Correcting Polarized-Neutron Data

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A polarized-beam data point is a collection of counts taken with specified flipper-states, and with all other experimental parameters *equal*. The analyst must have discretion over what *equal* means by setting the tolerances for equality testing, to satisfy the competing needs of increased couting statistics and coordinate definition to determine the neutron-polarization dependence of a scattering cross-section. For example, if the data are collected as a function of Q(wavevector transfer) and E(energy transfer), those values must be equal for all of the counts grouped into a polarized-beam data point. Similarly, the sample temperature and sample magnetic field, including horizontal or vertical guide field direction at the sample, must be the same for all the grouped counts. Once a group of counts is identified to make up a polarized-beam data point, the counts must be scaled so that all counting times are equal (if counting against time) or all monitor counts are equal (if counting against monitor). In addition to scaling, any fast-neutron background determined for the fixed counting time or monitor counts, should be subtracted, since that background is independent of the cross-sections of interest and does not depend on the flipper-state-settings. If the counts were obtained by counting against a monitor, there is an additional correction to be made, because a beam-monitor counts higher order neutrons in the beam as well. This correction will increase the count-rate as the monitor was counting too fast by including the higher orders. The fraction of higher-order neutrons in the beam is wavelength dependent, so that this correction is very importatnt for inelastic data. It is important to note whether the monitor is before or after the He-3 polarizer, since this will determine the higher-order neutron flux on the monitor. After these corrections the polarized beam data point is ready to be corrected for the He-3 transmissions, polarized beam transport loss and flipping efficiency. These corrections all together produce values for the flipper-state dependent scattering functions S_{uu}, S_{dd}, S_{du} and S_{ud} for the given experimental parameters. Note that these scattering functions will include all scattering that is not fast-background. The possible flipper states (FS) are,uu,dd,du and ud, where uu(UP-UP) is for both flippers OFF anddu(DOWN-UP) is for the front flipper ON. These results can be further analyzed to obtain, for example, information about the moment directions in the sample or the fraction of the scattering cross-section that is magnetic in origin, based on the selection rules which produce non-spin-flip magnetic scattering when the neutron polarization is parallel to the sample magnetic moment and spin-flip magnetic scattering when the neutron polarization is perpendicular to the sample magnetic moment, and only the sample magnetic moment components perpendicular to the scattering vector produce magnetic scattering. This analysis depends on the type of magnetic system. For example, if the magnetic structure is co-linear and the moment direction is effectively isotropic as in paramagnets and some antiferromagnets, $S_{uu} = S_{dd} = S_{nsf}$ and $S_{du} = S_{ud} = S_{sf}$. If the neutron polarization is parallel to the scattering vector, Q,

$$S_{sf,Q} = \sigma_{mag} + \frac{2}{3}\sigma_{si}$$

$$S_{nsf,Q} = \frac{1}{3}\sigma_{si} + \sigma_n.$$

If the neutron polarization is perpendicular to the scattering vector, Q,

$$S_{sf,\perp} = \frac{1}{2}\sigma_{mag} + \frac{2}{3}\sigma_{si}$$

$$S_{nsf,\perp} = \frac{1}{2}\sigma_{mag} + \frac{1}{3}\sigma_{si} + \sigma_n.$$

Here, $\sigma_{mag}$is from the magnetic scattering, σ_{si} is from the nuclear-spin-incoherent scattering, and $\sigma_n$is from the nuclear coherent and nuclear-isotopic-incoherent scattering.

When He-3 is used for the creation and detection of polarized neutron beams, the time at which data is taken must be recorded. Since the He-3 polarization is time dependent with a decay time on the order of 100 hours, and counting times are on the order of 1-10 minutes, recording a start, stop or average time for the measurement should be sufficient. In order to correct the data for the transmission of He-3 cells the wavelength(energy) of the neutrons traversing the cells must also be known. Thus the information required to correct polarized beam data for a given experiment setting must include the following

$\lambda_I$orE_I	$\lambda_F$orE_f	measured-count-rate,time-stamp,FS,He-3cells	...

For each count-rate measurement the incoming and outgoing wavelength, λ_I and λ_F, (or energy) will be the same, and the time-stamp, t, flipper state (FS), and polarized-beam transmission information will be recorded. The column marked ... indicates that any number of count-rates can be recorded at the same λ_I and λ_F, provided the time-stamp, flipper-state and polarized-beam transmission information are also recorded, and all other experiment settings are the same. Typically, at least one count-rate is measured for each polarized-beam cross-section (uu,dd,du or ud) of interest. This group of polarized-beam cross-section count-rate measurements at a fixed experiment setting is referred to as a polarized-beam data point for the given experimental setting, or $D_j(N, M)$, where j indexes the experiment setting (including λ_I and λ_F and other settings such as Q, sample guide-field and sample temperature), and N is the total number of count-rates collected for M unknown polarized-beam cross-sections.

The time stamps are in the UTC UNIX-time form which is integer seconds since January 1, 1970. Also some method must be provided for determining count-rate statistical errors.

Solving for the Underlying Cross-Section Count Rates

The model for the ith measurement count-rate in a polarized-beam datapoint, $C_0^{(m_i,X_i)}$, (where the data-point dependent flipper state index m_i corresponds to one of uu, dd, du, ud and X_i represents the scattering independent variable coordinates, and the only direct change given i is the measurement time, t_i and coordinate X_i) as a function of M unknown polarized-beam scattering cross-section count-rates, $S^n\left(X_i\right)$, (where the cross-section polarization state index, n, ranges in the set uu, dd, du, ud) is given by the linear equation

$$C_0^i = C_0^{(m_i,X_i)} = \sum_{n=1}^{M} T^{(m_i)n}(t_i, \lambda_I, \lambda_F, P_\mu; X_i)\, S^n\left(X_i\right) = T^{(m_i)n} S^n.$$

$$\overrightarrow{C_0} = \overleftrightarrow{T}\,\overrightarrow{S}$$

The transmission coefficients, $T^{(m_i)n}$, are functions of P_μ, which are the parameters of the polarizing and transport devices, as well as functions of time, t_i, and neutron incident and scattered wavelengths, λ_I and λ_F, and also possibly the scattering coordinate, X_i. The simplest case is to solve for S^n with X fixed. We shall look at the more complicated case later. If the data collection produces an exactly-determined system of linear equations, with the number of independent equations equal to the number of unknowns (for example, the counts are measured once for each unknown polarization state index $n = 1, M$), then the predicted counts are replaced by the measured counts in the above equation, and the T^{mn}matrix can be inverted to obtain the solution for underlying cross-section count rates.

$$\overrightarrow{S} = \overleftrightarrow{T^{-1}}\,\overrightarrow{C_0}$$

$$S^n = \sum^{m} \left(\overleftrightarrow{T^{-1}}\right)^{nm} \left(\overrightarrow{C_0}\right)^{m}$$

Note that S are the counts observed for a perfect instrument with an identity transmission matrix.

If this system of linear equations is over-determined, with the number of independent measurements greater than the number of unknowns, M, then the solution is generated by standard linear least-squares techniques. Handling the over-detrmined case is important because repeat measurements of polarized beam data using He-3 cannot be directly averaged due to the time dependence.

If there are constraints on the S^n, they should be put into the model equation before any least squares calculations are done.

Least-Squares Case

In the least-squares case, if C^i is the *ith* measured count-rate (where we drop the associated polarization state m), then the solution for the underlying cross-sections, $S^n$is obtained by minimizing χ^2given by

$$\chi^2 = \sum_{i=1}^{N} w_i \left(C^i - C_0^i\right)^2 ,$$

where N is the number of measurements contributing to the polarized-beam data point, and where the weight, $w_i = 1/\sigma_i^2$and $\sigma_i^2 = \sigma_{Ci}^2$. For Poisson counting statistics we have $\sigma_{Ci}^2 = C^i$ so that $w_i C^i = 1$. The normal equations for the solution of S^n are

$$\frac{\partial \chi^2}{\partial S^n} = 0 = \sum_{m=1}^{M} A^{nm} S^m - B^n,$$

where

$$A^{nm} = \sum_{i=1}^{N} w_i T^{in} T^{im} = A^{mn}$$

and

$$B^n = \sum_{i=1}^{N} w_i T^{in} C^i$$

$$S^\mu = \sum_{m=1}^{M} \left(A^{-1}\right)^{\mu m} B^m.$$

To compute the uncertainty in the solution,S^α, due to statistical fluctuation of the measured counts, C^i, we can write

$$\sigma_{S^\mu}^2 = \sum_{j=1}^{N} \left(\frac{\partial S^\mu}{\partial C^j}\right)^2 \sigma_{C^j}^2$$

with

$$\frac{\partial S^\mu}{\partial C^j} = \sum_{m=1}^{M} \left(A^{-1}\right)^{\mu m} w_j T^{jm}$$

$$\left(\frac{\partial S^\mu}{\partial C^j}\right)^2 = w_j^2 \sum_{m,n=1}^{M} \left(A^{-1}\right)^{\mu m} T^{jm} \left(A^{-1}\right)^{\mu n} T^{jn}$$

$$\sigma_{S^\mu}^2 = \sum_{m,n=1}^{M} \left(A^{-1}\right)^{\mu m} \left(A^{-1}\right)^{\mu n} \sum_{j=1}^{N} w_j T^{jm} T^{jn} = \sum_{m,n=1}^{M} \left(A^{-1}\right)^{\mu m} \left(A^{-1}\right)^{\mu n} A^{mn}.$$

This is the standard least-squares result that the statistical errors in the solution are equal to the diagonal elements of the so-called error matrix,

$$\sigma_{S^\mu}^2 = \left(A^{-1}\right)^{\mu\mu}.$$

In this problem, the parameters, P_α, that determine the transmission coefficients, T^{in}, also have uncertainties. Thus we need

$$\frac{\partial S^\mu}{\partial P_\alpha} = \sum_{m=1}^{M} \frac{\partial}{\partial P_\alpha} \left(A^{-1}\right)^{\mu m} B^m + \left(A^{-1}\right)^{\mu m} \frac{\partial}{\partial P_\alpha} B^m$$

$$\left(\frac{\partial S^\mu}{\partial P_\alpha}\right)^2 = \left(\sum_{m=1}^{M} \frac{\partial}{\partial P_\alpha} \left(A^{-1}\right)^{\mu m} B^m + \left(A^{-1}\right)^{\mu m} \frac{\partial}{\partial P_\alpha} B^m\right)^2.$$

To do this analysis, we require the partial derivative of an inverse matrix element with respect to its un-inverted matrix elements. This has been treated for example in *Nuclear Instruments and Methods in Physics Research A 451 (2000) 520-528*, Propagation of errors for matrix inversion, by M. Lefebvre, R.K. Keeler, R. Sobie and J. White. The result is

$$\frac{\partial \left(T^{-1}\right)^{nm}}{\partial T_{ab}} = -T_{na}^{-1} T_{bm}^{-1}.$$

This leads to

$$\frac{\partial \left(T^{-1}\right)^{\mu m}}{\partial P_\alpha} = \sum_{ab} \frac{\partial \left(T^{-1}\right)^{\mu m}}{\partial T_{ab}} \frac{\partial T^{ab}}{\partial P_\alpha} = -\sum_{ab} T_{\mu a}^{-1} T_{bm}^{-1} \frac{\partial T^{ab}}{\partial P_\alpha}.$$

In the lease-squares case the matrix, A, and vector, B are themselves functions of the transmission coefficients, and we have

$$\frac{\partial A^{ab}}{\partial P_\alpha} = \sum_{i=1}^{N} w_i \left(\frac{\partial T^{ia}}{\partial P_\alpha} T^{ib} + T^{ia} \frac{\partial T^{ib}}{\partial P_\alpha}\right)$$

$$\frac{\partial B^m}{\partial P_\alpha} = \sum_{i=1}^{N} w_i \frac{\partial T^{im}}{\partial P_\alpha} C^i.$$

Putting this all together

$$\left(\frac{\partial S^\mu}{\partial P_\alpha}\right)^2 = \left(\sum_{m=1}^{M} (-) \sum_{ab}^{M} A_{\mu a}^{-1} A_{bm}^{-1} \frac{\partial A^{ab}}{\partial P_\alpha} B^m + \left(A^{-1}\right)^{\mu m} \sum_{i=1}^{N} w_i \frac{\partial T^{im}}{\partial P_\alpha} C^i\right)^2$$

$$= \left(-\sum_n^M S^n \sum_m^M A^{-1}_{\mu m} \sum_{i=1}^N w_i \left(\frac{\partial T^{im}}{\partial P_\alpha} T^{in} + T^{im} \frac{\partial T^{in}}{\partial P_\alpha} \right) + \sum_m^M A^{-1}_{\mu m} \sum_{i=1}^N w_i \frac{\partial T^{im}}{\partial P_\alpha} C^i \right)^2 .$$

The full covariance matrix will look like

$$cov(S^\mu, S^\nu) = \sum_{\alpha\beta} \frac{\partial S^\mu}{\partial P_\alpha} \frac{\partial S^\nu}{\partial P_\beta} cov(P_\alpha, P_\beta) = \sum_\alpha$$

$$\left(-\sum_n^M S^n \sum_m^M A^{-1}_{\mu m} \sum_{i=1}^N w_i \left(\frac{\partial T^{im}}{\partial P_\alpha} T^{in} + T^{im} \frac{\partial T^{in}}{\partial P_\alpha} \right) + \sum_m^M A^{-1}_{\mu m} \sum_{i=1}^N w_i \frac{\partial T^{im}}{\partial P_\alpha} C^i \right)$$

$$\left(-\sum_q^M S^q \sum_p^M A^{-1}_{\nu p} \sum_{j=1}^N w_j \left(\frac{\partial T^{jp}}{\partial P_\alpha} T^{jq} + T^{jp} \frac{\partial T^{jq}}{\partial P_\alpha} \right) + \sum_p^M A^{-1}_{\nu p} \sum_{j=1}^N w_j \frac{\partial T^{jp}}{\partial P_\alpha} C^j \right) \sigma^2_{P\alpha}.$$

since we expect that the parameter errors should be uncorrelated so that

$$cov(P_\alpha, P_\beta) = \delta_{\alpha\beta} \sigma^2_{P\alpha}.$$

The parameter error for S^μ comes from the diagonal part of the covariance, $cov(S^\mu, S^\mu)$. Generating the terms of the covariance, using

$$cov(T^{im}, T^{jp}) = D^{im,jp} = \sum_{\alpha\beta} \left(\partial T^{im} / \partial P_\alpha \right) \left(\partial T^{jp} / \partial P_\beta \right) cov(P_\alpha, P_\beta)$$

$$= \sum_\alpha \left(\partial T^{im} / \partial P_\alpha \right) \left(\partial T^{jp} / \partial P_\alpha \right) \sigma^2_{P\alpha}$$

$$cov(S^\mu, S^\mu) =$$

$$\sum_{n,q}^M S^n S^q \sum_{m,p}^M A^{-1}_{\mu m} A^{-1}_{\mu p} \sum_{i,j=1}^N w_i w_j \left(T^{in} T^{jq} D^{im,jp} + T^{im} T^{jp} D^{in,jq} + T^{in} T^{jp} D^{im,jq} + T^{im} T^{jq} D^{in,jp} \right)$$

$$+ \sum_{m,p}^M A^{-1}_{\mu m} A^{-1}_{\mu p} \sum_{i,j=1}^N w_i C^i w_j C^j D^{im,jp}$$

$$-2 \sum_n^M S^n \sum_{m,p}^M A^{-1}_{\mu m} A^{-1}_{\mu p} \sum_{i,j=1}^N w_i w_j C^j \left(T^{in} D^{im,jp} + T^{im} D^{in,jp} \right)$$

$$= \sum_{m,p}^{M} A^{-1}_{\mu m} A^{-1}_{\mu p} \sum_{i,j=1}^{N} w_i w_j$$

$$\left\{ \sum_{n,q}^{M} S^n S^q \left(T^{in} T^{jq} D^{im,jp} + T^{im} T^{jp} D^{in,jq} + T^{in} T^{jp} D^{im,jq} + T^{im} T^{jq} D^{in,jp} \right) + C^i C^j D^{im,jp} - 2 \sum_{n}^{M} S^n C^j \right.$$

$$cov(S^\mu, S^\nu) =$$

$$\sum_{n,q}^{M} S^n S^q \sum_{m,p}^{M} A^{-1}_{\mu m} A^{-1}_{\nu p} \sum_{i,j=1}^{N} w_i w_j \left(T^{in} T^{jq} D^{im,jp} + T^{im} T^{jp} D^{in,jq} + T^{in} T^{jp} D^{im,jq} + T^{im} T^{jq} D^{in,jp} \right)$$

$$+ \sum_{m,p}^{M} A^{-1}_{\mu m} A^{-1}_{\nu p} \sum_{i,j=1}^{N} w_i C^i w_j C^j D^{im,jp}$$

$$- \sum_{n}^{M} S^n \sum_{m,p}^{M} A^{-1}_{\mu m} A^{-1}_{\nu p} \sum_{i,j=1}^{N} w_i w_j C^j \left(T^{in} D^{im,jp} + T^{im} D^{in,jp} + T^{in} D^{ip,jm} + T^{ip} D^{in,jm} \right)$$

Note that $\partial T^{im} / \partial P_\alpha = 0$ unless the parameter, P_α, belongs to the He-3 cell (or other device) associated with data-point i. The final result for the error analysis is

$$\sigma^2_{S^\mu} = cov(S^\mu, S^\mu) = \sum_{\alpha=1}^{NP} \left(\frac{\partial S^\mu}{\partial P_\alpha} \right)^2 \sigma^2_{P^\alpha} + \left(A^{-1} \right)^{\mu\mu} .$$

Also

$$cov(A^{ab}, A^{cd}) = \sum_{i,j,m,n}^{M} \frac{\partial A^{ab}}{\partial T^{im}} \frac{\partial A^{cd}}{\partial T^{jn}} cov(T^{im}, T^{jn})$$

$$A^{nm} = \sum_{i=1}^{N} w_i T^{in} T^{im} = A^{mn}$$

$$\frac{\partial A^{ab}}{\partial T^{im}} = \delta_{m,a} w_i T^{ib} + \delta_{m,b} w_i T^{ia}$$

$$cov(A^{ab}, A^{cd}) =$$

$$\sum_{i,j,m,n}^{M} \left(\delta_{m,a} w_i T^{ib} + \delta_{m,b} w_i T^{ia} \right) \left(\delta_{n,c} w_j T^{jd} + \delta_{n,d} w_j T^{jc} \right) cov(T^{im}, T^{jn})$$

$$= \sum_{i,j}^{M} w_i w_j \left(T^{ib} T^{jd} D^{iajc} + T^{ia} T^{jc} D^{ibjd} + T^{ib} T^{jc} D^{iajd} + T^{ia} T^{jd} D^{ibjc} \right)$$

Exact Case

In the exactly determined case

$$S^{\mu} = \sum_{m=1}^{M} \left(T^{-1}\right)^{\mu m} C^{m}.$$

$$\frac{\partial S^{\mu}}{\partial C^{j}} = \left(T^{-1}\right)^{\mu j}$$

$$\frac{\partial S^{\mu}}{\partial P_{\alpha}} = \sum_{m=1}^{M} \frac{\partial}{\partial P_{\alpha}} \left(T^{-1}\right)^{\mu m} C^{m}$$

$$= -\sum_{m=1}^{M} \sum_{ab} T^{-1}_{\mu a} T^{-1}_{bm} \frac{\partial T^{ab}}{\partial P_{\alpha}} C^{m} = -\sum_{n}^{M} S^{n} \sum_{m}^{M} T^{-1}_{\mu m} \frac{\partial T^{mn}}{\partial P_{\alpha}}.$$

Here the full covariance is

$$cov(S^{\mu}, S^{\nu}) = \left\{ \sum_{\alpha} \sum_{n}^{M} S^{n} \sum_{m}^{M} T^{-1}_{\mu m} \frac{\partial T^{mn}}{\partial P_{\alpha}} \sigma_{P\alpha} \right\} \left\{ \sum_{\alpha} \sum_{n}^{M} S^{n} \sum_{m}^{M} T^{-1}_{\nu m} \frac{\partial T^{mn}}{\partial P_{\alpha}} \sigma_{P\alpha} \right\}$$

$$= \sum_{n,q}^{M} S^{n} S^{q} \sum_{m,p}^{M} T^{-1}_{\mu m} T^{-1}_{\nu p} D^{mn,pq}_{\alpha\alpha} \sigma^{2}_{P^{\alpha}}$$

and

$$\sigma^{2}_{S^{\mu}} = cov(S^{\mu}, S^{\mu}) = \sum_{\alpha=1}^{NP} \left(\frac{\partial S^{\mu}}{\partial P_{\alpha}} \right)^{2} \sigma^{2}_{P^{\alpha}} + \sum_{m}^{M} \left(T^{-1}_{\mu m}\right)^{2} \sigma^{2}_{C^{m}}.$$

Comparing the Error Analysis for the Two Cases

We would like to make a connection between the error analysis for the two cases we are considering. To that end, consider a simple example, where the constraints are $S^{dd} = S^{uu}$ and $S^{ud} = S^{du}$. Suppose we measure C^{nsf} and C^{sf} each N times, the transmission coefficients are time-independent and each time we get exactly the same counts . Then

$$A^{nm} = N w_{nsf} T^{nsf,n} T^{nsf,m} + N w_{sf} T^{sf,n} T^{sf,m} = N w_{1} T^{1n} T^{1m} + N w_{2} T^{2n} T^{2m},$$

$$B^n = Nw_{nsf}T^{nsf,n}C^{nsf} + Nw_{sf}T^{sf,n}C^{sf} = Nw_1T^{1n}C^n + Nw_2T^{2n}C^s.$$

where m and n only have the values uu and du ($n = nonspinflip$ or $s = spinflip$ in the recast notation). Then rewriting

$$A = N \begin{bmatrix} w_n (T^{nn})^2 + w_s (T^{sn})^2 & w_nT^{nn}T^{ns} + w_sT^{sn}T^{ss} \\ w_nT^{nn}T^{ns} + w_sT^{sn}T^{ss} & w_n (T^{ns})^2 + w_s (T^{ss})^2 \end{bmatrix} = \begin{bmatrix} A^{nn} & A^{ns} \\ A^{sn} & A^{ss} \end{bmatrix}$$

$$B = N \begin{bmatrix} w_nT^{nn}C^n + w_sT^{sn}C^s \\ w_nT^{ns}C^n + w_sT^{ss}C^s \end{bmatrix}$$

Now we can calculate the determinant of A, using $\|T\| = D = T^{nn}T^{ss} - T^{ns}T^{sn}$

$$\|A\| = N^2 w_n w_s D^2$$

and we know the inverse of the two-by-two matrix is

$$A^{-1} = \begin{bmatrix} A^{ss} & -A^{ns} \\ -A^{sn} & A^{nn} \end{bmatrix} / \|A\|.$$

statistical error comparison

Using the preceeding example, find that the least-squares statistical errors are given by

$$\sigma^2_{Snsf} = A^{-1}_{11} = \frac{1}{ND^2} \left\{ (T^{ns})^2 / w_s + (T^{ss})^2 / w_n \right\}$$

$$\sigma^2_{Ssf} = A^{-1}_{22} = \frac{1}{ND^2} \left\{ (T^{nn})^2 / w_s + (T^{sn})^2 / w_n \right\}.$$

In the exact case of measuring $S^{dd} = S^{uu}$ and $S^{ud} = S^{du}$ each once, the statistical errors would be

$$\sigma^2_{Snsf} = \left(T^{-1}_{11}\right)^2 \sigma^2_{Cnsf} + \left(T^{-1}_{12}\right)^2 \sigma^2_{Csf}$$

$$\sigma^2_{Ssf} = \left(T^{-1}_{21}\right)^2 \sigma^2_{Cnsf} + \left(T^{-1}_{22}\right)^2 \sigma^2_{Csf}.$$

Since the exact-case matrix is

$$T = \begin{bmatrix} T^{nn} & T^{ns} \\ T^{sn} & T^{ss} \end{bmatrix}$$

the inverse is

$$T^{-1} = \begin{bmatrix} T^{ss} & -T^{ns} \\ -T^{sn} & T^{nn} \end{bmatrix} / D.$$

Substituting, find the exact case statistical errors

$$\sigma^2_{Snsf} = \left(T^{-1}_{11}\right)^2 \sigma^2_{Cnsf} + \left(T^{-1}_{12}\right)^2 \sigma^2_{Csf} = \frac{1}{D^2}\left\{\left(T^{ss}\right)^2 \sigma^2_{Cnsf} + \left(T^{ns}\right)^2 \sigma^2_{Csf}\right\}$$

$$\sigma^2_{Ssf} = \left(T^{-1}_{21}\right)^2 \sigma^2_{Cnsf} + \left(T^{-1}_{22}\right)^2 \sigma^2_{Csf} = \frac{1}{D^2}\left\{\left(T^{sn}\right)^2 \sigma^2_{Cnsf} + \left(T^{nn}\right)^2 \sigma^2_{Csf}\right\}.$$

We see that the statistical errors in the two cases, are matched when $N = 1$ (both cross-sections are measured once), although the least-squares problem becomes singular for $N = 1$. This just shows that the square of the statistical uncertainty in the results is reduced by $1/N$.

parameter error comparison

For simplicity, assume that there is a single parameter, but that each of the four transmission coefficients depends on it. We need to take the least-squares expression for the parameter error and modify it for the preceeding example. We had

$$\left(\frac{\partial S^\alpha}{\partial P_\mu}\right)^2 = \left(-\sum_b^M S^b \sum_a^M A^{-1}_{\alpha a} \sum_{i=1}^N w_i \left(\frac{\partial T^{ia}}{\partial P_\mu} T^{ib} + T^{ia}\frac{\partial T^{ib}}{\partial P_\mu}\right) + \sum_a^M A^{-1}_{\alpha a} \sum_{i=1}^N w_i \frac{\partial T^{ia}}{\partial P_\mu} C^i\right)^2.$$

First modfiy the sums over data-points for our example

$$\sum_{i=1}^N w_i \left(\frac{\partial T^{ia}}{\partial P_\mu} T^{ib} + T^{ia}\frac{\partial T^{ib}}{\partial P_\mu}\right) \to N w_n \left(\frac{\partial T^{na}}{\partial P} T^{nb} + T^{na}\frac{\partial T^{nb}}{\partial P}\right) + N w_s \left(\frac{\partial T^{sa}}{\partial P} T^{sb} + T^{sa}\frac{\partial T^{sb}}{\partial P}\right)$$

$$\sum_{i=1}^N w_i \frac{\partial T^{ia}}{\partial P_\mu} C^i \to N w_n \frac{\partial T^{na}}{\partial P} C^n + N w_s \frac{\partial T^{sa}}{\partial P} C^s$$

We also need the expressions for A^{-1} matrix elements which can be tabulated from the preceeding, using $\|T\| = D = T^{nn}T^{ss} - T^{ns}T^{sn}$,

$$A^{-1}_{11} = \frac{1}{ND^2}\left(\left(T^{ns}\right)^2/w_s + \left(T^{ss}\right)^2/w_n\right)$$

$$A^{-1}_{22} = \frac{1}{ND^2}\left(\left(T^{nn}\right)^2/w_s + \left(T^{sn}\right)^2/w_n\right)$$

$$A^{-1}_{12} = A^{-1}_{21} = -\frac{1}{ND^2}\left(T^{nn}T^{ns}/w_s + T^{sn}T^{ss}/w_n\right)$$

We have already written down B for this example

$$B = N \left[\begin{array}{c} w_n T^{nn} C^n + w_s T^{sn} C^s \\ w_n T^{ns} C^n + w_s T^{ss} C^s \end{array} \right]$$

so we can now solve for S^n and S^s.

$$S^n = \left(T^{ss} C^n - T^{ns} C^s\right) / D$$

$$S^s = \left(-T^{sn} C^n + T^{nn} C^s\right) / D.$$

We see that we get exactly the same solution as in the exact case (as we must since all the counts are the same). Now plugging in the solutions for S and A^{-1} and the data-point sums we have

$$\frac{\partial S^\alpha}{\partial P_\mu} = -\sum_b^M S^b \sum_a^M A^{-1}_{\alpha a} \sum_{i=1}^N w_i \left(\frac{\partial T^{ia}}{\partial P_\mu} T^{ib} + T^{ia} \frac{\partial T^{ib}}{\partial P_\mu} \right) + \sum_a^M A^{-1}_{\alpha a} \sum_{i=1}^N w_i \frac{\partial T^{ia}}{\partial P_\mu} C^i$$

Define the sum terms,

$$K^{nn} = 2 w_n \frac{\partial T^{nn}}{\partial P} T^{nn} + 2 w_s \frac{\partial T^{sn}}{\partial P} T^{sn}$$

$$K^{sn} = w_n \left(\frac{\partial T^{ns}}{\partial P} T^{nn} + T^{ns} \frac{\partial T^{nn}}{\partial P} \right) + w_s \left(\frac{\partial T^{ss}}{\partial P} T^{sn} + T^{ss} \frac{\partial T^{sn}}{\partial P} \right)$$

$$K^{ns} = w_n \left(\frac{\partial T^{nn}}{\partial P} T^{ns} + T^{nn} \frac{\partial T^{ns}}{\partial P} \right) + w_s \left(\frac{\partial T^{sn}}{\partial P} T^{ss} + T^{sn} \frac{\partial T^{ss}}{\partial P} \right)$$

$$K^{ss} = 2 w_n \frac{\partial T^{ns}}{\partial P} T^{ns} + 2 w_s \frac{\partial T^{ss}}{\partial P} T^{ss}$$

Then write out the terms for $\partial S^n / \partial P$,

$$\frac{\partial S^n}{\partial P} = -\frac{1}{D} \left(T^{ss} C^n - T^{ns} C^s\right) \left\{ \frac{1}{D^2} \left(\left(T^{ns}\right)^2 / w_s + \left(T^{ss}\right)^2 / w_n \right) K^{nn} \right\}$$

$$\frac{1}{D} \left(T^{ss} C^n - T^{ns} C^s\right) \left\{ \frac{1}{D^2} \left(T^{nn} T^{ns} / w_s + T^{sn} T^{ss} / w_n\right) K^{sn} \right\}$$

$$-\frac{1}{D} \left(-T^{sn} C^n + T^{nn} C^s\right) \left\{ \frac{1}{D^2} \left(\left(T^{ns}\right)^2 / w_s + \left(T^{ss}\right)^2 / w_n \right) K^{ns} \right\}$$

$$\frac{1}{D} \left(-T^{sn} C^n + T^{nn} C^s\right) \left\{ \frac{1}{D^2} \left(T^{nn} T^{ns} / w_s + T^{sn} T^{ss} / w_n\right) K^{ss} \right\}$$

$$\frac{1}{D^2}\left(\left(T^{ns}\right)^2/w_s+\left(T^{ss}\right)^2/w_n\right)\left[w_n\frac{\partial T^{nn}}{\partial P}C^n+w_s\frac{\partial T^{sn}}{\partial P}C^s\right]$$

$$-\frac{1}{D^2}\left(T^{nn}T^{ns}/w_s+T^{sn}T^{ss}/w_n\right)\left[w_n\frac{\partial T^{ns}}{\partial P}C^n+w_s\frac{\partial T^{ss}}{\partial P}C^s\right]$$

Note that for $\partial S^s/\partial P$, the only change is in the first index of A^{-1}. These expressions can be simplified using $D^{ab}=\partial T^{ab}/\partial P$,

$$D^2\frac{\partial S^n}{\partial P}=C^s\left\{T^{ns}\left(T^{nn}D^{ss}-T^{ns}D^{sn}+T^{ss}D^{nn}\right)-T^{nn}T^{ss}D^{ns}\right\}$$

$$+C^n\left\{T^{ss}\left(T^{ns}D^{sn}-T^{ss}D^{nn}+T^{sn}D^{ns}\right)-T^{ns}T^{sn}D^{ss}\right\}$$

$$D^2\frac{\partial S^s}{\partial P}=C^s\left\{T^{nn}\left(T^{ns}D^{sn}-T^{nn}D^{ss}+T^{sn}D^{ns}\right)-T^{ns}T^{sn}D^{nn}\right\}$$

$$+C^n\left\{T^{sn}\left(T^{nn}D^{ss}-T^{sn}D^{ns}+T^{ss}D^{nn}\right)-T^{nn}T^{ss}D^{sn}\right\}.$$

In the exact case this error due to a parameter was

$$\frac{\partial S^\alpha}{\partial P_\mu}=-\sum_n^M S^n\sum_m^M T^{-1}_{\alpha m}\frac{\partial T^{mn}}{\partial P_\mu}$$

and the inverse of the transmission coefficient matrix was

$$T^{-1}=\begin{bmatrix}T^{ss} & -T^{ns}\\ -T^{sn} & T^{nn}\end{bmatrix}/D.$$

Plugging in for S^n and T^{-1} we find

$$\frac{\partial S^n}{\partial P_\mu}=-S^n\left\{T^{-1}_{nn}\frac{\partial T^{nn}}{\partial P}+T^{-1}_{ns}\frac{\partial T^{sn}}{\partial P}\right\}-S^s\left\{T^{-1}_{nn}\frac{\partial T^{ns}}{\partial P}+T^{-1}_{ns}\frac{\partial T^{ss}}{\partial P}\right\}$$

$$=-\frac{1}{D}\left(T^{ss}C^n-T^{ns}C^s\right)\left\{T^{-1}_{nn}\frac{\partial T^{nn}}{\partial P}+T^{-1}_{ns}\frac{\partial T^{sn}}{\partial P}\right\}-\frac{1}{D}\left(-T^{sn}C^n+T^{nn}C^s\right)\left\{T^{-1}_{nn}\frac{\partial T^{ns}}{\partial P}+T^{-1}_{ns}\frac{\partial T^{ss}}{\partial P}\right\}$$

$$=-\frac{1}{D}\left(T^{ss}C^n-T^{ns}C^s\right)\left\{\frac{T^{ss}}{D}\frac{\partial T^{nn}}{\partial P}-\frac{T^{ns}}{D}\frac{\partial T^{sn}}{\partial P}\right\}-\frac{1}{D}\left(-T^{sn}C^n+T^{nn}C^s\right)\left\{\frac{T^{ss}}{D}\frac{\partial T^{ns}}{\partial P}-\frac{T^{ns}}{D}\frac{\partial T^{ss}}{\partial P}\right\}$$

$$\frac{\partial S^s}{\partial P_\mu}=-S^n\left\{T^{-1}_{sn}\frac{\partial T^{nn}}{\partial P}+T^{-1}_{ss}\frac{\partial T^{sn}}{\partial P}\right\}-S^s\left\{T^{-1}_{sn}\frac{\partial T^{ns}}{\partial P}+T^{-1}_{ss}\frac{\partial T^{ss}}{\partial P}\right\}$$

$$= -\frac{1}{D}\left(T^{ss}C^n - T^{ns}C^s\right)\left\{T^{-1}_{sn}\frac{\partial T^{nn}}{\partial P} + T^{-1}_{ss}\frac{\partial T^{sn}}{\partial P}\right\} - \frac{1}{D}\left(-T^{sn}C^n + T^{nn}C^s\right)\left\{T^{-1}_{sn}\frac{\partial T^{ns}}{\partial P} + T^{-1}_{ss}\frac{\partial T^{ss}}{\partial P}\right\}$$

$$= -\frac{1}{D}\left(T^{ss}C^n - T^{ns}C^s\right)\left\{-\frac{T^{sn}}{D}\frac{\partial T^{nn}}{\partial P} + \frac{T^{nn}}{D}\frac{\partial T^{sn}}{\partial P}\right\} - \frac{1}{D}\left(-T^{sn}C^n + T^{nn}C^s\right)\left\{-\frac{T^{sn}}{D}\frac{\partial T^{ns}}{\partial P} + \frac{T^{nn}}{D}\frac{\partial T^{ss}}{\partial P}\right\}$$

$$D^2\frac{\partial S^n}{\partial P_\mu} = C^n\left\{T^{ss}(-T^{ss}D^{nn} + T^{ns}D^{sn} + T^{sn}D^{ns}) - T^{sn}T^{ns}D^{ss}\right\}$$

$$+C^s\left\{T^{ns}\left(T^{ss}D^{nn} - T^{ns}D^{sn} + T^{nn}D^{ss}\right) - T^{nn}T^{ss}D^{ns}\right\}$$

$$D^2\frac{\partial S^s}{\partial P_\mu} = C^n\left\{T^{sn}(T^{ss}D^{nn} - T^{sn}D^{ns} + T^{nn}D^{ss}) - T^{ss}T^{nn}D^{sn}\right\}$$

$$+C^s\left\{T^{nn}\left(T^{ns}D^{sn} + T^{sn}D^{ns} - T^{nn}D^{ss}\right) - T^{ns}T^{sn}D^{nn}\right\}$$

the exact same expression as in the least-squares case. Note that the errors due to parameter uncertainty cannot be decreased with better counting statistics.

Matrix Inversion and Constraints

There are a number of techniques to perform the necessary matrix inversion. For example, determinants can be used to solve the equations, where the inverse is

$$T^{-1} = adj\,T/det\,T,$$

$$(adj\,T)^{nm} = U^{mn} = (-1)^{m+n} det\,T(m|n),$$

$$|T| = det\,T = \sum_i T^{in}U^{in}.$$

Also $det\,T(m|n)$ is the determinant of T with the mth row and nth column excluded. This leads to a recursive algorithm for obtaining the inverse T^{-1}. Note also that because the cofactor of a matrix element does not depend on that matrix element,

$$\frac{\partial\,|T|}{\partial T^{ab}} = U^{ab}.$$

This means that the uncertainty in the determinant is given by

$$\sigma_{|T|}^2 = \sum_{abcd} U^{ab} U^{cd} cov(T^{ab}, T^{cd}).$$

Alternatively, a numerical matrix inversion algorithm could be used (e.g. LU, QR or SVD decomposition) but for matrices limited to 4x4 the algebraic inversion is accurate and efficient. The determinant and SVD methods have specific ways to determine if a solution cannot be found, which means that the matrix to be inverted is rank-deficient or not invertible to some degree of accuracy. For example, the determinant method produces the cofactors necessary for calculating the uncertainty in the determinant (relevant for determining how close the uncertainties bring the matrix to singularity).

Now the uncertainties in the solution must be addressed. First of all, using known constraints on the scattering cross-sections can reduce the uncertainties in their solution. For example, as is often the case, $S^{du} = S^{ud}$. Thus, the data analysis may add linear constraints of the form

$$S^k = 0 + \sum_{n=free} a_{kn} S^n.$$

This reduces the number of unknowns by the number of constraint equations and changes the effective coefficients, so that

$$C_0^i = \sum_{n=free} \left(T^{in} + \sum_{k=cnst} a_{kn} T^{ik} \right) S^n = \sum_{n=free} \bar{T}^{in}\, S^n.$$

The resulting constrained coefficients, $\bar{T}^{in}$, are just linear combinations of the original coefficients at the same measurement point index, i. Thus when there are constraints, $T^{in} \to \overline{T}^{in}$. These become the coefficients used in the least-squares treatment.

The uncertainties in the count-rates, $C_i^m \pm \sigma_i^2$, and possible uncertainties in the transmission coefficient parameters, $P \pm \sigma_P$, must be taken into account to determine the uncertainty in the result, $S^n \pm \sigma_{S^n}$.

$$cov(C^\mu, C^\nu) = \delta^{\mu\nu} \sigma_{C^\mu}^2$$

This error propagation correctly handles the correlations between elements of the inverse matrix through their dependence on the original matrix elements. If the functional parameters of the transmission coefficients can be assumed to be independent then

$$cov(T^{ab}, T^{cd}) = \sum_{\gamma}^{L(a,c)} \frac{\partial T^{ab}}{\partial P_\gamma} \frac{\partial T^{cd}}{\partial P_\gamma} \sigma_{P_\gamma}^2 = D^{abcd},$$

where $L(a,c)$ is the number of independent parameters describing the coefficients T^{ab} and T^{cd}. L depends only on a and c since every coeficient in a given row of T depends on the same set of parameters. Recall that when there are constraints

$$T^{mn} \to \bar{T}^{mn} = T^{mn} + \sum_{k=cnst} a_{kn} T^{mk},$$

so that

$$\frac{\partial \bar{T}^{mn}}{\partial P_\gamma} = \frac{\partial T^{mn}}{\partial P_\gamma} + \sum_{k=cnst} a_{kn} \frac{\partial T^{mk}}{\partial P_\gamma}.$$

All of these coefficients are in the same row and so depend on the same set of parameters P_γ.

Finally, the covariance for the constrained S is

$$cov(S^k, S^k) = \sum_{i,j} \frac{\partial}{\partial S_i} \sum_{n=free} a_{kn} S^n \frac{\partial}{\partial S_j} \sum_{n=free} a_{kn} S^n cov(S^i, S^j).$$

or

$$cov(S^k, S^k) = \sum_{i,j=free} a_{ki} a_{kj} cov(S^i, S^j).$$

Invariably, there is only a single free S involved in a constraint, so take

$$cov(S^k, S^k) = \sum_{j=free} a_{kj}^2 \sigma_{S^j}^2.$$

In order to include the parameter errors in the calculation of the result uncertainty, it is necessary to calculate D^{iajb}. That is, given two measurement indices, i and j, which parameters, P_μ, do the transmission coefficients T_i and T_j have in common? This depends on which He-3 cells were used in common. Note that even when constraints on S are used, each row of T or A still depends on the same He-3 cells. To handle this, the data analysis will determine which He-3 cells were used for each measurement.

Generating the transmission coefficients, $T^{i(m)n}(t, \lambda_I, \lambda_F, P_\mu)$, and their uncertainties requires information about the He-3 cells and the polarized beam transport. In order to make this information available for correcting polarized-beam data, and to archive that information, an ASCII file containing one line for each He-3 cell setup used during an experiment is prepared. The fields in each line follow the format used in the He3logger spreadsheet application (Excel or open-office) as follows:

$name$	$PorA$	$iDate$	$iTime$	$iUNIXtime$	$E(meV)$	$lambda$
Zinfandel	P	01/01/08	00:00	1199163600	14.7	2.359

$iPol$	$iPolErr$	$T(hr)$	$Terr(hr)$	$A(cm)$	nsL	$nsLerr$
0.75	0.01	120	5	8	3.023	0

$trans$	$tErr$	$flip$	$fErr$	$tEmpty$	$tESlope$
1	0	1	0	0.86	0

$Pbar$	Lcm	$Diacm$	$rCRVcm$	$volcc$	$nsL0$	$nsL0err$	$nsLE$	$nsLEerr$
1.92	8.9	11.6	25	950	1.28	0	3.023	0

$resolName$	$Hmos'$	$Vmos'$	$dspA$	$Hcols'$	$Hcol2'$	$VcolsDeg$	$Vcol2Deg$
coarse	40	40	3.3542	40	40	2	2

$omRad$	$Hsig^2$	$Vsig^2$	$Xsig^2$	$curvCor$	$angCor$
0.3593	0.0001	0.0006	0.0005	1.0	0.822

$PorA$ indicates whether the cell was used as a polarizer or analyzer. $iDate$ and $iTime$ are the cell installation date and time with $iUNIXtime$ the equivalent UNIX time in seconds. $E(meV)$ and $lambda$ are the elastic condition neutron energy and equivalent wavelength used for flipping ratios and transmission measurements during the experiment and for the neutron measurement of nsL. $iPol$ is the initial installation He-3 polarization determined by transmission and NMR measurements, along with its error $iPolErr$. $T(hr)$ is the beam line decay time constant and $Terr(hr)$ its error. $A(cm2)$ is the beam cross-sectional area in the He-3 cell used to make small corrections to the effective nsL. nsL(dimensionless) is the beam-Area corrected $nsLE$ which is the wavelength corrected $nsL0$(dimensionless), which is the He-3 gas number density, times 1/2 the absorption cross-section for 1 Angstrom neutrons with spin opposite to the He-3 spin, times the path length through the He-3 gas. Using $\tau_\lambda = (1 - A/L/rCRV)(nsL0)\lambda$, the expression for the transmission of the two spin states of the neutron through the He-3 cell is

$$t_\pm = C_\pm t_E \exp\left(-\tau_\lambda[1 \mp P_{He3}]\right) \tag{1}$$

(- refers to the preferred transmission state) where t_E is the glass-only transmission, P_{He3} is the time dependent He-3 polarization, and $C_\pm$is a small correction coefficient depending on variation in path-length and wavelength. $trans$ is the transport efficiency associated with the pre-sample beam path (cell P) or post-sample beam path (cell A) and with error $tErr$. $flip$ is the flipper efficiency associated with the same beam path segment and $fErr$ is its error. $tEmp$ is the glass only transmission for neutrons at the $lambda$ wavelength and $tESlope$ gives the linear wavelength dependence of this transmission. $Pbar$ is the cell pressure in bars. Lcm is the maximal (straight through) gas thickness of the cell. $Diacm$ is the cell diameter which is the dimension perpendicular to the beam (for informational purposes only). $rCRVcm$ is the end window radius of curvature. $volcc$ is the cell gas volume in cm cubed. $nsL0$, $nsL0err$, $nsLE$, $nsLEerr$ were previously defined.

The information after the $resolName$ field describes the angular divergences of the spectrometer and is used to calculate the near unity correction coefficients $C_\pm$. In particular, $Hmos'$ and $Vmos'$ are the horizontal and vertical mosaics in minutes of the spectrometer crystal associated with the P or A beam path, $dspA$ is the d-spacing in Angstroms of that crystal. $Hcols'$ is the horizontal collimation in minutes on the sample side of the He-3 cell and $Hcol2'$ is the horizontal collimation on the other side of the cell. $VcolsDeg$ and $Vcol2Deg$ are the corresponding vertical collimations in degrees. $omRad$ is the spectrometer crystal setting angle in radians satisfying Bragg's law at the elastic condition energy $E(meV)$. $Hsig^2$, $Vsig^2$ and $Xsig^2$are calculated in the spreadsheet from the spectrometer divergence angles and are then used in the calculation of the correction coefficients $C_{\pm}$. $curvCor$ is the correction to nsL due to cell beam-Area. Note that the beam divergence parameters may be changed during an experiment, which means an additional line in the He-3 cell log must be prepared.

If you examine section 7 of the He3SpinTransport.pdf document, you will see that the corrections for pathlength variation are different than for the triple-axis case. We can use the same ascii configuration to handle the SANS case by redefining the meaning of some of the parameters. Thus if $dsp > 10$ or $Hmos <= 0$ a SANS correction will be performed instead of triple-axis. The dsp value is now the distance from sample to He-3 cell center in cm. $Hcols$ is now the detector distance (in m or cm), and $Hcol2$ is the wavelength spread $\Delta\lambda/\lambda$.

Typically only the total transport efficiency along the beam path can be measured, so that the individual transport efficiencies before and after the sample are estimated as the square-root of the total. The method for measuring both transport and flipper efficiencies is described in a separate document, *He3SpinTransport*. That document also contains the details of calculating the transmission coefficients $T_n^m(t_m, \lambda_I, \lambda_F, P_\mu)$ and their uncertainties. Note that the efficiencies may vary during data collection so that in the future provisions may be added to take this change into account.

The actual data correction procedure would begin by identifying the data files for each measured count-rate (uu, dd, du, ud). This will allow the grouping of all measured count-rates for a given experimental setting (including the sample guide field orientation). The data correction requires that all of the data are normalized for the same incident flux via beam monitoring or equal counting time for elastic data. Besides the cell information file, the only other information required is whether the data are counted using a beam monitor before or after the polarizer cell, or just using equal times. When using a beam monitor the amount of higher order wavelength contamination in the incident beam is required, and the correction software has several choices for this. Other data correction options include constraints on the cross-sections (e.g. $S^{du} = S^{ud}$).

What magnitude is expected for the extracted cross-section results? If the He-3 cells are perfectly polarized with a large nsL so that the preferred spin state has transmission unity and the non-preferred spin state has transmission zero, and there are no transport losses, then the extracted cross-section results will be exactly twice the input counts (with normalization against the unpolarized beam before the polarizer). The factor of two is due to the fact the perfect polarizer perfectly transmits only the preferred spin-state. As the He-3 cell transmissions become less ideal the extracted cross-sections will increase in magnitude compared to the measured counts.

Correcting Polarized-Beam Using Known Correlations

Often the X (scattering coordinate) dependence of the polarized-beam cross-section is known from previous experiments. Including the X dependence in the polarized-beam data analysis only makes sense if the X dependence of the polarized-beam cross-sections can be parameterized in a relatively simple way. Also we don't want to add more free parameters than measurments. Consider fitting polarized beam data at different values of X. Now the least squares problem at first looks the same, where C_0^i is the model value for datapoint counts C^i,

$$\chi^2 = \sum_{i=1}^{N} w_i \left(C^i - C_0^i\right)^2 ,$$

except that now the independent parameters include those that describe the X dependence of $S^n(X)$. One could take, for example, single Gaussian functions with flat background to describe the X dependence for the measured polarized-beam cross-sections.

$$S^n(X_i) = G^n(X_i, Q^n) + S^n_{bg}$$

where the Gaussian has height, S^n, position, Q^n_{x0} and standard deviation width, Q^n_σ

$$G^n(X_i, Q^n) = S^n \exp\left(-\frac{1}{2}\frac{(X_i - Q^n_{x0})^2}{(Q^n_{x\sigma})^2}\right) = S^n f^n(X_i)$$

where

$$f^n(X_i) = \exp\left(-\frac{1}{2}\frac{(X_i - Q^n_{x0})^2}{(Q^n_{x\sigma})^2}\right)$$

$$C_0^{(m_i,X_i)} = \sum_{n=1}^{M} T^{(m_i)n}(t_i, \lambda_I, \lambda_F, P_\mu; X_i)\, S^n(X_i) \,.$$

Note that without a parameterized background this model will force a partial Gaussian peak shape to fit the data. The peak width parameter could be made very large to approximate a flat background and the fitting with a peak or just background could be compared through chi-squared. Look at the case with a background parameter, where the positions and widths of the Gaussian functions are all fixed, so that problem is still linear equations with the model function,

$$C_0^{(m_i,X_i)} = \sum_{n=1}^{M} T^{(m_i)n}(t_i, \lambda_I, \lambda_F, P_\mu; X_i)\, \left[f^n(X_i)\, S^n + S^n_{bg}\right] .$$

$$\chi^2 = \sum_{i=1}^{N} w_i \left(C^i - \sum_{n=1}^{M} T^{(m_i)n}(t_i, \lambda_I, \lambda_F, P_\mu; X_i) \; \left[f^n \left(X_i \right) S^n + S^n_{bg} \right] \right)^2 ,$$

In this expression, it is usefule to divide the sum over measurement points i, into a sum over polarized-beam cross-sections, m, and a sub-sum over the X_i values for the given m.

$$\chi^2 = \sum_{m=1}^{M} \sum_{X_i(m)}^{N_{X(m)}} w \left(X_i \left(m \right) \right) \left(C^i - \sum_{n=1}^{M} T^{(m)n}(t_i, \lambda_I, \lambda_F, P_\mu; X_i \left(m \right)) \; \left[f^n \left(X_i \left(m \right) \right) S^n + S^n_{bg} \right] \right)^2 ,$$

The derivatives of χ^2 are needed to solve this equation,

$$\frac{\partial \chi^2}{\partial S^n} = 0 = \sum_{m=1}^{M} \sum_{X_i(m)}^{N_{X(m)}} w \left(X_i \left(m \right) \right) \left(C^i - \sum_{n'=1}^{M} T^{(m)n'}(t_i, \lambda_I, \lambda_F, P_\mu; X_i \left(m \right)) \; \left[f^{n'} \left(X_i \left(m \right) \right) S^{n'} + S^{n'}_{bg} \right] \right) (-)\, T$$

$$\frac{\partial \chi^2}{\partial S^n_{bg}} = 0 = \sum_{m=1}^{M} \sum_{X_i(m)}^{N_{X(m)}} w \left(X_i \left(m \right) \right) \left(C^i - \sum_{n'=1}^{M} T^{(m)n'}(t_i, \lambda_I, \lambda_F, P_\mu; X_i \left(m \right)) \; \left[f^{n'} \left(X_i \left(m \right) \right) S^{n'} + S^{n'}_{bg} \right] \right) (-)$$

Using the Gaussian weighted transmission

$$F^{(m)n} \left(X_i \left(m \right) \right) = T^{(m)n}(X_i \left(m \right)) \, f^n \left(X_i \left(m \right) \right) ,$$

for each m the sums over $X_i \left(m \right)$ in each term can be done to produce the following coeficients,

$$B^{(m)n}_{CF} = \sum_{X_i(m)}^{N_{X(m)}} w \left(X_i \left(m \right) \right) C^{(m, X_i(m))} F^{(m)n} \left(X_i \left(m \right) \right)$$

$$A^{(m)n'n}_{FF} = \sum_{X_i(m)}^{N_{X(m)}} w \left(X_i \left(m \right) \right) F^{(m)n'} \left(X_i \left(m \right) \right) F^{(m)n} \left(X_i \left(m \right) \right)$$

$$A^{(m)n'n}_{TF} = \sum_{X_i(m)}^{N_{X(m)}} w \left(X_i \left(m \right) \right) T^{(m)n'} \left(X_i \left(m \right) \right) F^{(m)n} \left(X_i \left(m \right) \right)$$

$$B^{(m)n}_{CT} = \sum_{X_i(m)}^{N_{X(m)}} w \left(X_i \left(m \right) \right) C^{(m, X_i(m))} T^{(m)n} \left(X_i \left(m \right) \right)$$

$$A_{FT}^{(m)n'n} = \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) F^{(m)n'}\left(X_i\left(m\right)\right) T^{(m)n}\left(X_i\left(m\right)\right) = A_{TF}^{(m)nn'}$$

$$A_{TT}^{(m)n'n} = \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) T^{(m)n'}\left(X_i\left(m\right)\right) T^{(m)n}\left(X_i\left(m\right)\right)$$

Then

$$\frac{\partial\chi^2}{\partial S^n} = 0 = \sum_{m=1}^{M}\left\{\sum_{n'=1}^{M} A_{FF}^{(m)n'n} S^{n'} + \sum_{n'=1}^{M} A_{TF}^{(m)n'n} S_{bg}^{n'} - B_{CF}^{(m)n}\right\}$$

$$\frac{\partial\chi^2}{\partial S_{bg}^n} = 0 = \sum_{m=1}^{M}\left\{\sum_{n'=1}^{M} A_{FT}^{(m)n'n} S^{n'} + \sum_{n'=1}^{M} A_{TT}^{(m)n'n} S_{bg}^{n'} - B_{CT}^{(m)n}\right\}$$

and doing the sums over m cross-sections, and noting that $w\left(m, X_i\left(m\right)\right) = 1/C^{(m,X_i(m))}$except when C==0

$$B_{CF}^{n} = \sum_{m=1}^{M} B_{CF}^{(m)n} = \sum_{m=1}^{M}\sum_{X_i(m)}^{N_{X(m)}} w\left(m, X_i\left(m\right)\right) C^{(m,X_i(m))} F^{(m)n}\left(X_i\left(m\right)\right)$$

$$A_{FF}^{n'n} = \sum_{m=1}^{M} A_{FF}^{(m)n'n} = \sum_{m=1}^{M}\sum_{X_i(m)}^{N_{X(m)}} w\left(m, X_i\left(m\right)\right) F^{(m)n'}\left(X_i\left(m\right)\right) F^{(m)n}\left(X_i\left(m\right)\right) = A_{FF}^{nn'}$$

$$A_{TF}^{n'n} = \sum_{m=1}^{M} A_{TF}^{(m)n'n} = \sum_{m=1}^{M}\sum_{X_i(m)}^{N_{X(m)}} w\left(m, X_i\left(m\right)\right) T^{(m)n'}\left(X_i\left(m\right)\right) F^{(m)n}\left(X_i\left(m\right)\right)$$

$$B_{CT}^{n} = \sum_{m=1}^{M} B_{CT}^{(m)n} = \sum_{m=1}^{M}\sum_{X_i(m)}^{N_{X(m)}} w\left(m, X_i\left(m\right)\right) C^{(m,X_i(m))} T^{(m)n}\left(X_i\left(m\right)\right)$$

$$A_{FT}^{n'n} = \sum_{m=1}^{M} A_{FT}^{(m)n'n} = \sum_{m=1}^{M}\sum_{X_i(m)}^{N_{X(m)}} w\left(m, X_i\left(m\right)\right) F^{(m)n'}\left(X_i\left(m\right)\right) T^{(m)n}\left(X_i\left(m\right)\right) = A_{TF}^{nn'}$$

$$A_{TT}^{n'n} = \sum_{m=1}^{M} A_{TT}^{(m)n'n} = \sum_{m=1}^{M} \sum_{X_i(m)}^{N_{X(m)}} w\left(m, X_i\left(m\right)\right) T^{(m)n'}\left(X_i\left(m\right)\right) T^{(m)n}\left(X_i\left(m\right)\right) = A_{TT}^{nn'}$$

$$\frac{\partial \chi^2}{\partial S^n} = 0 = \left\{ \sum_{n'=1}^{M} A_{FF}^{n'n} S^{n'} + \sum_{n'=1}^{M} A_{TF}^{n'n} S_{bg}^{n'} - B_{CF}^{n} \right\}$$

$$\frac{\partial \chi^2}{\partial S_{bg}^n} = 0 = \left\{ \sum_{n'=1}^{M} A_{FT}^{n'n} S^{n'} + \sum_{n'=1}^{M} A_{TT}^{n'n} S_{bg}^{n'} - B_{CT}^{n} \right\}$$

In matrix notation, and using the transpose properties,

$$\begin{bmatrix} A_{FF} & A_{FT} \\ A_{TF} & A_{TT} \end{bmatrix} \begin{pmatrix} S \\ S_{bg} \end{pmatrix} = \begin{pmatrix} B_{CF} \\ B_{CT} \end{pmatrix}$$

This can be solved by variable elimination. For example first solve for the S_{bg} as a function of S, using the bottom row,

$$S_{bg} = -A_{TT}^{-1} A_{TF} S + A_{TT}^{-1} B_{CT}$$

and substitute in the top row to solve for S,

$$A_{FF} S + A_{FT} \left(-A_{TT}^{-1} A_{TF} S + A_{TT}^{-1} B_{CT}\right) = B_{CF}$$

$$\left(A_{FF} - A_{FT} A_{TT}^{-1} A_{TF}\right) S = B_{CF} - A_{FT} A_{TT}^{-1} B_{CT}$$

$$S = \left(A_{FF} - A_{FT} A_{TT}^{-1} A_{TF}\right)^{-1} \left(B_{CF} - A_{FT} A_{TT}^{-1} B_{CT}\right)$$

This is a complicated solution. If this model for S is used over the entire data range, then the solution requires just two vectors, S^n and S_{bg}^ninstead of the per datapoint solution which solves for one vector at each datapoint. We also don"t propagate errors from He3 parameters to individual datapoints (e.g. He3 polarization).

The problem looks much simpler if we can assume that $S_{bg} = 0$, but then the Gaussian endpoints must match any actual background value of S for the solution to make sense. If $S_{bg}$is assumed zero then the solution comes from,

$$A_{FF} S = B_{CF}$$

In the non-Gaussian least-squares case we had,

$$A^{nm} = \sum_{i=1}^{N} w_i T^{in} T^{im} = A^{mn}$$

and

$$B^n = \sum_{i=1}^{N} w_i T^{in} C^i$$

In this expression, it is usefule to divide the sum over measurement points i, into a sum over polarized-beam cross-sections, m, and a sub-sum over the X_i values for the given m.

$$\chi^2 = \sum_{m=1}^{M} \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) \left(C^i - \sum_{n=1}^{M} T^{(m)n}(t_i, \lambda_I, \lambda_F, P_\mu; X_i\left(m\right)) \; \left(S_{bg}^n + f^n\left(X_i\left(m\right)\right) S^n\right) \right)^2 ,$$

$$\frac{\partial \chi^2}{\partial S_{bg}^n} = 0 = \sum_{m=1}^{M} \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) \left(C^i - \sum_{n'=1}^{M} T^{(m)n'}(t_i, \lambda_I, \lambda_F, P_\mu; X_i\left(m\right)) \; \left(S_{bg}^{n'} + f^{n'}\left(X_i\left(m\right)\right) S^{n'}\right) \right) (-$$

The derivatives of χ^2 are needed to solve these equations,

$$\frac{\partial \chi^2}{\partial S^n} = 0 = \sum_{m=1}^{M} \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) \left(C^i - \sum_{n'=1}^{M} T^{(m)n'}(t_i, \lambda_I, \lambda_F, P_\mu; X_i\left(m\right)) \; \left(S_{bg}^{n'} + f^{n'}\left(X_i\left(m\right)\right) S^{n'}\right) \right) (-)$$

Using the Gaussian weighted transmission

$$F^{(m)n}\left(X_i\left(m\right)\right) = T^{(m)n}(X_i\left(m\right)) \, f^n\left(X_i\left(m\right)\right),$$

for each m the sums over $X_i\left(m\right)$ in each term can be done to produce the following coeficients,

$$B_{CF}^{(m)n} = \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) C^{(m,X_i(m))} F^{(m)n}\left(X_i\left(m\right)\right)$$

$$A_{FT}^{(m)nn'} = \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) F^{(m)n}\left(X_i\left(m\right)\right) T^{(m)n'}\left(X_i\left(m\right)\right)$$

$$A_{FF}^{(m)nn'} = \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) F^{(m)n}\left(X_i\left(m\right)\right) F^{(m)n'}\left(X_i\left(m\right)\right)$$

$$B_{CT}^{(m)n} = \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) C^{(m,X_i(m))} T^{(m)n}(X_i\left(m\right))$$

$$A_{TT}^{(m)nn'} = \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) T^{(m)n}(X_i\left(m\right)) \, T^{(m)n'}\left(X_i\left(m\right)\right)$$

$$A_{TF}^{(m)nn'} = \sum_{X_i(m)}^{N_{X(m)}} w\left(X_i\left(m\right)\right) T^{(m)n}(X_i\left(m\right))F^{(m)n^{'}}\left(X_i\left(m\right)\right).$$

Then

$$\frac{\partial \chi^2}{\partial S^n} = 0 = \sum_{m=1}^{M} \left\{ \sum_{n'=1}^{M} \left(A_{FT}^{(m)nn'} S_{bg}^{n^{'}} + A_{FF}^{(m)nn'} S^{n^{'}} \right) - B_{CF}^{(m)n} \right\}$$

$$\frac{\partial \chi^2}{\partial S_{bg}^n} = 0 = \sum_{m=1}^{M} \left\{ \sum_{n'=1}^{M} \left(A_{TT}^{(m)nn'} S_{bg}^{n^{'}} + A_{TF}^{(m)nn'} S^{n^{'}} \right) - B_{CT}^{(m)n} \right\}$$

followed by the sum over m for each coeficient,

$$\frac{\partial \chi^2}{\partial S^n} = 0 = \sum_{n'=1}^{M} \left(A_{FT}^{nn'} S_{bg}^{n^{'}} + A_{FF}^{nn'} S^{n^{'}} \right) - B_{CF}^n$$

$$\frac{\partial \chi^2}{\partial S_{bg}^n} = 0 = \sum_{n'=1}^{M} \left(A_{TT}^{nn'} S_{bg}^{n^{'}} + A_{TF}^{nn'} S^{n^{'}} \right) - B_{CT}^n$$

produces a set of $2M$ linear equations in $2M$ variables, S^n and S_{bg}^n. Note that the X dependence must be described by a single variable, S^n(in addition to the background S_{bg}^n) for this linear equations solution to work. Adding more complicated X dependence or asking for minimization of χ^2 in terms of cross-section positions or widths leads to non-linear sets of equations.

$$\frac{\partial \chi^2}{\partial S^n} = 0 = \sum_{m=1}^{M} A^{nm} S^m - B^n,$$

where

$$A^{nm} = \sum_{i=1}^{N} w_i T^{in} T^{im} = A^{mn}$$

and

$$B^n = \sum_{i=1}^{N} w_i T^{in} C^i$$

$$S^{\mu} = \sum_{m=1}^{M} \left(A^{-1}\right)^{\mu m} B^m.$$