Spectral Analysis by Neural Networks for Compound Identification in Ion Mobility Spectrometry toward Small Tandem IMS Architectures

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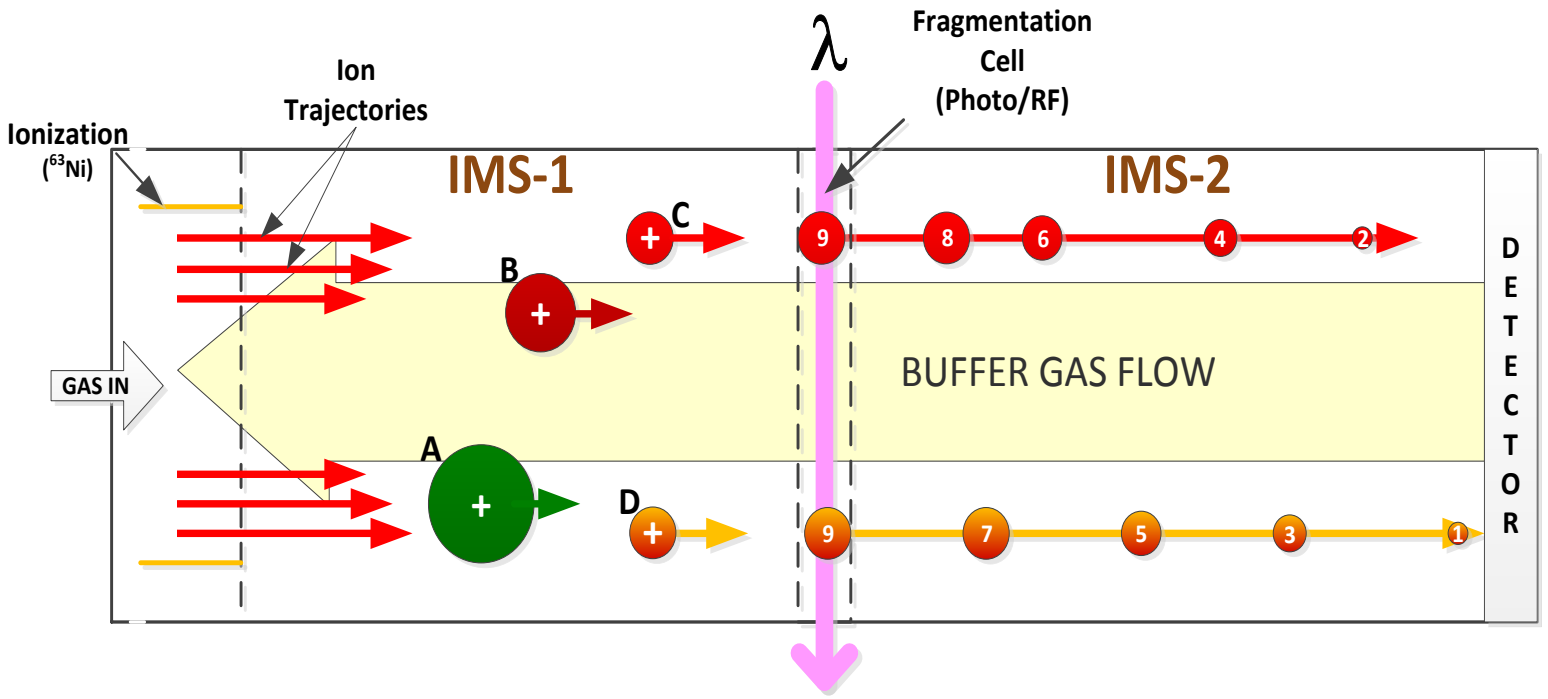
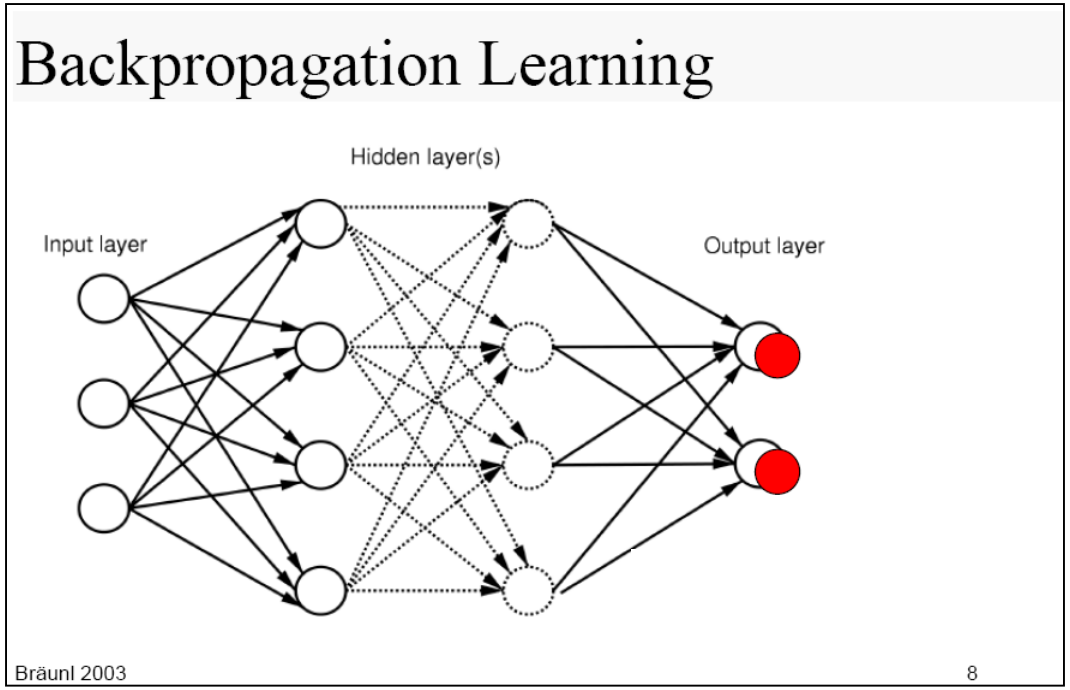


- TIMS (Tandem Ion Mobility Spectrometry) design and manufacturing by MAEGLIN (IARPA),
  and Dr. Eiceman's research group from NMSU
- Goal: To separate the ion of interest by shutter 2 in IMS 2, and fragmenting by high RF
- Provide spectra libraries for 140 compounds from different chemical families

- Use of a neural network for chemical classification of familiar and unfamiliar compounds at different low and high temperatures
- Back propagation NN is used.



Previous research results with no RF fragmentation, at different temperatures

- AAVs (average adjusted values: NN performance criteria) for all familiar compounds were 0.89 at low temperature, and 0.99 at high temperature
- For unfamiliar compounds, overall AAVs were 0.55 at low temperature, and 0.79 at high temperature