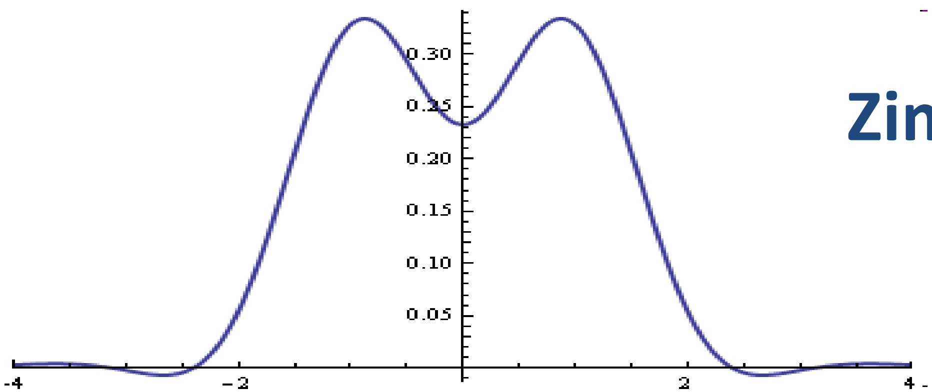
Gram-Charlier and Edgeworth expansions for nongaussian correlations in femtoscopy



Zimányi 2009 Winter School on Heavy Ion Physics

Michiel de Kock
University of Stellenbosch
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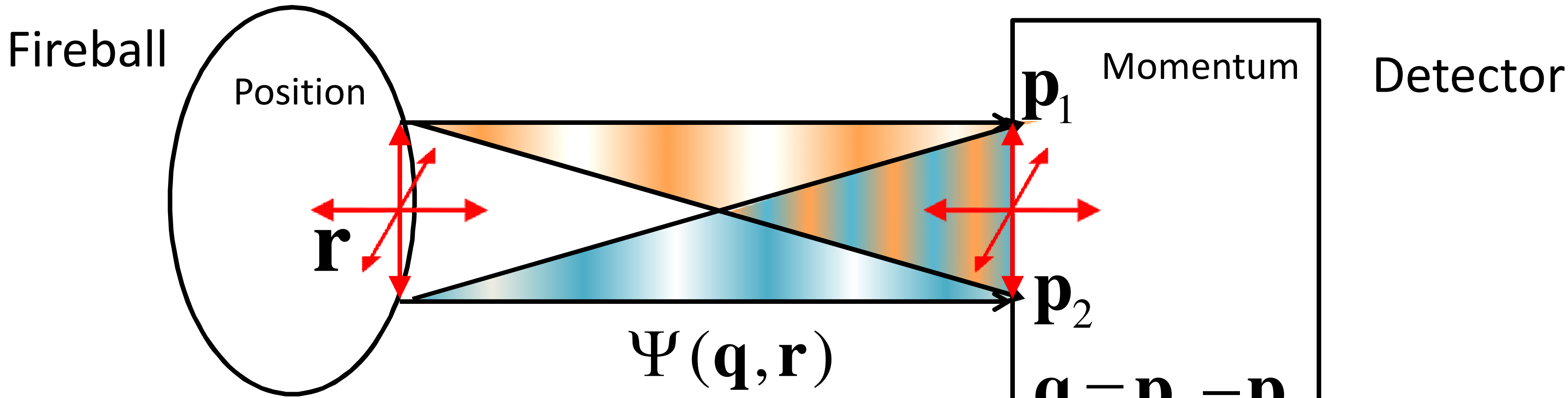
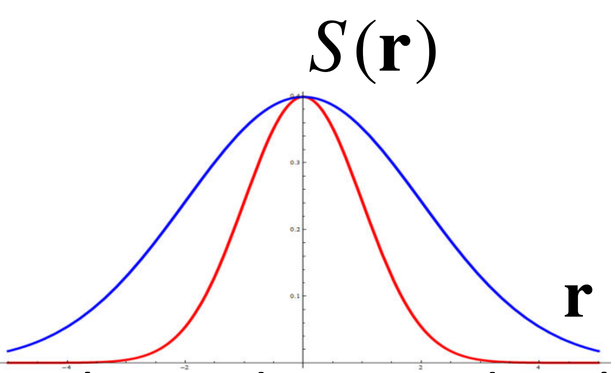
Experimental Femtoscopy



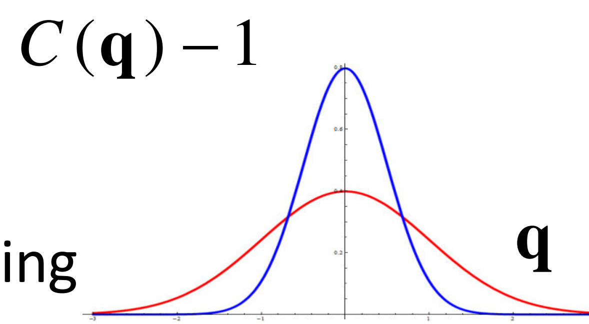
Wave function



Relative distance distribution

Fourier Transform

Identical,non-interacting particles



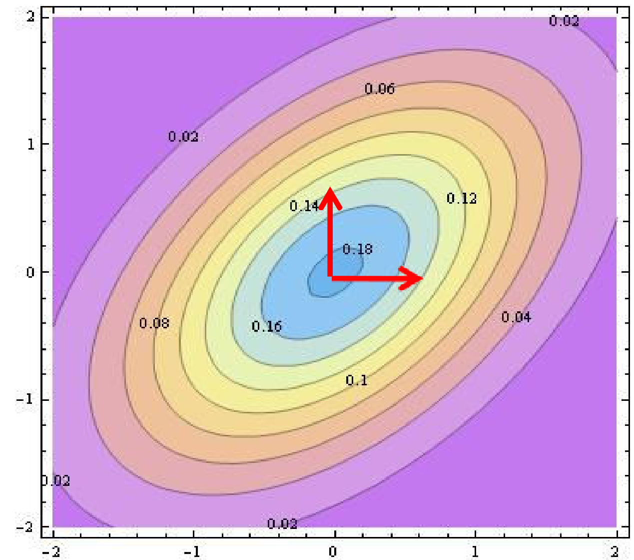
Correlation function

$$C(\mathbf{q})-1=\int d^3\mathbf{r}\, S(\mathbf{r})\left[\left|\Psi(\mathbf{q},\mathbf{r})\right|^2-1\right]$$

First Approximation: Gaussian

- Assume Gaussian shape for correlator:

$$C(\mathbf{q})-1=\lambda\exp\left(-\sum_{ij} q_i R_{ij}^2 q_j\right)$$



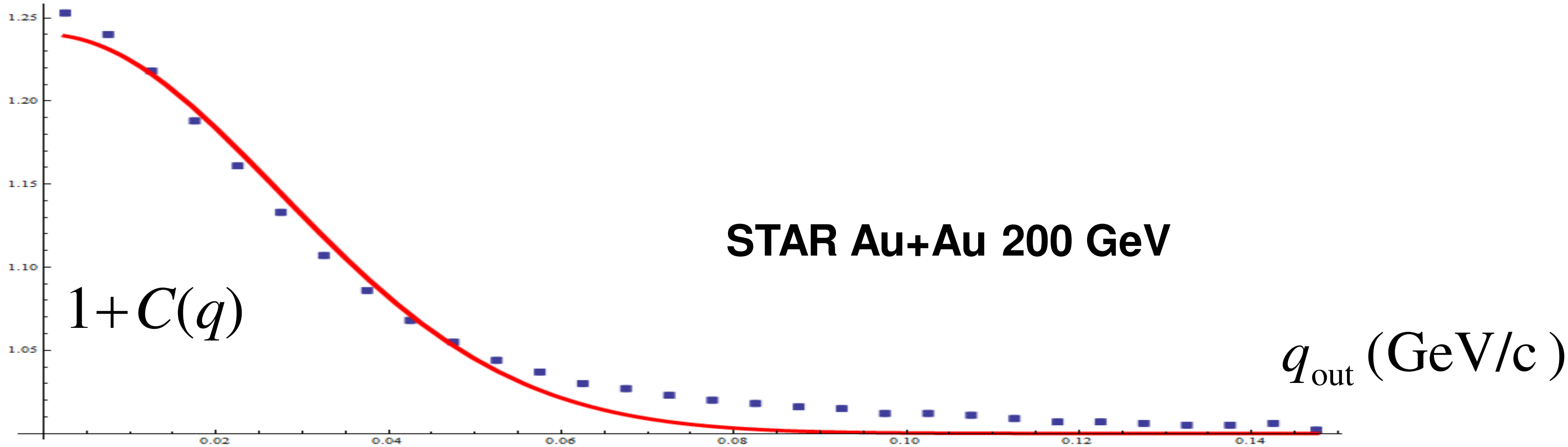
- Out, long and side

$$\mathbf{q}=(q_{\text{out}},q_{\text{long}},q_{\text{side}})$$

- Measuring Gaussian Radii through fitting

$$\left(R_{ij}^2\right)^{-1}=\begin{pmatrix} \langle q_{\text{out}}^2\rangle & 0 & \langle q_{\text{out}}q_{\text{long}}\rangle \\ 0 & \langle q_{\text{side}}^2\rangle & 0 \\ \langle q_{\text{out}}q_{\text{long}}\rangle & 0 & \langle q_{\text{long}}^2\rangle \end{pmatrix}$$

High-Statistics Experimental Correlation functions: Not Gaussian!



Data: http://drupl.star.bnl.gov/STAR/files/starpublications/50/data.htm

- Measured 3D Correlation function are not Gaussian.
- The traditional approach: fitting of non-Gaussian functions.
- Systematic descriptions beyond Gaussian:

Harmonics (Pratt & Danielewicz, http://arxiv.org/abs/nucl-th/0612076v1)

Edgeworth and Gram-Charlier series

Reference: T. Csörgő and S. Hegyi, Phys. Lett. B **489**, 15 (2000).

Derivation of Gram-Charlier series

- Assume one dimension, $C(\mathbf{q}) - 1 \rightarrow g(q)$

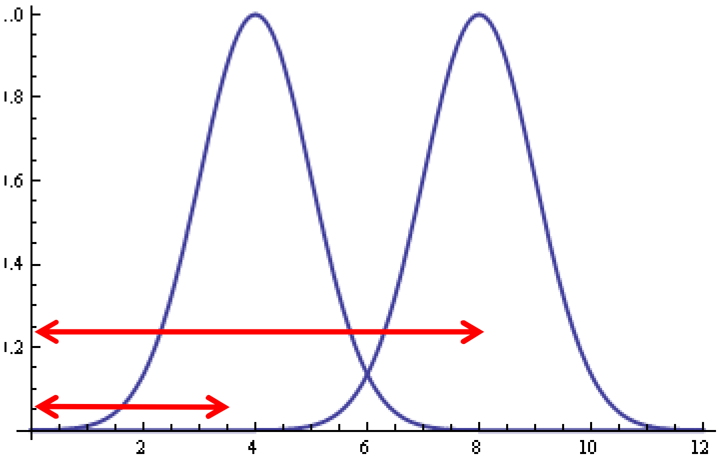
  with $\int g(q)\,dq = 1$
- Moments: $\mu_r = \mathrm{E}[q^r] = \int q^r g(q)\,dq = \langle q^r \rangle$
- Cumulants: $\kappa_1 = \mathrm{E}[q] \quad \kappa_2 = \mathrm{E}[q^2] - \mathrm{E}[q]^2$

We want to use cumulants to go beyond the Gaussian.

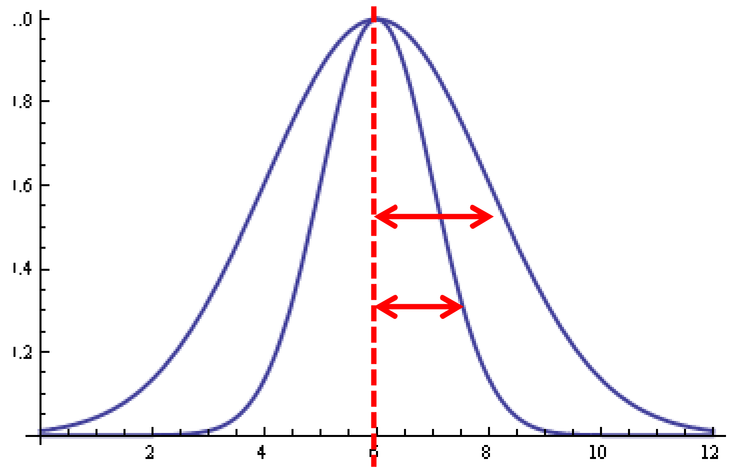
$$K_{ij} = \left(R_{ij}^2\right)^{-1} = \begin{pmatrix} \langle q_{\mathrm{out}}^2 \rangle & 0 & \langle q_{\mathrm{out}} q_{\mathrm{long}} \rangle \\ 0 & \langle q_{\mathrm{side}}^2 \rangle & 0 \\ \langle q_{\mathrm{out}} q_{\mathrm{long}} \rangle & 0 & \langle q_{\mathrm{long}}^2 \rangle \end{pmatrix}$$

First four Cumulants

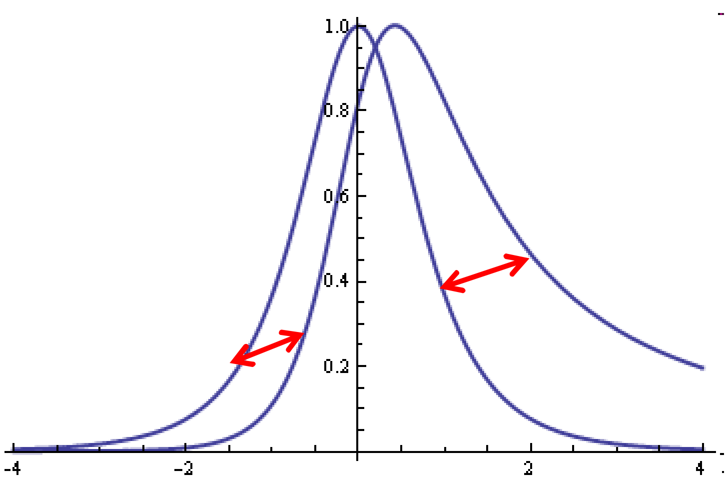
Mean κ_1



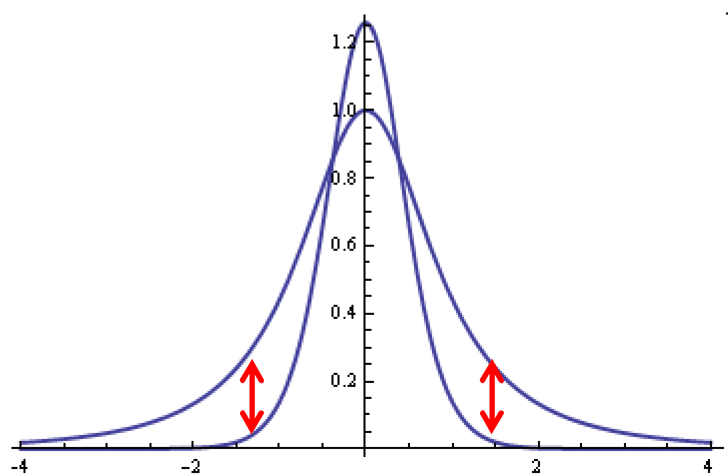
Variance κ_2



Skewness κ_3



Kurtosis κ_4



Why Cumulants?

- Cumulants are invariant under translation $q \rightarrow q + c$
- Cumulants are simpler than moments

One-dimensional Gaussian: $g(q) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(q-\mu)^2}{2\sigma^2} \right)$

Moments of a Gaussian	Cumulants
$\mu_1 = \mu$	$\kappa_1 = \mu$
$\mu_2 = \mu^2 + \sigma^2$	$\kappa_2 = \sigma^2$
$\mu_3 = \mu^3 + 3\mu\sigma^2$	$\kappa_3 = 0$
$\mu_4 = \mu^4 + 6\mu^2\sigma^2 + 3\sigma^4$	$\kappa_4 = 0$

Generating function $G(x)$

Moment generating function (Fourier Transform).

$$G(x) = 1 + (ix)\mu_1 + \tfrac{1}{2!}(ix)^2\mu_2 + \ldots = \sum_{j=0}^{\infty} \frac{(ix)^j}{j!}\mu_j = \int g(q)e^{iqx}dq$$

Cumulant generating function (Log of Fourier Transform).

$$\log[G(x)] = (ix)\kappa_1 + \tfrac{1}{2!}(ix)^2\kappa_2 + \tfrac{1}{3!}(ix)^3\kappa_3 + \ldots = \sum_{j=1}^{\infty} \frac{(ix)^j}{j!}\kappa_j$$

Moments:

$$\mu_r = \left(\frac{d}{d(ix)}\right)^r G(x)\Bigg|_{x=0}$$

Cumulants:

$$\kappa_r = \left(\frac{d}{d(ix)}\right)^r \log G(x)\Bigg|_{x=0}$$

Moments to Cumulants:

$$\mu_1 = \kappa_1$$

$$\mu_2 = \kappa_2 + \kappa_1^2$$

$$\mu_3 = \kappa_3 + 3\kappa_1\kappa_2 + \kappa_1^3$$

$$\mu_4 = \kappa_4 + 4\kappa_1\kappa_3 + \kappa_1^4 + 6\kappa_1^2\kappa_2 + 3\kappa_2^2$$

Reference function

Measured correlation function $g(q)$

- Want to approximate g in terms of a reference function $f(q)$

Generating functions of g and f:

$$G(x) = \int g(q) e^{ixq} dq = \sum_{j=0}^{\infty} \frac{(ix)^j}{j!} \mu_j = \exp\left(\sum_{j=1}^{\infty} \frac{(ix)^j}{j!} \kappa_j \right)$$

$$F(x) = \int f(q) e^{ixq} dq = \sum_{j=0}^{\infty} \frac{(ix)^j}{j!} \mu_j^* = \exp\left(\sum_{j=1}^{\infty} \frac{(ix)^j}{j!} \kappa_j^* \right)$$

Start with a Taylor expansion in the Fourier Space

$$\frac{G(x)}{F(x)} = 1 + \frac{c_1}{1!} x + \frac{c_2}{2!} x^2 + \frac{c_3}{3!} x^3 + \ldots$$

Gram-Charlier Series

Useful property of Fourier transforms

$$f(x) \Leftrightarrow F(x) \qquad f'(q) \Leftrightarrow (-ix)F(x)$$

$$f''(q) \Leftrightarrow (-ix)^2 F(x) \qquad f^{(3)}(q) \Leftrightarrow (-ix)^3 F(x)$$

$$\frac{G(x)}{F(x)} = 1 + \frac{c_1}{1!}x + \frac{c_2}{2!}x^2 + \frac{c_3}{3!}x^3 + \ldots$$

Expansion in the derivatives of a reference function

Coefficients are determined by the moments/cumulants

$$g(q) = f(q) - \frac{c_1}{1!}f'(q) + \frac{c_2}{2!}f''(q) - \frac{c_3}{3!}f^{(3)}(q) + \ldots$$

Determining the Coefficients

$$\frac{G(x)}{F(x)} = 1 + \frac{c_1}{1!}x + \frac{c_2}{2!}x^2 + \frac{c_3}{3!}x^3 + \ldots$$

Taking logs on both sides and expanding

$$\log F(x) - \log G(x) = \sum_{j=0}^{\infty} \frac{x^j}{j!}\Delta_j$$

Coefficients in terms of Cumulant Differences:

$$c_j \rightarrow \Delta_j = \kappa_j - \kappa_j^*$$

Cumulant differences to Coefficients

$$c_1 = \Delta_1$$

$$c_2 = \Delta_2 + \Delta_1^2$$

$$c_3 = \Delta_3 + 3\Delta_1\Delta_2 + \Delta_1^3$$

$$c_4 = \Delta_4 + 4\Delta_1\Delta_3 + \Delta_1^4 + 6\Delta_1^2\Delta_2 + 3\Delta_2^2$$

Partial Sums

Infinite Formal Series

$$g(q) = \sum_{j=0}^{\infty} (-1)^j \frac{c_j}{j!} \left(\frac{d}{dq} \right)^j f(q)$$

Truncate series to form a partial sum, from infinity to *k*

$$g(q) \approx \sum_{j=0}^{k} (-1)^j \frac{c_j}{j!} \left(\frac{d}{dq} \right)^j f(q)$$

$$\approx f_k(q)$$

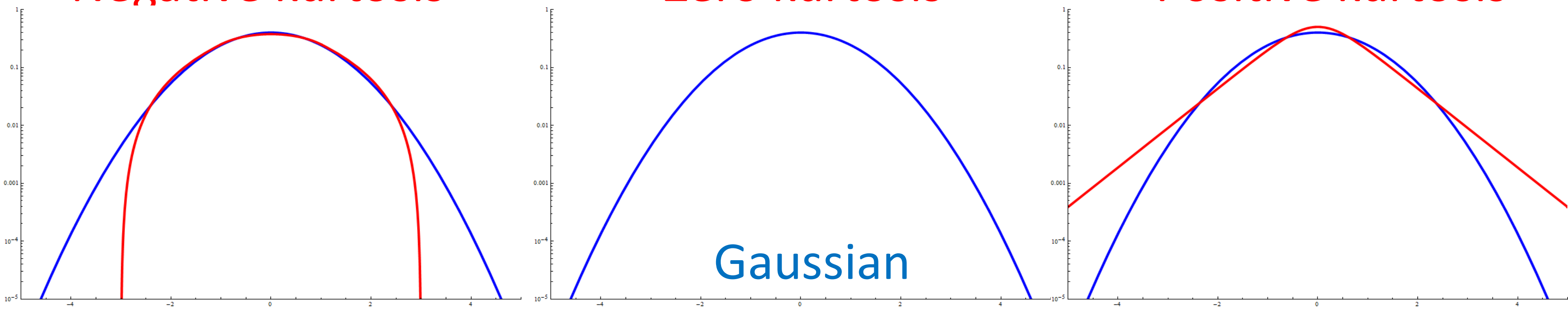
← Truncate to *k* terms

How good is this approximation in practice?

Kurtosis

We will now use analytical functions for the correlator to test the Gram-Charlier expansion.

Negative kurtosis | Zero kurtosis | Positive kurtosis



$$\log\left[f(q)\right] \text{ vs. } q$$

Negative Kurtosis	Zero Kurtosis	Positive Kurtosis
Beta Distribution	Gaussian	Hypersecant
		Student's t
		Normal Inverse Gaussian

Gram-Charlier Type A Series: Gaussian reference function

$$f(q)=\frac{1}{\sqrt{2\pi\sigma}}\exp\left(-\frac{(q-\mu)^2}{2\sigma^2}\right)$$

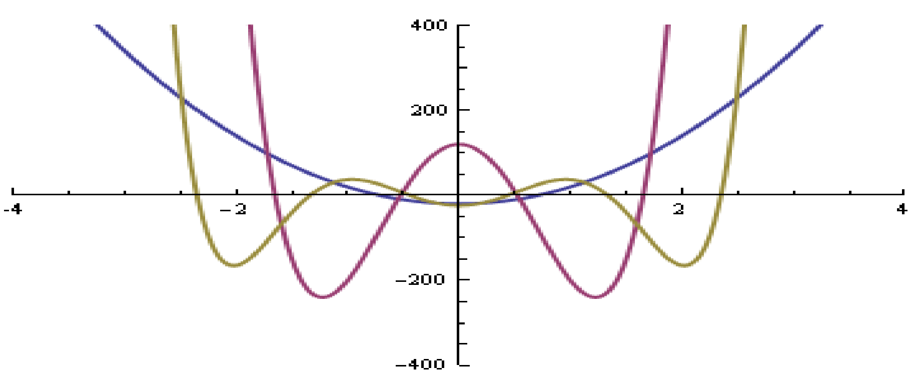
Gaussian gives Orthogonal Polynomials; $H_r(q)=\frac{1}{f(q)}(\frac{d}{dq})^r[f(q)]$
Rodrigues formula for Hermite polynomials.
Gram-Charlier Series is not necessarily orthogonal!

$$g(q)=f(q)[1-\frac{c_1}{1!}H_1(q)+\frac{c_2}{2!}H_2(q)-\frac{c_3}{3!}H_3(q)+\ldots]$$

$$H_2(q)=q^2-1$$

$$H_4(q)=q^4-6q^2+3$$

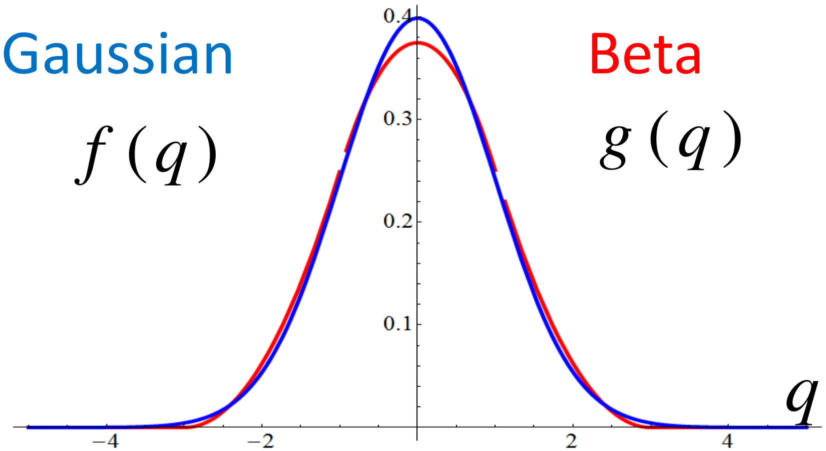
$$H_6(q)=q^6-15q^4+45q^2-15$$



Negative-Kurtosis g(q)

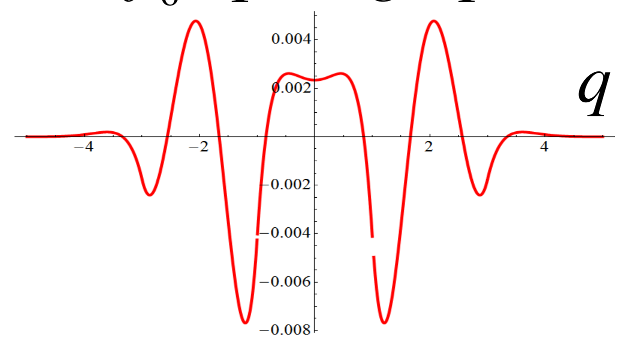
Gaussian $f(q)$

Beta $g(q)$



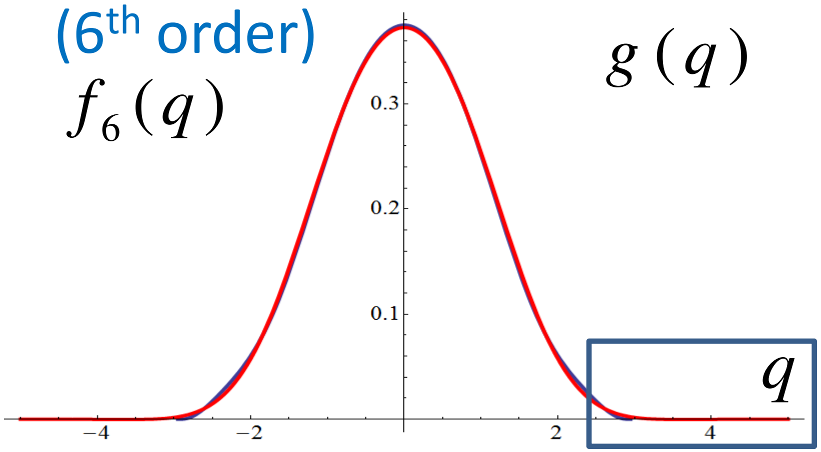
$$f_k(q) = \sum_{j=0}^{k} (-1)^j \frac{c_j}{j!} H_j(q) f(q)$$

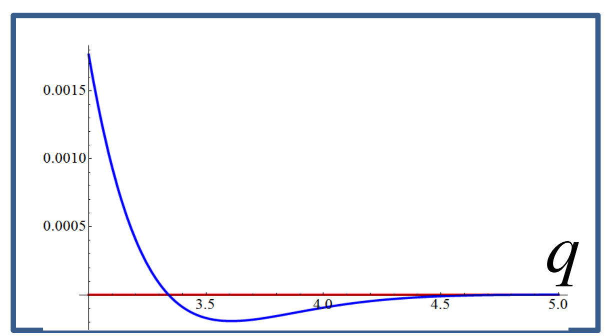
$f_6(q) - g(q)$



Gram-Charlier (6th order) $f_6(q)$

Beta $g(q)$





Negative probabilities

Positive-kurtosis g(q)

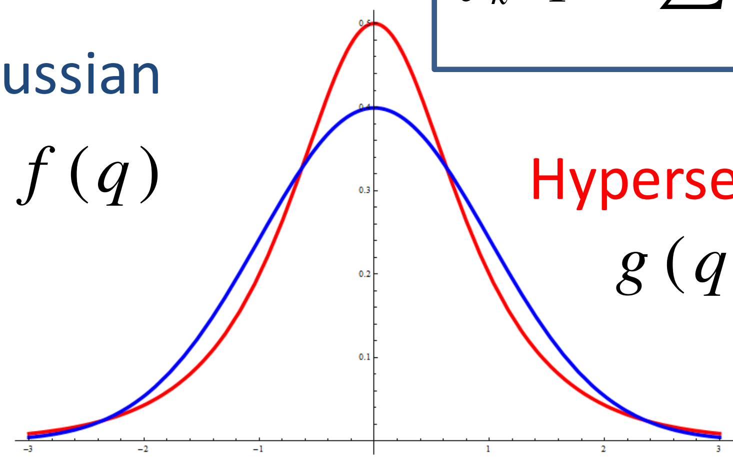
$$f_k(q) = \sum^{k} (-1)^j \frac{c_j}{j} H_j(q)\, f(q)$$

Gaussian

$f(q)$

Hypersecant

$g(q)$



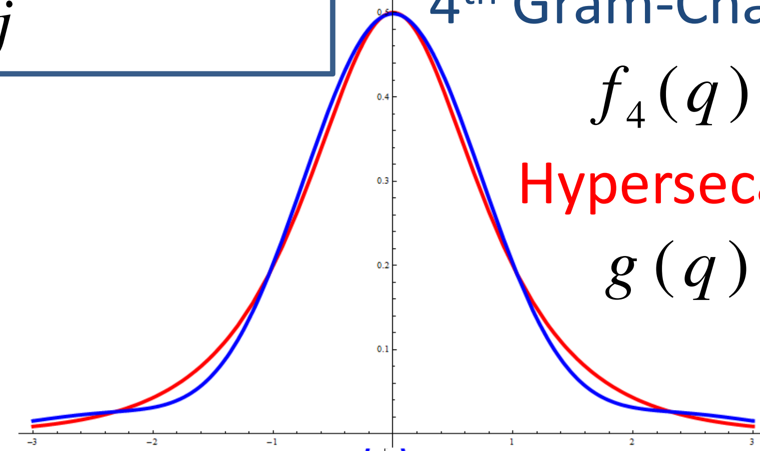
q

4th Gram-Charlier

$f_4(q)$

Hypersecant

$g(q)$



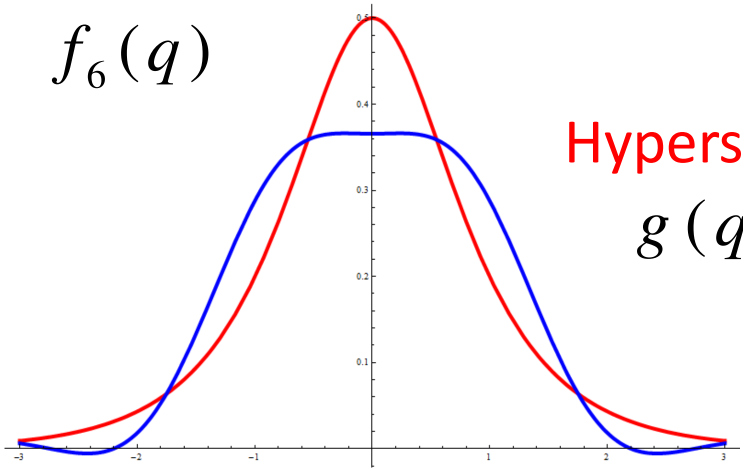
q

6th Gram-Charlier is worse

$f_6(q)$

Hypersecant

$g(q)$



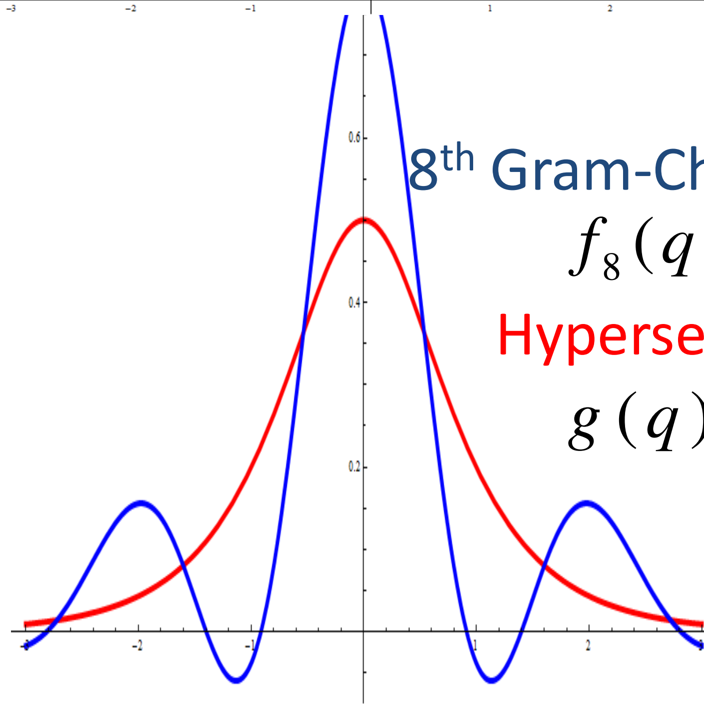
q

8th Gram-Charlier

$f_8(q)$

Hypersecant

$g(q)$



q

Edgeworth Expansion

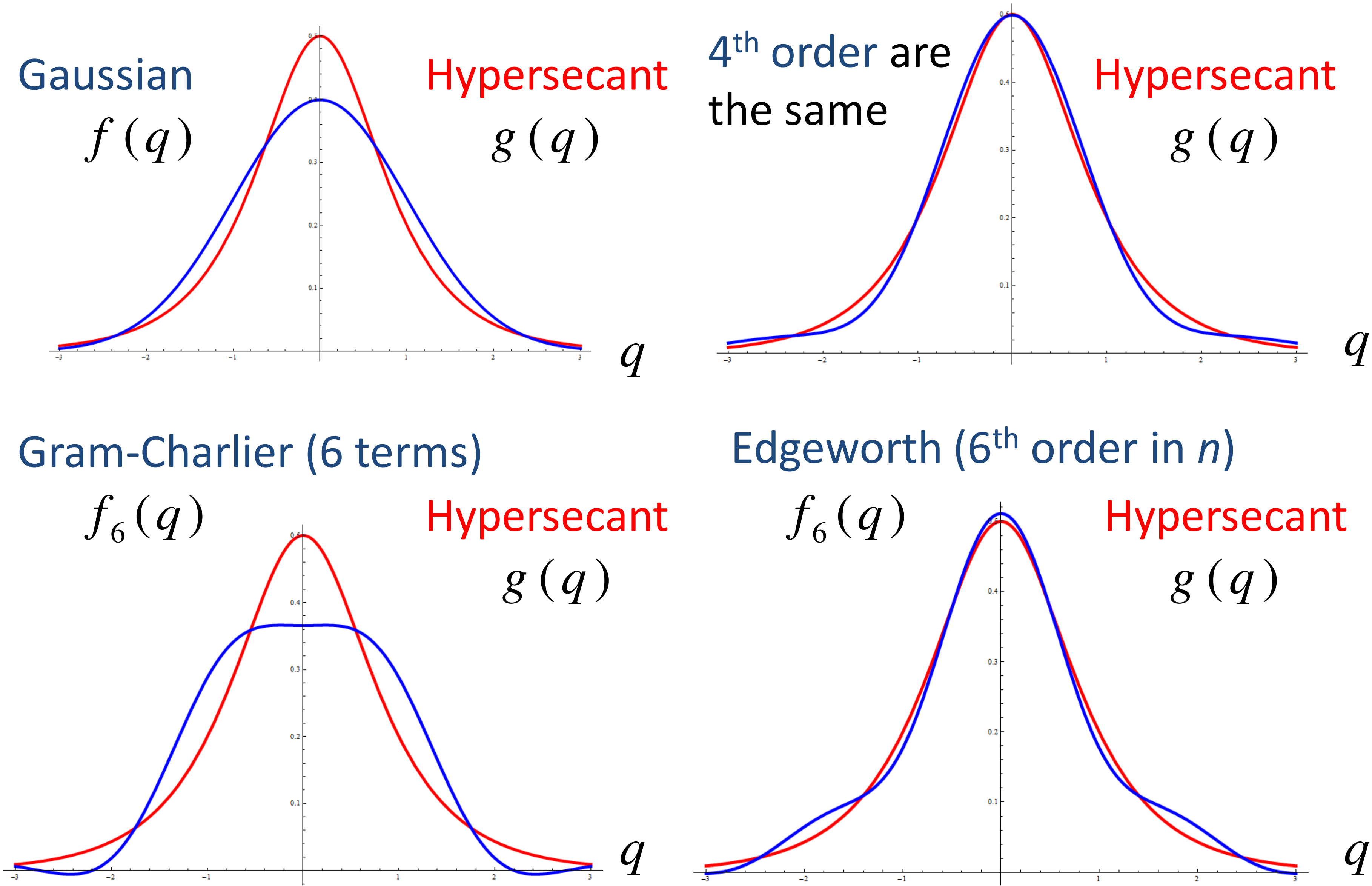
- Same series; different truncation
- Assume that unknown correlator g(q) is the sum of *n* variables.

$$G(x \mid n) = \left[G\left(\frac{x}{\sigma\sqrt{n}} \right) \right]^n = \exp\left[n \sum_{j=1}^{\infty} \left(\frac{ix}{\sigma\sqrt{n}} \right)^j \frac{\kappa_j}{j!} \right]$$

Truncate according to order in *n* instead of a number of terms (Reordering of terms).

Gram-Charlier	Edgeworth
$\frac{1}{3!}\kappa_3 H_3(q)$	$\frac{1}{3!}\kappa_3 H_3(q)$
$\frac{1}{4!}\kappa_4 H_4(q)$	$\kappa_4 \frac{1}{4!} H_4(q) + 10\kappa_3^2 \frac{1}{6!} H_6(q)$
$\frac{1}{5!}\kappa_5 H_5(x)$	$\kappa_5 \frac{1}{5!} H_5(q) + 35\kappa_3\kappa_4 \frac{1}{7!} H_7(q) + 280\kappa_3^3 \frac{1}{9!} H_9(q)$
$\frac{1}{6!}(\kappa_6 + 10\kappa_3^2) H_6(q)$	$\kappa_6 \frac{1}{6!} H_6(q) + \frac{1}{8!}\left(56\kappa_3\kappa_5 + 35\kappa_4^2\right) H_8(q) + \ldots$

Edgeworth does better



Interim Summary

- Asymptotic Series
- Edgeworth and Gram-Charlier have the same convergence
  - Gaussian reference will not converge for positive kurtosis.
  - Negative kurtosis will converge, but will have negative tails.

Different reference function for different measured kurtosis

- Negative kurtosis g(q): use Beta Distribution for f(q)
  1. Solves negative probabilities.
  2. Great convergence .
- Small positive kurtosis g(q): use Edgeworth Expansion for f(q)
- Large positive kurtosis g(q): use Student's t Distribution for f(q) and Hildebrandt polynomials, investigate further...

Hildebrandt Polynomials

$$f(q) = \frac{1}{aB(\tfrac{1}{2}, m)}\left(1 + \frac{q^2}{a^2}\right)^{-m-\tfrac{1}{2}}$$

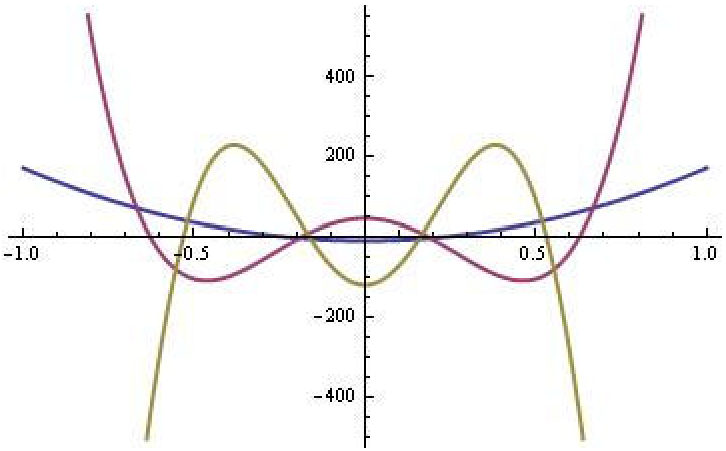
Student's t distribtion:

Orthogonal polynomials:

$$S_2 = 2m(m-1)q^2 - m$$

$$S_4 = \tfrac{2}{3}m(m-1)(m-2)(m-3)q^4 - 2m(m-1)(m-2)q^2 + \tfrac{1}{2}m(m-1)$$

$$S_6 = \Gamma(m)\left(\tfrac{4}{45}\frac{q^6}{\Gamma(m-6)} - \tfrac{2}{3}\frac{q^4}{\Gamma(m-4)} - \tfrac{1}{6}\frac{q^2}{\Gamma(m-4)}\right)$$



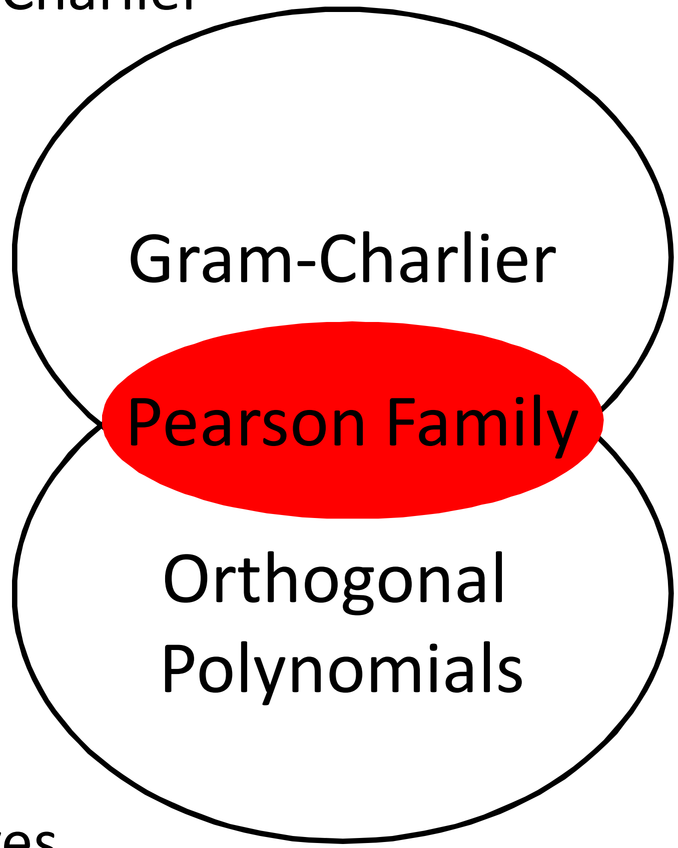
- Student's t distribution has limited number of moments (2m-1).
- Hildebrandt polynomials don't exist for higher orders.

Orthogonality vs. Gram-Charlier

- Pearson family: Orthogonal **and** Gram-Charlier
- Choose: **Either** Gram-Charlier

(derivatives of reference)

or Orthogonal Polynomials

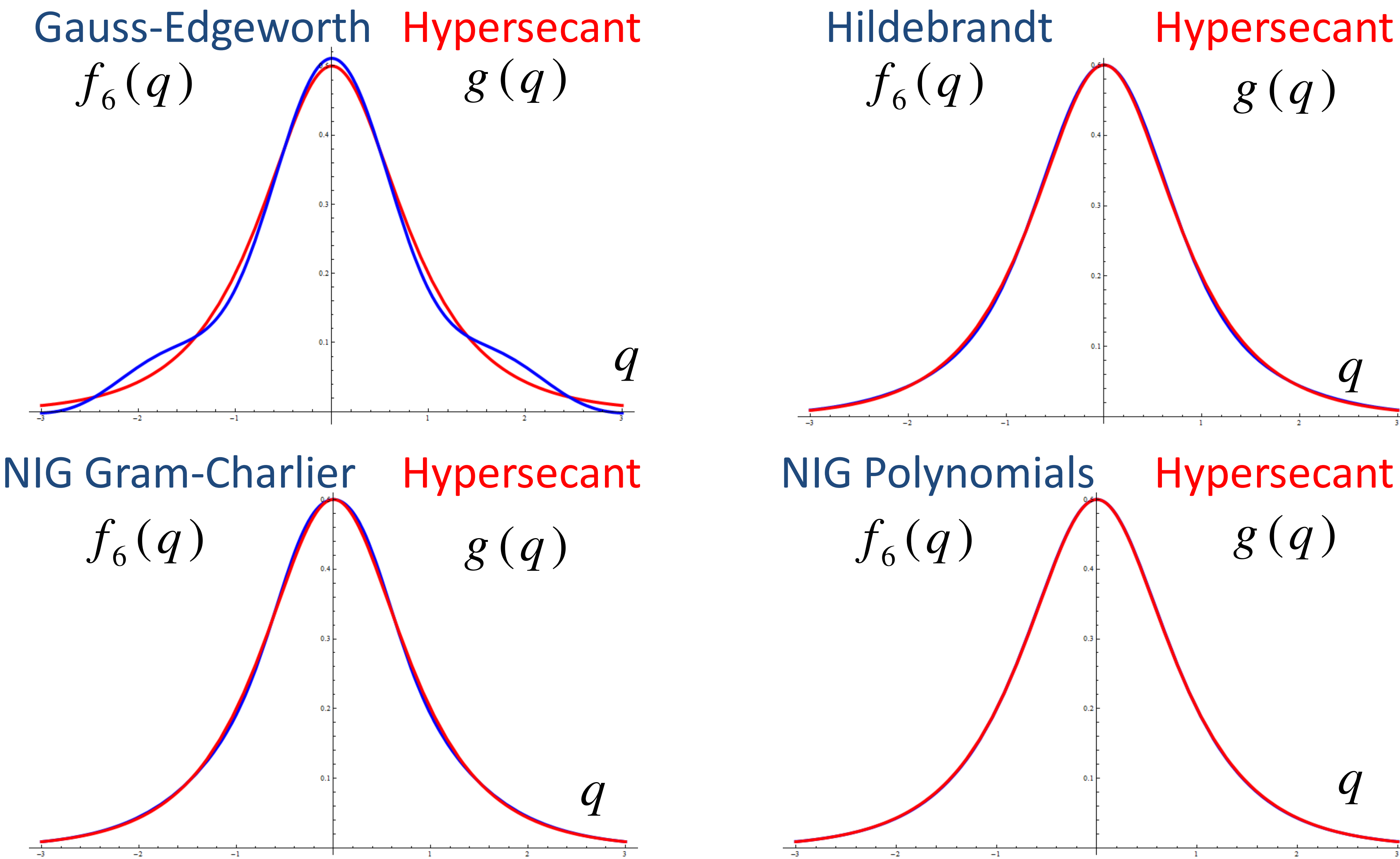


$$f(x) = \frac{\alpha\delta e^{\alpha\delta} K_1\left(a\sqrt{\delta^2 + q^2}\right)}{\pi\sqrt{\delta^2 + q^2}}$$

Normal Inverse Gaussian

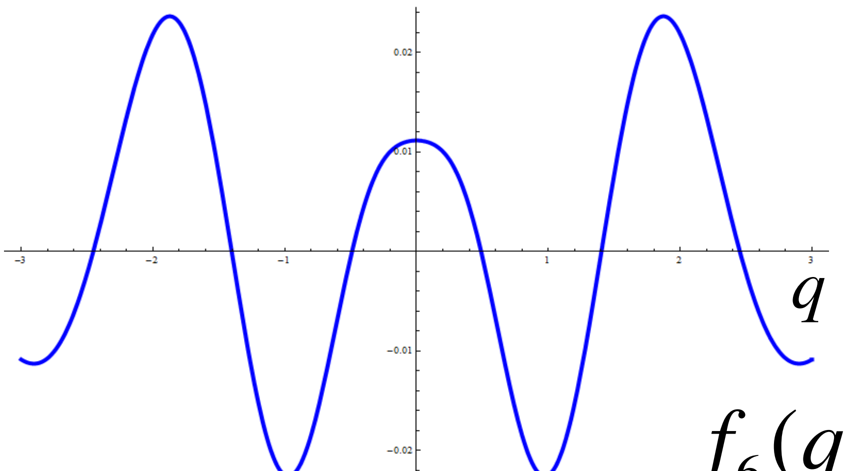
- Finite moments and simple cumulants
- Construct polynomials or take derivatives

Strategies for Positive kurtosis: Comparison

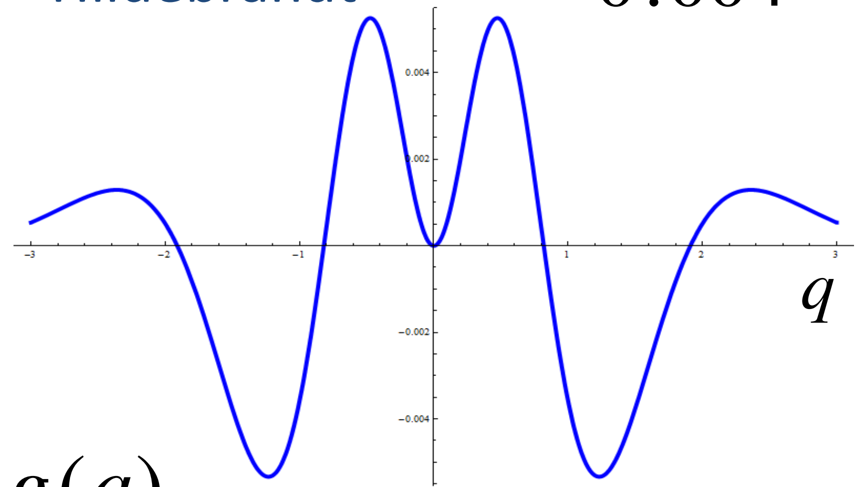


Strategies for Positive kurtosis: Difference

Gauss-Edgeworth ≈ 0.02

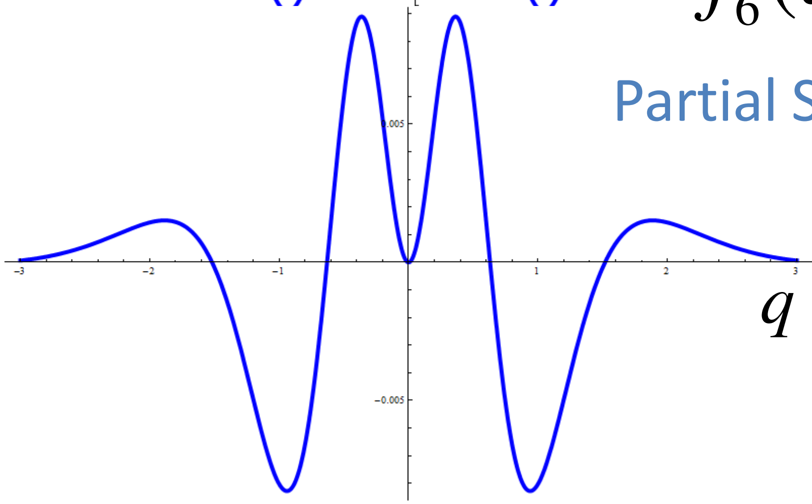


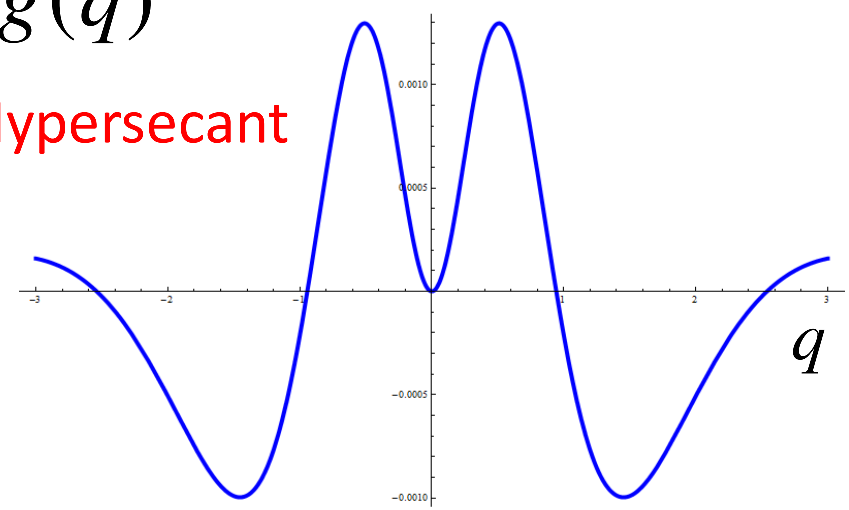
Hildebrandt ≈ 0.004



$$f_6(q) - g(q)$$

Partial Sum-Hypersecant





NIG Gram-Charlier ≈ 0.005

NIG Polynomials ≈ 0.001

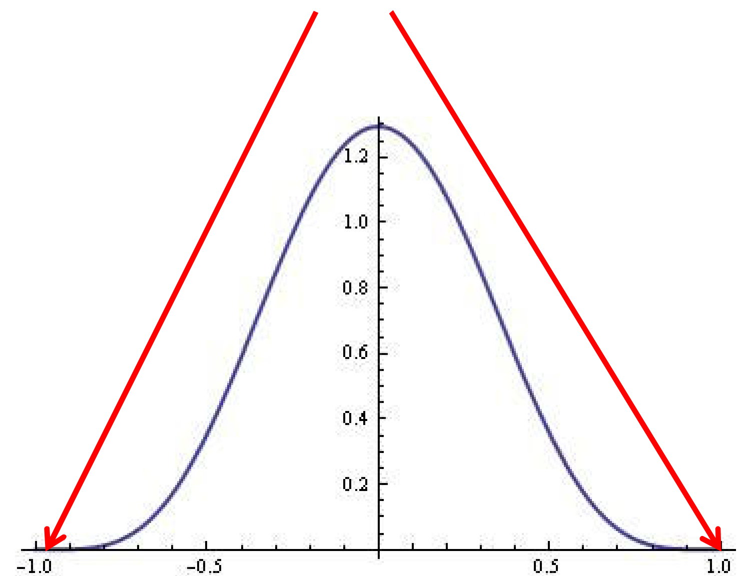
Conclusions

- The expansions are not based on fitting; this might be an advantage in higher dimensions.
- For measured distributions g(q) close to Gaussian, the Edgeworth expansion performs better than Gram-Charlier.
- For highly nongaussian distributions g(q), both series expansions fail.
- Choosing nongaussian reference functions f(q) can significantly improve description.
  - Negative kurtosis g(q): use Beta distribution for f(q)
  - Positive kurtosis g(q): choose reference f(q) to closely resemble g(q)
- Cumulants and Moments are only a good idea if the shape is nearly Gaussian.

Smoothness property

- All derivatives should be zero at the endpoints of the reference function
- No “surface terms” in partial integration.
- Ensures coefficient are only dependent on the moments/cumulants

f	1	μ_1	μ_2	μ_3
f'	0	μ_1	μ_2	μ_3
f''	0	0	μ_2	μ_3
$f^{(3)}$	0	0	0	μ_3



Orthogonality?

Rodrigues formula: Orthogonal Polynomials

$$P_n(q) = \frac{1}{f(q)} \left(\frac{d}{dq}\right)^n \left[f(q) w(q)^n \right]$$

Correction function to ensure smooth contact

$$\frac{d}{dq}\left(f(q) w(q) \frac{dy}{dq} \right) - \lambda_n f(q) y = 0$$

Sturm-Liouville Equation

$$\int \frac{g(q)}{\sqrt{f(q)}} dq$$

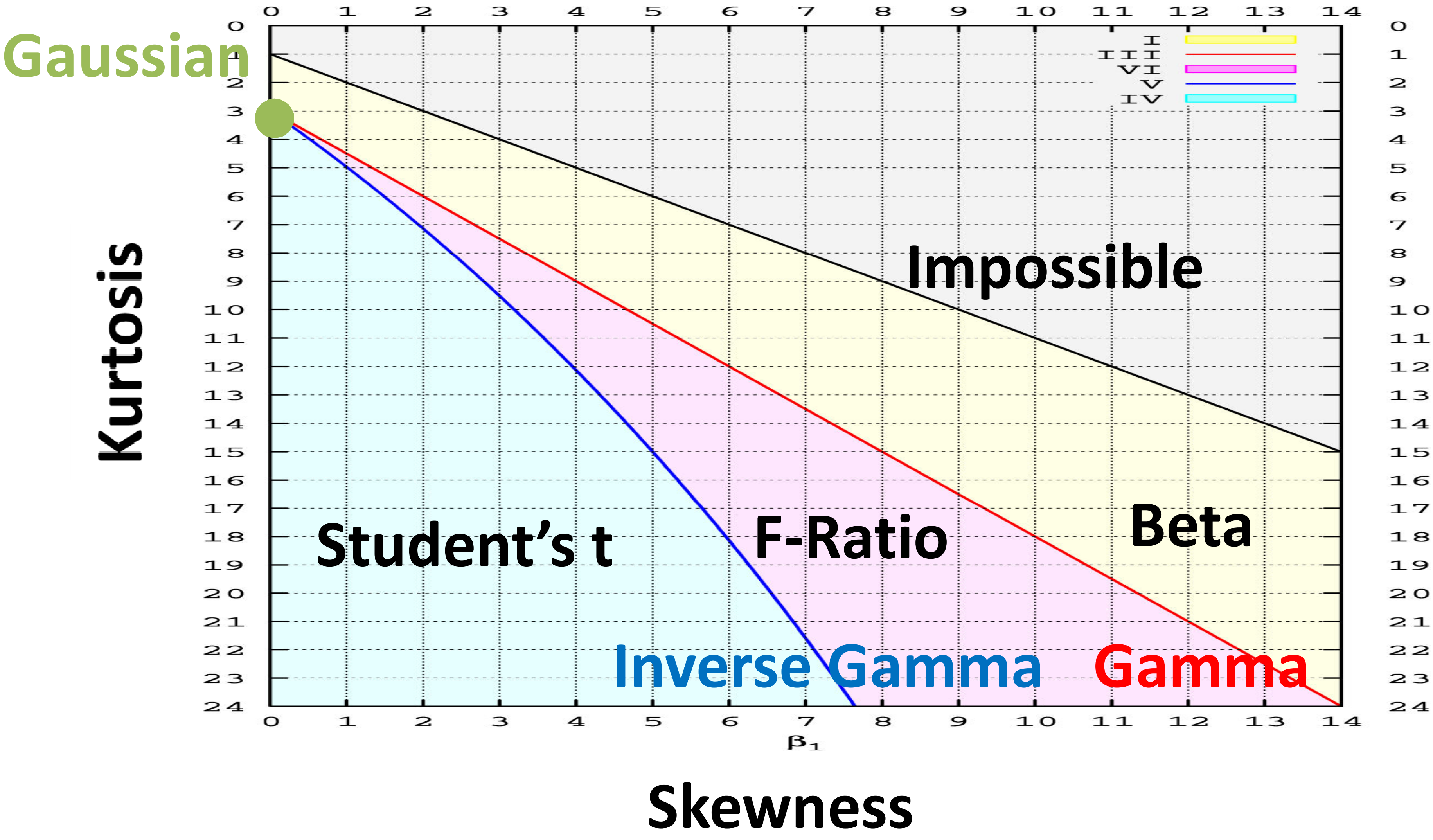
Pearson’s Differential Equation

$$
\begin{aligned}
\#_2 P_2 f &= D^2\left(f w^2\right) \\
&= f\left[w D^2 w + D\left(\#_1 P_1 w\right) + \left(\#_1 P_1\right)^2\right]
\end{aligned}
$$

If the degree of the correction function *w* is greater than 2, the last equation would be impossible.

$$
\frac{f'(q)}{f(q)} = \frac{a_0 + a_1 q}{b_0 + b_1 q + b_2 q^2} = \frac{a_0 + a_1 q}{w(q)}
$$

Pearson Family



http://en.wikipedia.org/wiki/Pearson_distribution