Deconvolution of Post-Detonation Mixtures of Soot

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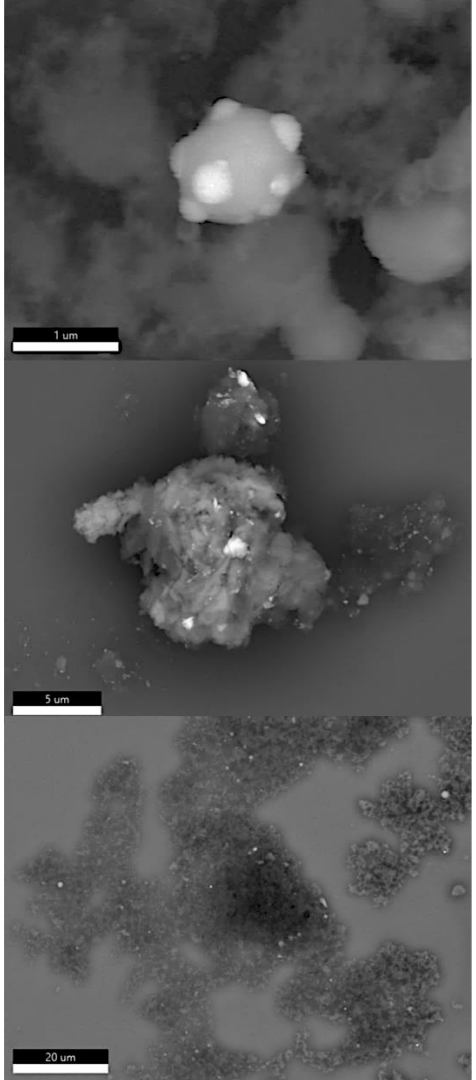
27 October 2024

LA-UR-24-31465

Sources of Soot

- **Atmospheric Soot**
  - Formed through incomplete combustion
  - Submicron Particles
- **Detonation Soot**
  - Produced by shock-driven decomposition
  - Much higher temperature and pressure regimes
  - Chemical properties dependent on the fuel, detonation conditions, and environment



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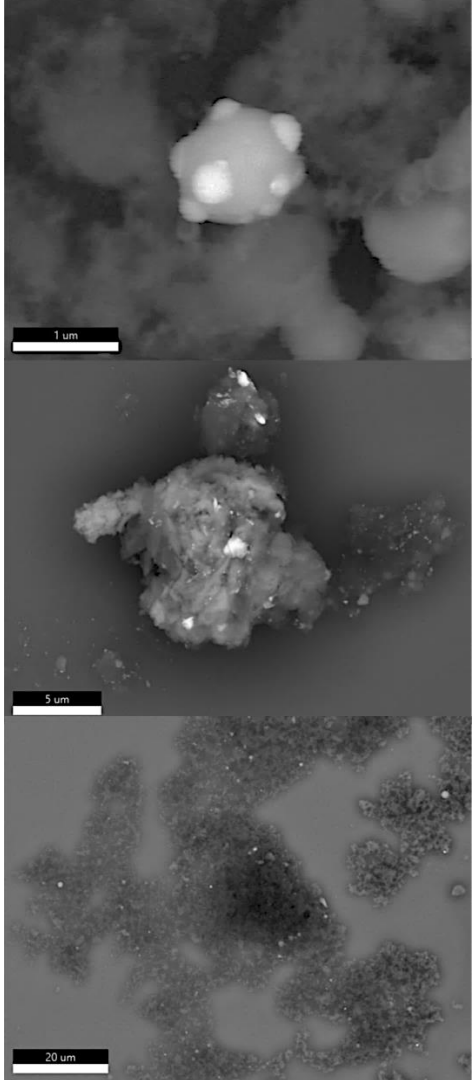
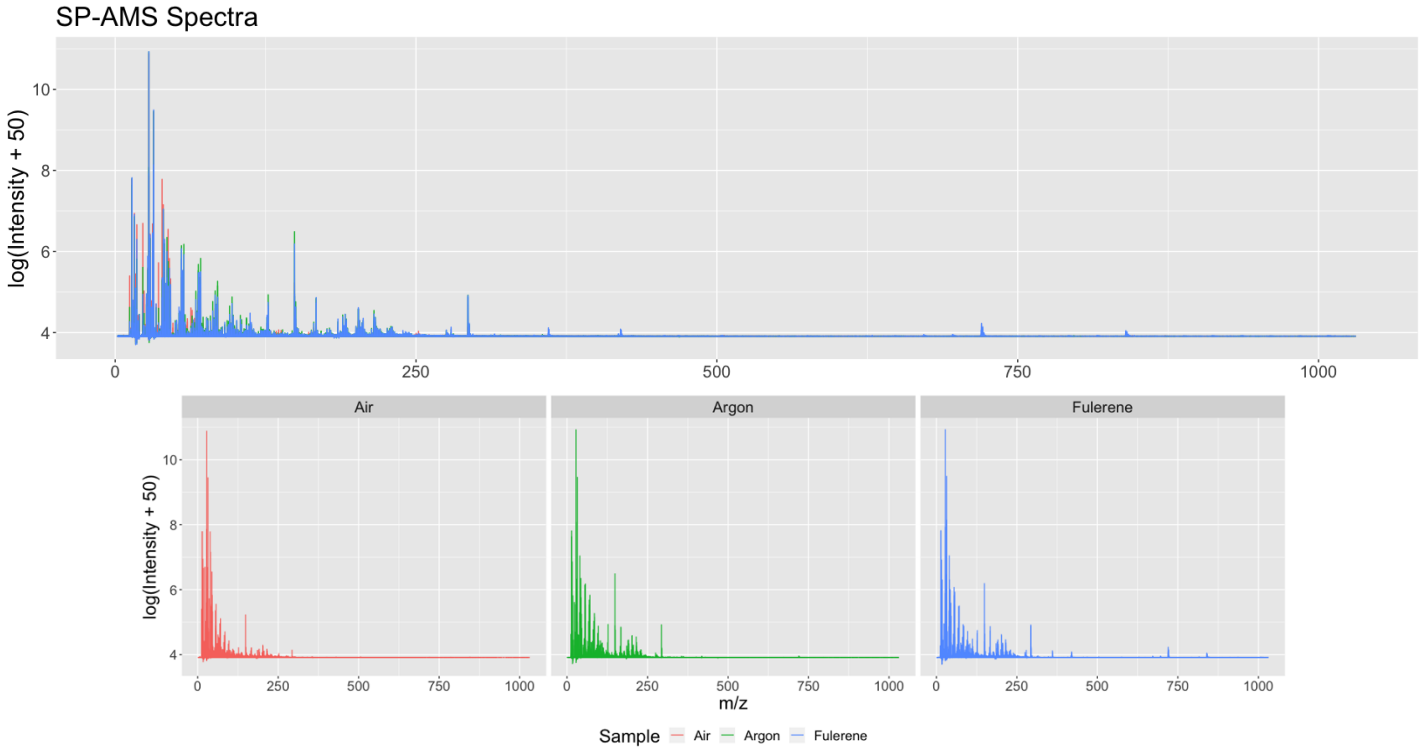
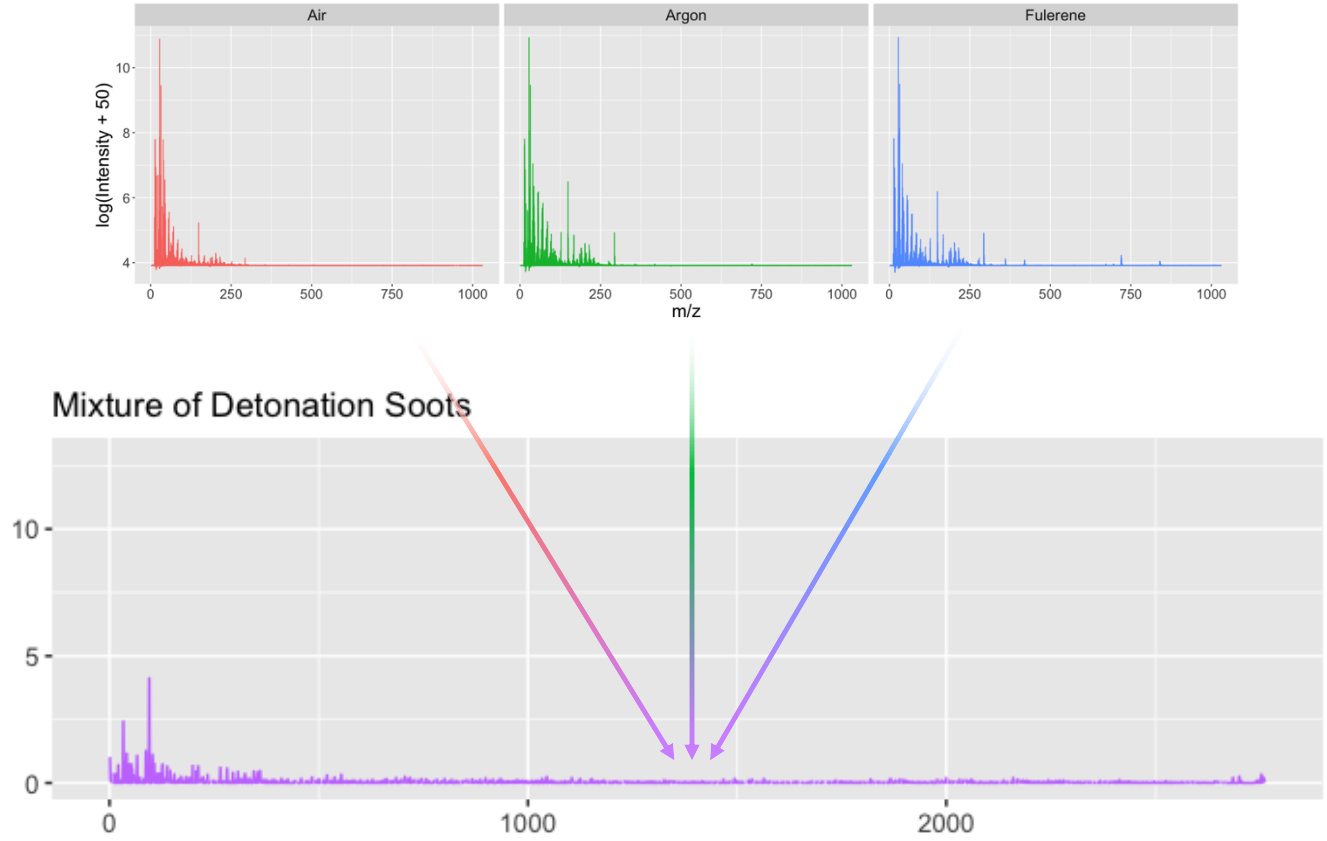
These factors are useful for defining source-dependent features



Source-Dependent Signatures

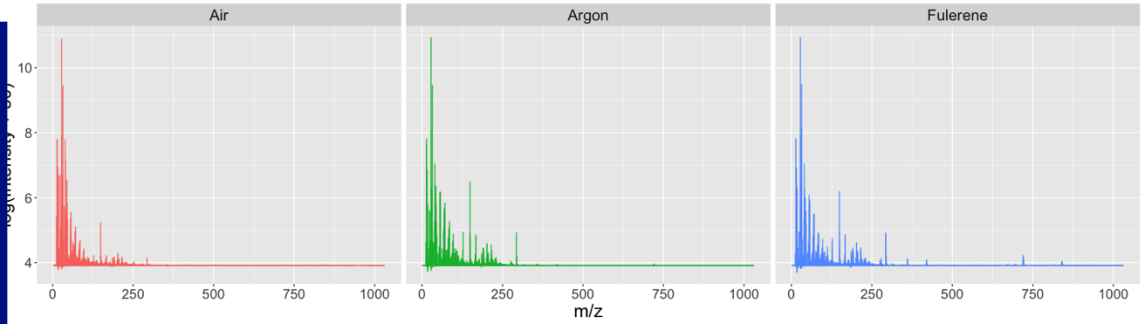


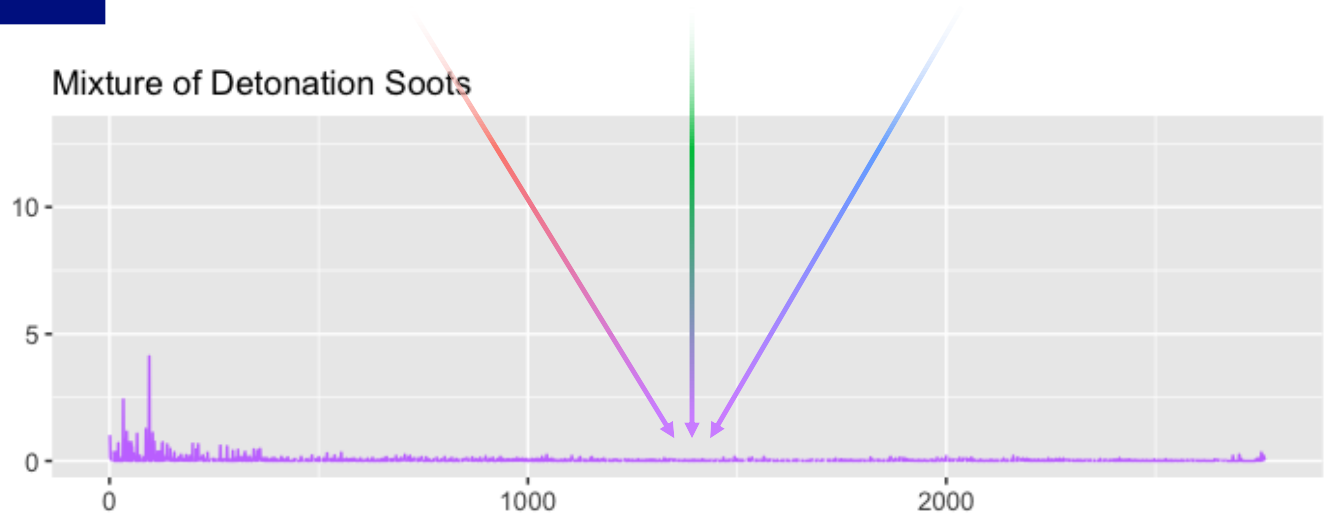
Mixture of Signatures



Mixture of Signatures

Is there another way we can represent this data?

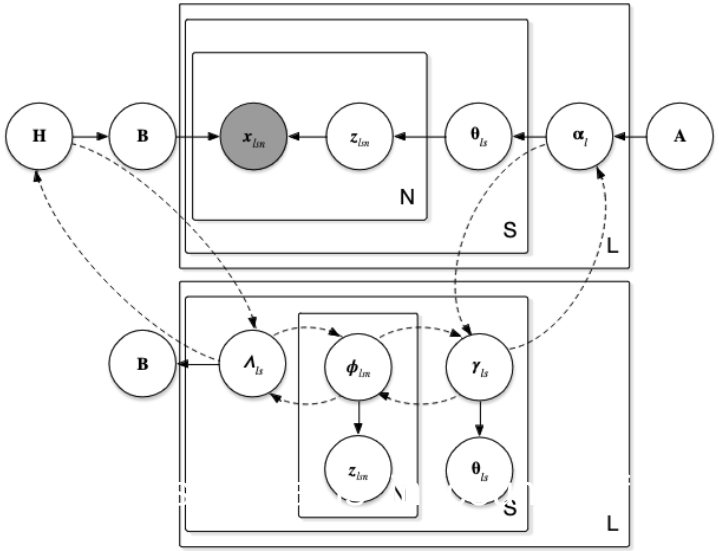




Latent Dirichlet Allocation

Key Points

- Statistical technique
- Specifically designed for **mixtures**
- Originally designed for **topic modelling**
  - **Topics**, characterized by **words**;
  - **Soot** characterized by **moiety families**;



$$q(\Theta, \mathbf{B}, \mathbf{Z}|\mathbf{\Gamma}, \mathbf{\Lambda}, \mathbf{\Phi}) = \prod_{l=1}^{L} \prod_{s=1}^{S} \left[q_{ls}(\boldsymbol{\theta}_{ls}|\boldsymbol{\gamma}_{ls}) \prod_{n=1}^{N} q_{ls}(\mathbf{z}_{lsn}|\boldsymbol{\phi}_{lsn}) \prod_{m=1}^{M} q_m(\boldsymbol{\beta}_m|\boldsymbol{\lambda}_{lsm}) \right]$$

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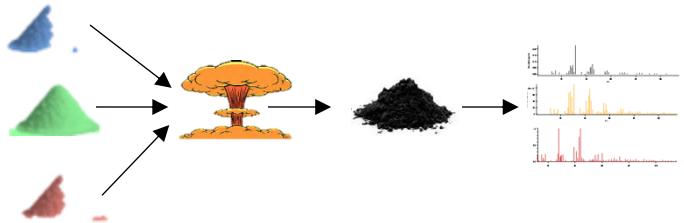


- Extension to **mixtures of mixtures**:
  - Originally designed for various types of dust particles (data is in counts of **dust particle types** associated with different **locations**)
  - Extension to soot: use peak heights as “proportions”, and use these to sample “particles” (**moiety families**) from a given “location” (**detonation soot**)
  - Multiple soot types, each defined by their own mixture of moiety families

Convert Magnitudes of Spectra into Count Data

	Air1	Air2	Air3	Air4	Air5	Air6	Air7	Ar1	Ar2	Ar3	Ar4	Ar5	Ar6	Ful1	Ful2	TR1	TR2	TR3
HRBC_FullereneC	1	1	1	1	1	1	1	44	42	55	34	42	43	299	230	211	293	294
HRBC_LowC	471	470	473	524	451	479	433	502	448	382	450	525	529	47	35	125	130	140
HRBC_MidC	3	3	4	4	6	4	3	5	0	3	0	0	0	0	0	0	1	1
HRChl	7	8	8	8	8	6	8	4	3	3	2	2	2	16	19	16	17	17
HRMxM_familyOther	626	615	620	621	628	619	634	530	544	560	534	501	510	35	39	142	136	135
HRNH4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HRNO3	10	10	8	9	9	9	10	4	5	0	2	8	2	15	16	12	13	12
HROrg_CH	343	390	388	385	394	433	419	1062	1071	997	1028	1150	1166	2769	3152	2629	2532	2527
HROrg_CHN	24	35	26	29	35	27	29	91	13	48	35	7	30	259	112	94	116	121
HROrg_CHO1	302	312	298	255	238	247	215	246	207	234	264	247	246	1277	1093	997	985	983
HROrg_CHOgt1	108	112	100	99	108	114	101	0	0	0	38	18	5	144	140	114	123	123
HRSO4	3	2	2	2	3	2	2	3	22	7	7	6	5	4	6	3	4	4
HRmetal	3102	3042	3072	3063	3119	3060	3144	2511	2659	2717	2607	2493	2462	137	160	656	651	643

1. Partition the data into moiety families;
2. Use peak heights as proportions used to sample particles
3. Get Particle Counts

A Case Study

Suppose that…

- We have a library of three types of detonation soots:
  1. Composition B detonated in Air
  2. Composition B detonated in Argon
  3. Fullerene

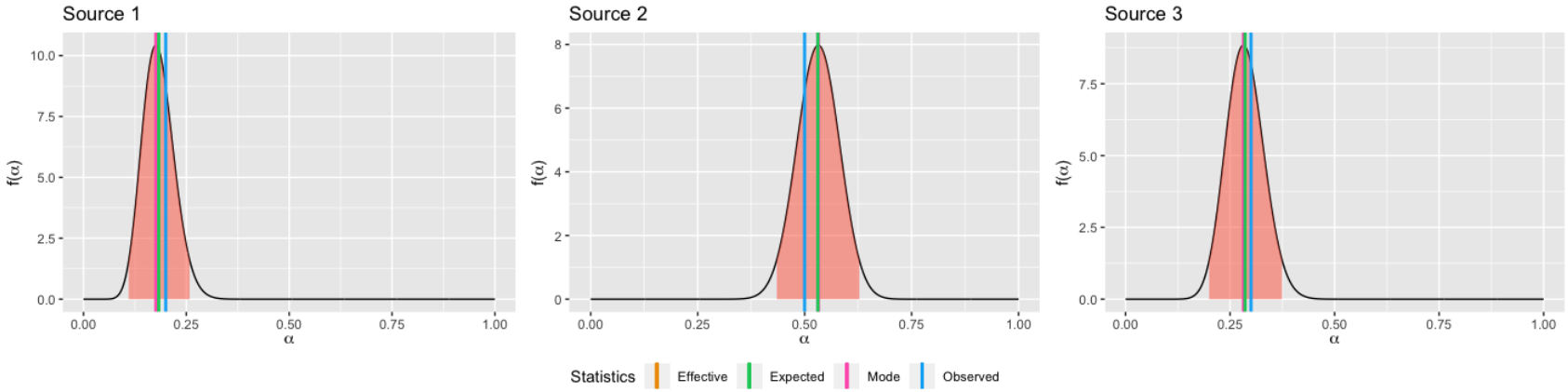
this is what we use to **train our model**

- We can only observe **pure samples** of potential sources (from our library)
- We have observed three samples of trace soot (from the same detonation)
- Our trace source is a **mixture** of the three sources
  - 20% Composition B in Air
  - 50% Composition B in Argon
  - 30% Fullerene

we don't know this… this is what we **want to learn**!

A Case Study

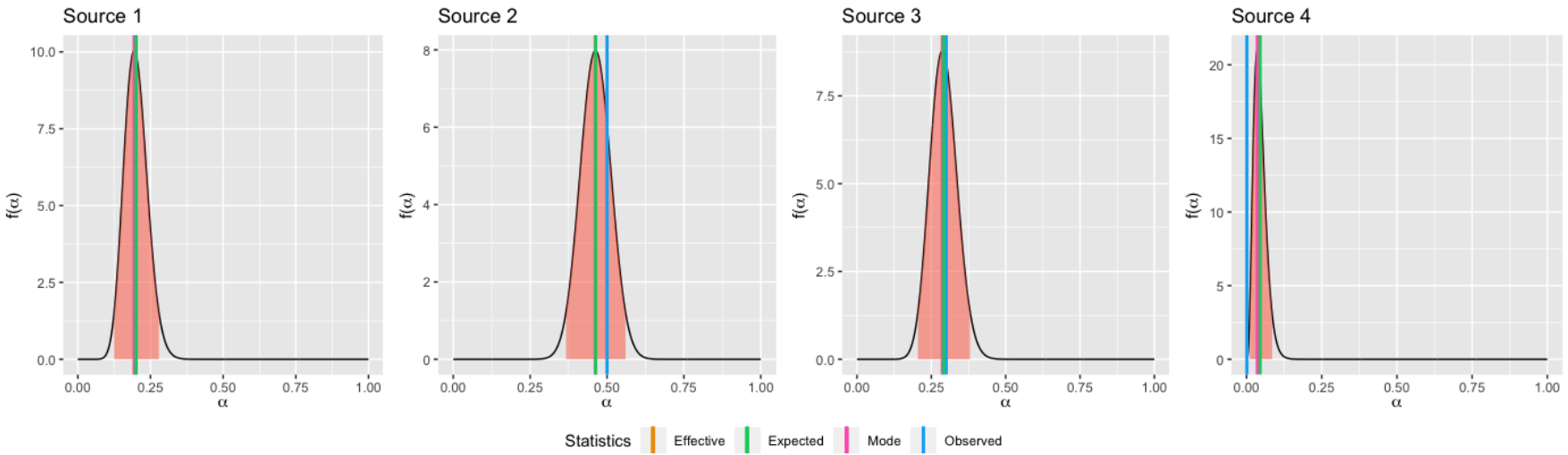
When we train on all three sources:



A Case Study

When we give the model a little more flexibility

(What if our sample has a source that our library doesn't know about?):



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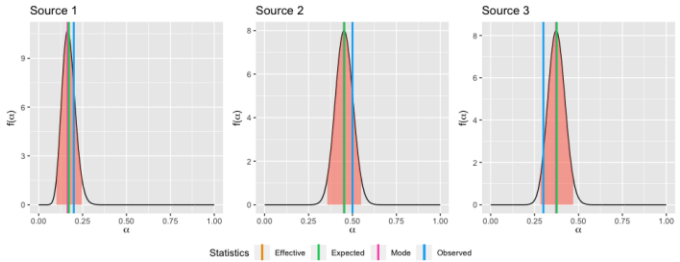
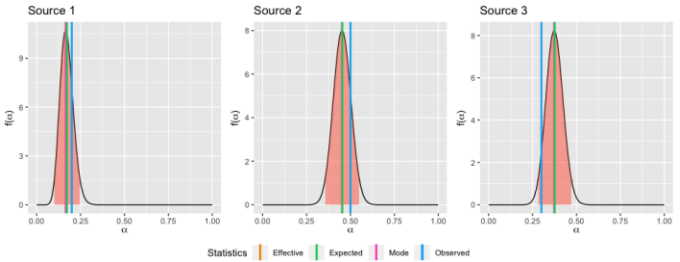
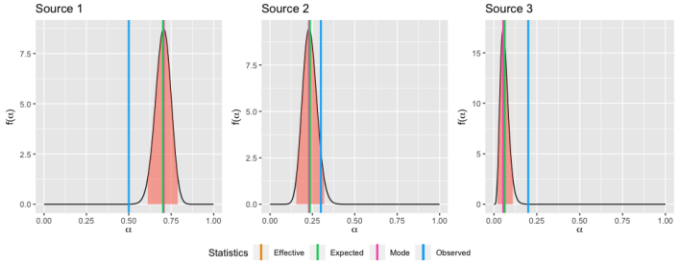


Fullerene not in library



Ar not in library

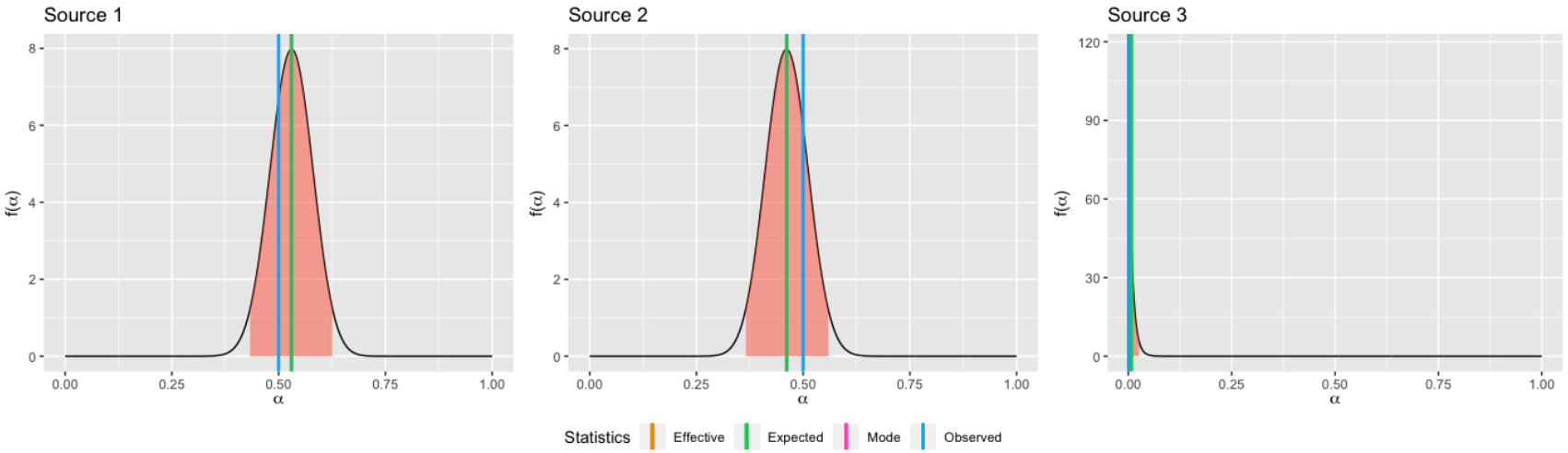


Air not in library

A Case Study

When not all of the sources are in the sample

(What if our sample doesn't contain all of the sources in our library?):



Takeaways:

- Given a library of potential sources, we can identify which sources are present (and in which proportions) in a mixture of soot
  - When all sources are present in the mixture
  - When only some sources are present in the mixture
- Even if a source is missing from that library, we can identify which sources are present (and in which proportions) in a mixture of soot