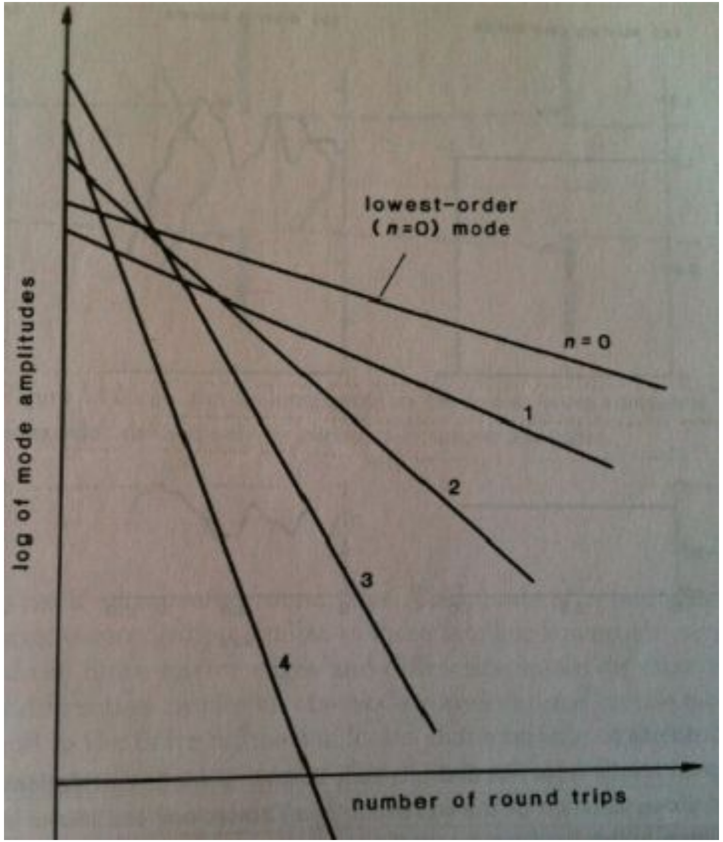
Fast Refinement of the PDF

Lasing Modes

Optical Eigenmodes

What is a common laser pulse shape?

- We can split a propagating pulse into the sum of solitons
- Within an optical cavity, radiation is lost by all modes
  - Lowest loss mode has eigenvalue closest to one
- For a laser that has built up over many periods in a cavity, we only care about the highest order mode (Fox and Li)



Paraxial Wave

- Consider the wave equation for a wave propagating in the z-direction

- Apply the paraxial approximation: changes in z-direction tiny compared to gradients in other directions

$$\tilde{E}(x, y, z) \equiv \tilde{u}(x, y, z)e^{i(\omega t - kz)}$$

Pulse Propagating in z

$$\Delta \tilde{E}(x, y, z, t) = \mu_0 \epsilon_0 \frac{\partial^2}{\partial t^2} \tilde{E}(x, y, z, t)$$

$$\Delta \tilde{E}(x, y, z, t) = -k^2 \tilde{E}(x, y, z, t)$$

$$[\Delta + k^2]\tilde{E}(x, y, z) = 0$$

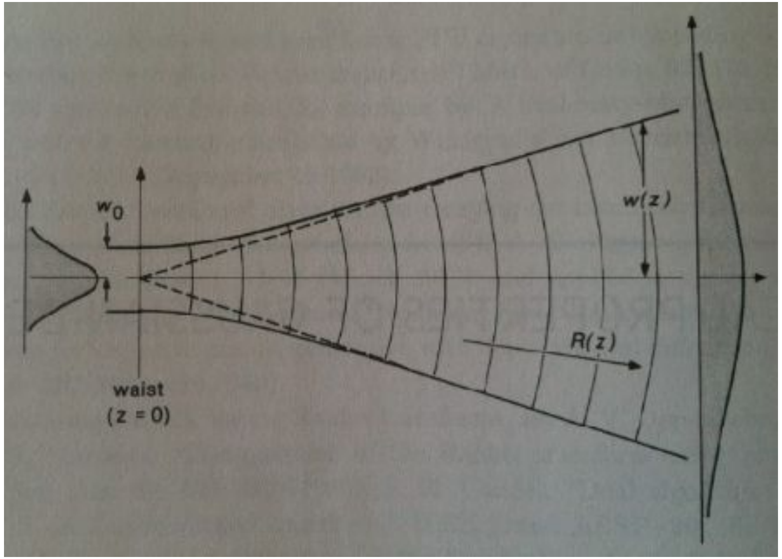
Wave Equation

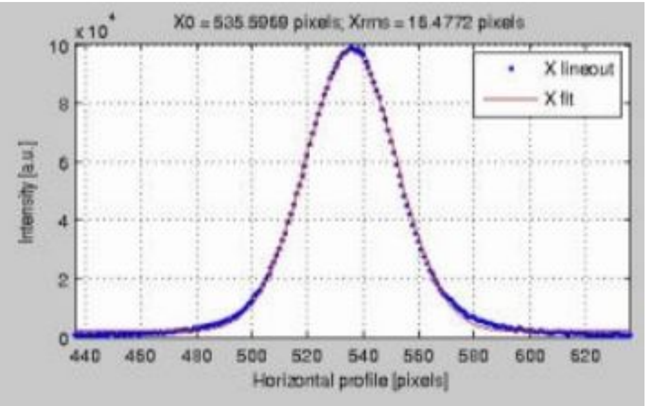
$$\frac{\partial^2 \tilde{u}}{\partial x^2} + \frac{\partial^2 \tilde{u}}{\partial y^2} - 2ik\frac{\partial \tilde{u}}{\partial z} = 0$$

Paraxial Approximation

Analytical Solution

$$\tilde{u}(x,y,z) = \sqrt{\frac{2}{\pi}} \frac{\exp\left[-ikz + i\psi(z)\right]}{w(z)} \exp\left[-\frac{x^2+y^2}{w^2(z)} - ik\frac{x^2+y^2}{2R(z)}\right]$$

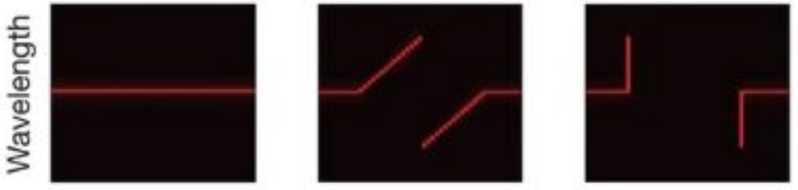




https://www.osti.gov/servlets/purl/1505100

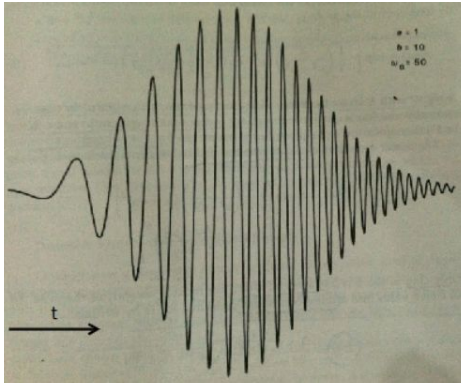
Chirping

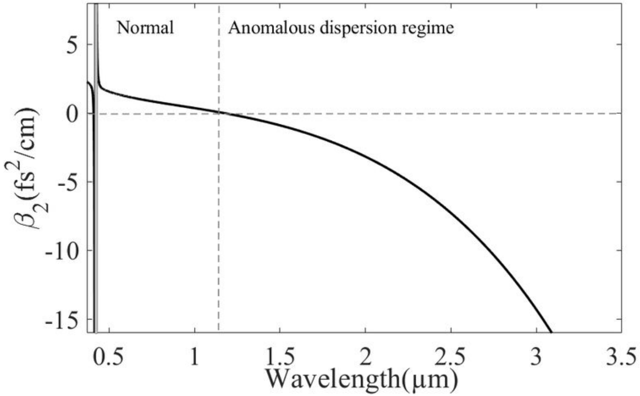
- BNL ATF uses chirping to intensify their lasers
  - Only Gaussian pulses have no fringe effects when chirped



https://www.nature.com/articles/nature10695

https://opg.optica.org/optica/fulltext.cfm?uri=optica-2-8-675&id=323254

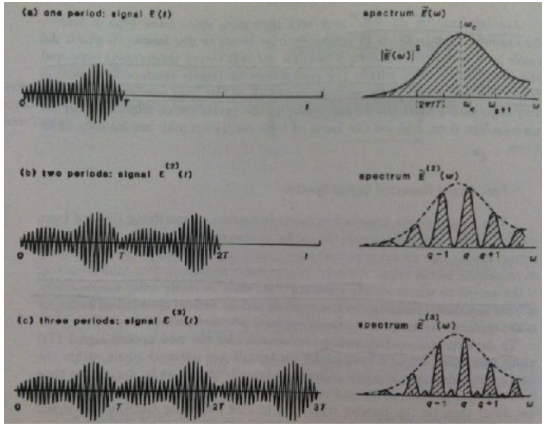


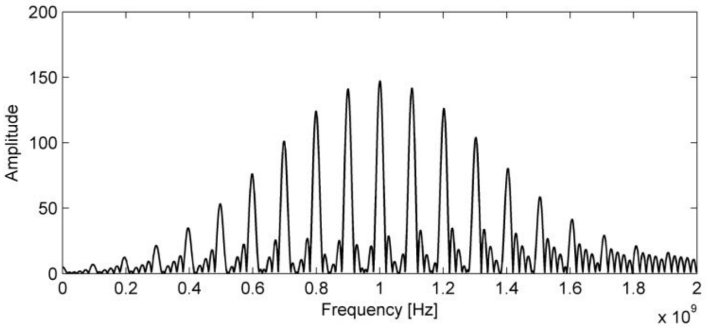


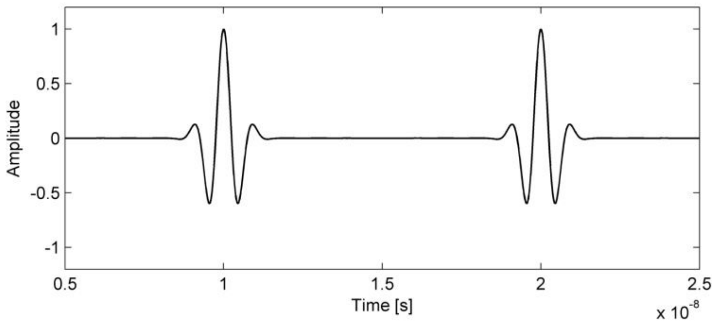
https://www.mdpi.com/2079-6439/9/4/21

Inhomogeneous Broadening

- Caused by doppler shift in gases or nonuniform strain in solids
  - Gaussian lineshape in frequency domain
- Frequency comb is a natural result of periodic cavity signals





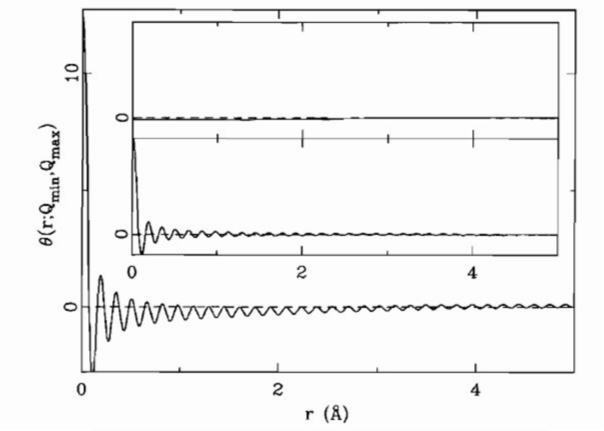


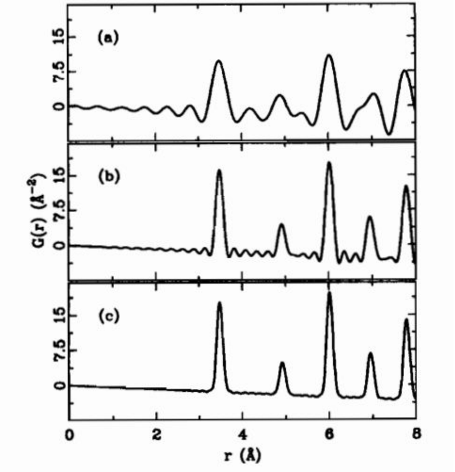
https://www.intechopen.com/chapters/6880

Convolution

F(Q) to g(r)

- Because we only consider F(Q) up to a certain Qmax, our observed g(r) becomes convoluted with a termination function
- Removing the termination function requires:
  - Fourier transforming the signal
  - Dividing by the termination function at each point
  - Fourier transforming back





https://www.sciencedirect.com/bookseries/pergamon-materials-series/vol/16/suppl/C

g(r) to F(Q) Convolution

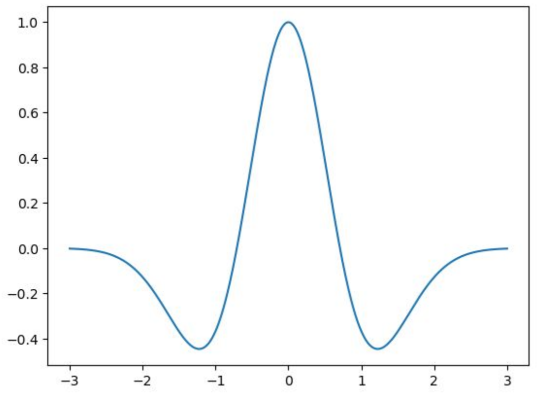
- A g(r) with delta peaks is strongly affected by the termination function
- Gaussian peaks are less affected
  - Acts as a low pass filter (Weierstrass transform)
  - Will naturally have Gaussian dampening of frequencies in the Q domain

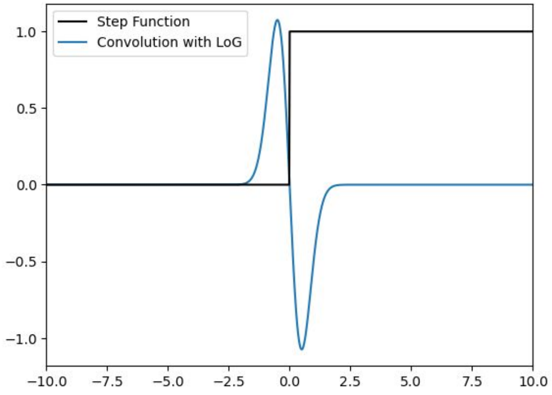
$$\frac{1}{\sqrt{4\pi}}\int_{-\infty}^{\infty}\cos(bx)e^{-\frac{(x-y)^2}{4}}\,dy = e^{-b^2}\cos(bx)$$

https://www.sciencedirect.com/science/article/pii/S0734189X87801536

Signal Enhancing

- Attempts to deblur a Gaussian led to the Laplacian of Gaussians (LoG)
- When convolved with functions, has sharp intensity spikes at edges
- Can be approximated by difference of two Gaussian blurs (DoG)

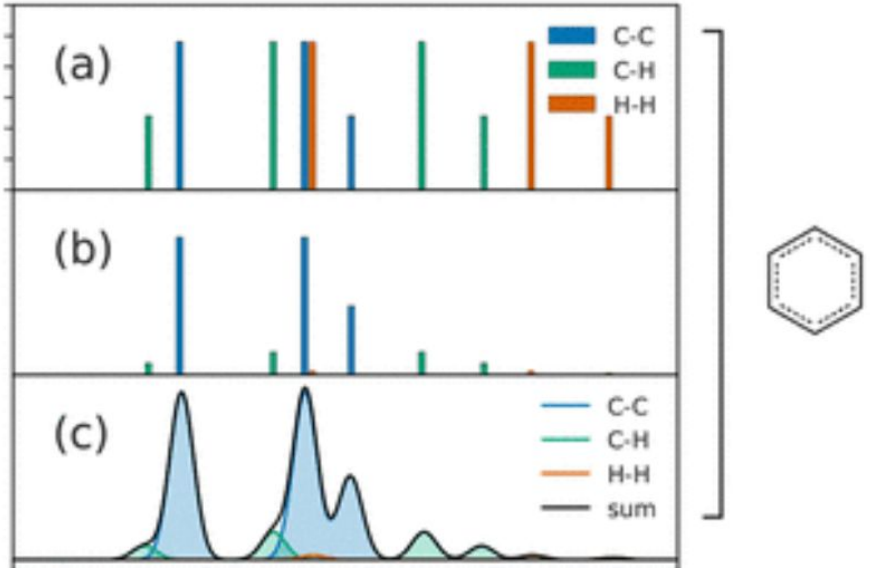




PDF Refinement

Constructing a RDF

- Count number of pairs, scale by atomic form factor, and convolute each stick with the proper Gaussian
- If the RDF has a Gaussian convolution, our I(Q) should have a product with a Gaussian



https://pubs.acs.org/doi/10.1021/acs.chemrev.1c00237

$$A\,(\mathbf{h}) = \sum_{j=1}^{n} f_j(h) \exp\,(2\pi i \mathbf{h} \cdot \mathbf{r}_j)$$

https://onlinelibrary.wiley.com/iucr/itc/doi/10.1107/97809553602060000935

$$f(|\vec{G}|) = \sum_{i=1}^{4} a_i \exp\left(-b_i \left(\frac{G}{4\pi}\right)^2\right) + c,$$

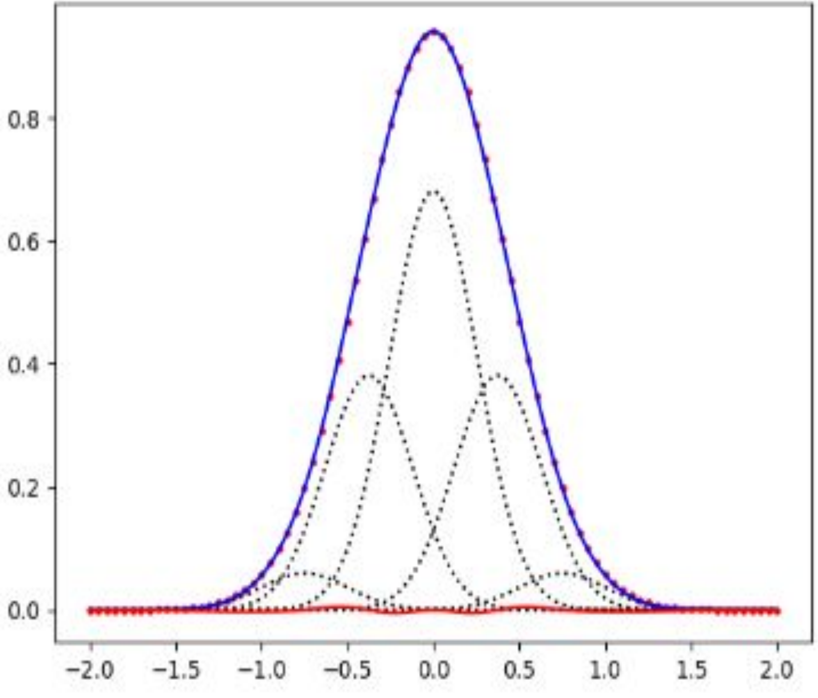
https://lampx.tugraz.at/~hadley/ss1/crystaldiffraction/atomicformfactors/formfactors.php

Radial Basis Function Interpolation

- Sufficiently smooth functions can be approximated by a linear combination of some RBFs

https://www.sciencedirect.com/science/article/pii/S0021999109001156

- Guidelines:
    - Choose spacing of Rmin=0.6
    - While the FWHM ratio between the thin and target gaussians is below Rmin, decrease Rmin and increase N (number of gaussians)
    - Measure maximum error percent



https://journals.iucr.org/j/issues/2015/03/00/to5109/to5109.pdf

Three Gaussian Approximation

$$I_0[A_1 e^{-\frac{(x+r)^2}{2s^2}} + A_0 e^{-\frac{x^2}{2s^2}} + A_1 e^{-\frac{(x-r)^2}{2s^2}}] = I_0 e^{-\frac{x^2}{2o^2}}$$

We want to approximate some Gaussian with STD 'o' as the sum of three Gaussians with STD 's'

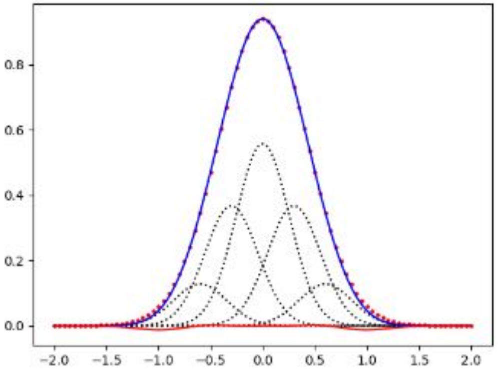
$$\begin{bmatrix} 1 & e^{-\frac{r^2}{2s^2}} & e^{-\frac{2r^2}{s^2}} \\ e^{-\frac{r^2}{2s^2}} & 1 & e^{-\frac{r^2}{2s^2}} \\ e^{-\frac{2r^2}{s^2}} & e^{-\frac{r^2}{2s^2}} & 1 \end{bmatrix} \begin{bmatrix} A_1 \\ A_0 \\ A_1 \end{bmatrix} = \begin{bmatrix} e^{-\frac{r^2}{2o^2}} \\ 1 \\ e^{-\frac{r^2}{2o^2}} \end{bmatrix} \qquad \begin{cases} A_0 = 1 - 2A_1 e^{-\frac{r^2}{2s^2}} \\ A_1 = \frac{e^{-\frac{r^2}{2o^2}} - e^{-\frac{r^2}{2s^2}}}{[1-e^{-\frac{r^2}{s^2}}]^2} \end{cases}$$

The interpolation matrix and solution

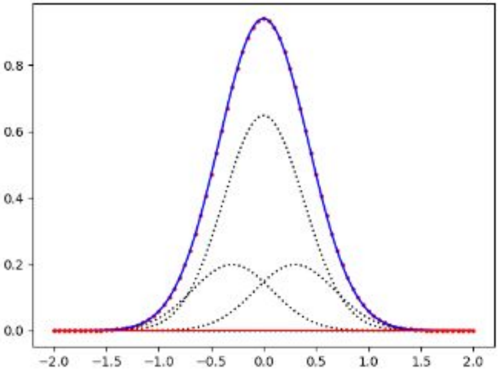
Comparing Errors

$$R_{\min} \leq f_{\mathrm{p}}/f_{\mathrm{a}} \leq 1.0$$

- R_min is the distance between the two closest sticks to the center scaled by f_a
- Strict requirements for R_min given ratio between approximating Gaussian and actual Gaussian
- Worst case scenario when R_min equals the ratio



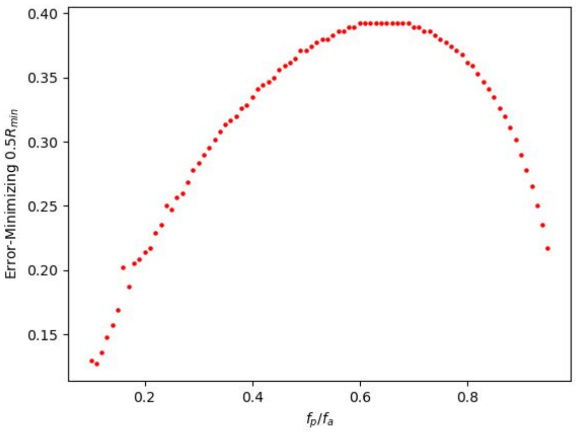
fp/fa = 0.6
Absolute Error: 0.33%
Relative Error: 0.16%

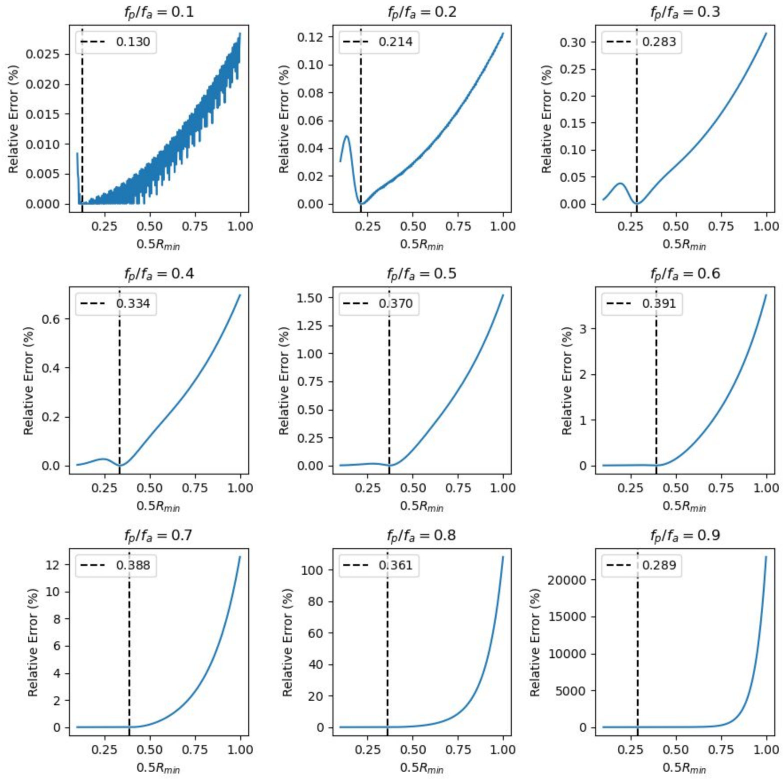


fp/fa = 0.9
Absolute Error: 0.04%
Relative Error: <0.01%

Error Minimization

- The rule R_min < fp/fa generally works, and a good baseline R_min to use is 0.8
- Following plots generated with fa=1

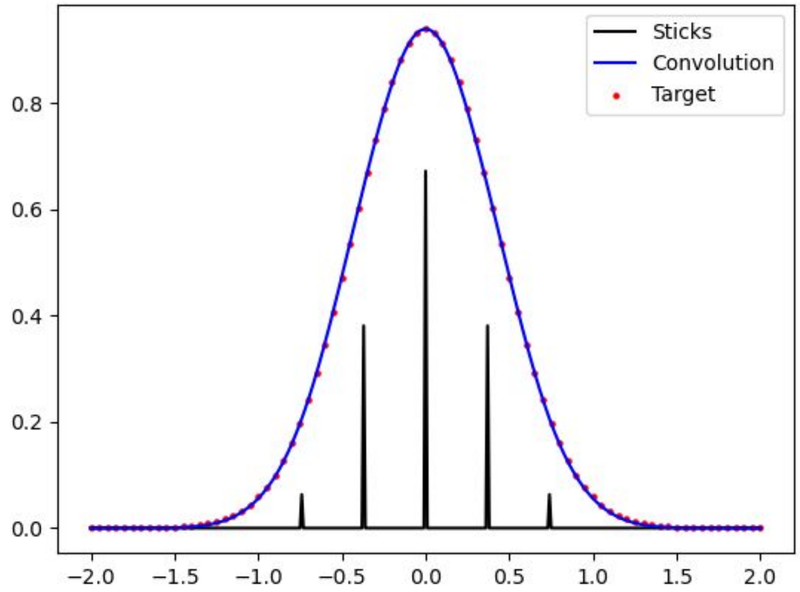




Splitting Sticks

- Instead of summing Gaussians, we want to convolute a single Gaussian with a stick pattern of delta-ish patterns

- We then convolve the stick pattern with a Gaussian of a single width to recreate the wider Gaussian



Saving Analytic Expressions

- We can come up with general analytic expressions for the heights of the sticks given separation distance r, target FWHM o, and convolution FWHM s
- We can decide on a cutoff n (such as n=5) where any ratio beyond such a cutoff is computed numerically instead

```
a2 = (e**(17*r**2/s**2) - 2*e**(16*r**2/s**2) + e**(15*r**2/s**2) +
e**(2*r**2*(6*o**2 + s**2)/(o**2*s**2)) + e**(2*r**2*(8*o**2 +
s**2)/(o**2*s**2)) - e**(3*r**2*(11*o**2 + s**2)/(2*o**2*s**2)) -
e**(r**2*(13*o**2 + 2*s**2)/(o**2*s**2)) - e**(r**2*(15*o**2 +
2*s**2)/(o**2*s**2)) - e**(r**2*(25*o**2 + 3*s**2)/(2*o**2*s**2)) +
2*e**(r**2*(29*o**2 + 3*s**2)/(2*o**2*s**2)))/(e**(r**2*(7/s**2 +
2/o**2))*(e**(10*r**2/s**2) - 3*e**(9*r**2/s**2) + e**(8*r**2/s**2) +
4*e**(7*r**2/s**2) - 2*e**(6*r**2/s**2) - 2*e**(5*r**2/s**2) -
2*e**(4*r**2/s**2) + 4*e**(3*r**2/s**2) + e**(2*r**2/s**2) -
3*e**(r**2/s**2) + 1))
```

```
[A_0] Analytic: 0.715477620791366, Numerical: 0.7154776207913877
[A_1] Analytic: 0.405462459777574, Numerical: 0.40546245977758283
[A_2] Analytic: 0.0672460216657563, Numerical: 0.06724602166575397
```

Questions?