Searching for Complex Organic Molecules in Space

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NAS
NASA Ames
Moffett Field CA

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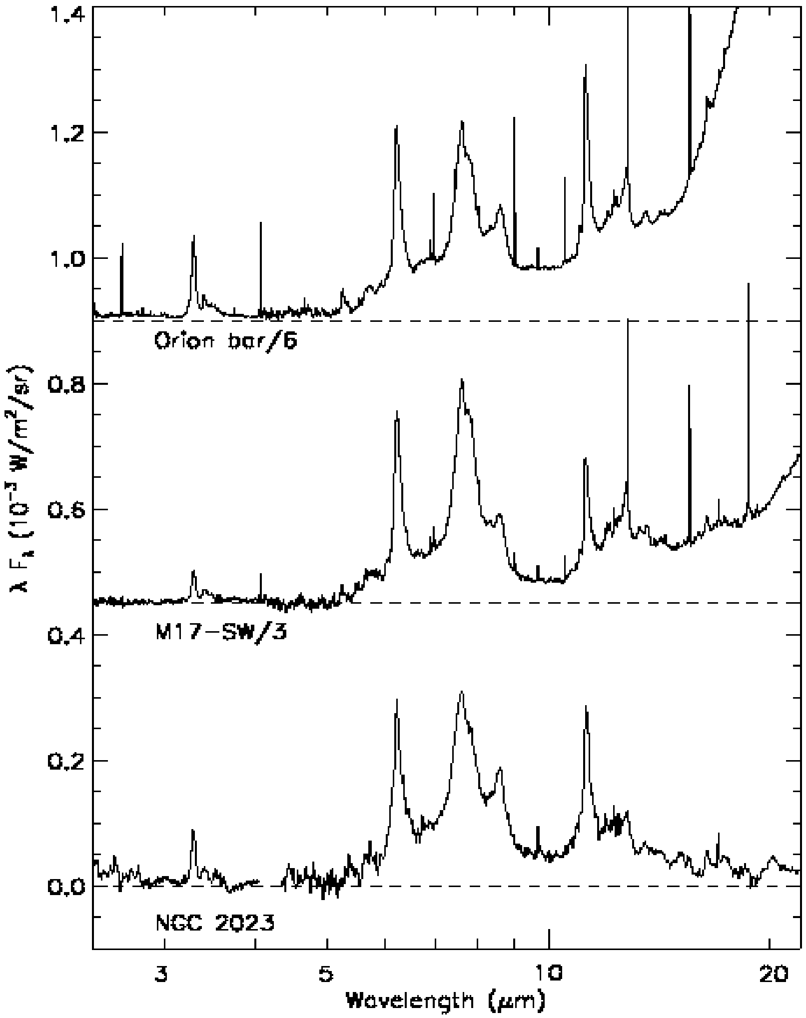
Unidentified InfraRed (UIR) Emission

- UIR emission when there is UV-lit dust
- emission near 3.3, 6.2, 7.7, 8.6 and 11.2 μm.
- dying stars, forming stars/planetary systems, ISM
- other galaxies, z = 2.8



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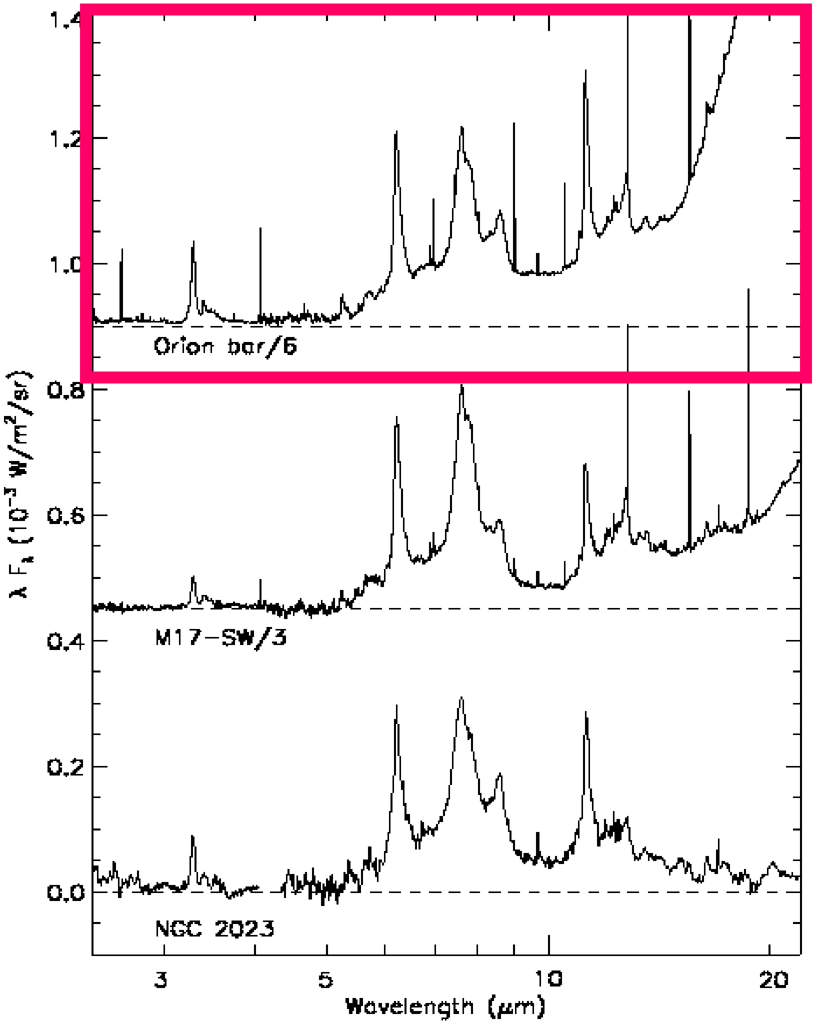
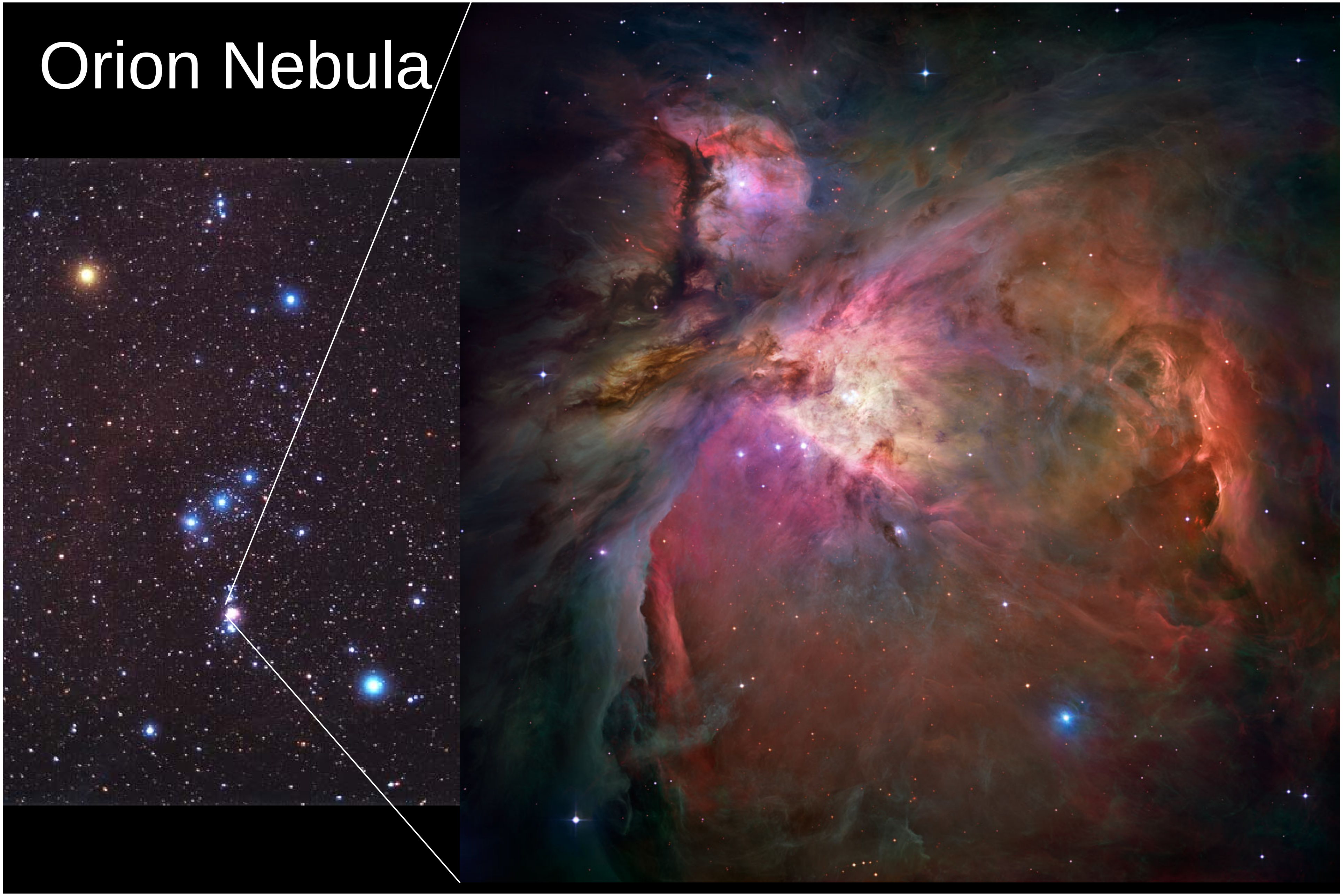
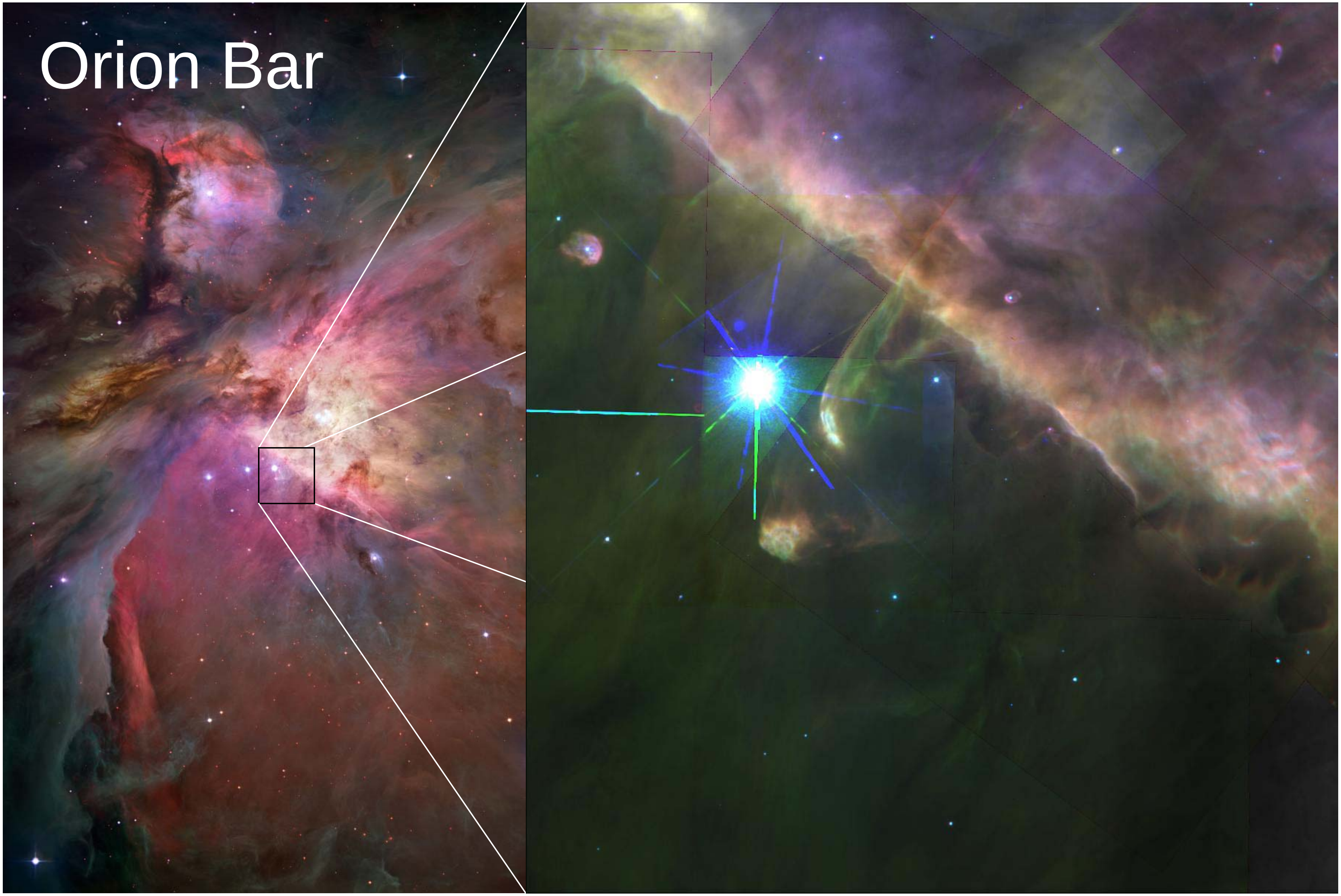


Orion

Photo Credit: Matthew Spinelli

Orion Nebula




Orion Bar

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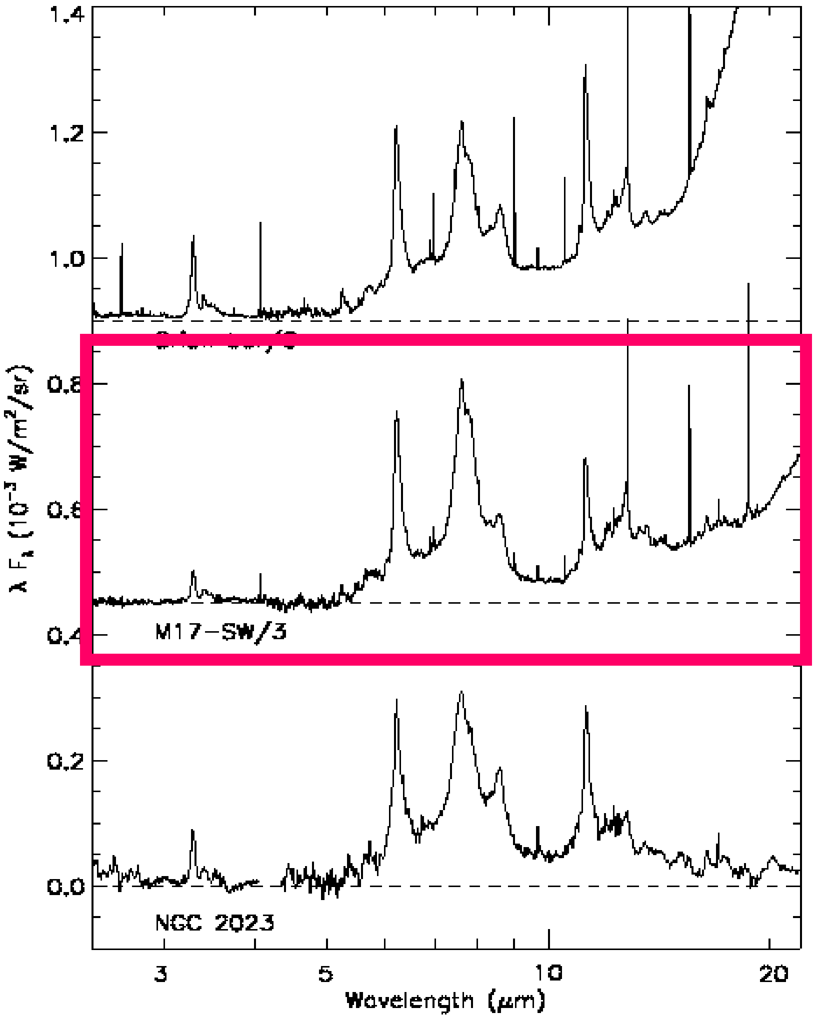
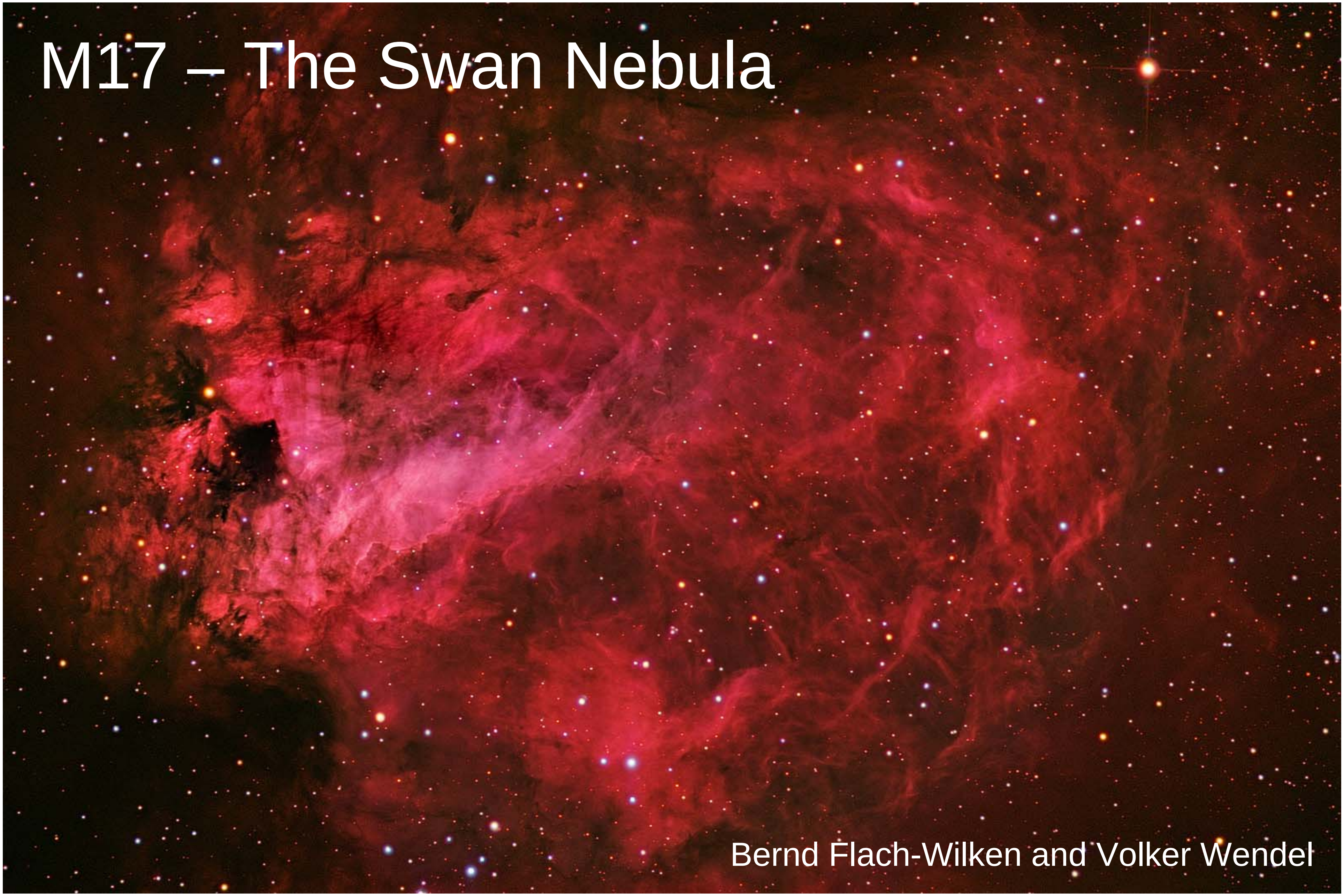


M17 – The Swan Nebula



Bernd Flach-Wilken and Volker Wendel

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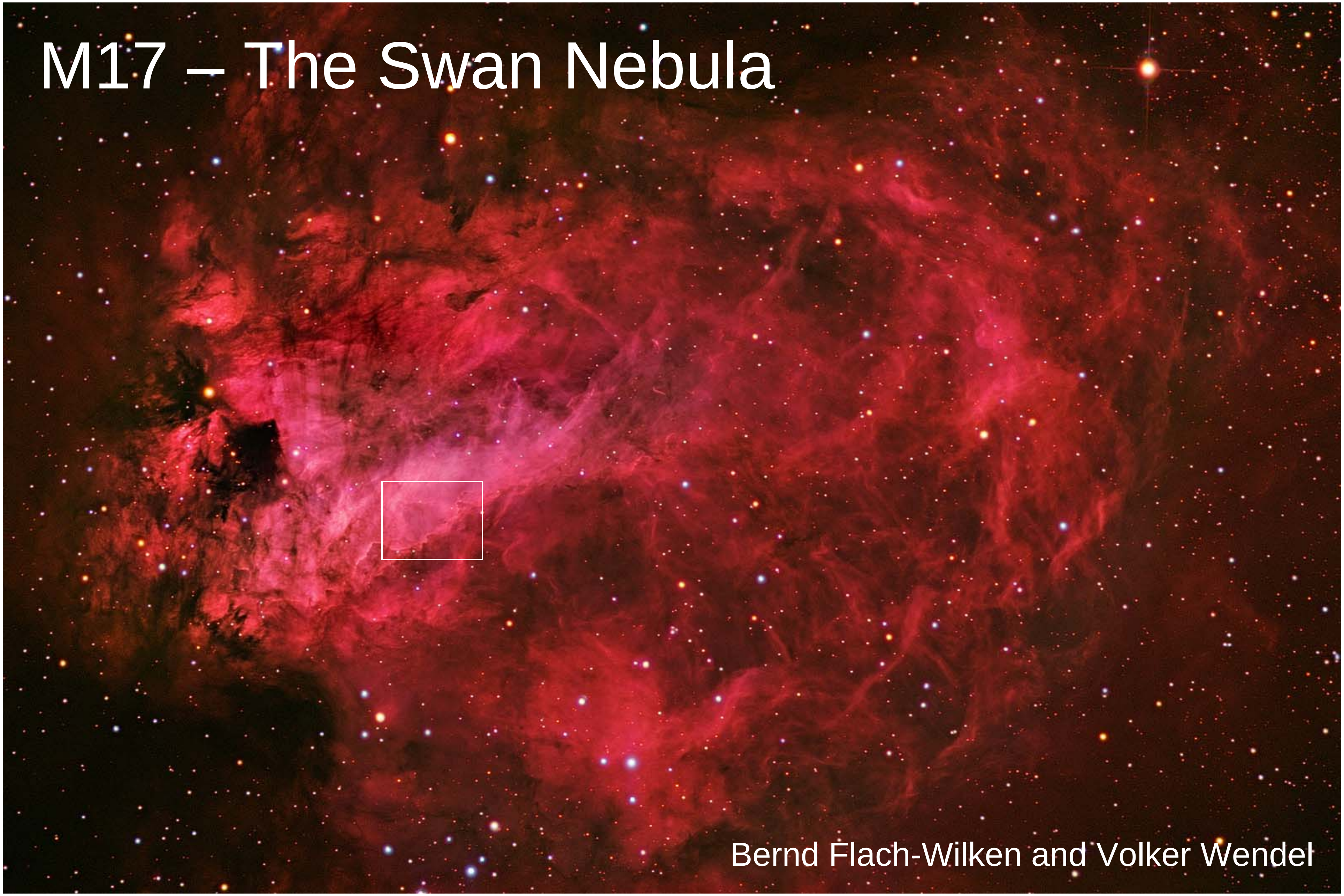

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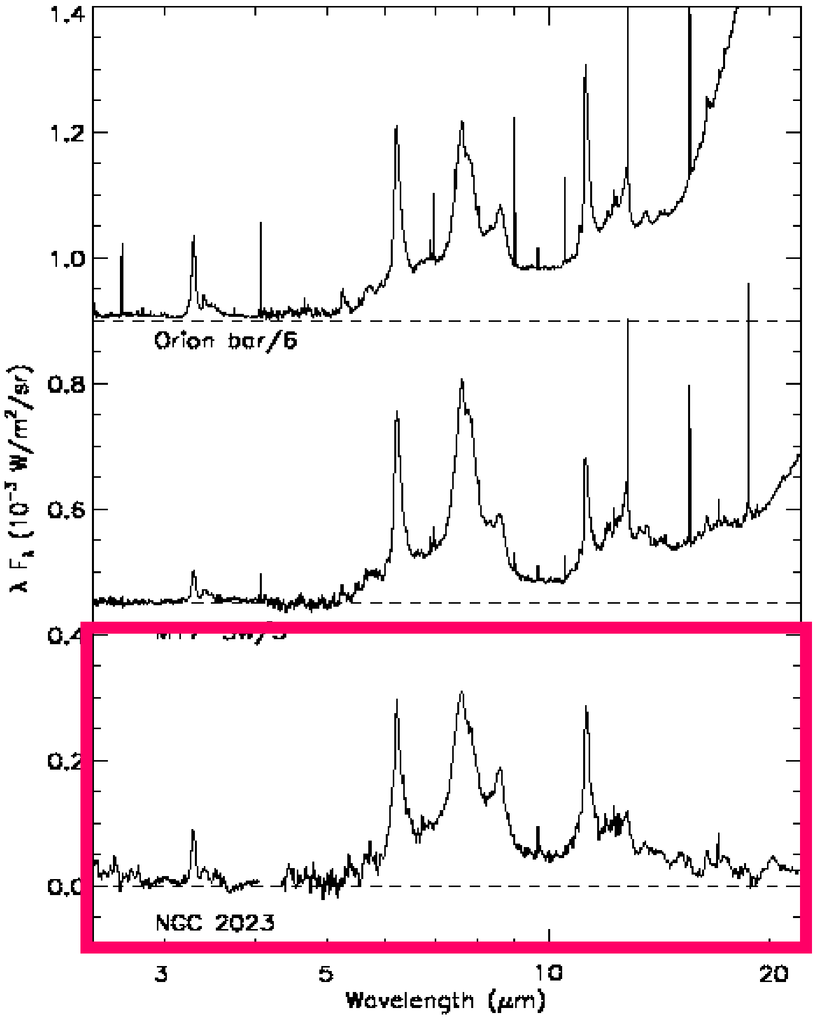
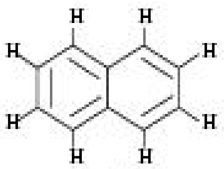


NGC 2023

Russell Croman

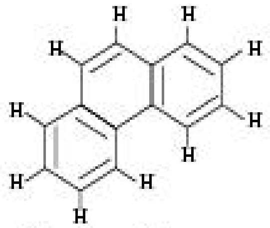
PAHs: Source of the UIR Emission?

Polycyclic Aromatic Hydrocarbons



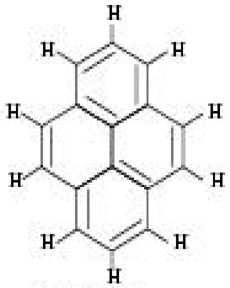
Naphthalene

$C_{10}H_8$



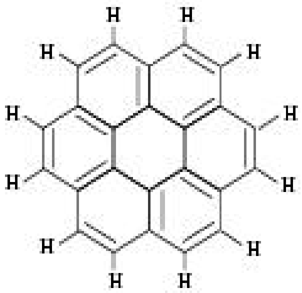
Phenanthrene

$C_{14}H_{10}$



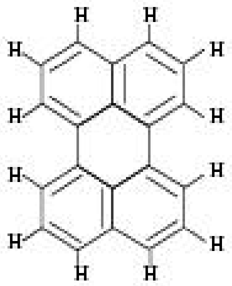
Pyrene

$C_{16}H_{10}$



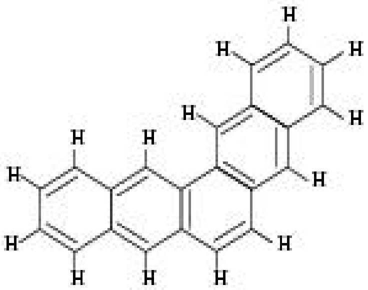
Coronene

$C_{24}H_{12}$



Perylene

$C_{22}H_{14}$



Pentaphene

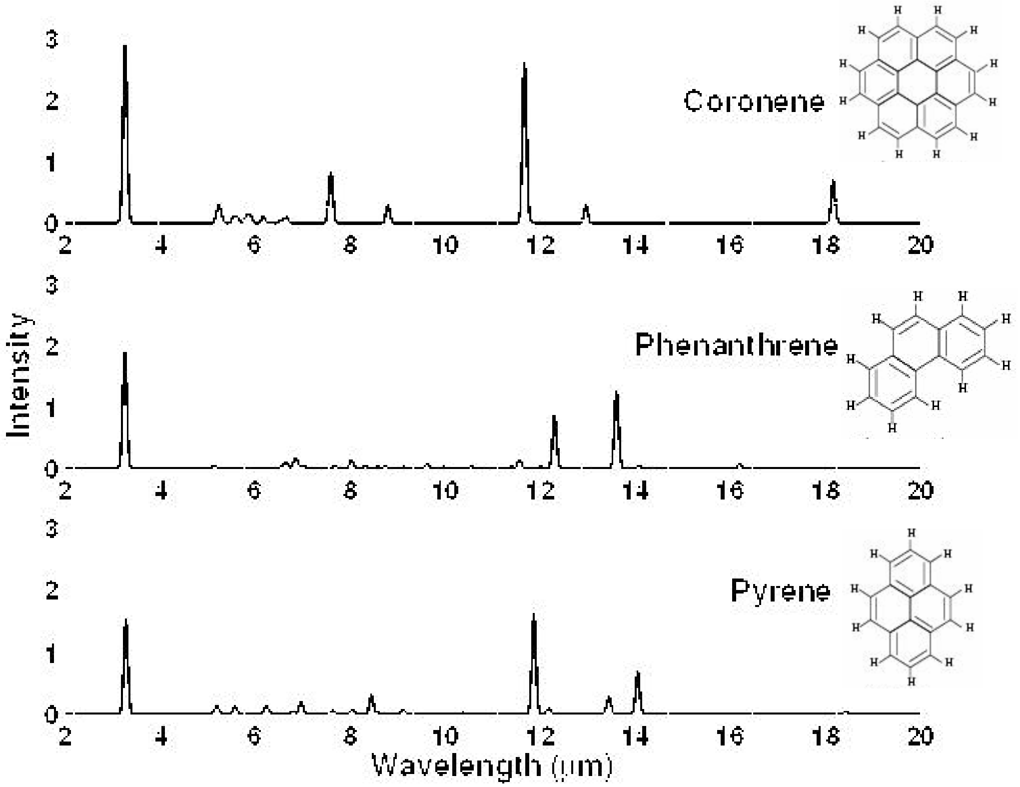
$C_{20}H_{14}$

- Molecular bands near correct wavelengths
- Reasonable physical model for UV-driven IR emission

Every PAH is an Individual

- Spectra for ~1000 PAH species known from lab or theoretical work
  - – neutral, ions, and D, N, Fe, Mg-substituted

- Each PAH has unique spectral features



Why are PAHs so Interesting?

10-20% of all carbon atoms in the Interstellar Medium (ISM) are in PAH molecules

For this reason, PAH emissions are found in almost every cosmic environment in which there are concentrations of dust illuminated by ultraviolet radiation

They could be used to characterize the conditions of the ISM, and could be used as a tracer of star formation in the Milky Way

PAHs now appear to be important molecules on the pathway to life

The PAH Identification Problem

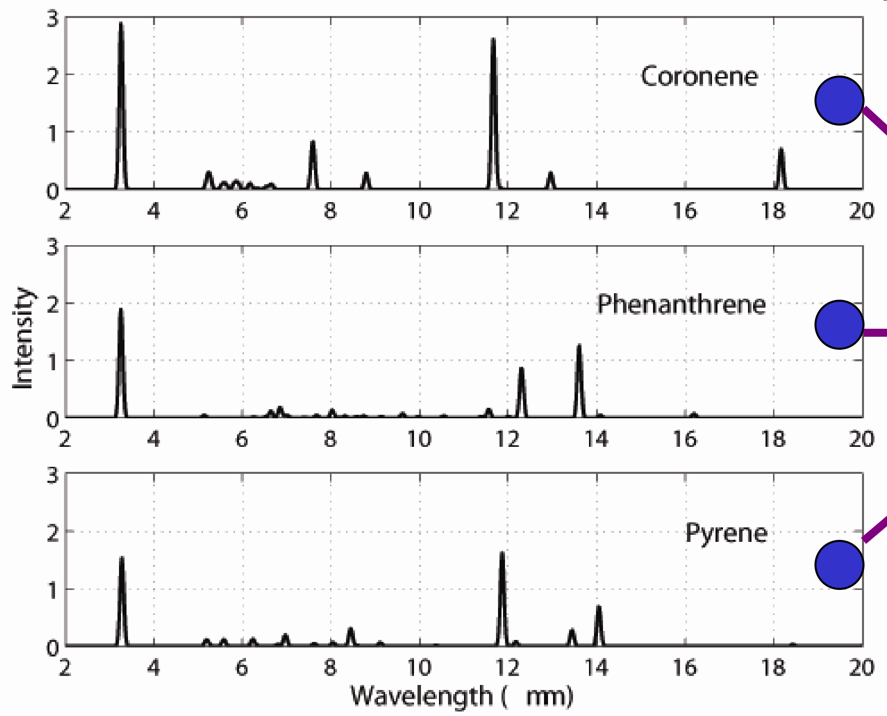
No astrophysical source shows the unique signature of any identifiable known PAH

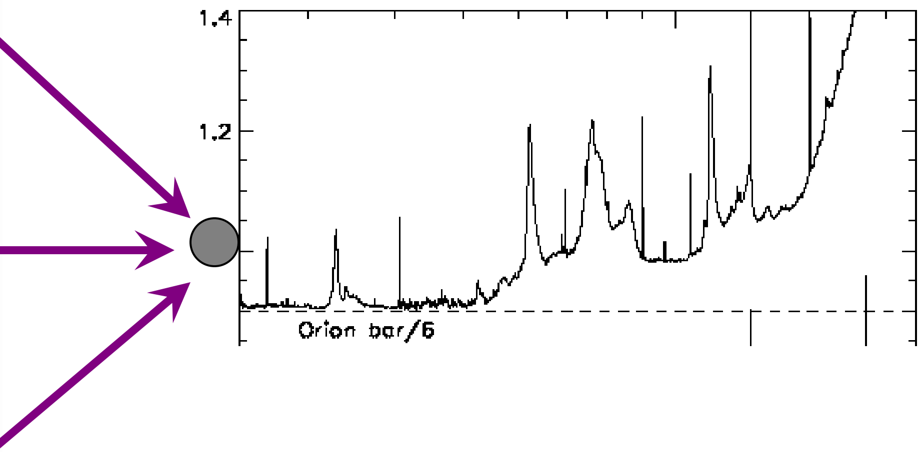
Astrophysical sources appear to have:

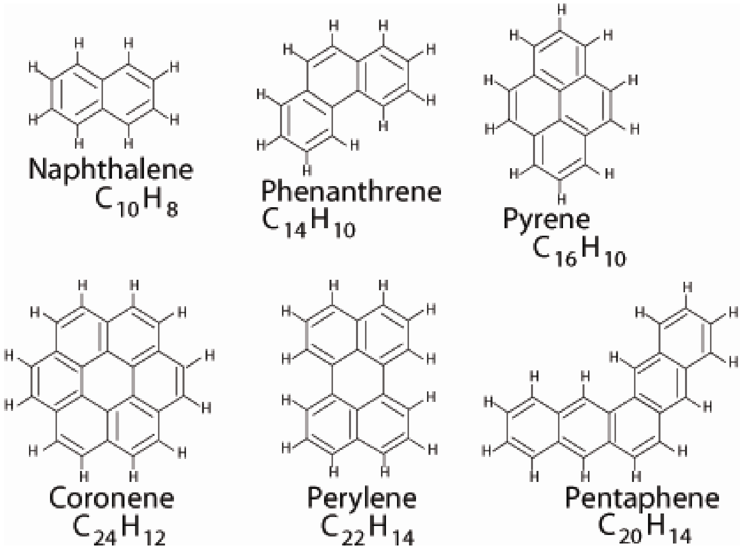
- multiple PAH species present
- different PAH-species concentrations depending on:
  - UV-intensity, temperature, and composition

Source Separation
of Spectra

Numerous PAH Species

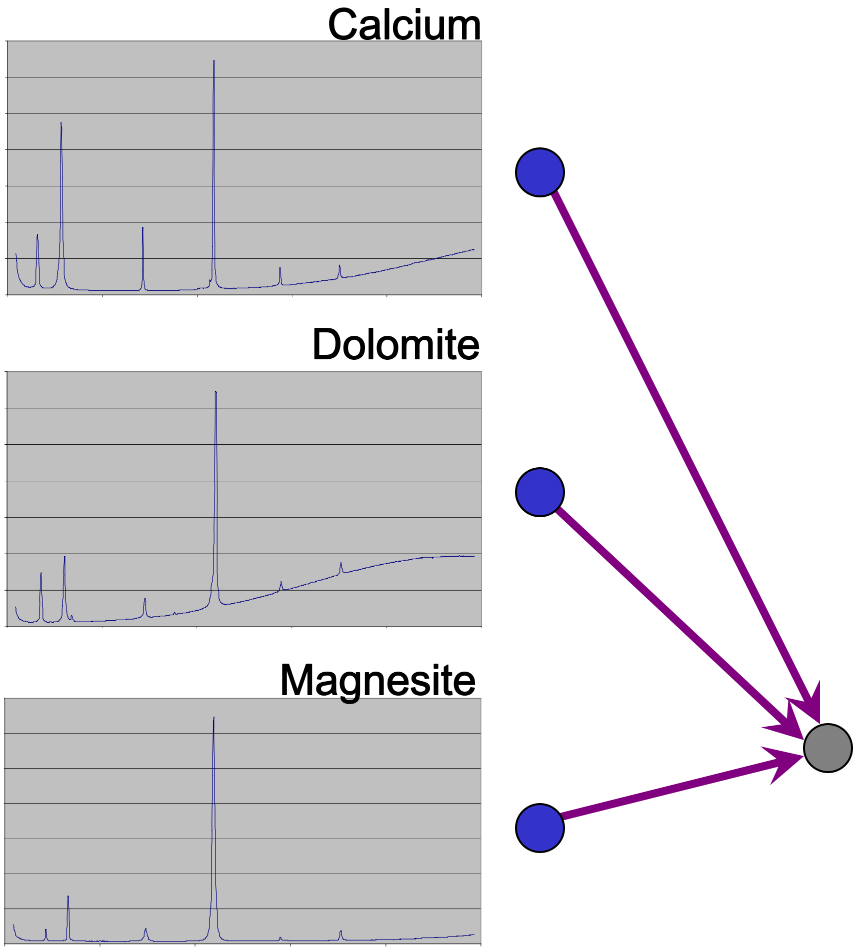


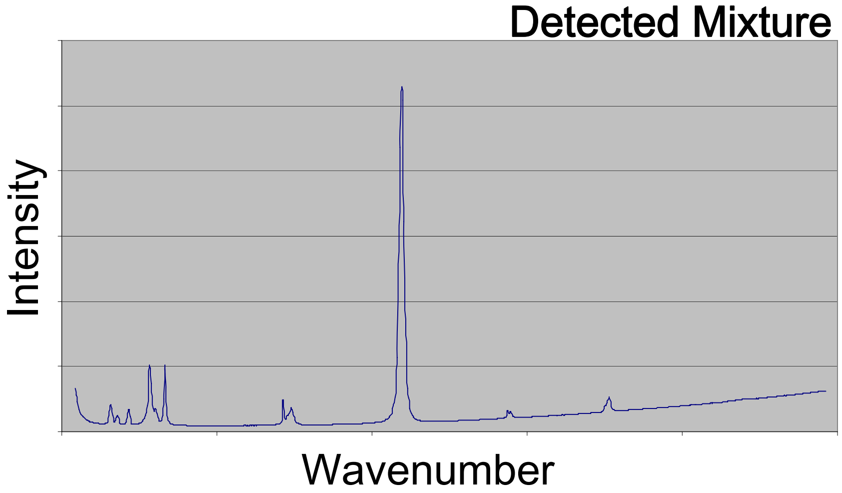




Any number of **thousands** of PAH species can contribute to an observed spectrum.

Numerous Applications





Data from: Mary Garland, University of Toronto
Raman Spectrum Excitation: 514 nm argon ion laser.
http://minerals.gps.caltech.edu/files/raman/toronto/toronto.htm

PAHs Pose Unique Difficulties

Most source separation problems consist of multiple mixtures and a handful of unknown sources with unknown contributions.

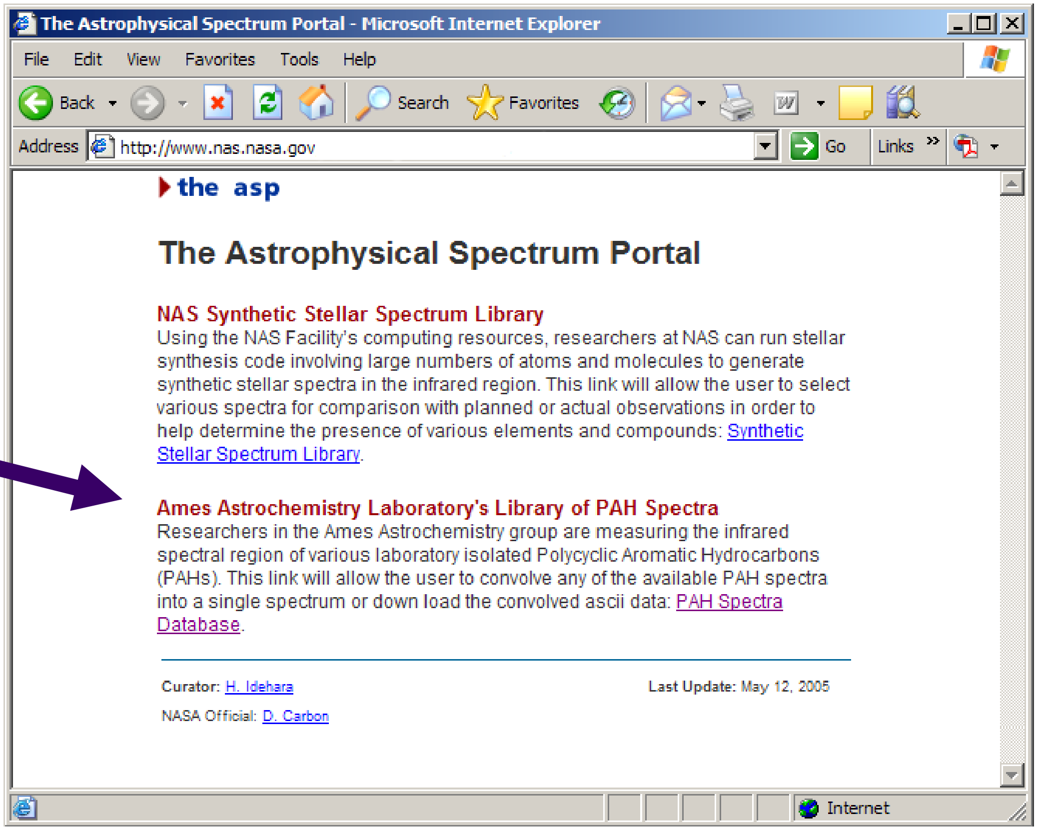
PAH spectral source separation consists of one mixture and numerous known sources with unknown contributions (and even some unknown sources).

There are potentially 100s to 1000s of species present.

- How do we tell which ones?
- How do we deal with the large number of spectra?

Astrophysical Spectrum Portal

The PAH spectra database at NASA Ames Research Center will contain ~1000 PAH spectra



The Astrophysical Spectrum Portal

NAS Synthetic Stellar Spectrum Library

Using the NAS Facility's computing resources, researchers at NAS can run stellar synthesis code involving large numbers of atoms and molecules to generate synthetic stellar spectra in the infrared region. This link will allow the user to select various spectra for comparison with planned or actual observations in order to help determine the presence of various elements and compounds: Synthetic Stellar Spectrum Library.

Ames Astrochemistry Laboratory's Library of PAH Spectra

Researchers in the Ames Astrochemistry group are measuring the infrared spectral region of various laboratory isolated Polycyclic Aromatic Hydrocarbons (PAHs). This link will allow the user to convolve any of the available PAH spectra into a single spectrum or down load the convolved ascii data: PAH Spectra Database.

Curator: H. Idehara

Last Update: May 12, 2005

NASA Official: D. Carbon

Three Approaches

1) Hand-fitting by eye

- widely applied

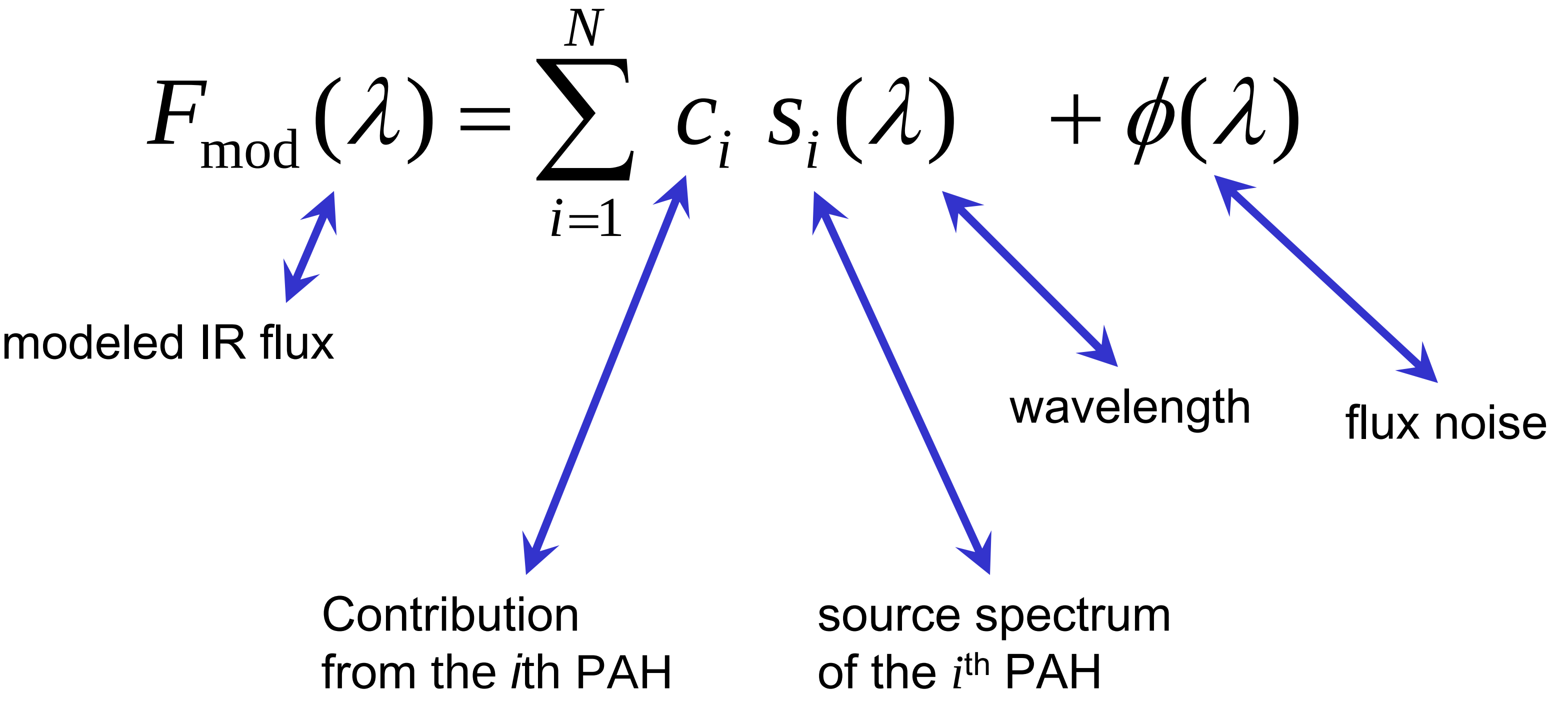
2) Non-Negative Least Squares

- two applications to PAHs (N < 12)

3) Bayesian Source Separation with Sampling

- work in progress

A Straightforward PAH Model



$$F_{\mathrm{mod}}(\lambda) = \sum_{i=1}^{N} c_i \; s_i(\lambda) \quad + \phi(\lambda)$$

modeled IR flux

wavelength

flux noise

Contribution
from the *i*th PAH

source spectrum
of the i^{th} PAH

ignores line-of-sight variations and
various thermal and radiative effects

Non-Negative Least Squares

Minimize: χ^2

Subject to: $c_i > 0$

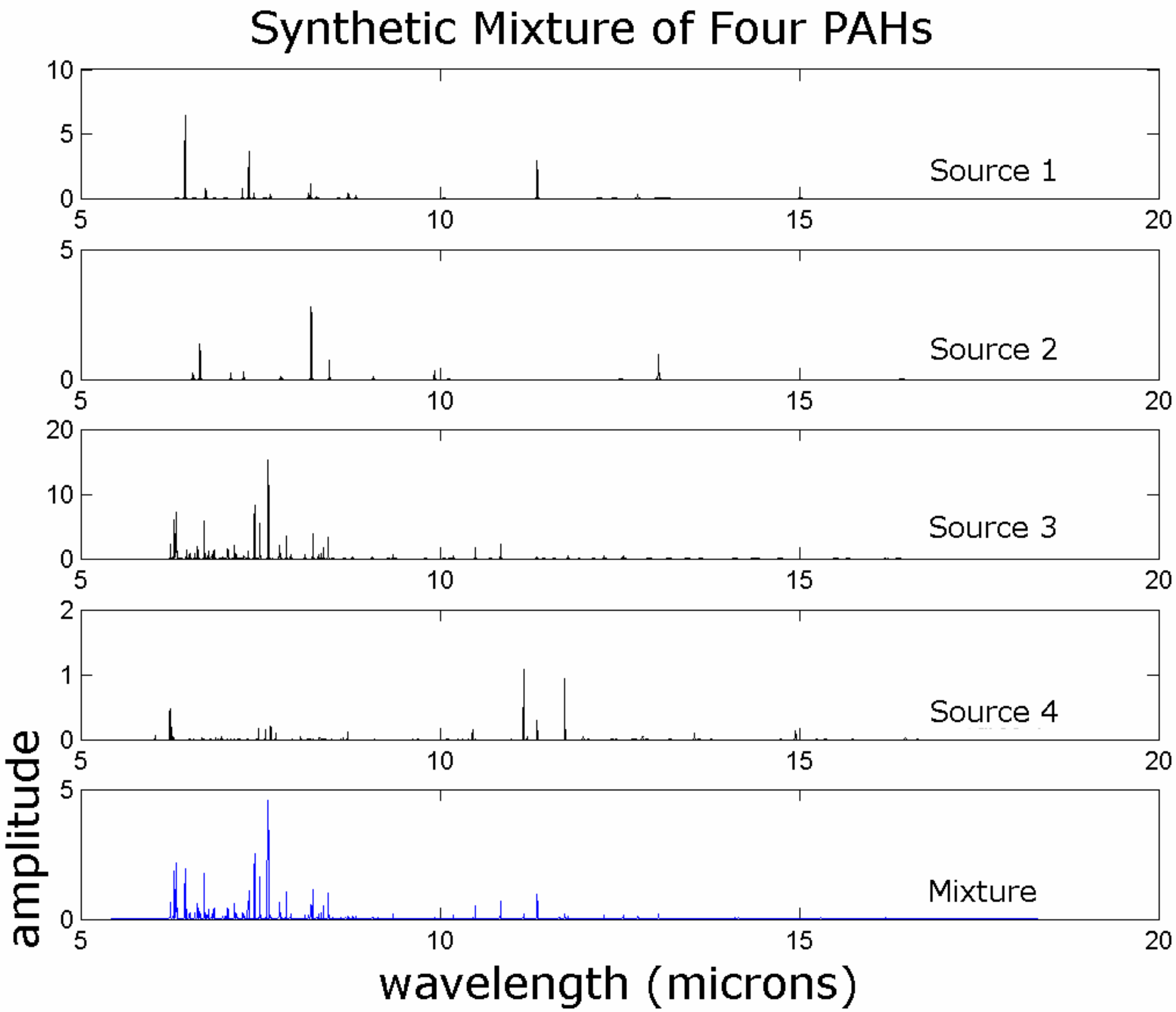
$$\chi^2 = \sum_{l=1}^{L} \left(F_{\text{obs}}(\lambda_l) - F_{\text{mod}}(\lambda_l)\right)^2$$

$$\chi^2 = \sum_{l=1}^{L} \left(F_{\text{obs}}(\lambda_l) - \sum_i c_i s_i(\lambda_l) \right)^2$$

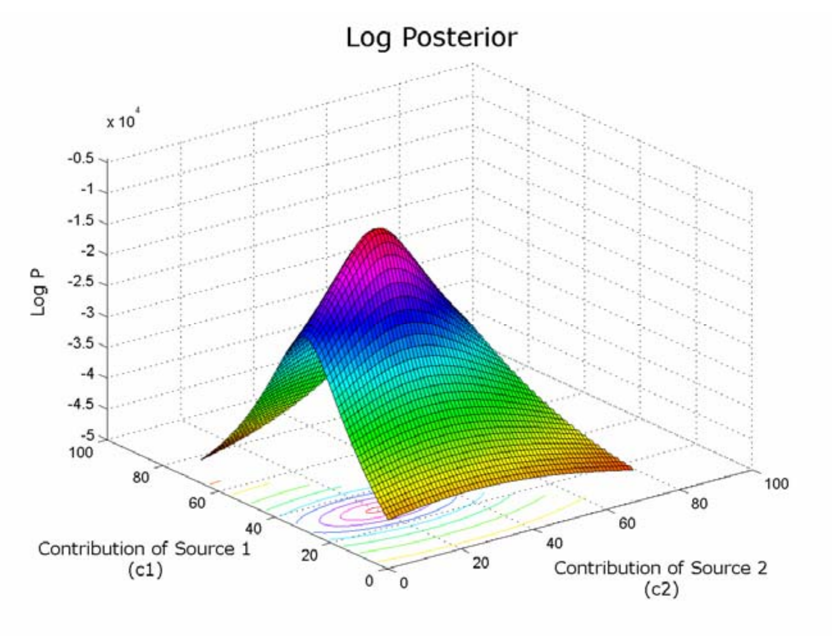
Estimate PAH contributions

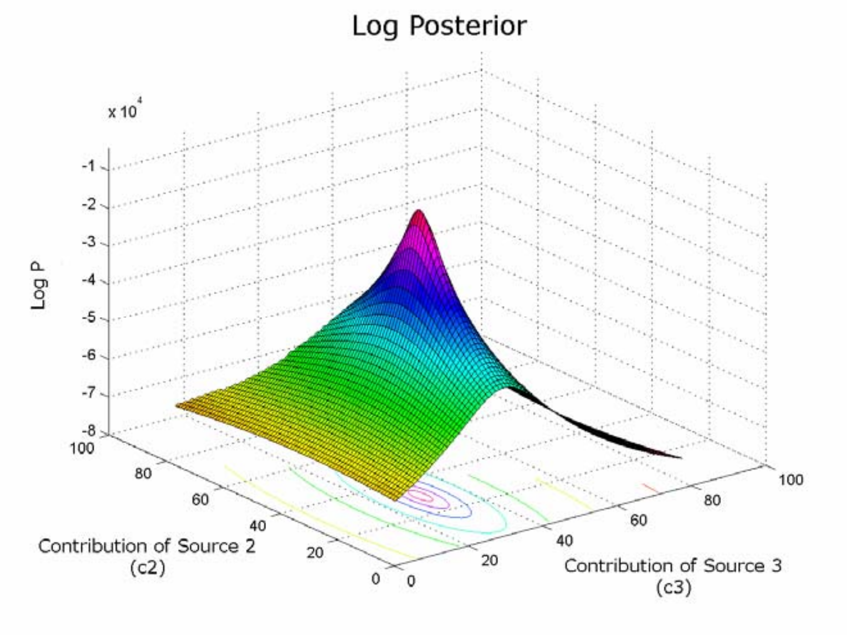
Works alright, but with only small numbers of PAHs and with little spectral overlap.

Mixing Four PAHs



Slices Through the Space

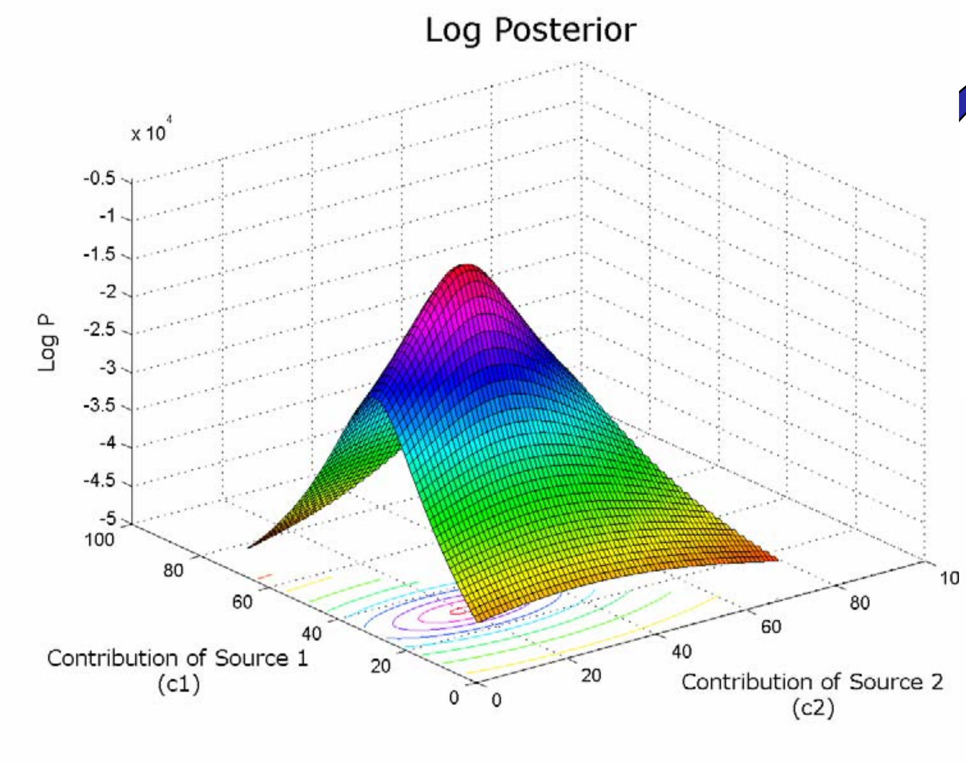


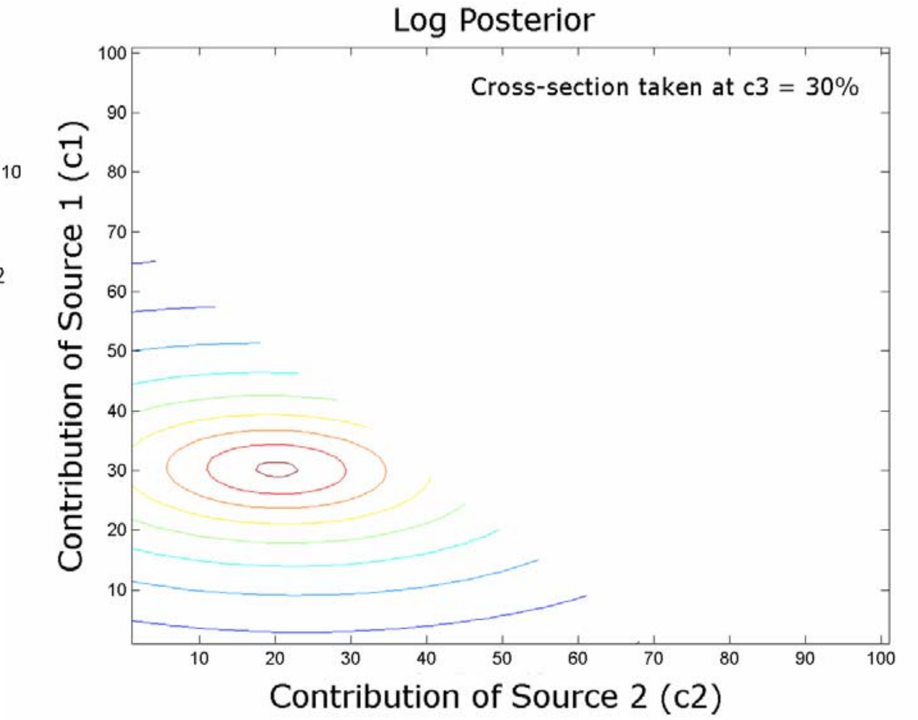


These are cross-sections of a three-dimensional probability space with c1, c2, c3 being the three variables. c4 is constrained by
c4 = 1-(c1+c2+c3)

Note the variations in the ellipsoidal contour eccentricities

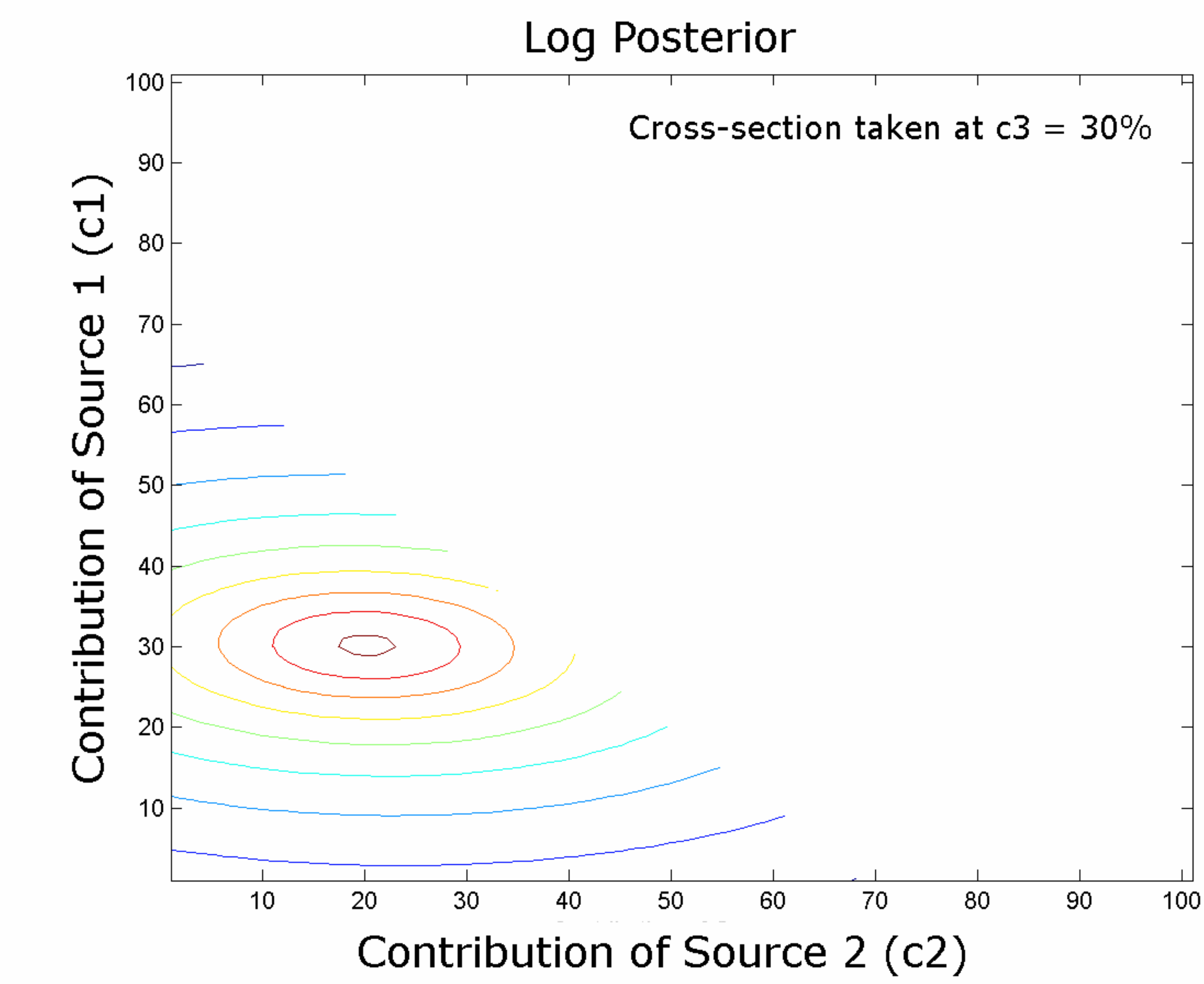
Cross-Section for c1 and c2





This cross-section showing the probabilities for c1 and c2 was taken at the correct value for c3 = 0.3

Why is c1 More Accurate?



The ratio of the semi-minor to semi-major axes is related to the relative accuracy to which we can estimate the contributions.

In this case:

w1/w2 = 0.4722

The best predictor seems to be the inverse of the ratio of the number of lines in the spectrum

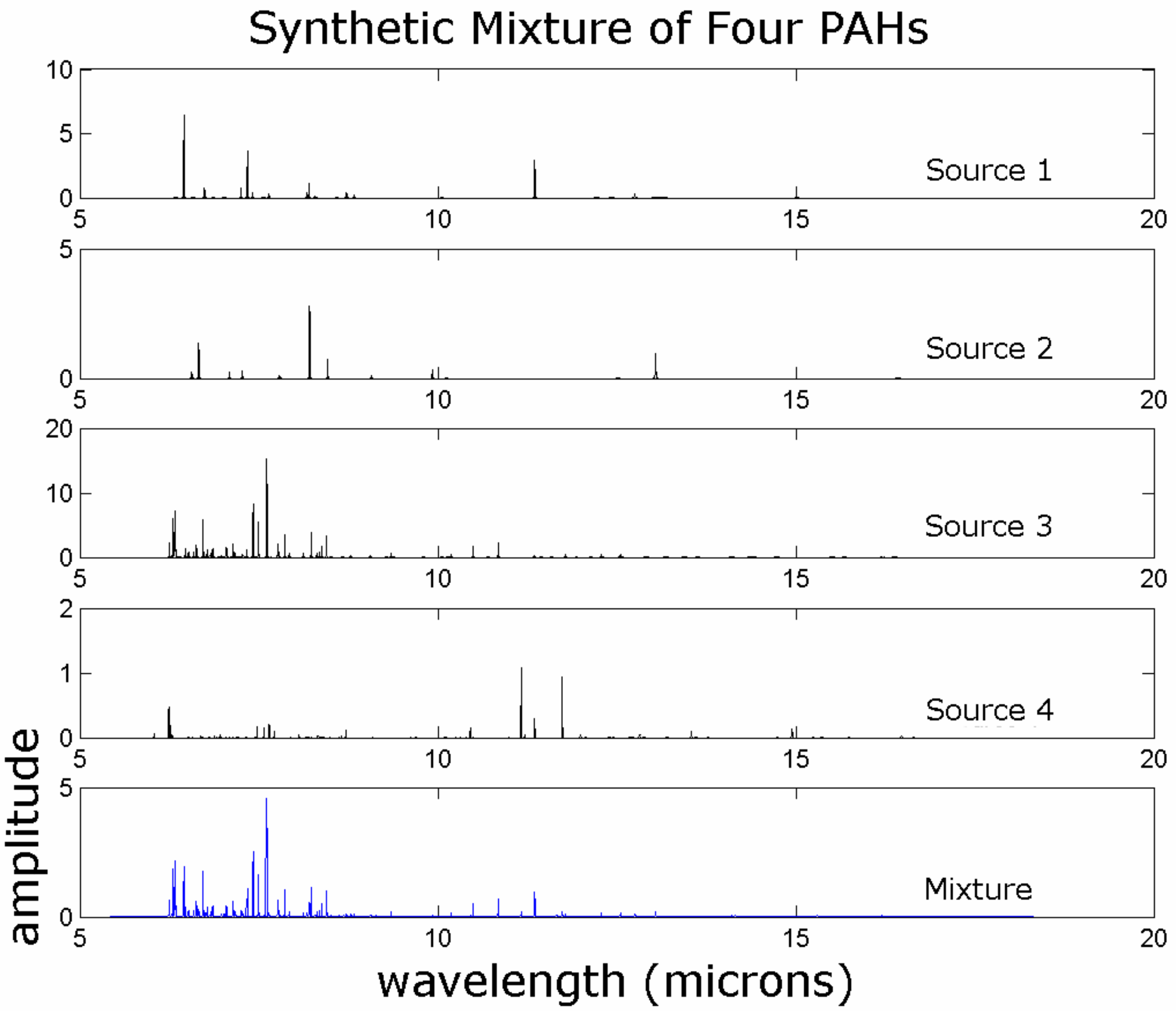
L2/L1 = 13/28
= 0.4643

Comparing Spectral Lines

PAH 1 has about twice as many spectral lines than PAH 2.

It is thus two times more quantifiable.

We should expect the PAH 3 estimate of c3 to be very accurate.

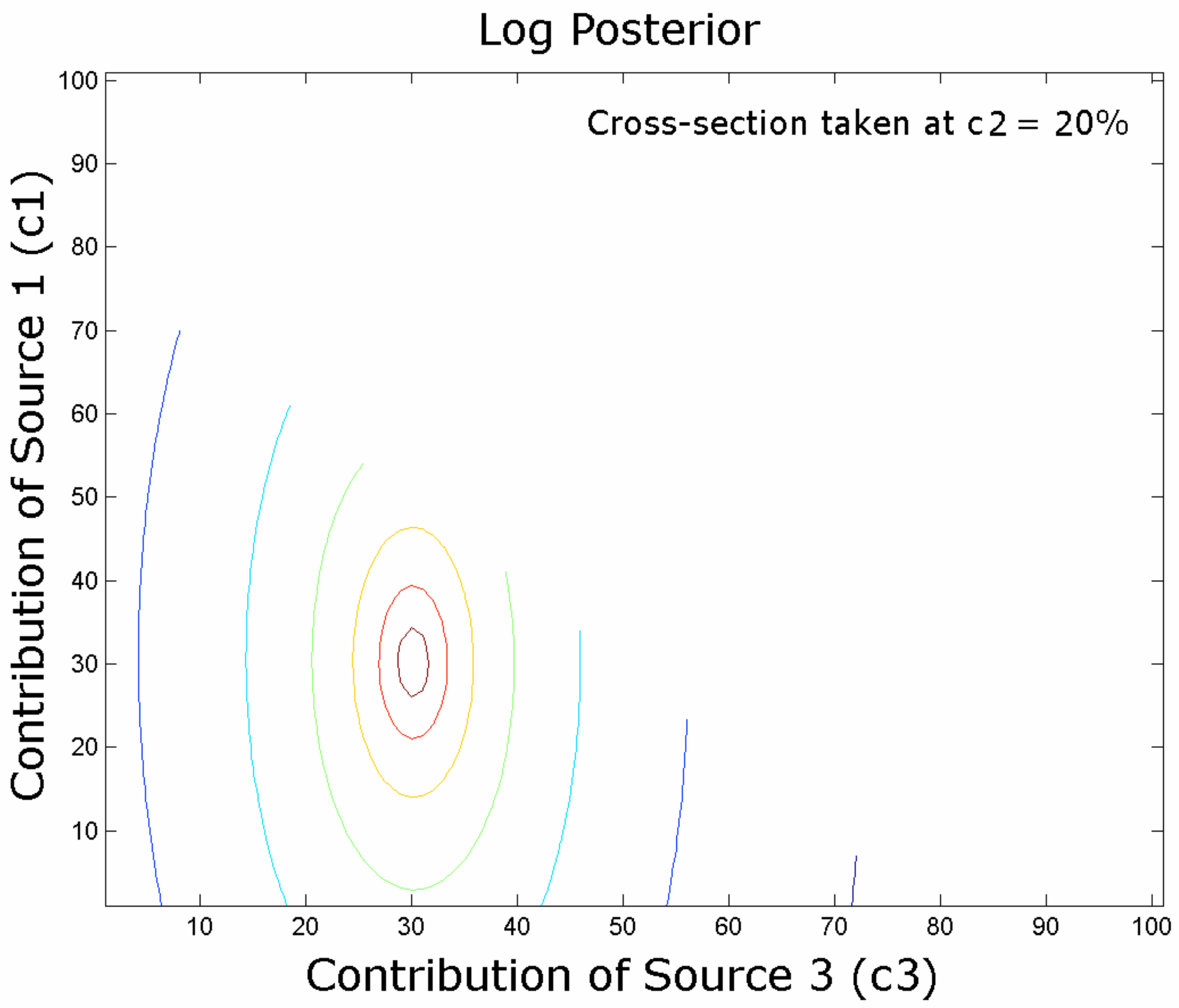


28

13

82

Cross-Section for c1 and c3



Here

w3/w1 = 0.3538

The best predictor seems to be the inverse of the ratio of the number of lines in the spectrum

L1/L3 = 28/82
= 0.3415

Early Findings and Expectations

Non-negative least squares always assigns a positive value for the PAH contribution in even mild noise conditions.

Non-contributing PAHs steal spectral energy from contributing PAHs.

The accuracy to which we are able to detect PAH contributions is roughly related to the number of unique spectral lines.

This is expected to break down as many PAHs superimpose.

Nested Sampling

Nested Sampling with ON/OFF

ON/OFF

$$F(\lambda) = \sum_{i=1}^{N} \delta_i \, c_i \, s_i(\lambda) + bkgnd(\lambda) + \phi(\lambda)$$

contribution

Implementing a Nested Sampling algorithm utilizing ON/OFF switches.

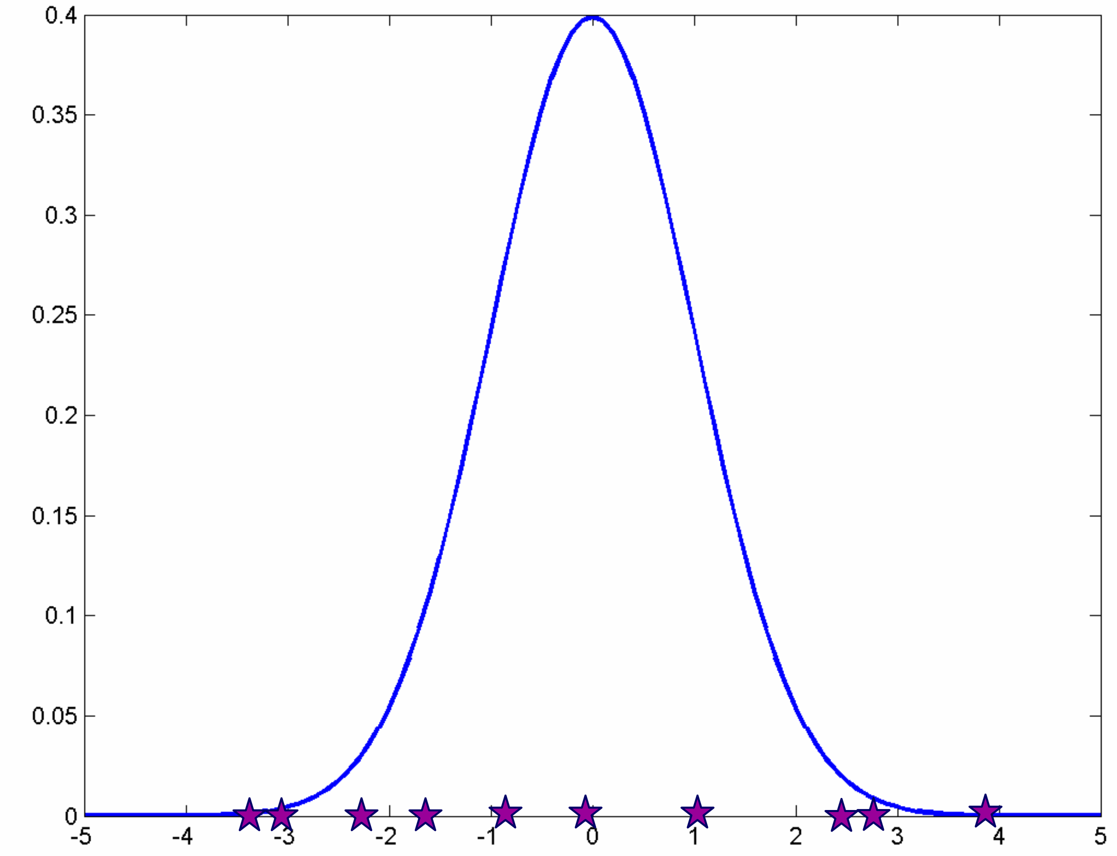
Estimate contribution independently from the probability the PAH is present or not present

Compute the evidence that the data provides about the PAH contributions

At worst we expect to be able to rule out classes of PAHs or identify classes (eg. mass, ionization, etc)

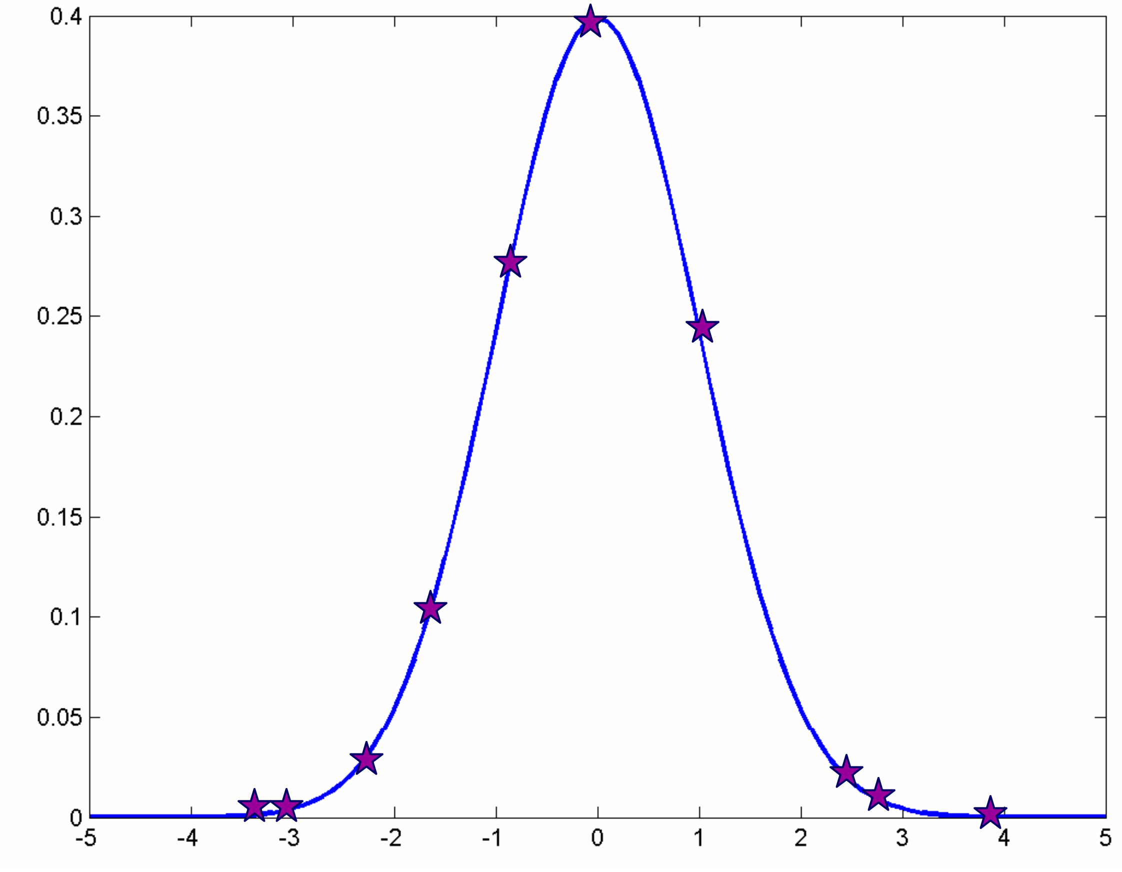
How Stochastic Integration Works

Uniformly draw samples from the interval



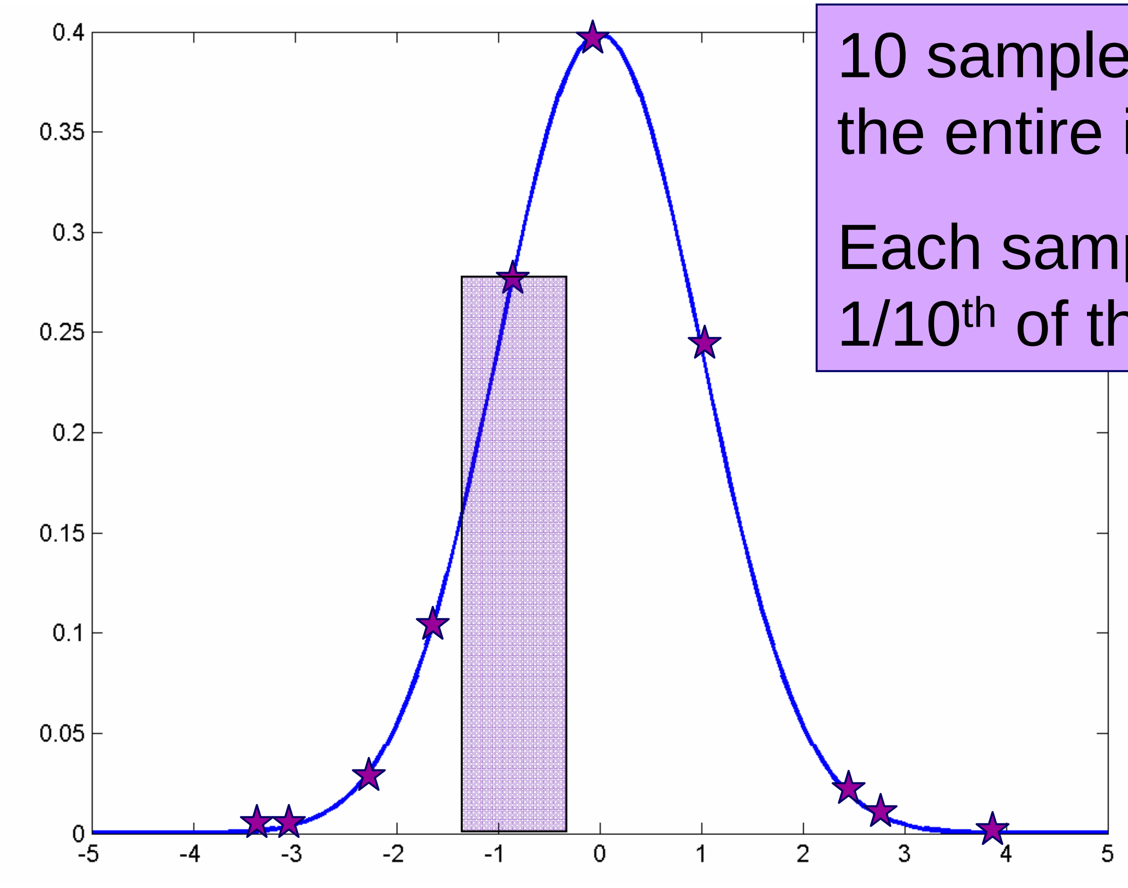
Stochastic Integration

Uniformly drawn samples are used to approximate an integral



Stochastic Integration

Each sample represents an area

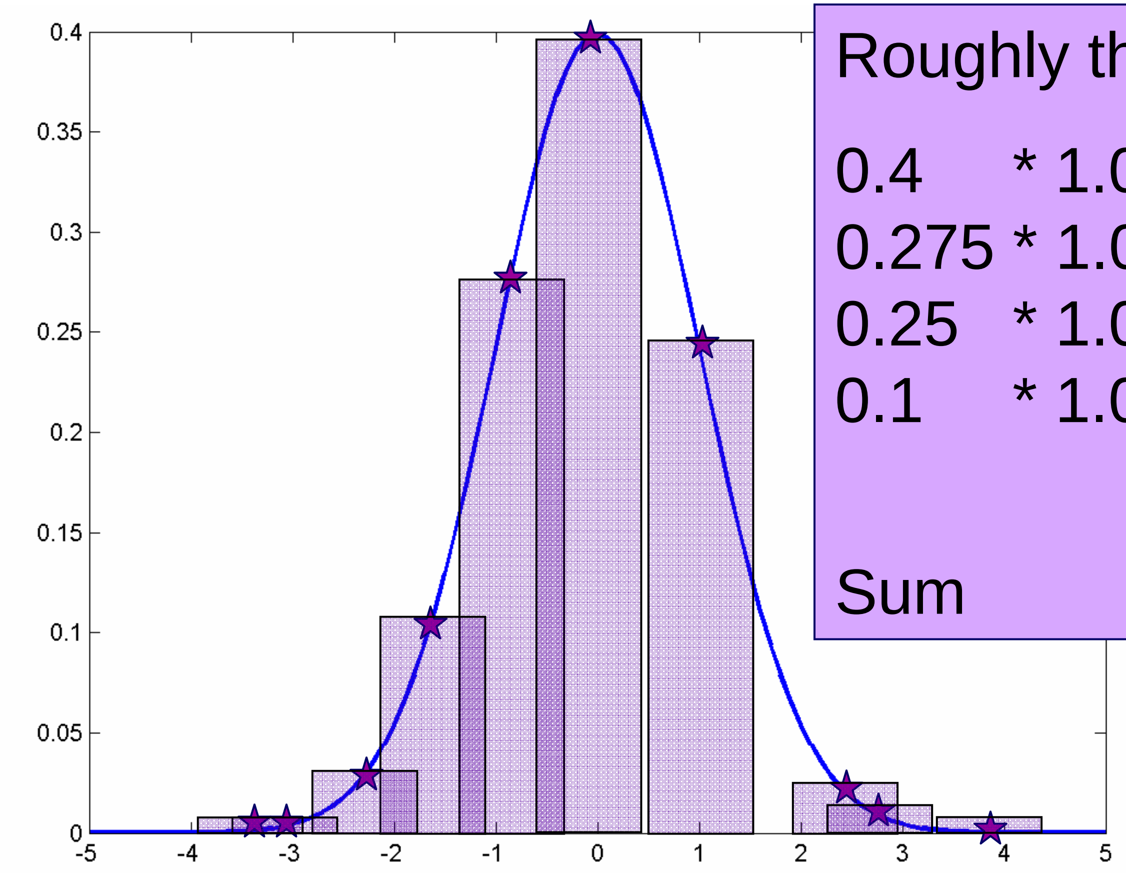


10 samples cover the entire interval

Each sample covers 1/10th of the interval

Stochastic Integration

Add up the areas



Roughly this is:

0.4 * 1.0 = 0.4
0.275 * 1.0 = 0.275
0.25 * 1.0 = 0.25
0.1 * 1.0 = 0.1

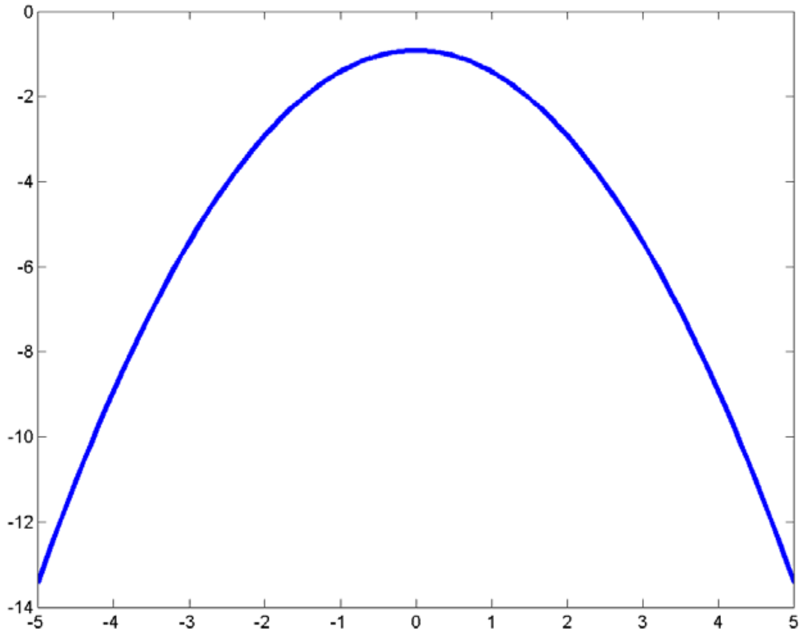
Sum ~ 1.1

Skillings Nested Sampling

John Skilling's **Nested Sampling** is a variation on this theme.

The idea is:

0. work with the log posterior
1. start with N samples
2. find the least probable sample
3. use it to define logPstar
4. duplicate one other sample
5. constrained exploration
6. N uniform samples
   over smaller interval
7. goto 2



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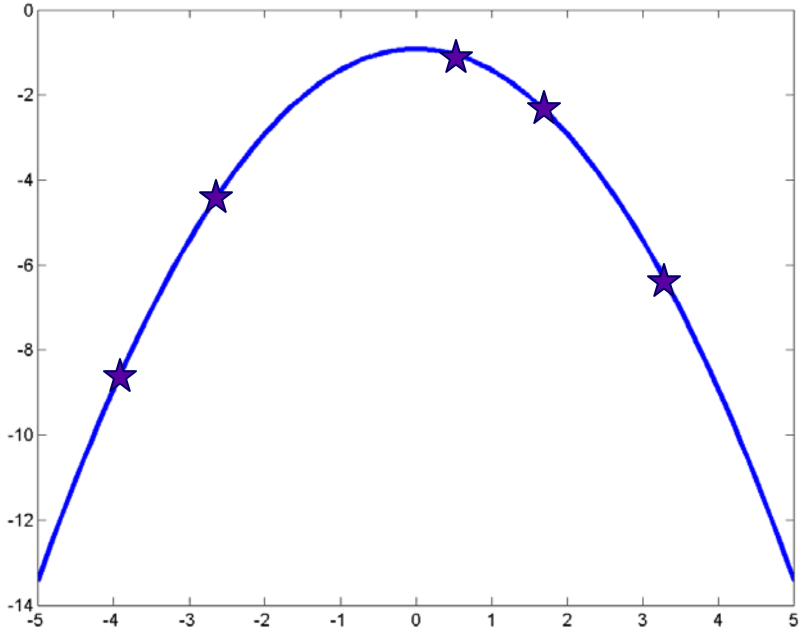

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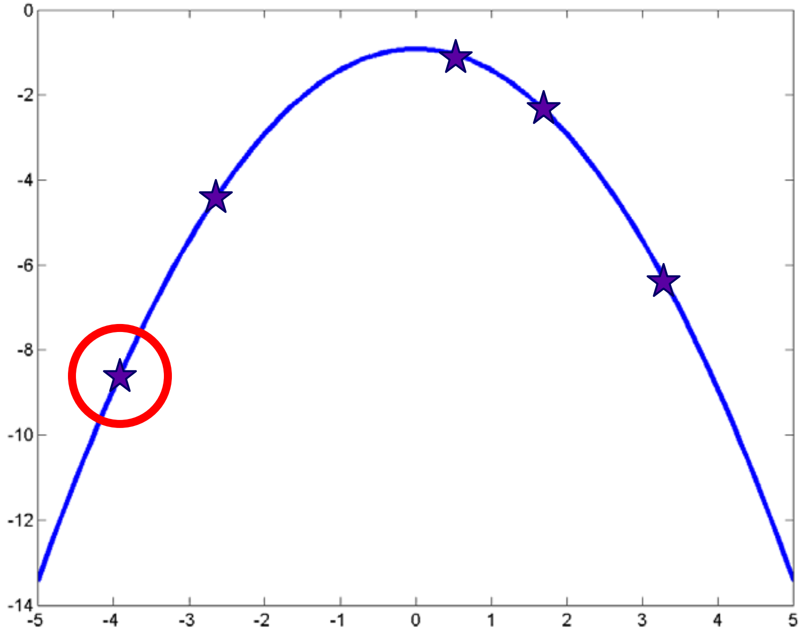

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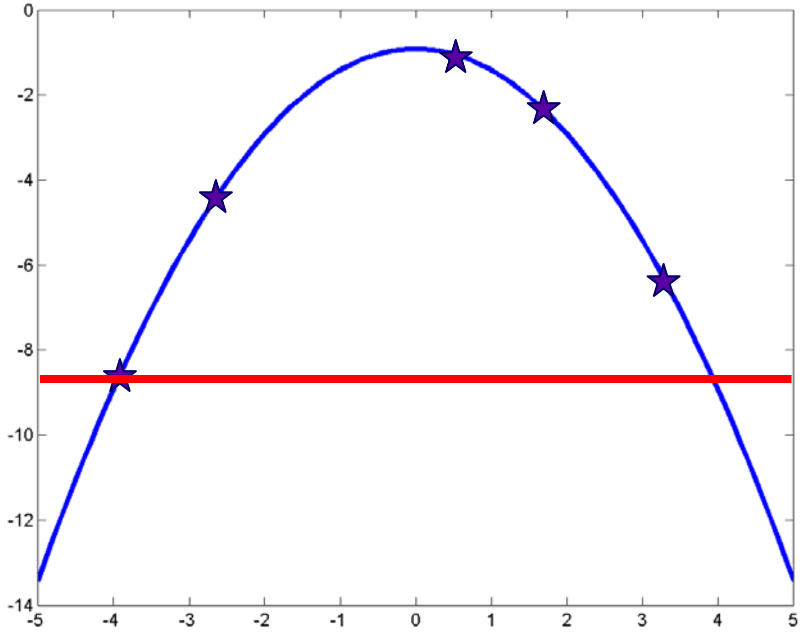

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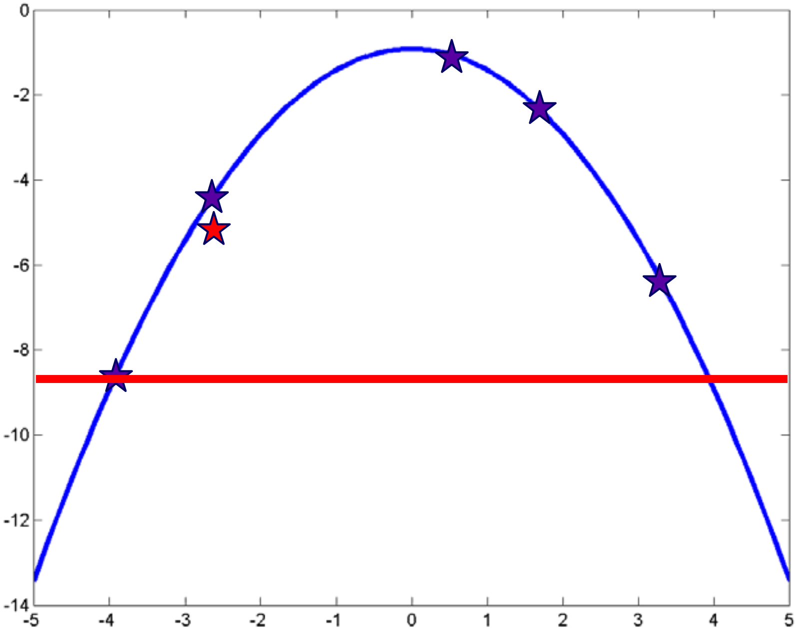

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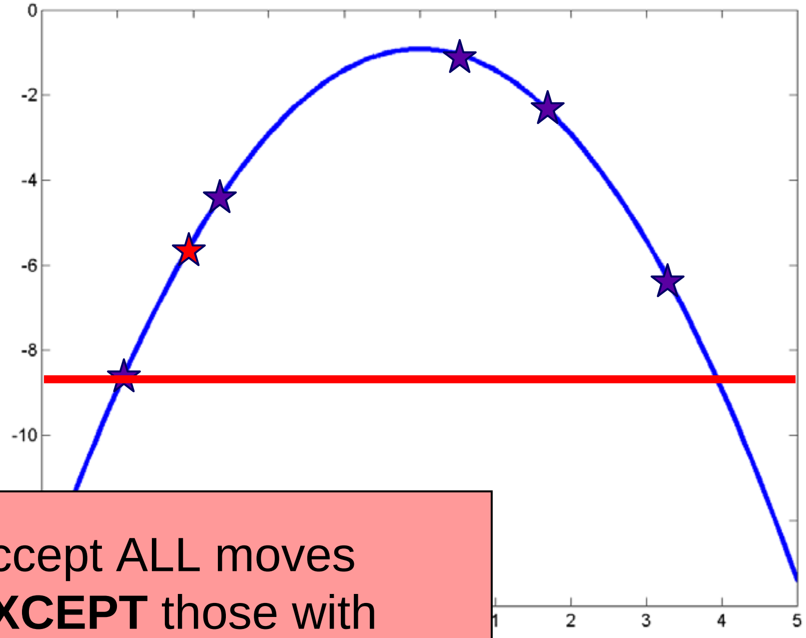

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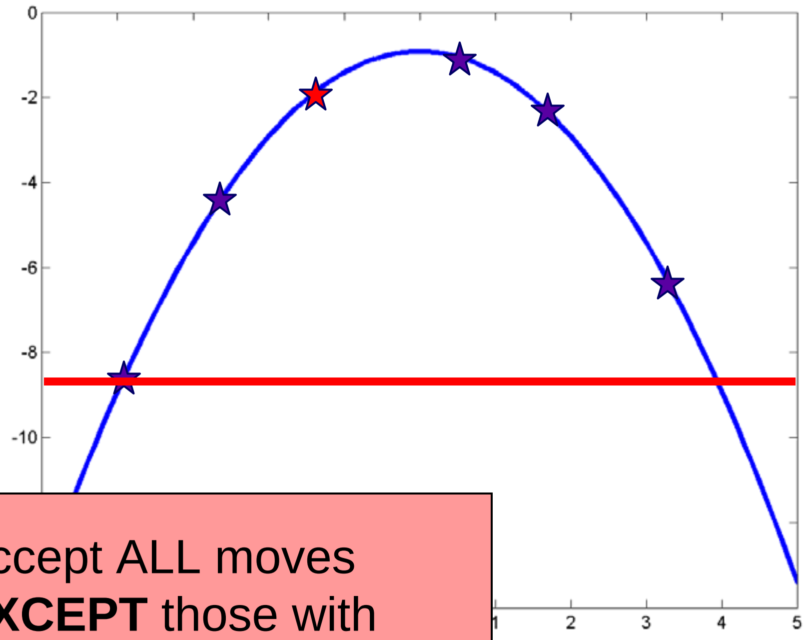

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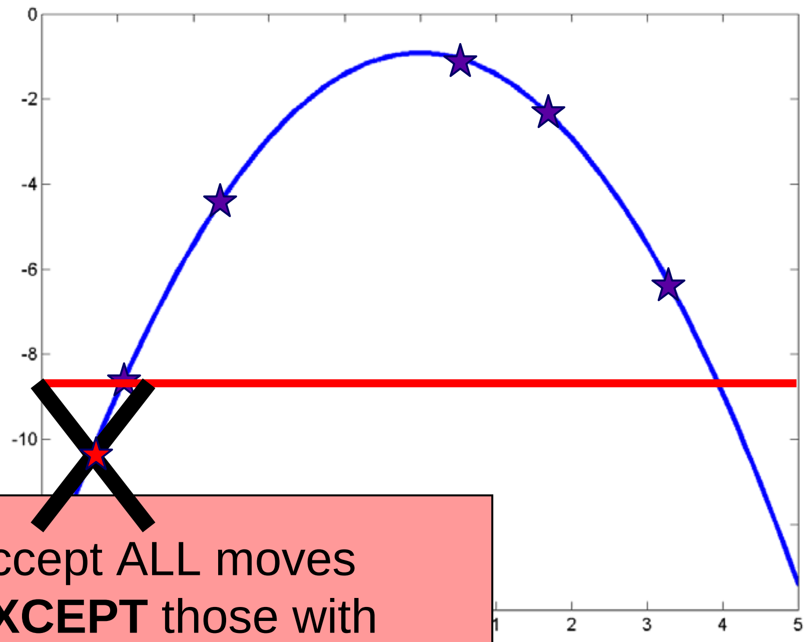

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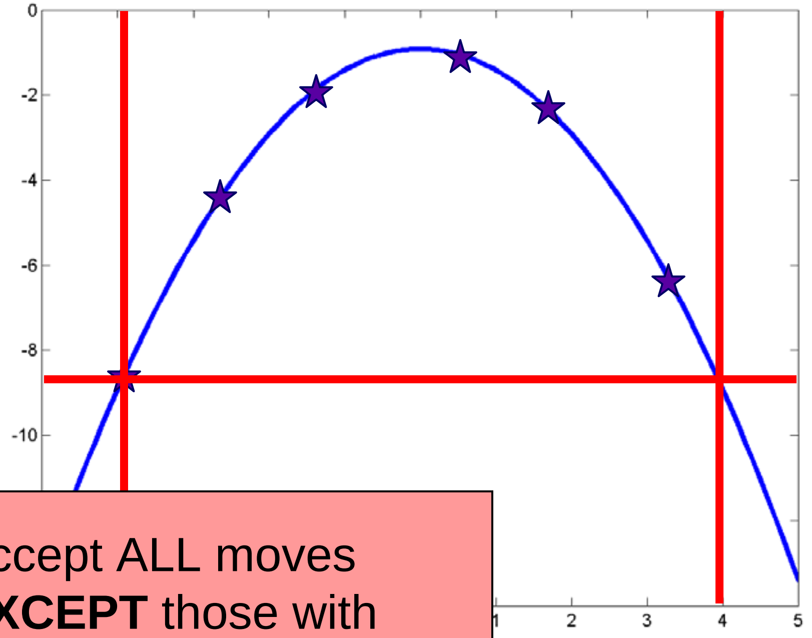

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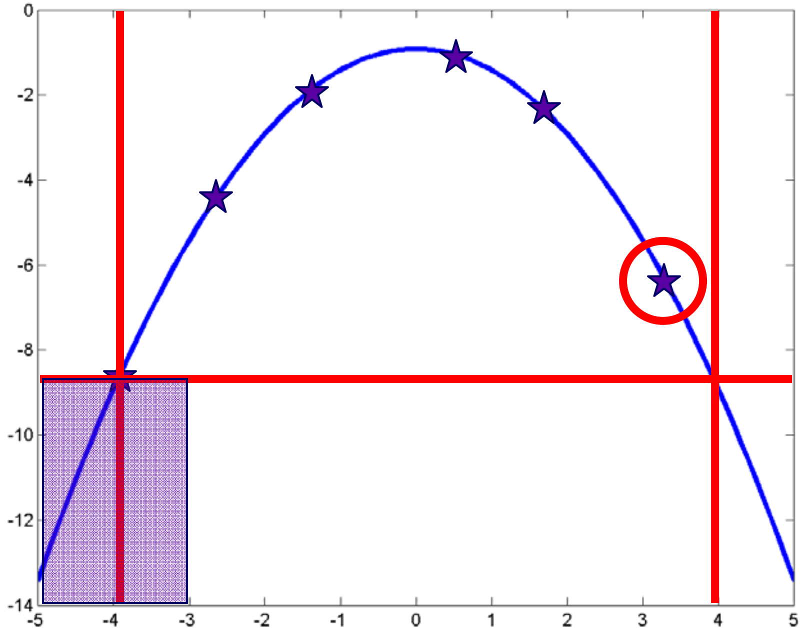

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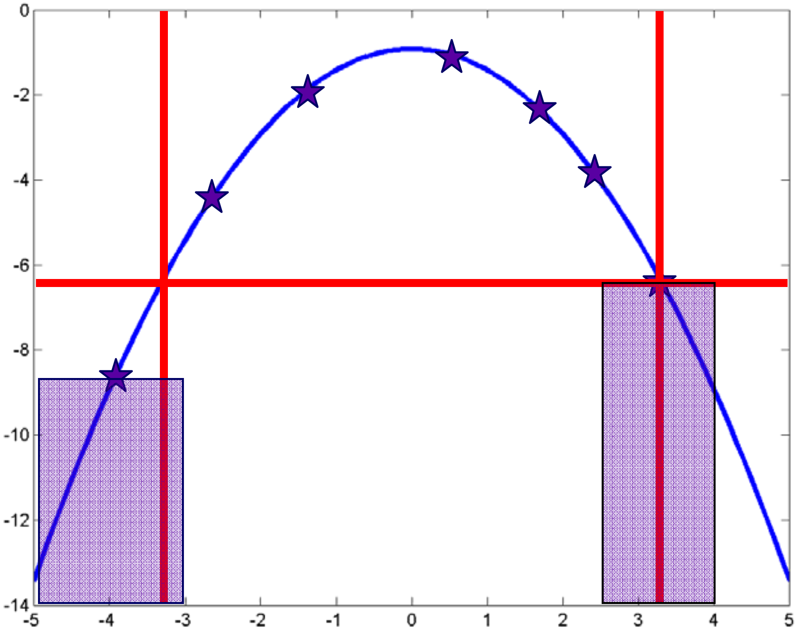
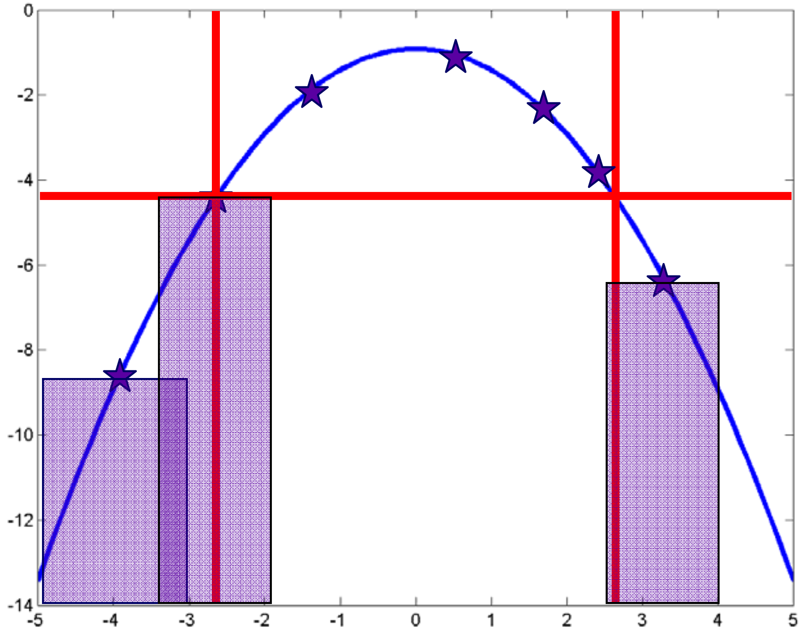
6. N uniform samples
   over smaller interval
7. goto 2



Skillings Nested Sampling

Notice that the interval shrinks as we iterate and contracts to high probability regions.

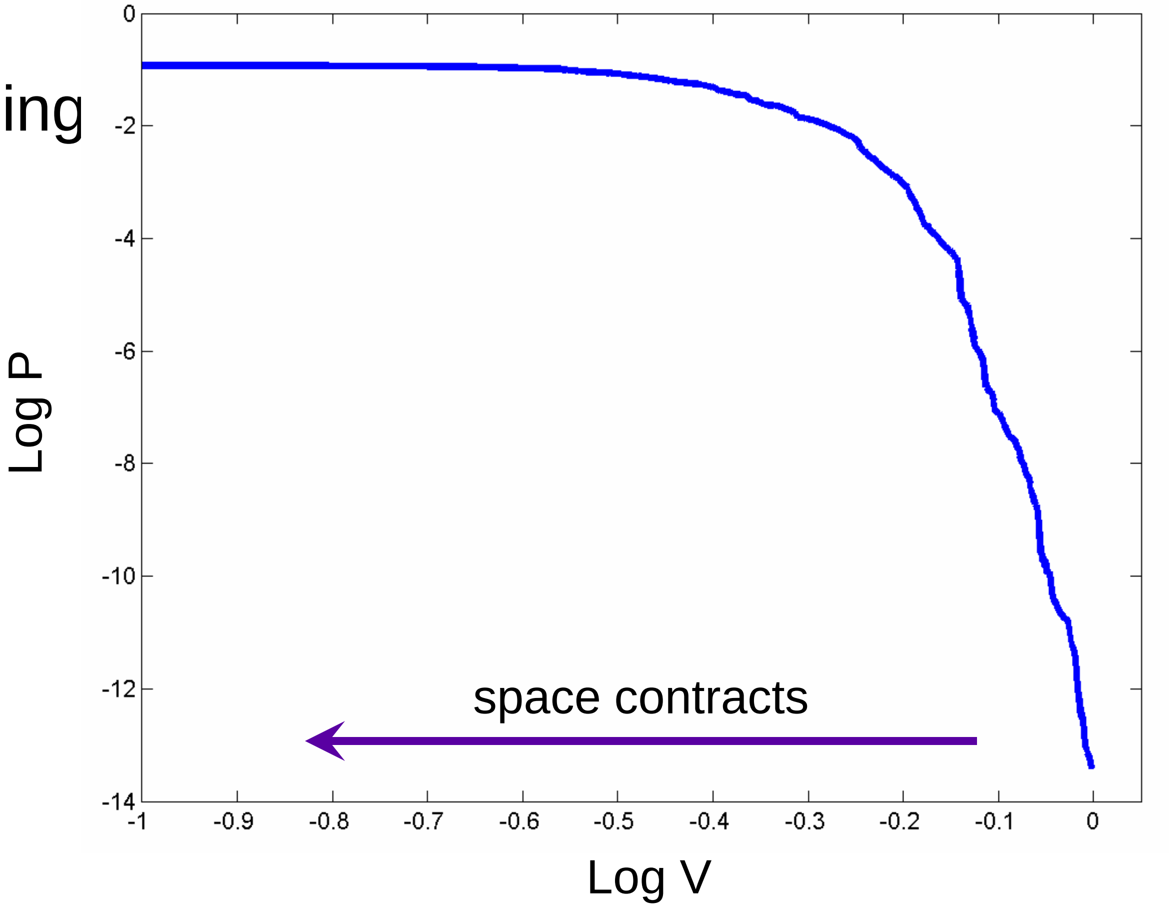
Also, the area associated with each sample decreases as we refine our integral in regions that matter.



Typical Behavior

In a well-behaved problem the log probability increases monotonically with a monotonically decreasing rate.

Since we are ordering according to the probability, this turns all problems into ONE-DIMENSIONAL problems!!!



Movie of
Acoustic Source Separation

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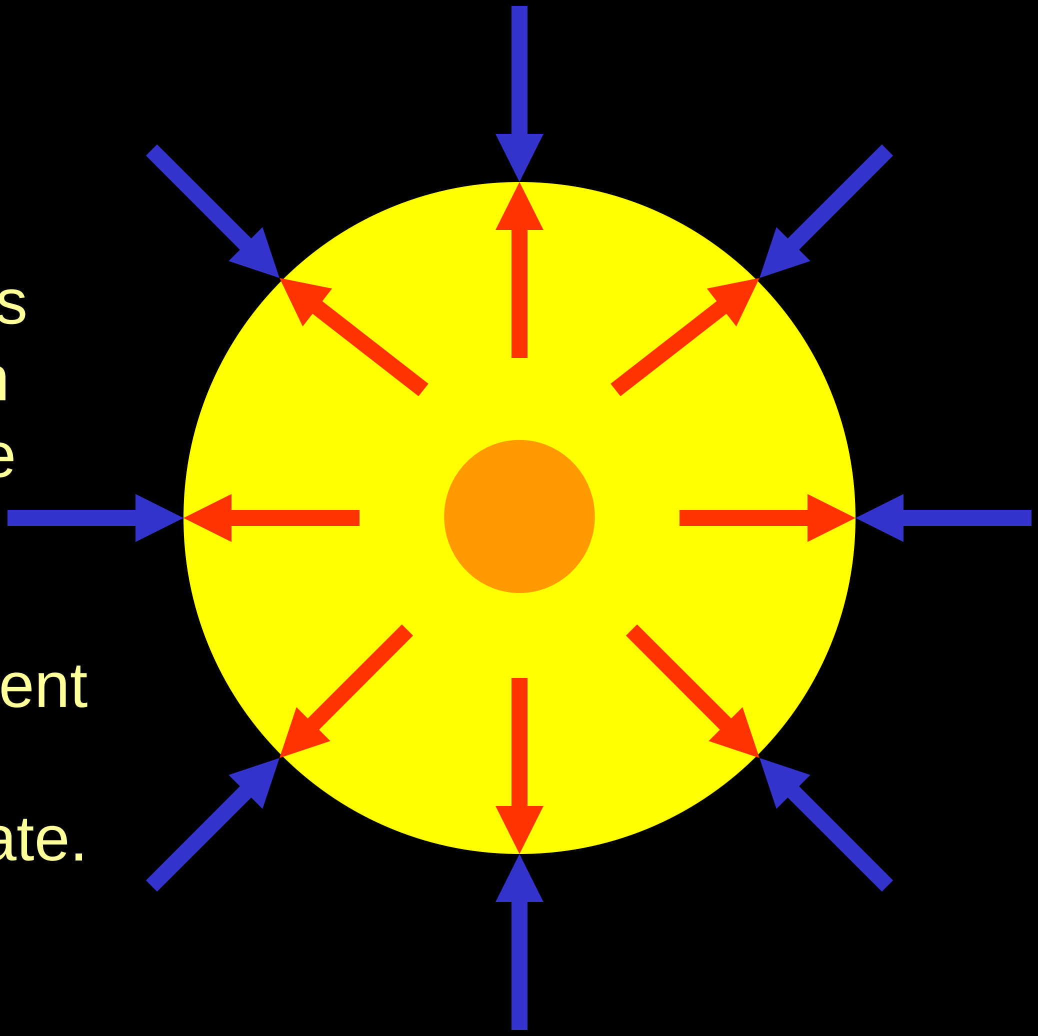
If So, How Did PAHs Get There?

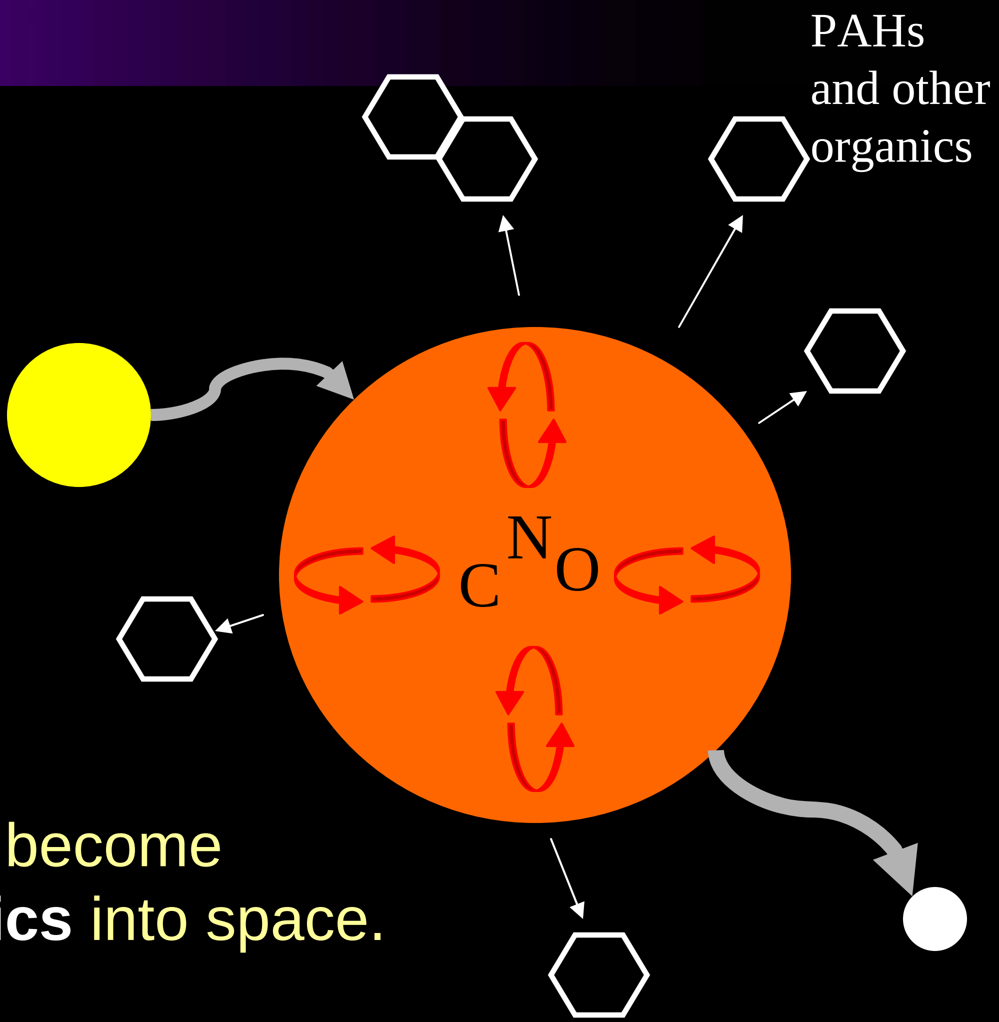
Forces Governing Stellar Structure

Nuclear fusion occurs
in the high temperature
and density present
in the **core** and generates
thermal pressure, which
acts against the attractive
gravitational forces.

As long as there is sufficient
fuel in the core, the star
remains in this steady-state.



Stellar Evolution



Stars eventually run out of Hydrogen to fuse, and begin to collapse cramming more matter into the core.

The greater densities and pressures allow creation of C N and O.
The star swells and cools to become a Red Giant spewing **organics** into space.

When fuel finally runs out, the star collapses into a **hot** White Dwarf

Why are PAHs so Interesting?

10-20% of all carbon atoms in the Interstellar Medium (ISM) are in PAH molecules

For this reason, PAH emissions are found in almost every cosmic environment in which there are concentrations of dust illuminated by ultraviolet radiation

They could be used to characterize the conditions of the ISM, and could be used as a tracer of star formation in the Milky Way

PAHs now appear to be important molecules on the pathway to life