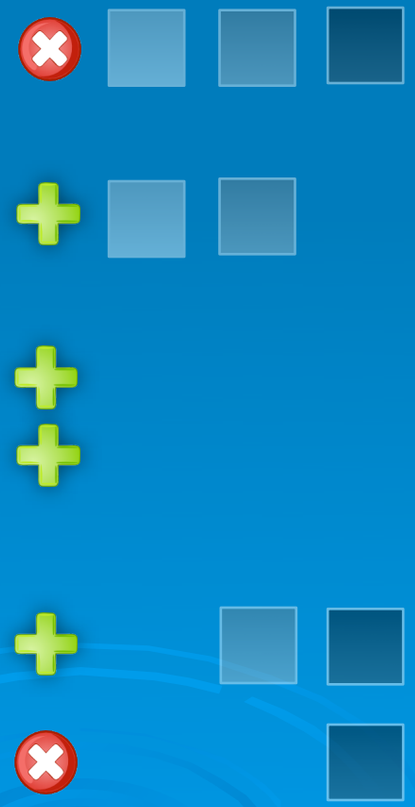
p_1 p_2



- patterns applied to **all** data

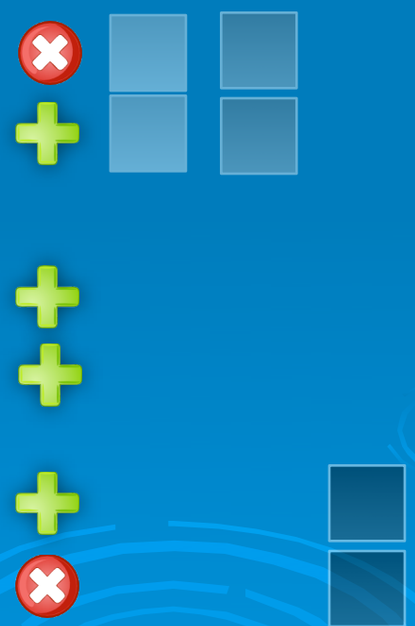
mine local, use global

p_1 p_2 p_3



mine local, use local

p_1 p_2 p_3



- patterns mined on **subset**

another tale of two paradigms

mine global, use global

p_1 p_2

mine local, use global

p_1 p_2 p_3

mine local, use local

p_1 p_2 p_3

introducing **remine**

- patterns applied to **all** data
- patterns mined on **subset**

experimental evaluation

measure	expected	actual	
# equivalence classes	remine ~ dtm	remine ~ dtm	✓
# features (prec slide)	remine < dtm	remine < dtm	✓
	remine ? fcork	remine > fcork	
# correspondences	remine ~ dtm	remine < dtm	⚠
auc	remine ~ dtm	remine ~ dtm	✓
running times	remine < dtm	remine < dtm	✓
	remine ? fcork	remine < fcork	☺

getting picky

measure	evaluation
# correspondences	remine < dtm
# equivalence classes	remine < dtm
auc	remine < dtm

getting picky

measure	evaluation	exploration
# correspondences	remine < dtm	dtm ~ fcork
# equivalence classes	remine < dtm	dtm > fcork
auc	remine < dtm	dtm >> fcork

getting picky

measure	evaluation	exploration
# correspondences	remine < dtm	dtm ~ fcork
# equivalence classes	remine < dtm	dtm > fcork
auc	remine < dtm	dtm >> fcork

⇒ **Unsupervised**

getting picky

measure	evaluation	exploration
# correspondences	remine < dtm	dtm ~ fcork
# equivalence classes	remine < dtm	dtm > fcork
auc	remine < dtm	dtm >> fcork

⇒ **Unsupervised**

# features	fcork < remine < dtm

getting picky

measure	evaluation	exploration
# correspondences	remine < dtm	dtm ~ fcork
# equivalence classes	remine < dtm	dtm > fcork
auc	remine < dtm	dtm >> fcork

⇒ **Unsupervised**

# features/auc	fcork < remine < dtm

getting picky

measure	evaluation	exploration
# correspondences	remine < dtm	dtm ~ fcork
# equivalence classes	remine < dtm	dtm > fcork
auc	remine < dtm	dtm >> fcork

⇒ **Unsupervised**

# features/auc	fcork < remine < dtm

⇒ **overfitting?!**

conclusions

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preliminary evidence that

Unsupervised > **Supervised**

conclusions

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Unsupervised > **Supervised**

& class information can improve partition-scores

conclusions

preliminary evidence that

Unsupervised > **Supervised**

& class information can improve partition-scores

mine global, use global — Trade-off → **remine** ← Trade-off — **mine local, use local**

conclusions

preliminary evidence that

Unsupervised > **Supervised**

& class information can improve partition-scores

mine global, use global — Trade-off → **remine** ← Trade-off — **mine local, use local**

further evidence of importance partition

but also of **overfitting?!**

Thank You for Your Attention