Automated evaluation of crystallisation experiments
SUMMARY

image -> mask -> objects -> classification variables

classify objects

image score
crystals

piles of crystals

very interesting

quite interesting

precipitate

rubbish

empty
The programme is now written in C rather than fortran

- gave the whole thing a revamp
- will allow different image formats to be used easily
- caused a few problems!

Circular mask is no longer used
Ok the problem at the moment is that the test set that I have has been poorly classified - the human classes that I have are: empty, precipitate, interesting precipitate and crystal. Having looked through all the images in the test set the two precipitate classes were not consistent enough to be trustworthy so we have blocked them together into a middle "interesting" class. So to build up an assessment of the results from your classifier I have reduced them down to a similar three levels (see I told you the results should not be relied on!) then I created a truth table (like the one you have asked for below) and this is where I have got the results I have sent...
Here is the full table:

The woolly level altering is using simply

- If JW Score $\geq 4$ - class 2
- If JW Score $\leq 2$ - class 0
- Otherwise class 1

<table>
<thead>
<tr>
<th></th>
<th>Human</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Machine 0 (empty)</td>
<td>850</td>
<td>446</td>
<td>363</td>
<td>51%</td>
<td></td>
</tr>
<tr>
<td>Machine 1 (stuff)</td>
<td>11</td>
<td>25</td>
<td>21</td>
<td>37%</td>
<td></td>
</tr>
<tr>
<td>Machine 2 (xtal)</td>
<td>129</td>
<td>369</td>
<td>1410</td>
<td>75%</td>
<td></td>
</tr>
</tbody>
</table>

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</table>

|                |       | 86%  | 23%  | 79%  |

86% 23% 79%
WHAT DOES THIS MEAN?

There are far too many drops being classified as empty!

Actually this is not necessarily true….but if it was

It could only be due to …
    …having the wrong cut-off level and not finding the objects
      (dark shadows or badly focussed drops)
    …no objects being classified (if SOM and Bayes classifier
      disagree by too much an object is not classified)
WHAT DOES THIS MEAN?

79% of images containing crystals are classified as crystals

86% of empty drops are classified as empty

74% of drops classified as crystals really contain crystals

? % of drops classified as empty really are empty
How can it be improved?

Use information from the whole image as well as object-based classification

Overall image statistics
Texture analysis - local variance
  - Fourier transforms (frequencies)
  - wavelet analysis

More pre-processing
  - histogram equalization
  - contrast stretching
barcoded trays → images → crystallisation conditions → positive and negative results → automated screening protocol → prior knowledge of protein

- images
- crystallisation conditions
- positive and negative results
- automated screening protocol
- prior knowledge of protein