

# *Data Stream Mining with Limited Validation Opportunity: Towards Instrument Failure Prediction*

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Knowledge Transfer  
Partnerships



# Motivation

- Analytical instruments routinely quantify many metals and some non-metals at high speeds in liquids.



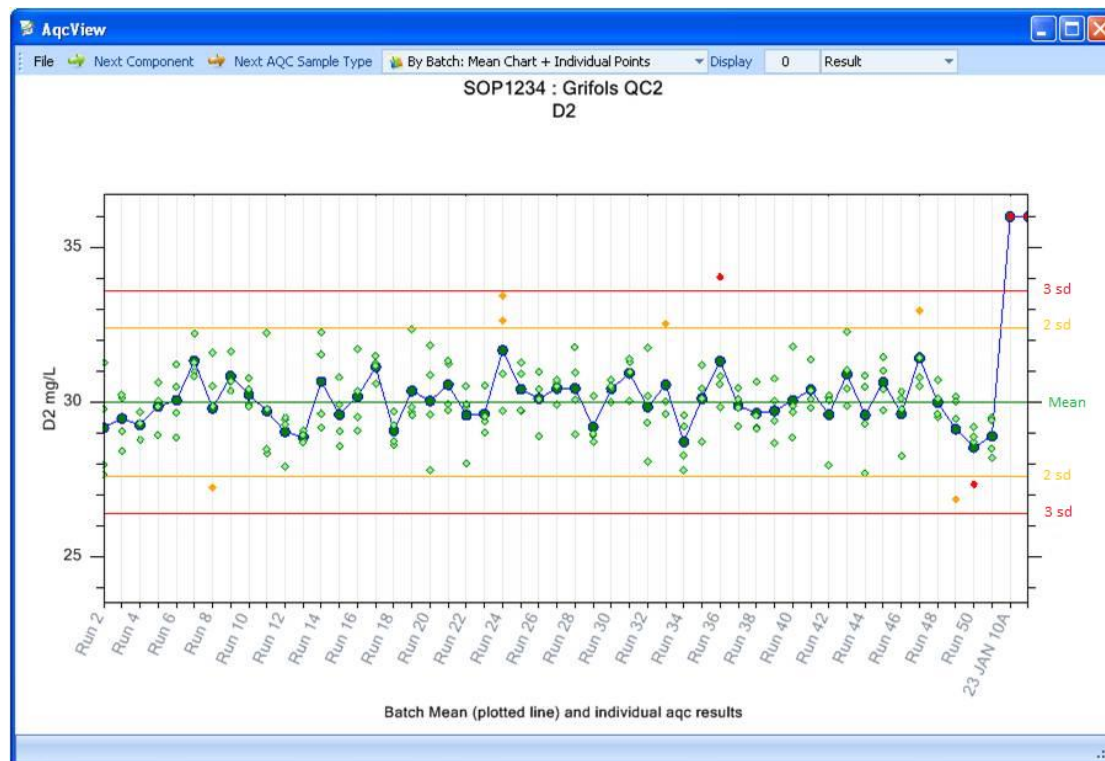
**But...** How does an analyst know that these readings are correct?

# Methods to Detect Instrument Errors

- Declining Instrument Sensitivity
- Inconsistent results for Analytical Standards
- System Suitability

# Inconsistent Results for Analytical Standards

- The most effective way of monitoring an instrument's performance is to regularly use control samples with independently verified results



# Initial Summary

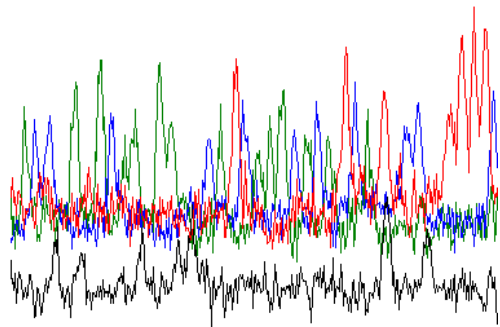
- The paper describes a model that can predict instrument failure so that some mitigation can be invoked so as to prevent failure.
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- **Specifically:** This paper presents a probabilistic time-series analysis technique applied to data stream subsequences to predict instrument failure, where significant attributes in the data stream are separated from noise attributes using a probabilistic learning approach

# Challenges

- Streamed data

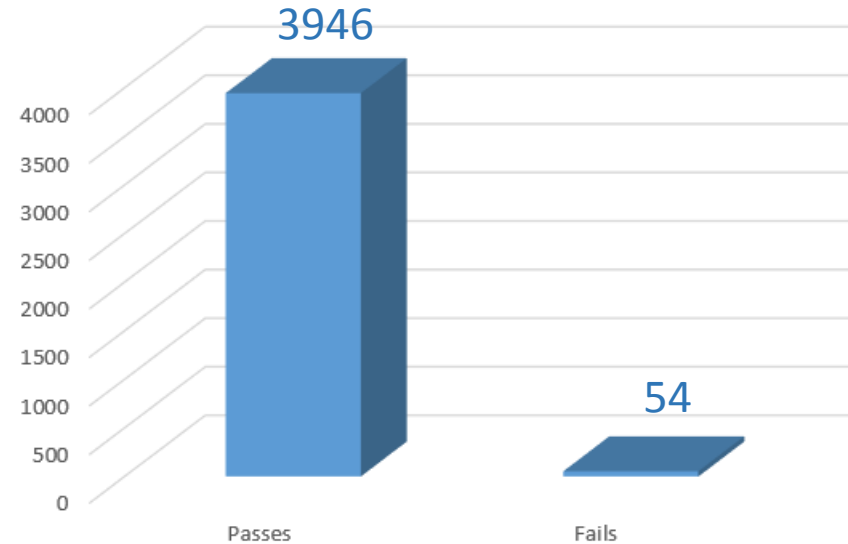


- Noisy data



How to pick out the **significant** attribute?

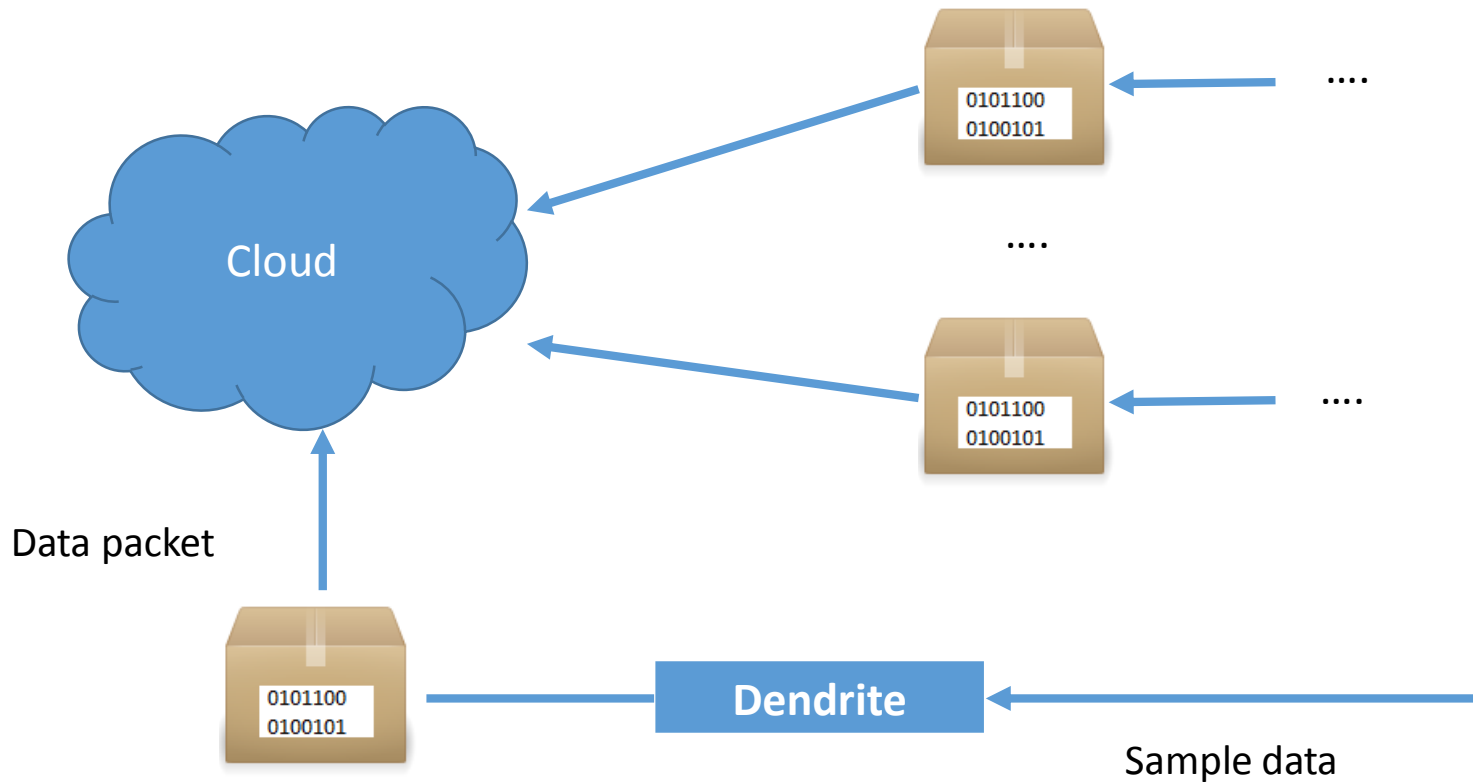
- Unbalanced data



- Also cannot confirm the instrument failed



# System Setup



A **Data packet** contains:

A set of **attributes**

A set of **values**

(1-to-1 mapping)

Principle challenge here:

Data is potentially infinite yet  
only a fixed proportion can be  
stored



Two classes of data packets:

**Failure** and **non-failure**

# System Setup (2)



The data packets are processed to produce **continuous time series**

One continuous time series for every **attribute** on every **instrument**

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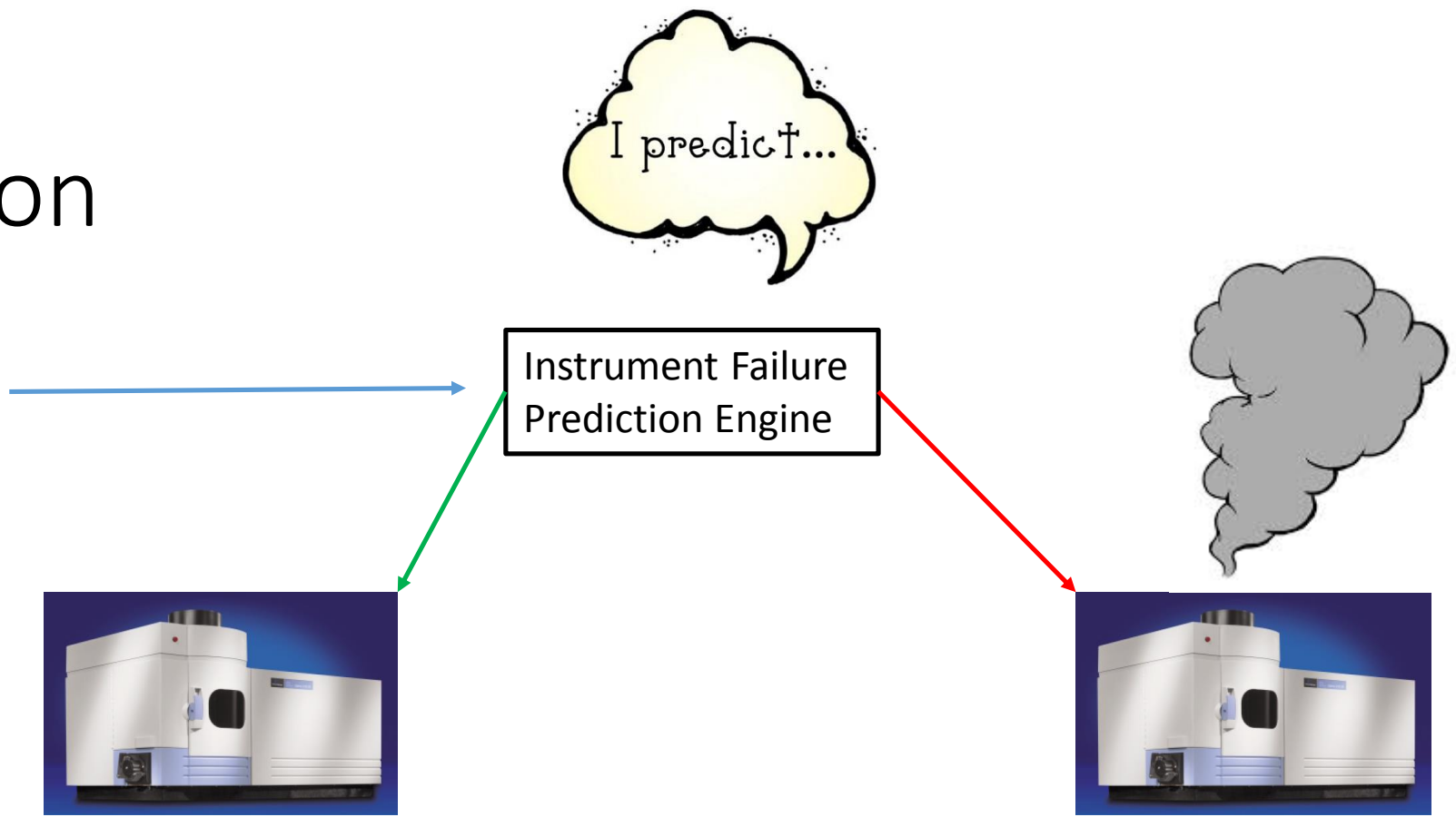
Note:

- All instruments are assumed to have the same attributes
- The length of the time series may not be the same across all the instruments
- The time series can be broken up into subsequences



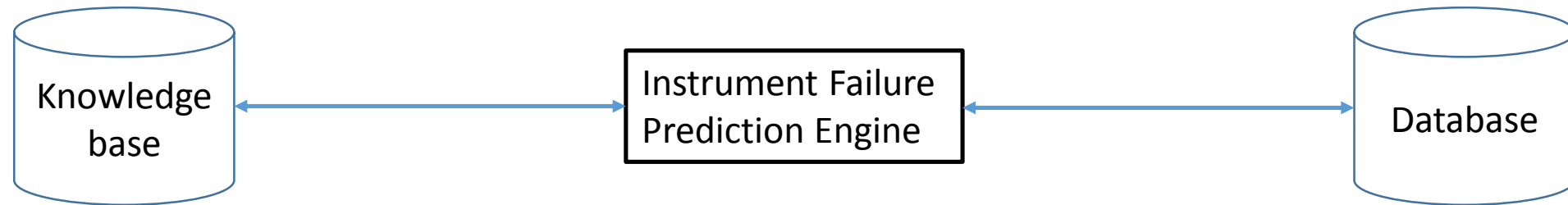
# Failure Prediction

- Given a subsequence



- A learning phase is required.
- We can learn the nature (shape) of subsequences that are good predictors of failure from observing the subsequences associated with the instruments that have failed

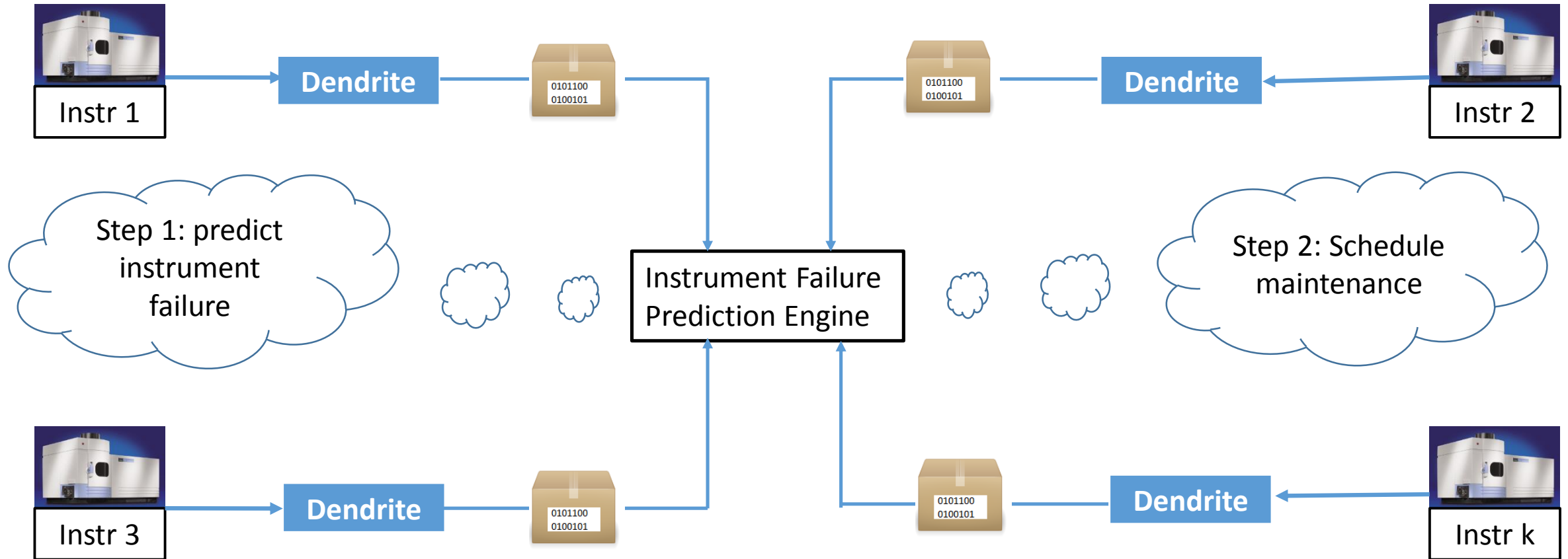
# Instrument Failure Prediction Engine



- The **database** stores subsequences of length **p** for all possible attributes of each instrument.
- The **knowledge base** stores subsequences also of length **p** that are associated with instrument failure.
- Both the database and the knowledge base are **empty on startup**.

# Simulation Environment (Diagram)

A multi-agent based simulation environment was used:



# Instrument Failure Prediction Engine

**Main()**

If **Datapacket = empty** then  
    addSubsequencesToKB()  
    pruneKB()

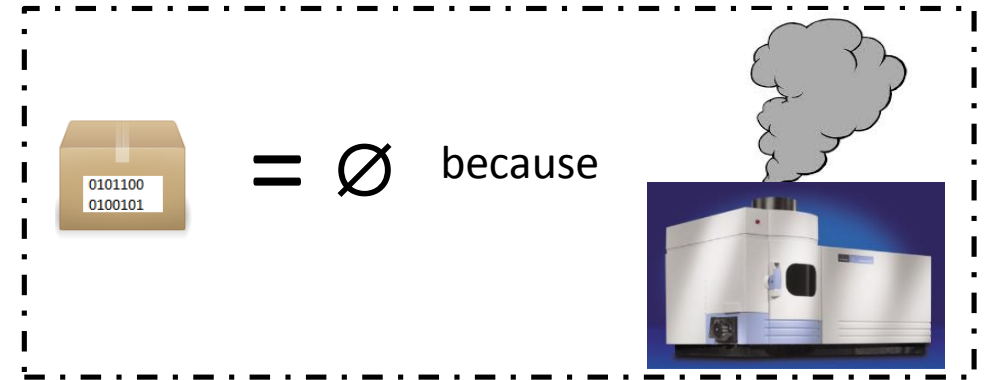
Else

Update each time series in DB by **adding the new attribute values** and **removing the last value**

If **Not in learning phase** then  
    prediction(instr\_i)

End If

End If



# Adding Subsequences to the KB

## **AddSubsequenceToKB(instrumentsSubsequence)**

For each **attribute in the subsequence**:

    If the attribute's Subsequence  $\in$  KB then

**increase count** of attribute's subsequence

    Else

**add attribute's subsequence** to the KB

    End If

End For

For each **subsequence in the knowledge base**:

**recalculate weight** =  $\frac{\text{times the subsequence has been recorded as a result of instrument failure}}{|\text{KB}|}$

End For

# Knowledge Base Pruning

## **pruneKB(instrumentsSubsequence)**

For each instruments and instrument's attribute:

If an attribute's subsequence's **weight is  $< \omega$**  then

**remove** the subsequence from the KB

End If

End For

If KB has changed:

**recalculate** weight as described in AddSubsequenceToKB()

End If

Selection of the most appropriate value for  $\omega$  is thus important and discussed later

# Making a prediction: comparing subsequences

- To predict failure, a comparison between subsequences is required

Subsequences:

$$M = \{m_1, m_2, \dots, m_l\}$$

$$N = \{n_1, n_2, \dots, n_l\}$$

$$\text{dist}(M, N) = \sum_{i=1}^{i=l} (m_i - n_i)^2$$

- We compare the subsequences via Euclidean distance

# How to predict failure?

**prediction(instr\_i)**

For each attribute subsequence in the database

if  $\text{dist}(\text{attribute subsequence in DB}, \text{attribute's subsequence in KB}) \leq \sigma$  then

**Predict failure** for instr\_i

End If

End For

$\sigma$  is a pre-set similarity threshold. Selection of the most appropriate threshold value is discussed later



# The Simulation Environment

- $k$  instruments with  $n$  attributes each
- The simulation operated on a loop
- Each iteration, each instrument may perform a sampling activity
- Two attribute types: (a) activity **dependant**; and (b) activity **independent**
- **One** attribute was chosen as the **sentinel attribute**, others provided noise
- The sentinel attribute was an activity **dependant** attribute and was designated to cause **instrument failure** once a **particular value** was reached

# Evaluation Metrics

- As we wish to intervene prior to failure, we have no information as to whether our predictions were correct or not.
- Instead we use an accumulated gross profit measure.
- When a **sample is completed**, a **profit** of  $g_{\text{sample}}$  is made.
- When **instrument maintenance** occurs, a **cost** of  $g_{\text{maint}}$  is incurred.
- When **instrument replacement** occurs, a **cost** of  $g_{\text{replace}}$  is incurred.

$$g_{\text{sample}} < g_{\text{maint}} < g_{\text{replace}}$$

# Single Sentinel Attribute Evaluation

- The aim of these experiments was to determine the effect of different:
  - Similarity thresholds ( $\sigma$ )
  - Subsequence lengths ( $p$ )

Clear correlation between  $\sigma$  and  $p$ : A larger  $p$  value requires a larger  $\sigma$  for best results.

Best overall result had the lowest  $\sigma$  and  $p$  values

$p$	Similarity threshold $\sigma$									
	0	1	2	3	4	5	6	7	8	9
2	<b>711</b>	706	687	657	627	593	561	528	504	480
3	691	<b>696</b>	692	683	666	650	623	601	583	557
4	650	683	<b>687</b>	677	672	663	654	639	622	605
5	575	657	<b>677</b>	675	667	660	654	645	640	627
6	470	615	659	<b>668</b>	667	661	650	644	636	633
7	351	558	634	657	<b>660</b>	658	651	644	636	632
8	248	479	595	635	650	<b>655</b>	653	646	639	632
9	167	389	540	606	635	646	<b>648</b>	645	641	634

Each parameter combination had:  
1000 simulations.  
200 iterations in each.

$p$	Similarity threshold $\sigma$									
	0	1	2	3	4	5	6	7	8	9
2	<b>1445</b>	1425	1381	1319	1260	1186	1126	1064	1014	967
3	<b>1425</b>	1409	1396	1374	1338	1300	1256	1210	1167	1120
4	1381	<b>1400</b>	1395	1369	1352	1333	1312	1277	1245	1211
5	1299	1374	<b>1387</b>	1368	1343	1330	1310	1299	1285	1259
6	1156	1326	<b>1369</b>	1364	1348	1331	1306	1291	1277	1268
7	949	1250	1338	<b>1353</b>	1347	1336	1316	1291	1276	1262
8	712	1136	1292	1332	<b>1340</b>	1334	1321	1303	1284	1265
9	501	986	1223	1299	1325	<b>1328</b>	1320	1308	1291	1275

Table 2. Comparison in terms of gross profit ( $k = 40$ ).

Table 1. Comparison in terms of gross profit ( $k = 20$ ).

# Maintained/Failed Instruments

$p$	Similarity threshold $\sigma$									
	0	1	2	3	4	5	6	7	8	9
2	<b>2</b>	1	1	1	1	1	1	1	1	1
3	<b>3</b>	2	1	1	1	1	1	1	1	1
4	<b>7</b>	3	2	2	1	1	1	1	1	1
5	<b>12</b>	5	3	2	2	2	1	1	1	1
6	<b>20</b>	9	5	3	2	2	2	2	1	1
7	<b>29</b>	13	7	4	3	2	2	2	2	2
8	<b>37</b>	19	10	6	4	3	3	2	2	2
9	<b>44</b>	26	14	9	6	4	4	3	2	2

$p$	Similarity threshold $\sigma$									
	0	1	2	3	4	5	6	7	8	9
2	<b>2</b>	1	1	1	1	1	1	1	1	1
3	<b>4</b>	2	1	1	1	1	1	1	1	1
4	<b>7</b>	3	2	2	1	1	1	1	1	1
5	<b>13</b>	6	3	2	2	2	1	1	1	1
6	<b>24</b>	10	5	3	2	2	2	2	1	1
7	<b>39</b>	16	8	5	3	3	2	2	2	2
8	<b>57</b>	25	12	7	5	4	3	2	2	2
9	<b>74</b>	36	18	10	7	5	4	3	3	2

Note – the **average** number of **failed instruments** when maintenance was not scheduled (with 1000 simulations and 200 iterations), was as follows:  
**54** (when  $k = 20$ )  
**109** (when  $k = 40$ )

Table 3. Comparison in terms of number of failed machines ( $k = 20$ ).

Table 4. Comparison in terms of number of failed machines ( $k = 40$ ).

$p$	Similarity threshold $\sigma$									
	0	1	2	3	4	5	6	7	8	9
2	60	62	63	66	68	70	73	75	76	<b>78</b>
3	58	61	62	64	65	66	68	70	71	<b>73</b>
4	55	60	62	63	64	65	66	67	68	<b>69</b>
5	48	57	60	62	63	64	65	66	<b>67</b>	<b>67</b>
6	40	53	58	61	63	64	65	66	<b>67</b>	<b>67</b>
7	30	47	55	59	61	63	64	65	66	<b>67</b>
8	21	41	51	56	59	61	63	64	65	<b>66</b>
9	13	33	46	53	57	60	61	63	64	<b>65</b>

$p$	Similarity threshold $\sigma$									
	0	1	2	3	4	5	6	7	8	9
2	122	125	129	133	138	143	147	151	155	<b>158</b>
3	120	125	127	129	132	135	138	141	144	<b>148</b>
4	116	123	126	129	131	132	134	136	139	<b>141</b>
5	109	119	124	127	130	131	133	134	136	<b>138</b>
6	97	115	121	125	128	131	133	135	136	<b>137</b>
7	80	107	118	123	126	129	131	133	135	<b>137</b>
8	60	97	112	119	124	127	130	132	134	<b>136</b>
9	42	84	106	115	121	125	128	130	132	<b>134</b>

Table 5. Comparison in terms of number of maintained machines ( $k = 20$ ).

Table 6. Comparison in terms of number of maintained machines ( $k = 40$ ).

The **higher** the  $\sigma$ , the **least precise** the prediction, resulting in **maintenance** frequently being conducted when it was **not necessary**.

This is why the lower  $\sigma$ , the more likely that an instrument will fail.

# Knowledge base size

$p$	Similarity threshold $\sigma$									
	0	1	2	3	4	5	6	7	8	9
2	<b>2</b>	1	1	1	1	1	1	1	1	1
3	<b>3</b>	2	1	1	1	1	1	1	1	1
4	<b>6</b>	3	2	2	1	1	1	1	1	1
5	<b>12</b>	5	3	2	2	2	1	1	1	1
6	<b>20</b>	9	4	3	2	2	2	2	1	1
7	<b>29</b>	13	7	4	3	2	2	2	2	2
8	<b>37</b>	19	10	6	4	3	3	2	2	2
9	<b>44</b>	26	14	9	6	4	4	3	2	2

Table 7. Comparison in terms of *KB* size ( $k = 20$ ).

$p$	Similarity threshold $\sigma$									
	0	1	2	3	4	5	6	7	8	9
2	<b>2</b>	1	1	1	1	1	1	1	1	1
3	<b>3</b>	2	1	1	1	1	1	1	1	1
4	<b>6</b>	3	2	2	1	1	1	1	1	1
5	<b>13</b>	6	3	2	2	2	1	1	1	1
6	<b>23</b>	10	5	3	2	2	2	2	1	1
7	<b>39</b>	16	8	5	3	3	2	2	2	2
8	<b>57</b>	25	12	7	5	4	3	2	2	2
9	<b>74</b>	36	17	11	7	5	4	3	3	2

Table 8. Comparison in terms of *KB* size ( $k = 40$ ).

- The number of subsequences in KB decreases as the  $\sigma$  value increases. This is because as  $\sigma$  is increased the prediction becomes less precise so the KB requires fewer subsequences.
- The number of subsequences in the KB also decreases as  $p$  decreases; this is because as the  $p$  value is reduced the number of possible value combinations making up a time series subsequence also decreases

# Finding the best parameter settings for different number of attributes

# Atts. (n)	$\sigma$	$p$	$\omega$	$\lambda$	# Fail. Inst.	# Main. Inst.	Final KB Size	# KB Values Pruned	GP
2	1	2	0.250	22	23	319	1	28	2884
3	1	2	0.225	25	26	323	1	60	2727
4	1	2	0.250	27	28	320	1	93	2701
5	1	2	0.175	31	32	325	1	137	2527
6	1	2	0.150	29	30	342	1	160	2333
7	1	2	0.125	30	31	352	1	194	2176
8	1	2	0.125	35	36	332	1	261	2308
9	1	2	0.100	36	37	352	1	300	2009
10	2	2	0.100	33	34	394	1	313	1502

**Table 9.** Best parameter settings for a range of attribute set sizes, and  $k = 20$ . Average results obtained from 500 simulation runs per parameter permutation, 1000 iterations per simulation

**Note** – the **average** number of **failed instruments** when maintenance was not scheduled (with 1000 simulations and 1000 iterations), was **281** and the average GP was **-140**.

As  $n$  **was increased**, the number of noise attributes were increased and it **became harder to predict instrument failure**, hence the value of  $\lambda$  (learning window size) increases with  $n$ .

# learning window and weighting threshold value

$\omega$	Learning window size ( $\lambda$ )							
	24	26	28	30	32	34	36	38
0.050	-14543	-14492	-13685	-13652	-13360	-13448	<b>-12686</b>	-12774
0.075	-6801	-6072	-5522	-5010	-5033	-4498	<b>-4460</b>	-4518
0.100	-1131	-1056	-529	-637	-173	-12	<b>22</b>	12
0.125	890	<b>1540</b>	1174	1377	1359	1306	1373	1245
0.150	1913	1788	2049	2097	2194	2061	<b>2245</b>	2125
0.175	2251	2291	2307	2355	<b>2401</b>	2377	2393	2285
0.200	2276	2406	2364	2292	2454	2428	<b>2481</b>	2448
0.225	-138	-140	-139	-138	-139	<b>-137</b>	-139	-138
0.250	-139	<b>-137</b>	-138	-137	-138	-138	-139	-139

**Table 10.** Learning window size ( $\lambda$ ) versus Weighting threshold ( $\omega$ ), comparison in terms of gross profit ( $k = 20$ ,  $n = 5$ ,  $\sigma = 1$  and  $p = 2$ )

For the experiments,  $\omega = 1$  and  $p = 2$  were used as these setting had produced the best results.

Experiments show that **the choice of  $\omega$  is important**, either side of the optimum value, GP quickly starts to fall.

Yet the **size of  $\lambda$  can still influence the results**.

**Reminder:**  $\omega$  is the threshold for pruning a subsequence from the KB

# Conclusions

- A mechanism, founded on time series analysis, for predicting instrument failure using data stream mining has been proposed.
- The presented evaluation indicated that **best results** are obtained **when the similarity threshold  $\sigma = 1$**  (almost exact matching between current time series subsequences associated with individual instruments and subsequences in KB) and **the size of the subsequences are  $p = 2$** .
- The **optimum value** for **the learning window size  $\lambda$**  increases with  $n$ .



# Future work

- Lowering the sensitivity associated with the KB pruning threshold value  $\omega$ .
- Investigate scenarios where we have several sentinel/significant attributes
- Investigate alternative prediction mechanisms, e.g.: dynamic classification, association rule or decision tree based techniques.
- Predict non-failure and well as failure.
- Implement this functionality into a real world app via CSols Dendrite instrument interfaces.
- Finding more accurate valuations for the profit of a sample, the cost of maintenance and the cost of replacement.

Any questions?

