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STRATEGIES FOR INTERPRETING TWO DIMENSIONAL MICROWAVE SPECTRA

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ISMS – WE11

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Microwave Spectroscopy

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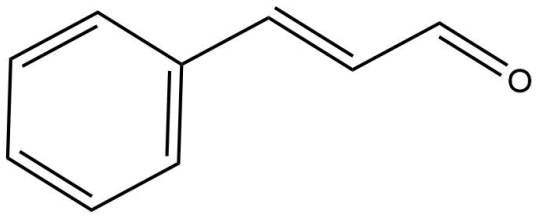
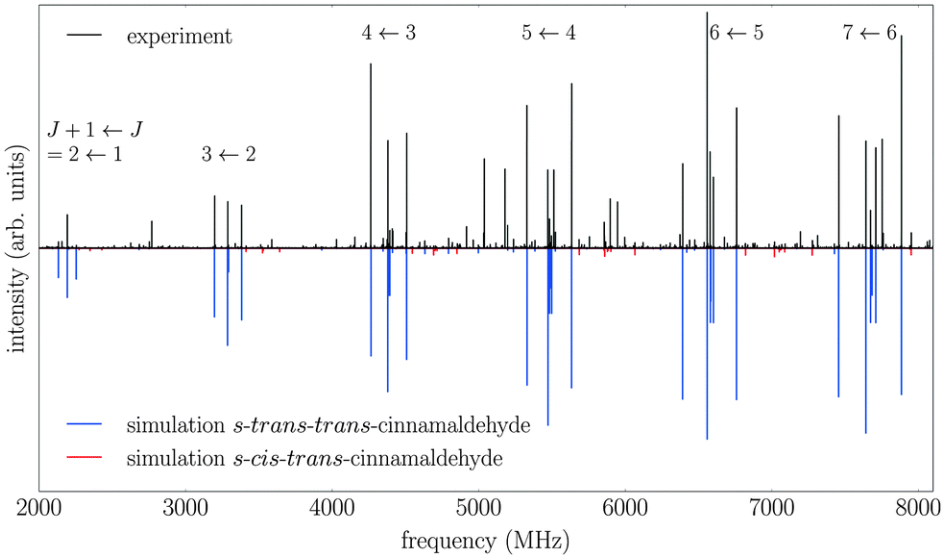
Gives a unique fingerprint of molecules based off of 1, 2 or 3 moments of inertia

Traditionally, slow to get high bandwidth, solved by CP-FTMW

Very little usage as a “real” analytical technique due to the difficulty in decoding the spectra

Our goal is to make microwave spectroscopy accessible as an analytical identifying technique.





What makes a technique accessible?

1. Fast
2. Doesn’t take a specialist to analyze data

Zinn, Sabrina et al, Phys. Chem. Chem. Phys, 2015, 17, 16080-16085

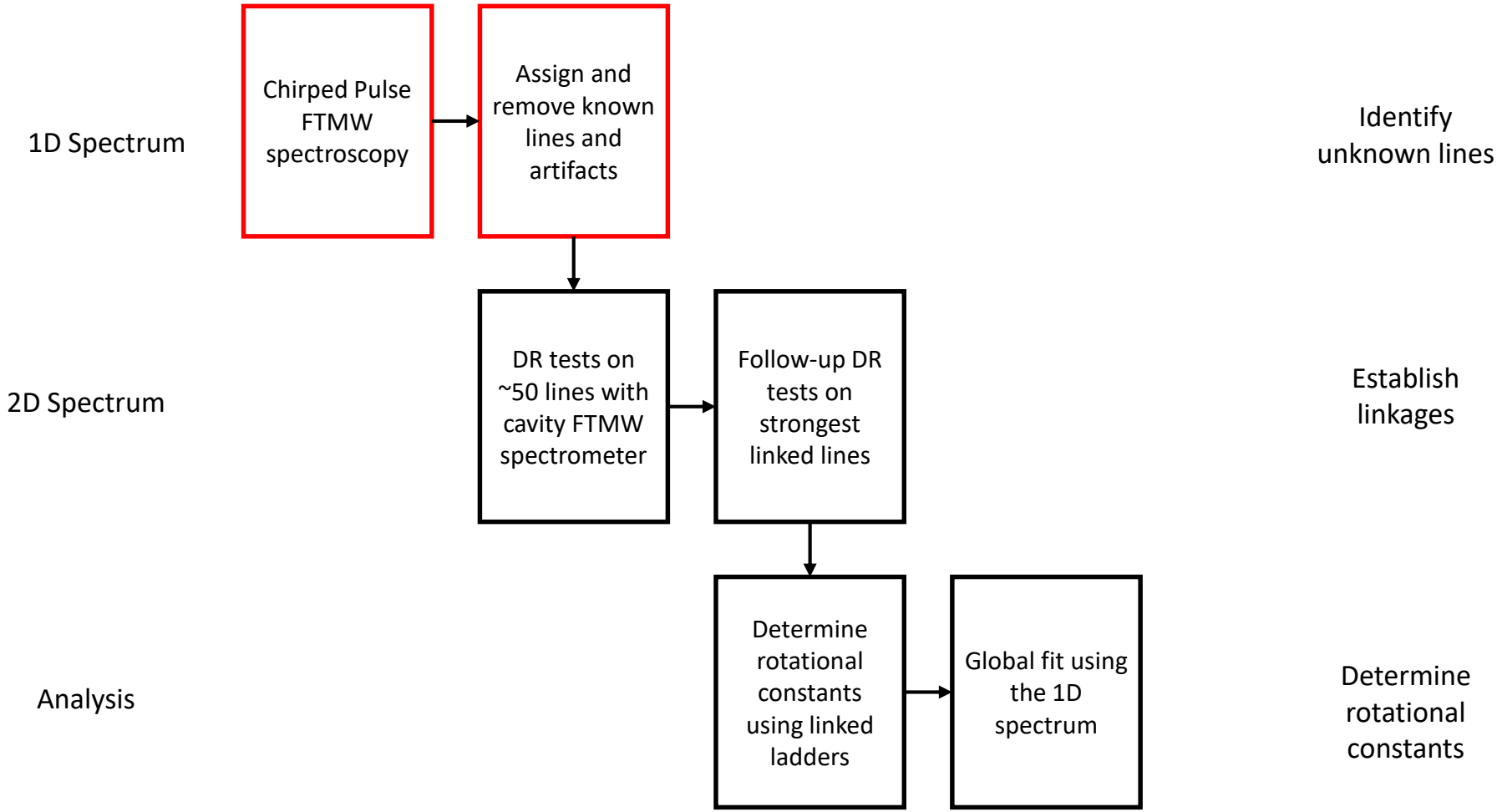
Past work

- Automated microwave double resonance spectroscopy (AMDOR)

New Work

- New algorithm for measuring data
- AMDOR Neural Network

AMDOR workflow



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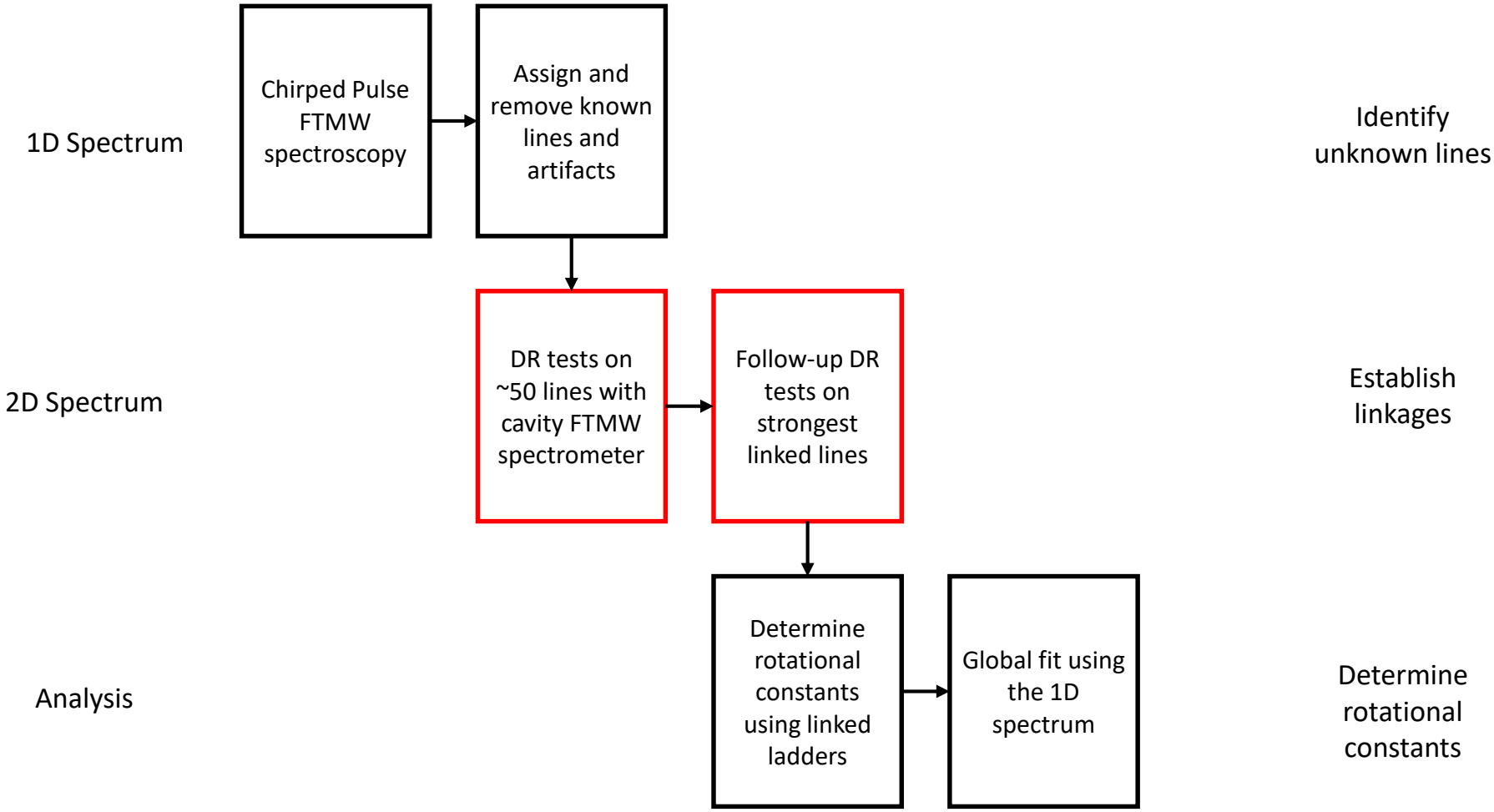
AMDOR workflow



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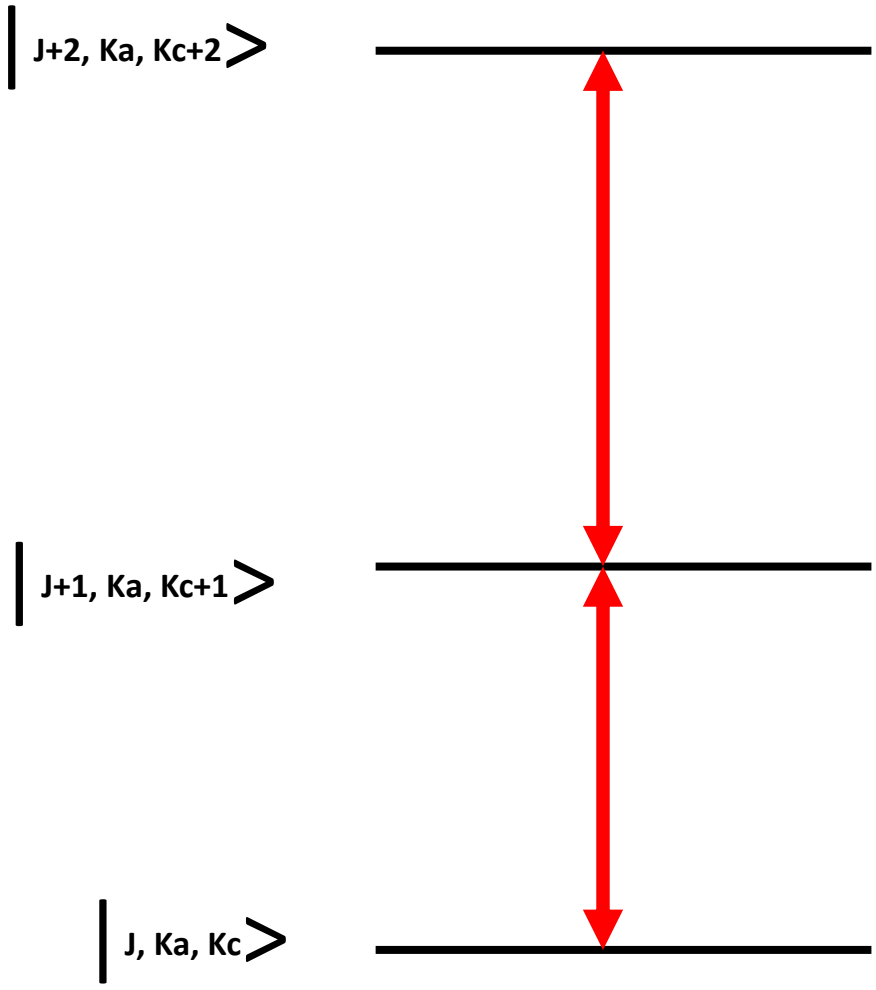
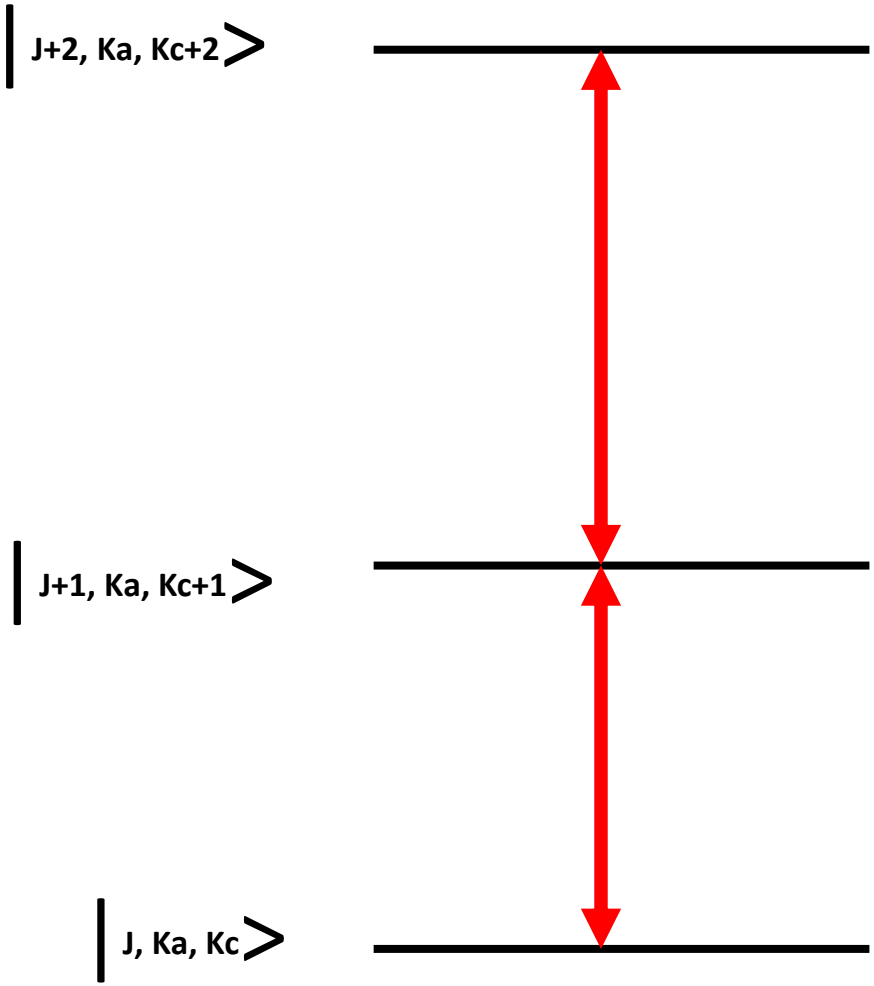

J+2, Ka, Kc+2
J+1, Ka, Kc+1
J, Ka, Kc

AMDOR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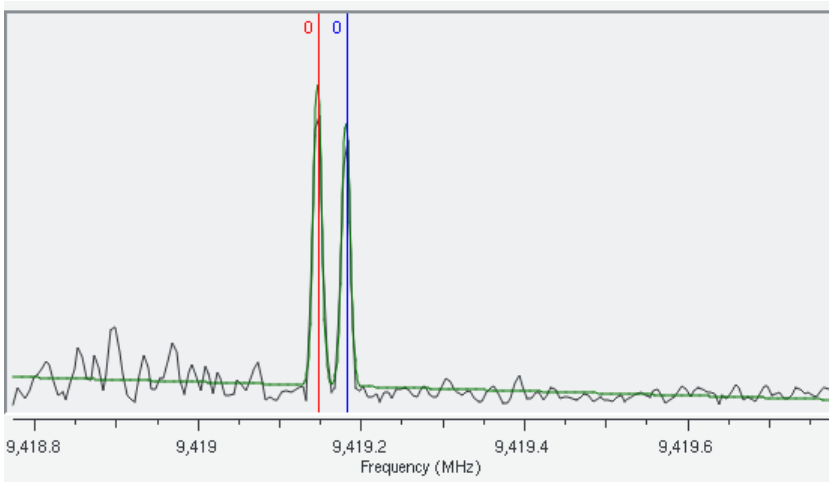
J, Ka, Kc


0
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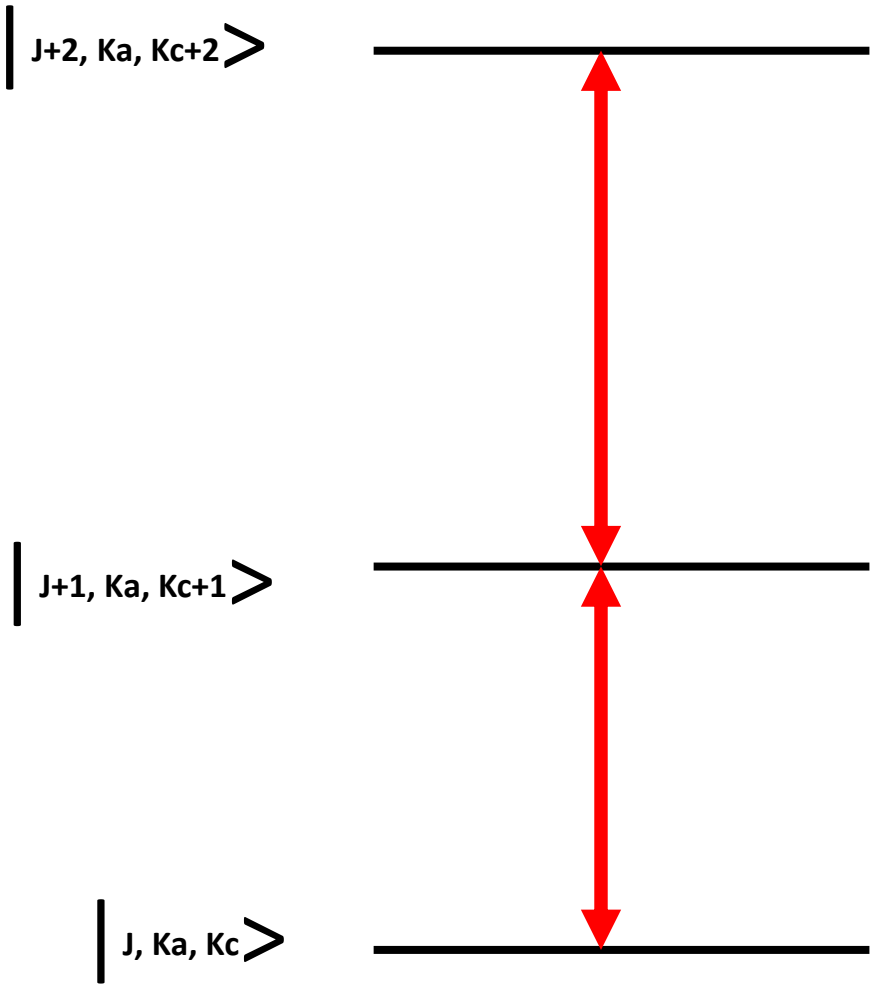
9,418.8
9,419
9,419.2
9,419.4
9,419.6
Frequency (MHz)

AMDOR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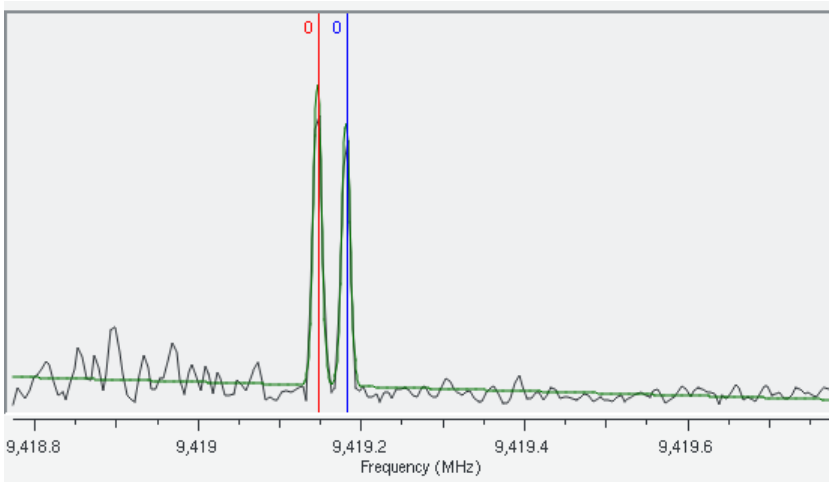
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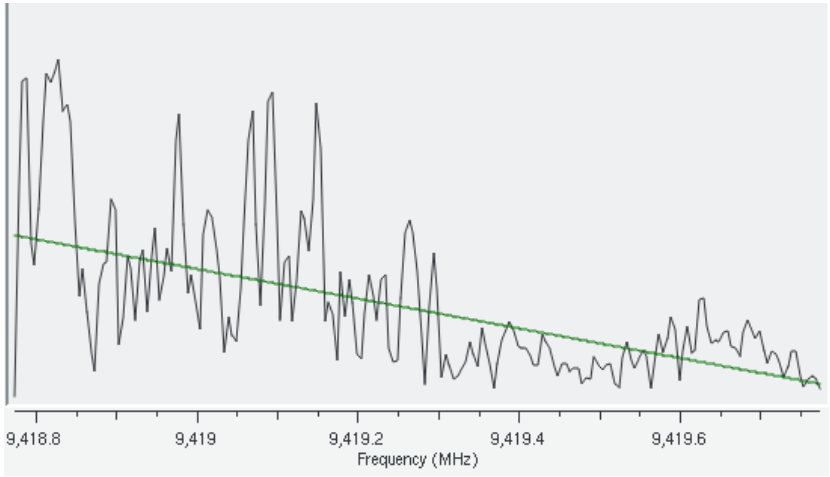
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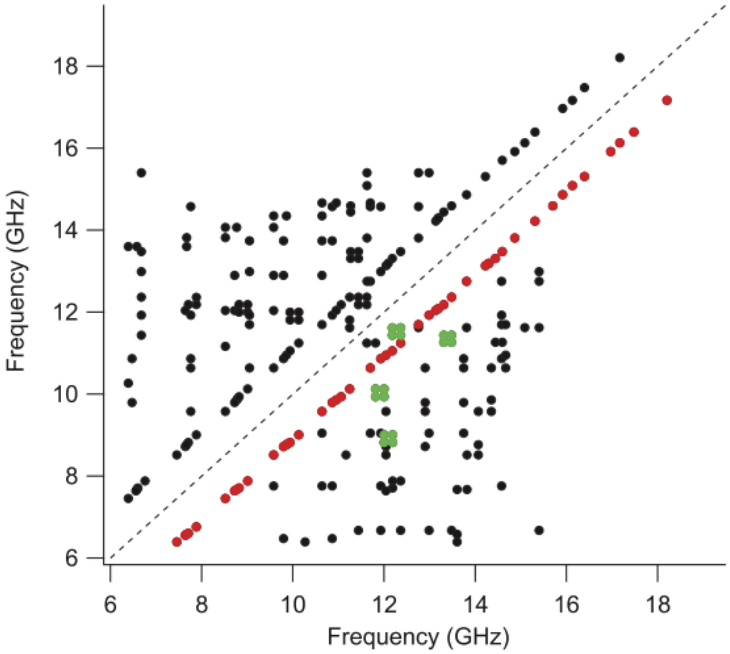

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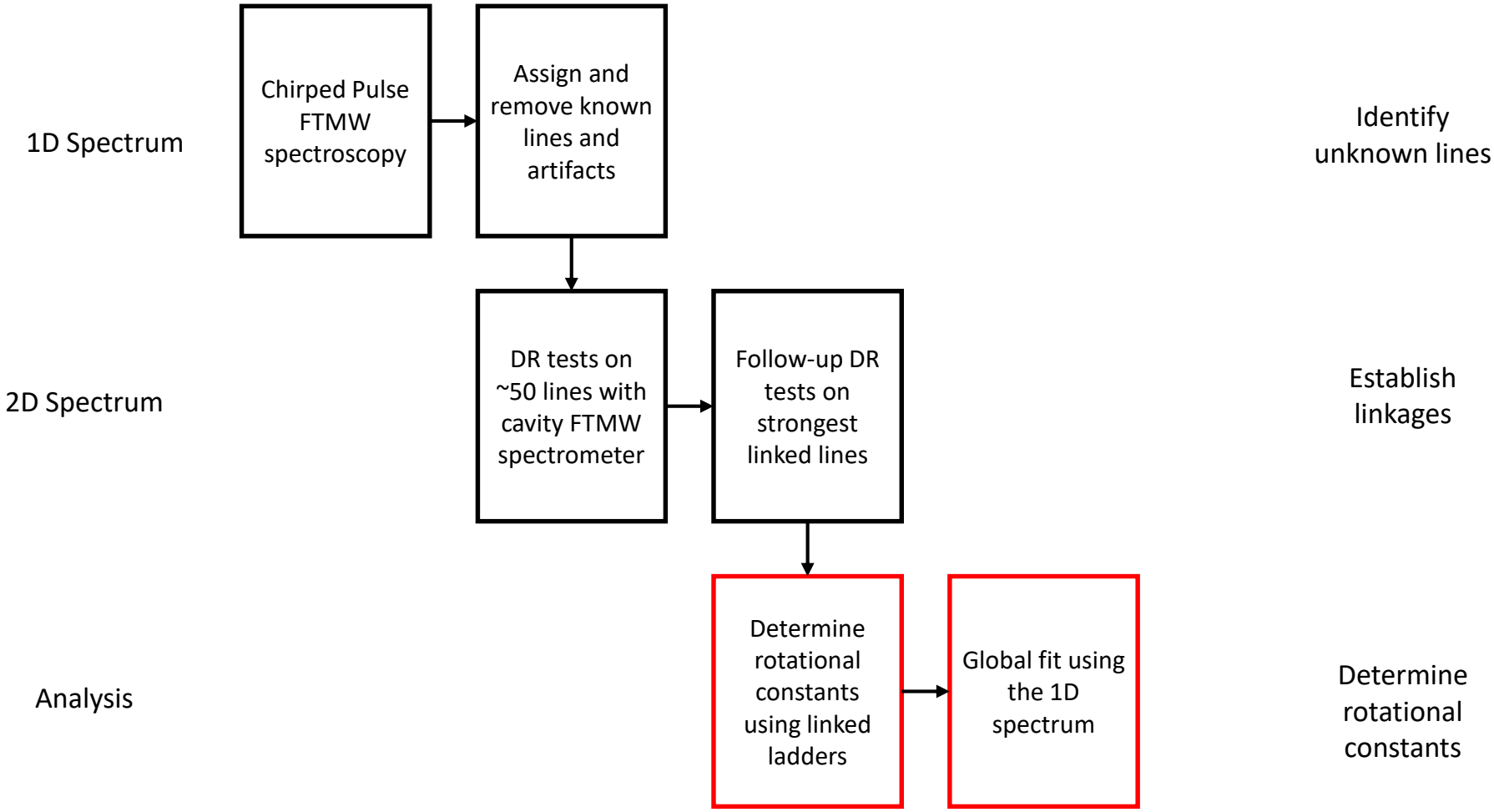
AMDOR workflow



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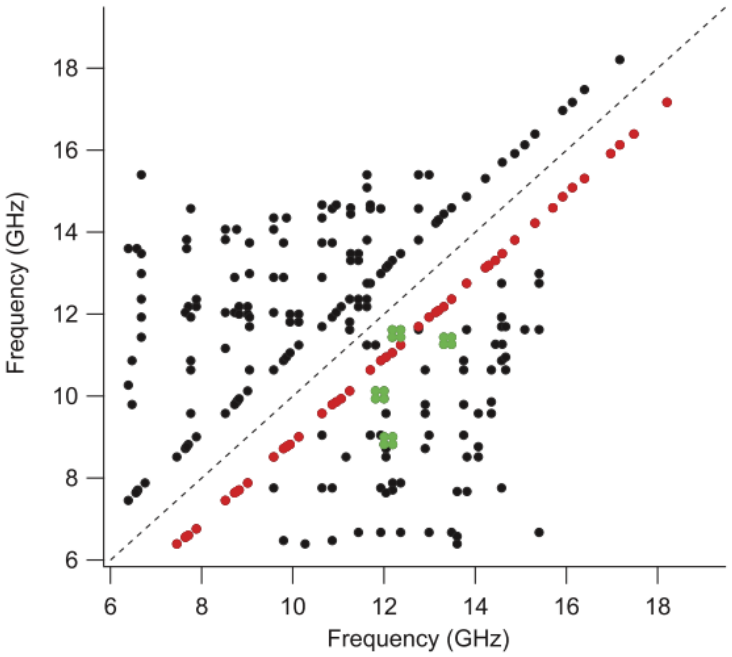

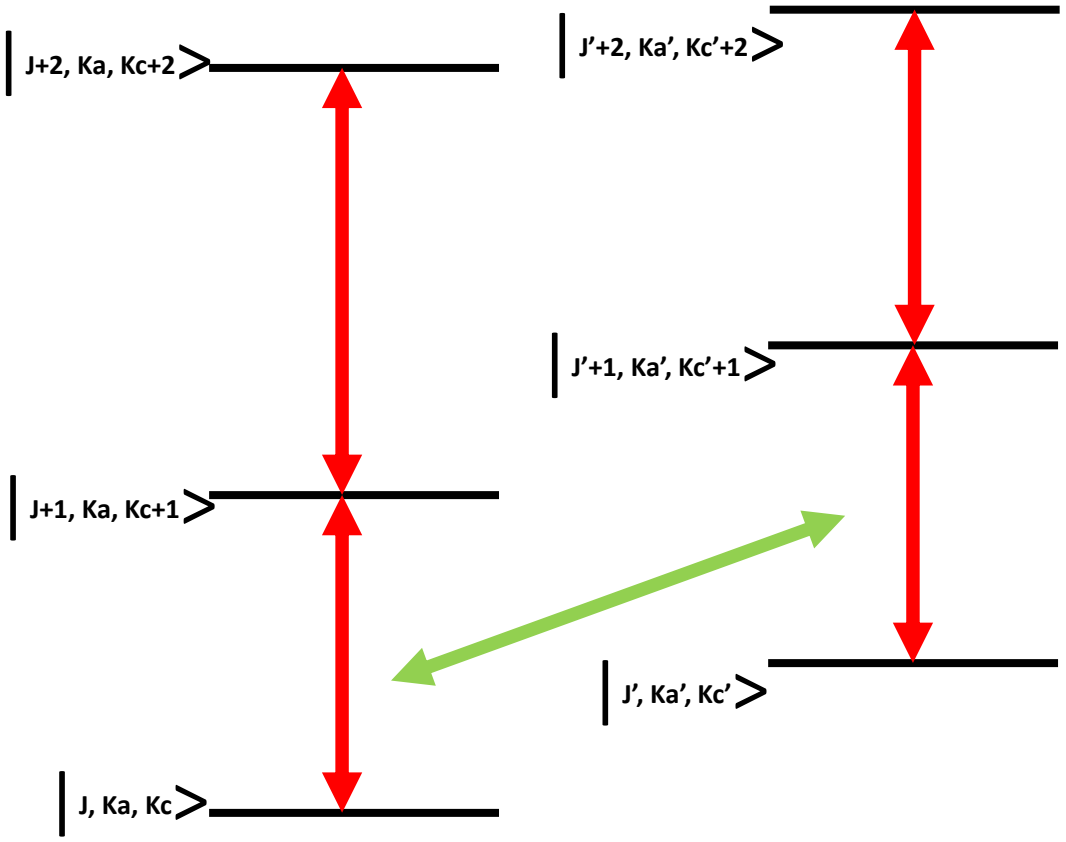

a-ladder 1

a-ladder 2

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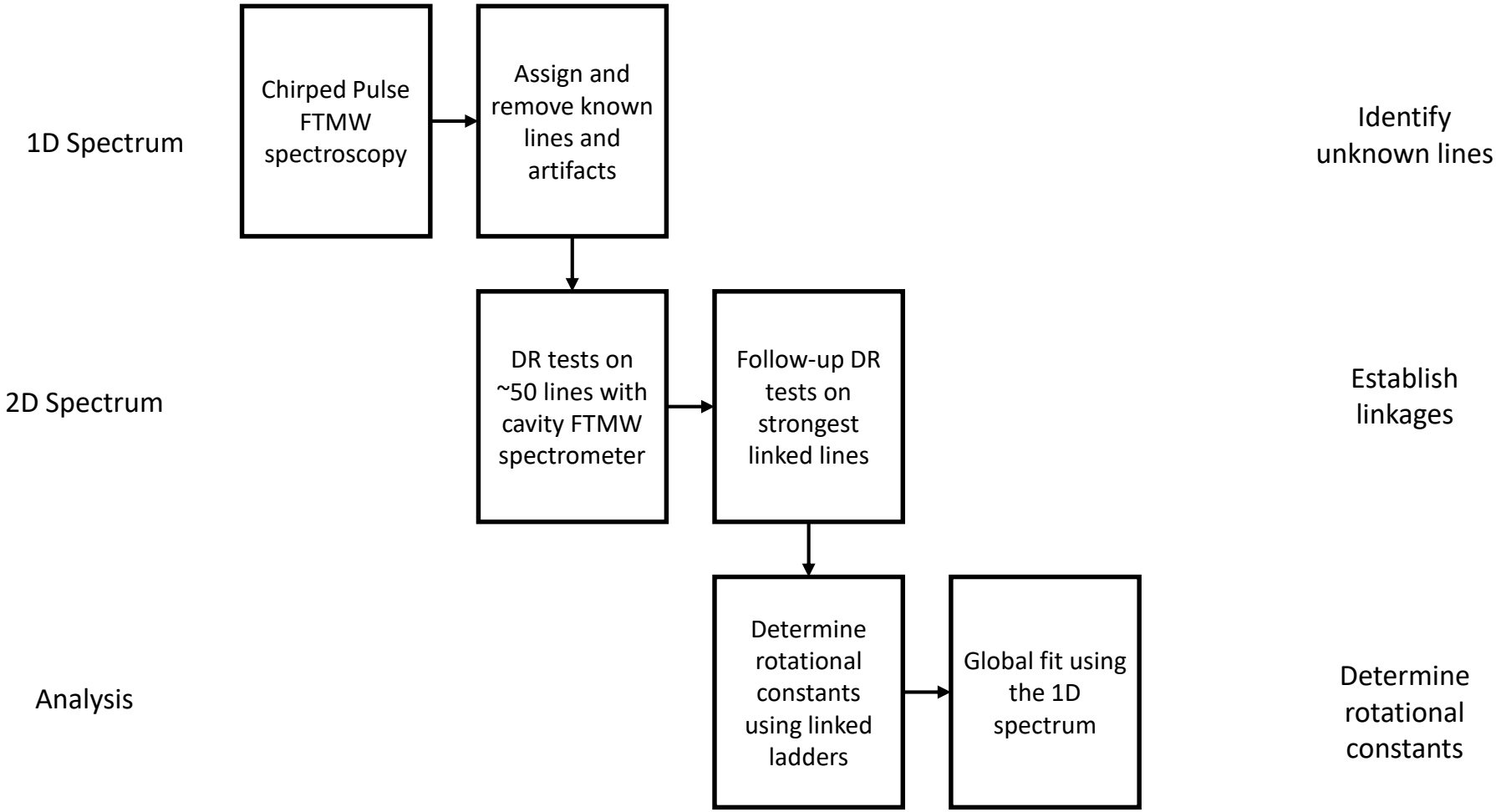
AMDOR workflow



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AMDOR – New Measurement Algorithm

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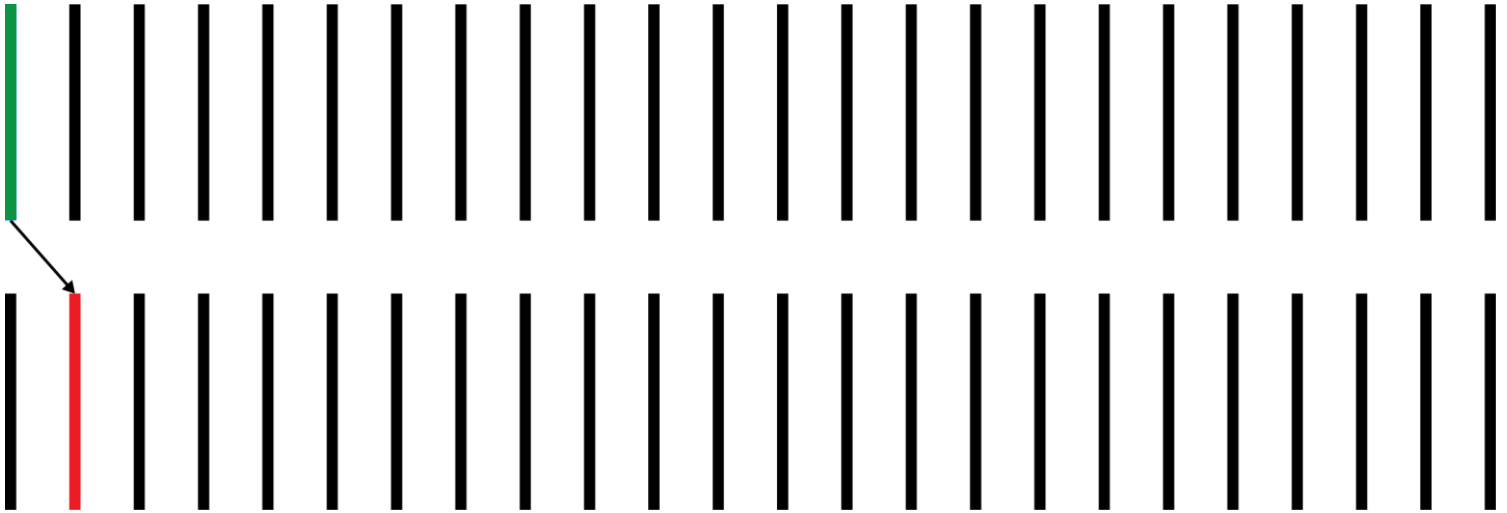

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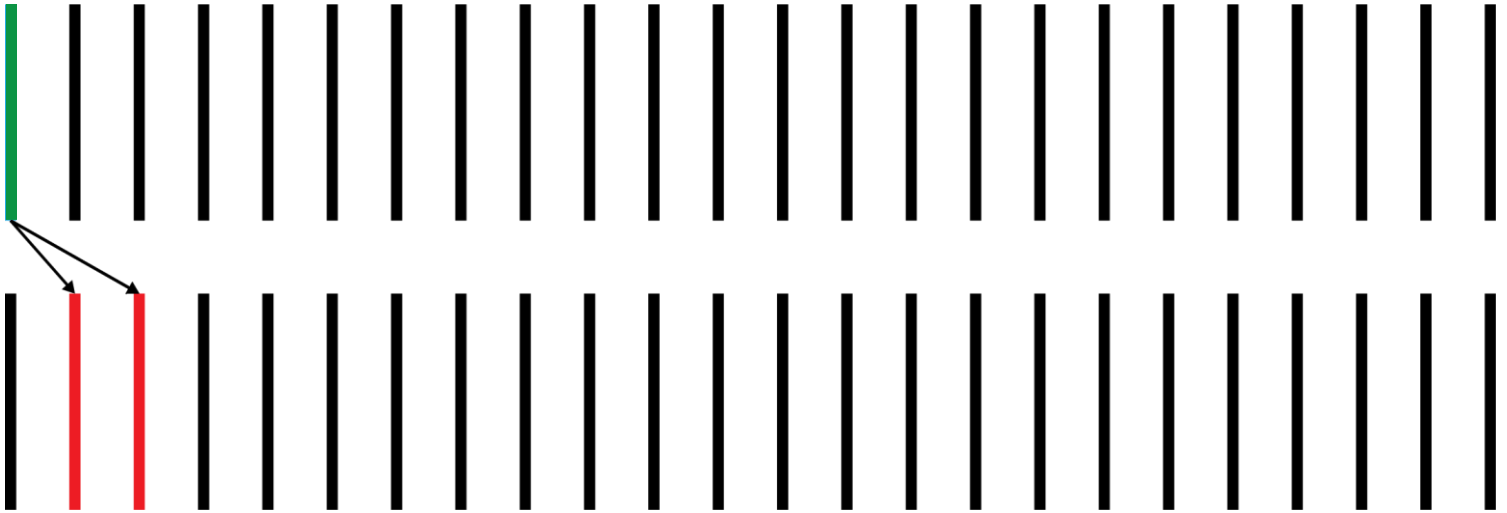

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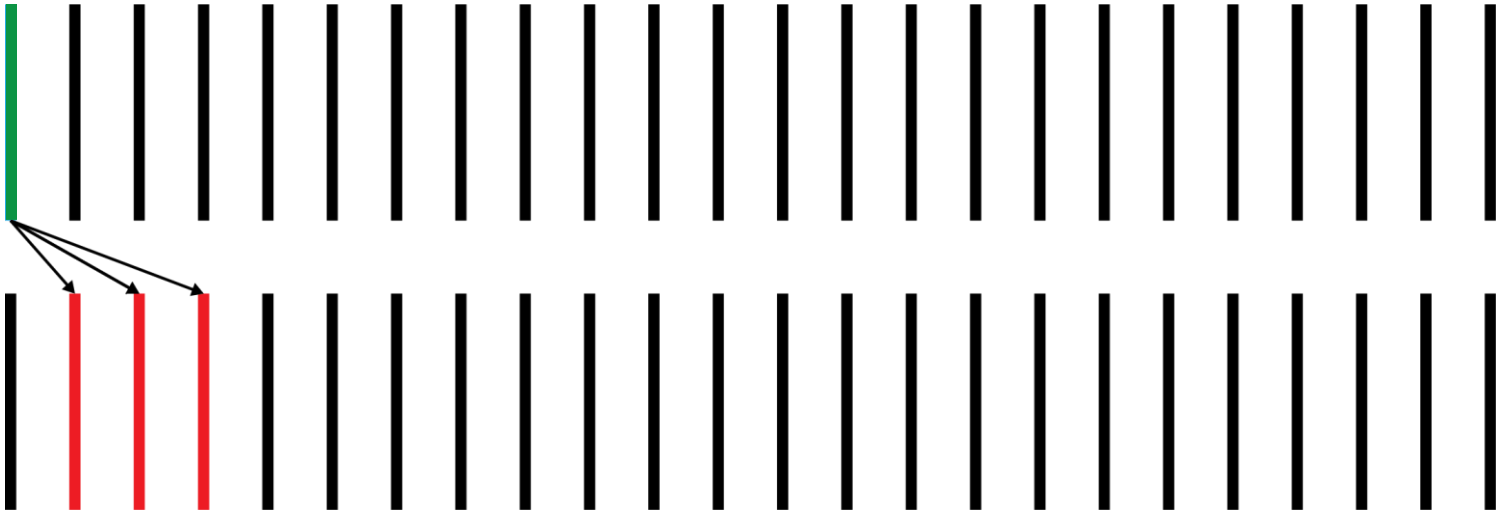

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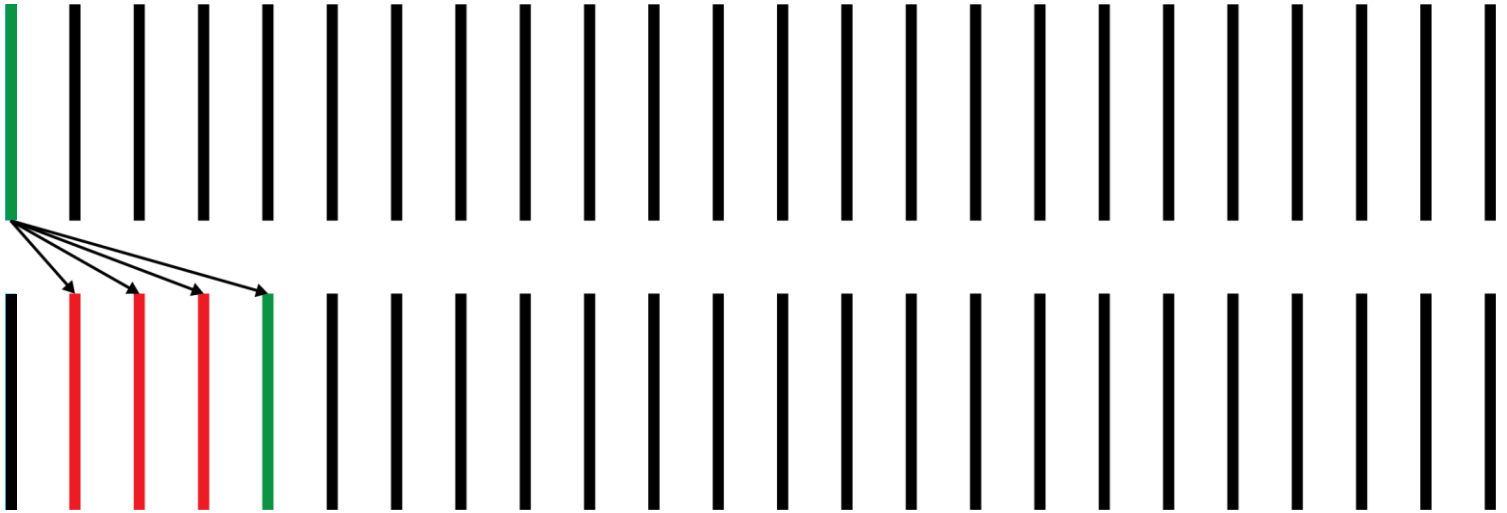

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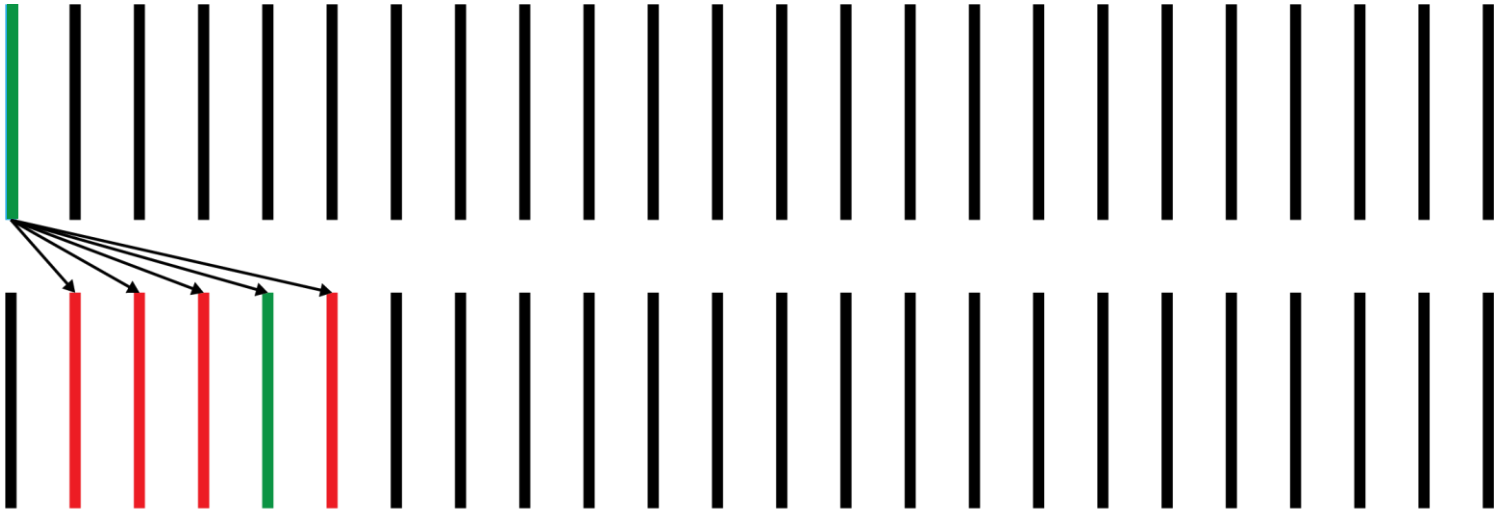

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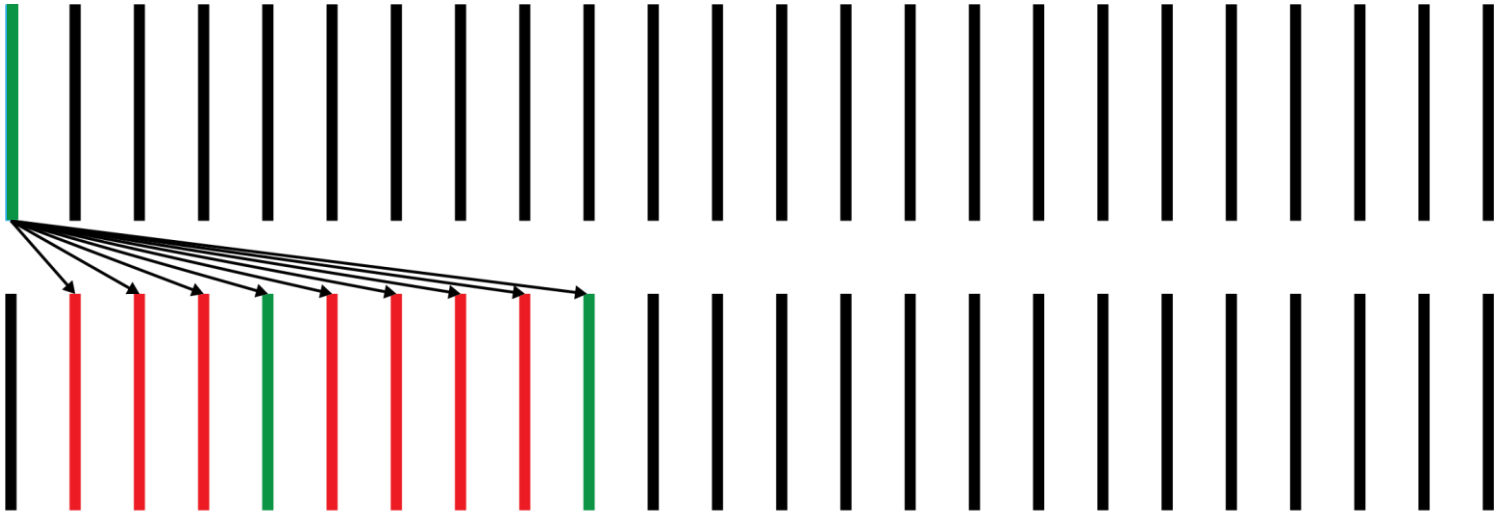

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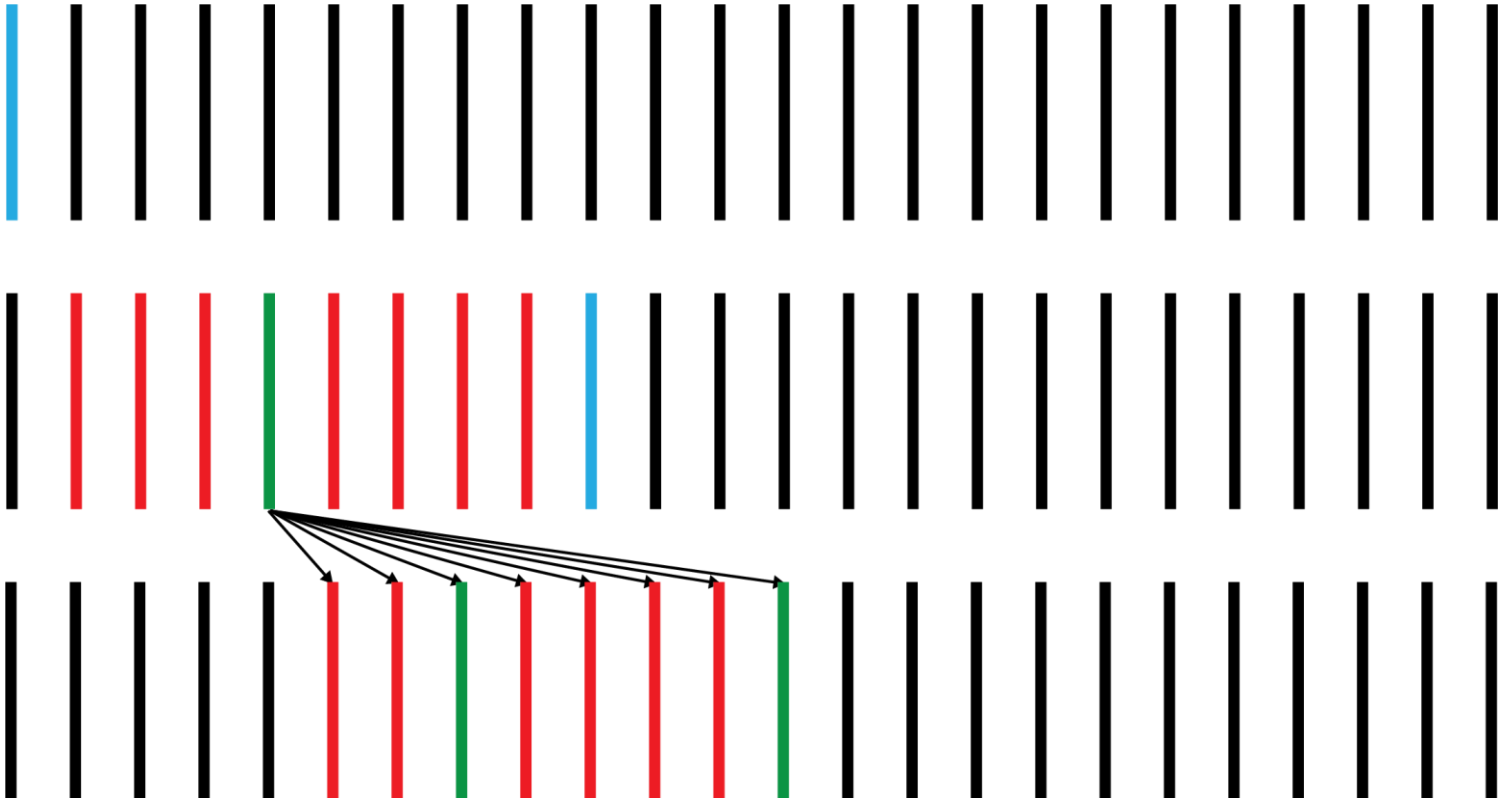

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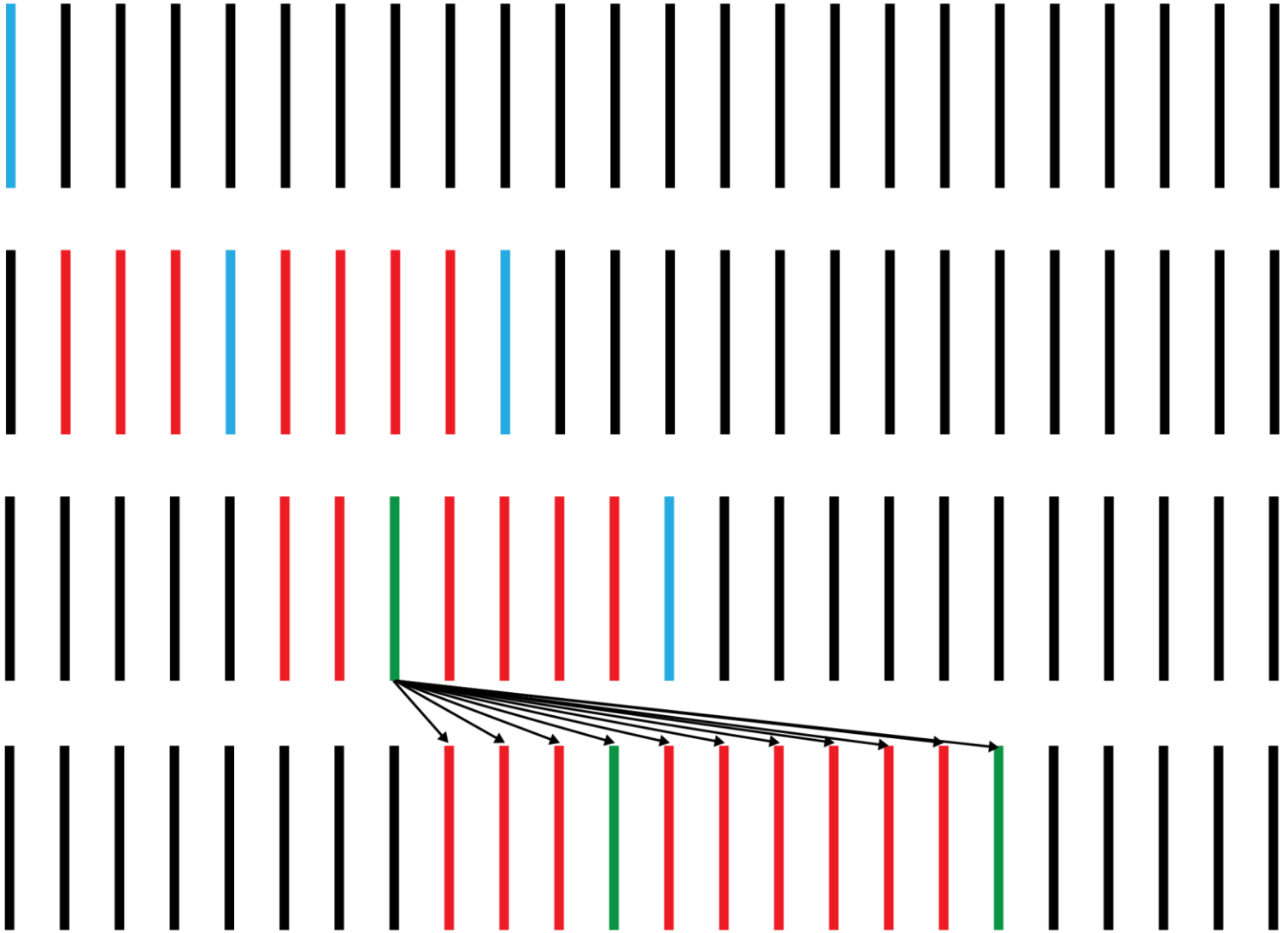

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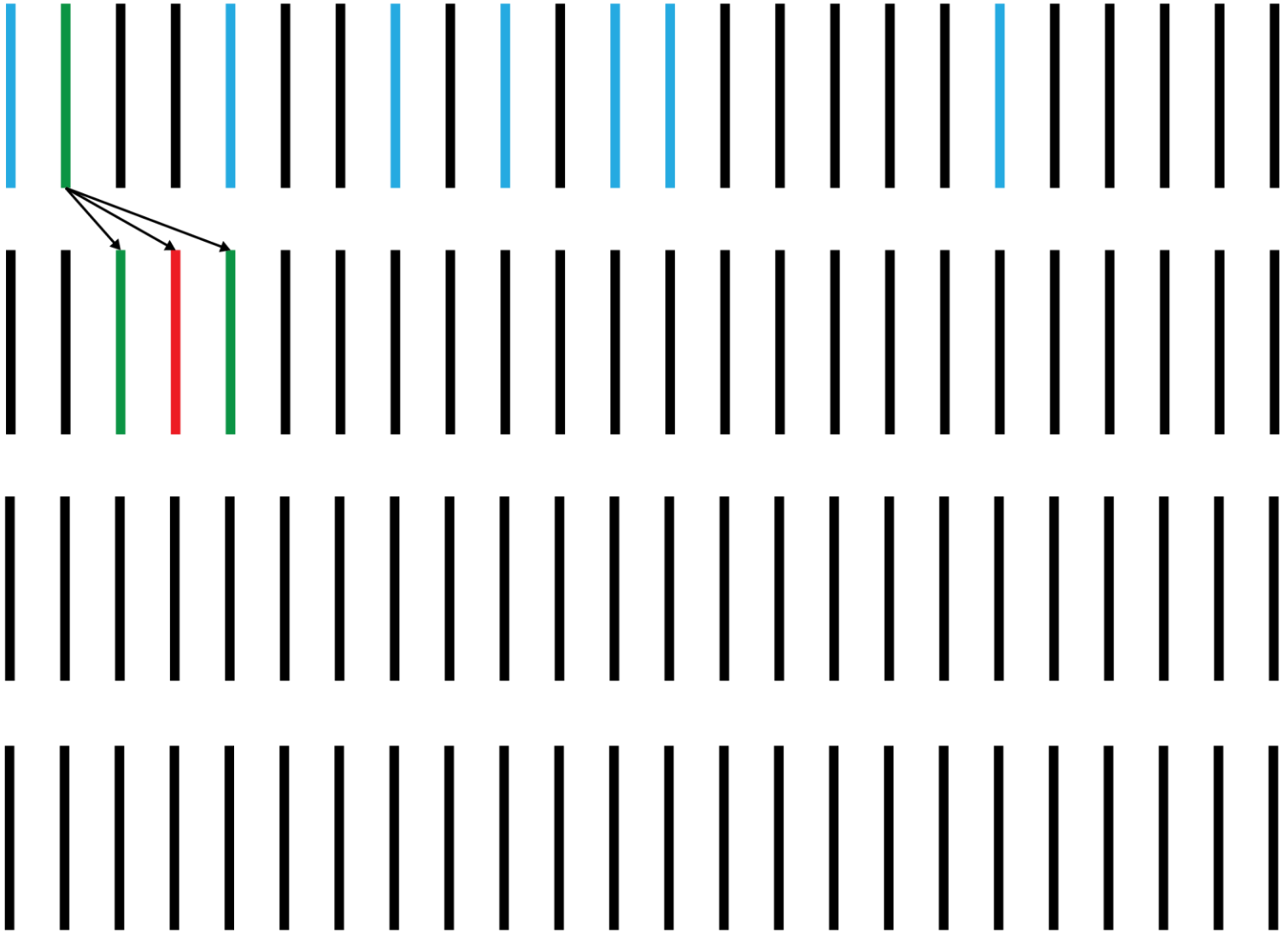

AMDOR - Eugenol

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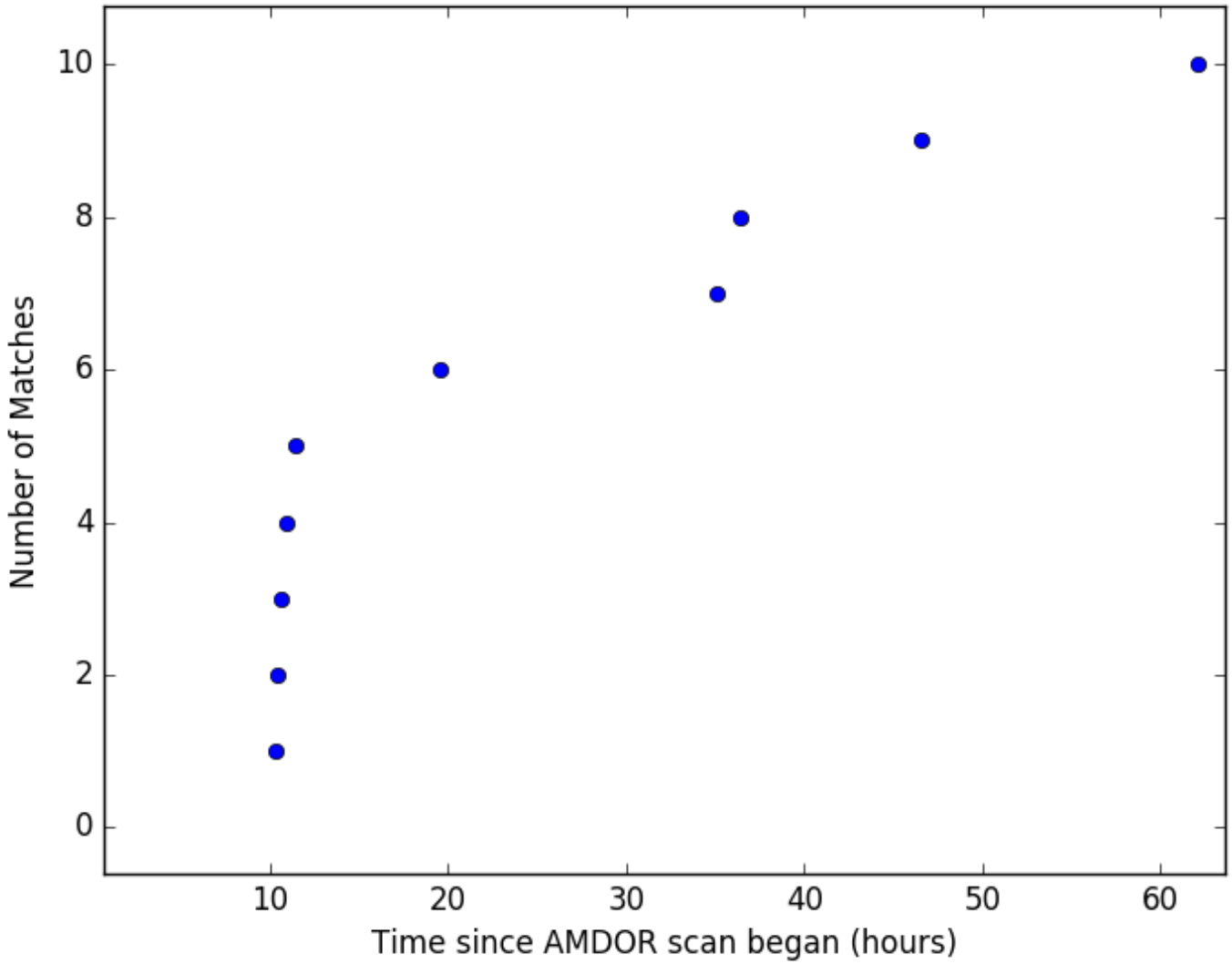

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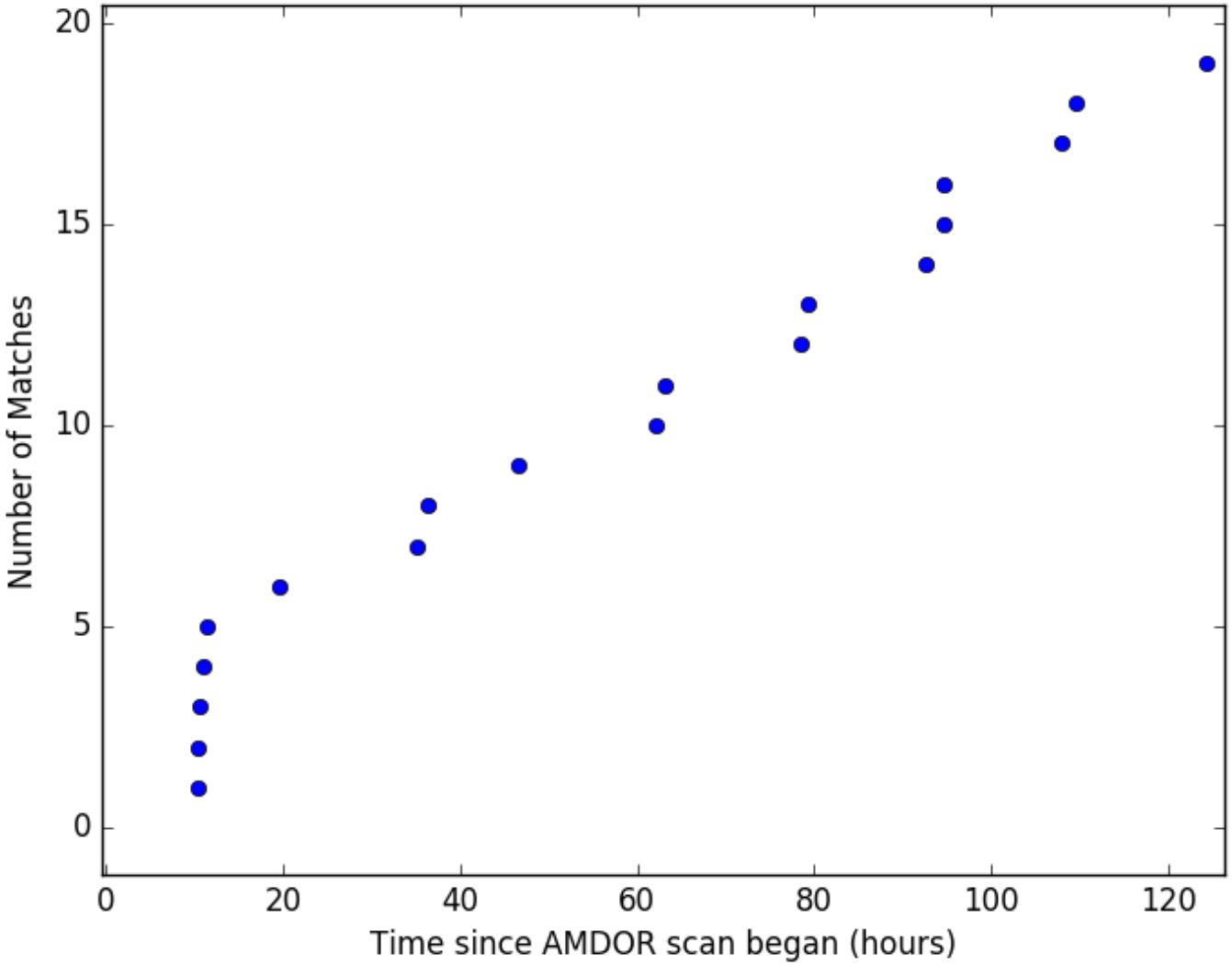

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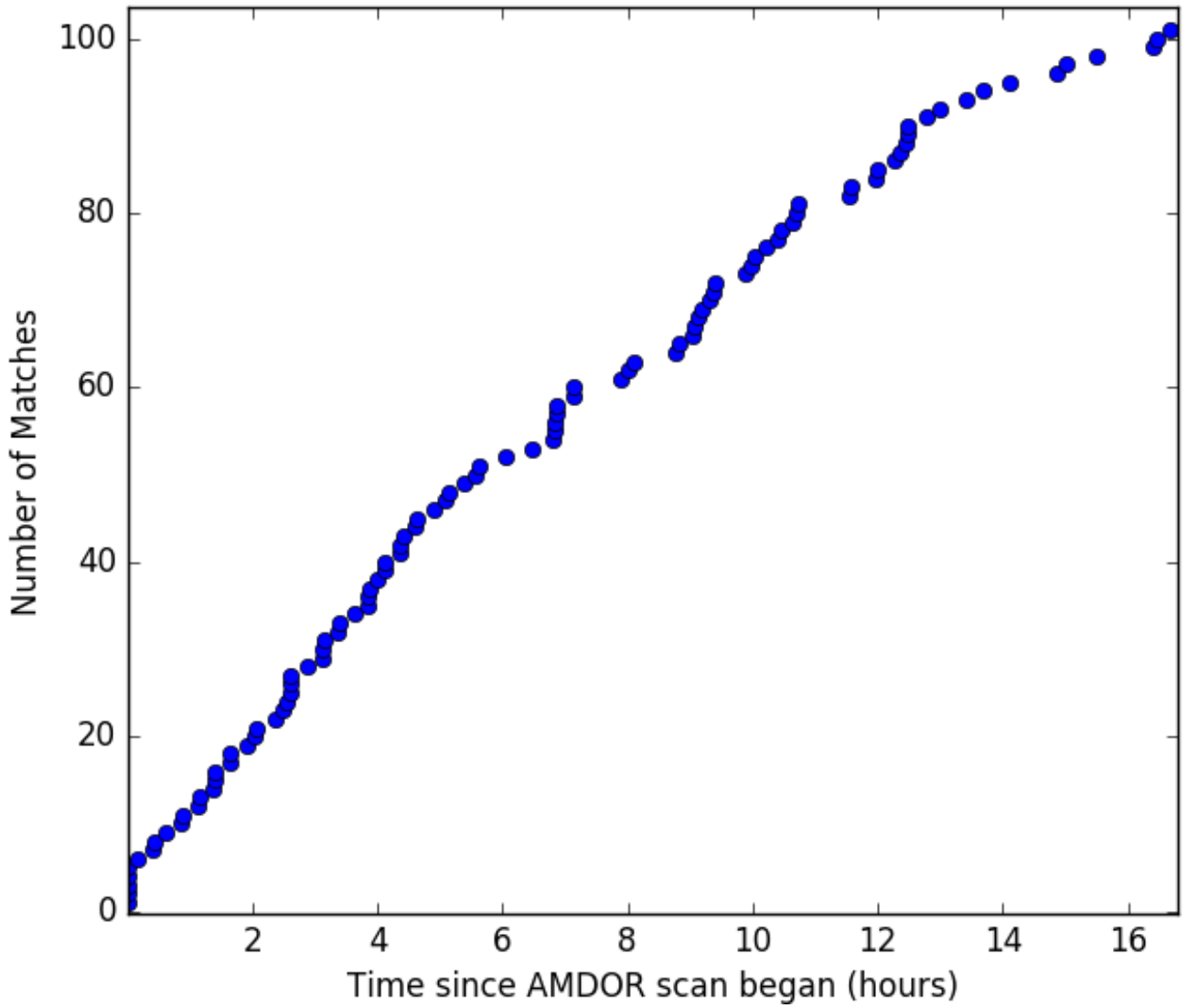
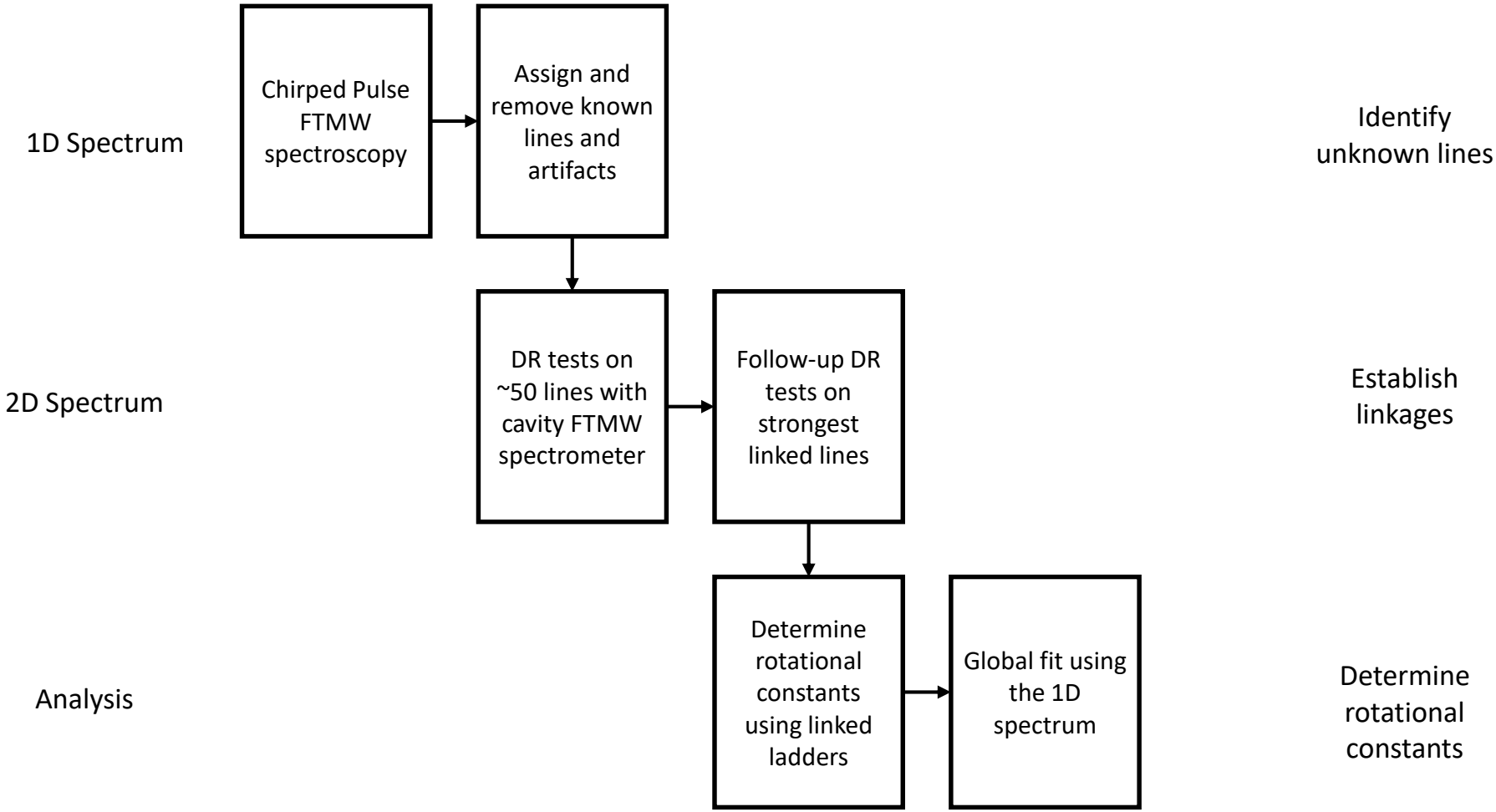


AMDOR workflow



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Machine Learning

"A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E."

Machine Learning, Tom Mitchell, McGraw Hill, 1997.

Supervised Learning

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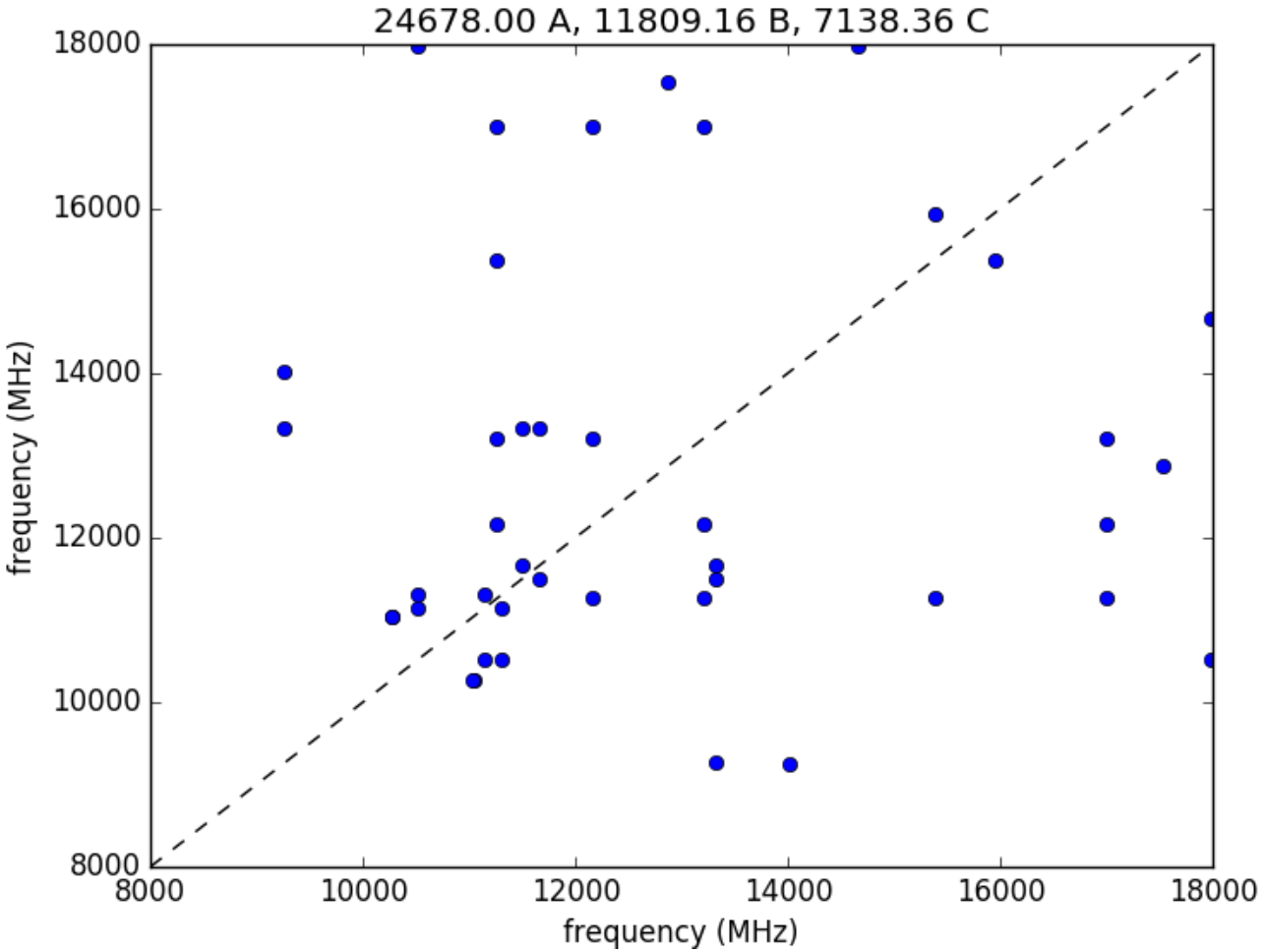
- Supervised Learning = Labeled training set



Supervised Learning - Cost

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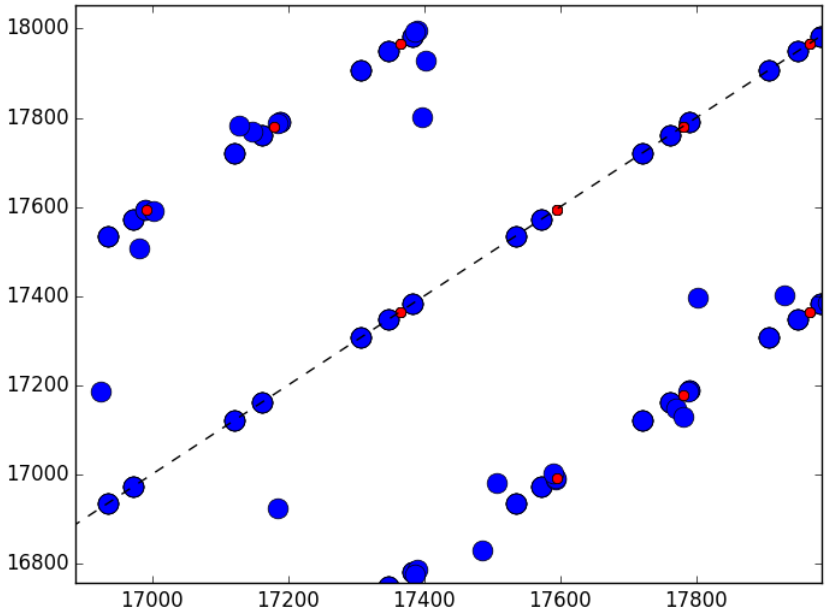
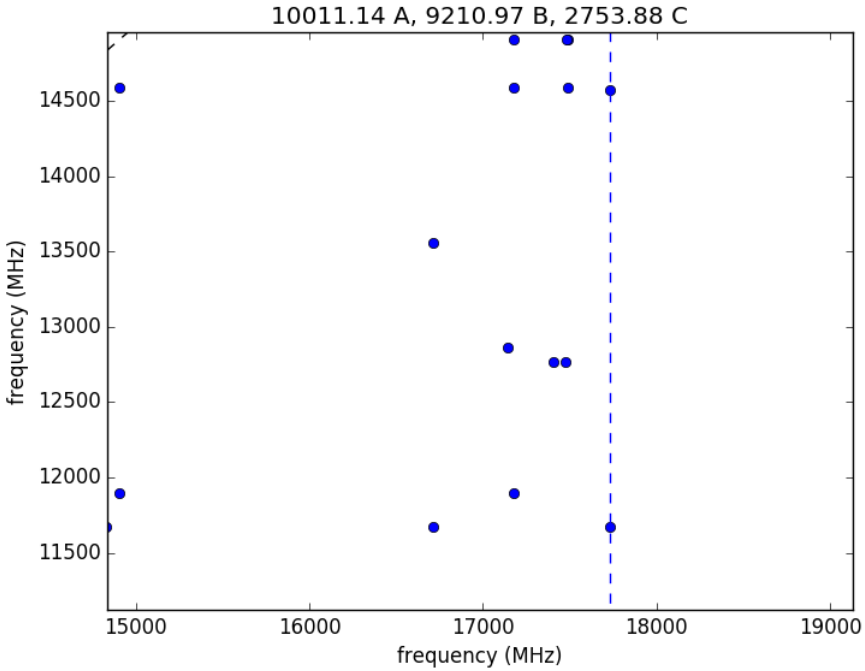
- P, the measured performance is often called the “cost” or “loss.” This is a measurement of how far the model is off from the training data





Supervised Learning - Output

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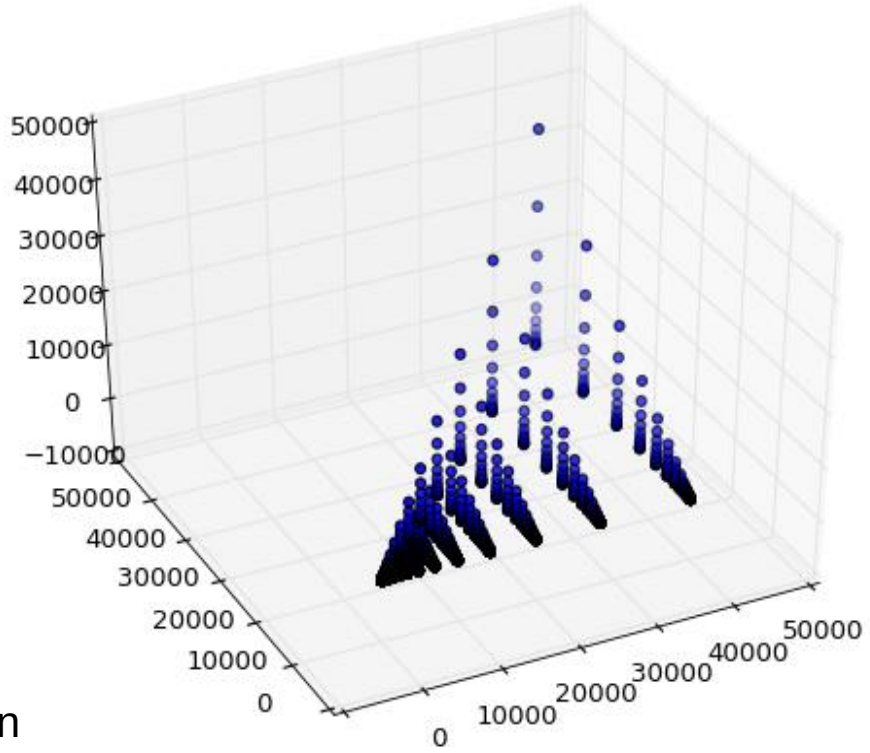
- We've built a database of ~3400 simulated AMDOR spectra with rotation constants ranging from 100 MHz to 40000 MHz logarithmically spaced.
- The output from our model will be a normalized ~3400x1 vector with weights for each "answer" in the database.
- These guesses at initial rotational constants can be used as a starting point for use in the previously developed algorithms



Conclusion

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- AMDOR has proven that it has the potential to extract rotational constants without *a priori* knowledge
- New developments in data acquisition algorithms allow for quick screening of lines to find sets of linked lines.
- Machine learning is being implemented to identify potential rotational constants for unknown molecules

Acknowledgements

- Kyle Crabtree
- Marie-Aline Martin-Drumel
- Michael C McCarthy
- Crabtree Research Group