Fitting data (ch15)

Comparing theory and experiment
\{p_j\} inputs parameter set
\sigma^{\text{exp}}(i) experimental data (\Delta \sigma \text{ standard deviation})

Measure of discrepancy
\[ \chi^2 = \sum_{i=1}^{N} \frac{(\sigma^{\text{th}}(i) - \sigma^{\text{exp}}(i))^2}{\Delta \sigma(i)^2}. \]

If theory agrees exactly with experiment \( \chi^2 = 0 \) (very unlikely!)
What is statistically reasonable \( \sigma^{\text{th}}(i) \sim \sigma^{\text{exp}}(i) \sim \Delta \sigma(i) \) so \( \chi^2 \sim N \) (or \( \chi^2/N \sim 1 \))
If \( \chi^2/N >> 1 \) then theory needs improvement
If \( \chi^2/N << 1 \) errors have been overestimated

Fitting data (including an overall scale)

Comparing theory and experiment
\{p_j, s\} inputs parameter set (s is overall scale)
\sigma^{\text{exp}}(i) experimental data (\Delta \sigma \text{ standard deviation})

Measure of discrepancy
\[ \chi^2 = \frac{(s - E[s])^2}{\Delta s^2} + \sum_{i=1}^{N} \frac{(\sigma^{\text{th}}(i) - s \sigma^{\text{exp}}(i))^2}{\Delta \sigma(i)^2}. \]

If theory agrees exactly with experiment \( \chi^2 = 0 \) (very unlikely!)
What is statistically reasonable \( \sigma^{\text{th}}(i) \sim s \sigma^{\text{exp}}(i) \sim \Delta \sigma(i) \) so \( \chi^2 \sim N+1 \) (or \( \chi^2/(N+1) \sim 1 \))
Multivariate theory

Probability distribution for a set of random variables
(normal distribution)

\[ f(x) = \frac{1}{\sqrt{2\pi \Delta}} \exp \left[ -\frac{(x - \mu)^2}{2\Delta^2} \right] \]

Mean \( \mu = E[x] \)

Standard deviation \( \Delta \)

\[ \Delta^2 = E[(x - \mu)^2] = E[x^2] - 2\mu E[x] + \mu^2 = E[x^2] - \mu^2 \]

\[ E[X] = \int X f(x) \, dx \]

Multivariate theory (many correlated variables)

Probability distribution for a set of correlated variables \( x = \{x_1, \ldots, x_N\} \)

might no longer be normal

\[ f(x) = (2\pi)^{-\frac{N}{2}} |\mathbf{V}|^{-\frac{1}{2}} \exp \left[ -\frac{1}{2} (x - \mu)^T \mathbf{V}^{-1} (x - \mu) \right] \]

Symmetric covariance matrix

\[ \mathbf{V}_{ij} = E[(x_i - \mu_i)(x_j - \mu_j)] \]

Diagonal terms are the standard deviations squared

Off diagonal depend on correlation coefficients \( \rho_{ij} \Delta_i \Delta_j \)
Chi2 and the covariance matrix

Probability that a data point \( x_i \) with variance \( \Delta^2_i \) is correctly fitted by theory \( y_i \)

\[
f_i(y_i) = \frac{1}{\sqrt{2\pi \Delta_i}} \exp \left[ -\frac{(x_i - y_i)^2}{2\Delta^2_i} \right]
\]

For many statistically independent points the joint probability is:

\[
P_{\text{tot}} = (2\pi)^{-\frac{N}{2}} \Delta^{-1} \exp \left[ -\frac{1}{2} \sum_{i=1}^{N} \frac{(x_i - y_i)^2}{\Delta^2_i} \right]
\]

\[
= (2\pi)^{-\frac{N}{2}} \Delta^{-1} \exp \left[ -\frac{1}{2} \chi^2 \right]
\]

\[\Delta = \prod_{i}^{N} \Delta_i \]

\[\chi^2 = \sum_{i}^{N} \frac{(x_i - y_i)^2}{\Delta^2_i}\]

Using this we can generalize the Chi2 definition by:

\[
\chi^2 = (x - y)^T V^{-1} (x - y)
\]

\[\chi^2 = \sum_{j \neq i}^{N} (x_i - y_j) V^{-1} (x_j - y_j)\]

Chi2 distribution

Adding together \( N \)-squares of independent normal distributions \( z_i^2 \) with zero mean and unit variance

\[\chi^2 = \sum_{i=1}^{N} z_i^2\]

\[f(\chi^2) = \frac{1}{2\Gamma(N/2)} \left( \frac{\chi^2}{2} \right)^{N/2 - 1} e^{-\chi^2/2}\]

\[E[\chi^2] = N; \quad V(\chi^2) = 2N; \quad \sigma(\chi^2) = \sqrt{2N}\]

For \( N > 20 \) the Chi2 distribution becomes close to the normal distribution.
What is a perfect fit?

When theory predicts exactly the statistical mean of experiment

\[ y_i = E[x_i] = \mu_i \]

\[ z_i^2 = \frac{(x_i - y_i)^2}{\Delta_i^2} = \frac{(x_i - \mu_i)^2}{\Delta_i^2} \]

have zero means and unit variances

If \( z_i \) have normal distributions \( \chi^2 \) follows ch2 distribution

mean N and variance 2N

Thus our reasoning \( \chi^2/N \sim 1 \)

Expanding chi2 around a minimum

Let us consider the expansion of chi2 around a minimum found for the set of parameters \( \{p^0\} \)

\[ \chi^2(p_1, \ldots, p_P) \approx \chi^2(p^0_1, \ldots, p^0_P) + \frac{1}{2} \sum_{m,n=1}^{P} H_{mn}(p_m - p^0_m)(p_n - p^0_n) \]

\[ \equiv \chi^2(p^0) + \frac{1}{2}(p - p^0)^T H (p - p^0) \]

Hesse matrix

\[ H_{mn} = \frac{\partial^2}{\partial p_m \partial p_n} \chi^2(p_1, \ldots, p_P) \]

Covariance matrix

\[ (V_P)^{-1} = \frac{1}{2}H \quad \text{or} \quad V_P = 2H^{-1} \]

The fitting probability can be defined in terms of the Hesse matrix:

\[ P_{tot} = \frac{1}{(2\pi)^{P/2} \Delta} e^{-\chi^2(p^0)/2} \exp \left[ -\frac{1}{4} \sum_{mn} (p_m - p^0_m)H_{mn}(p_n - p^0_n) \right] \]
Allowed parameters within 1sigma

This happens with argument of exp is 1/2

\[ \frac{1}{2} \sum_{mn}^{p} (p_m - p_m^0) H_{mn}(p_n - p_n^0) = 1 \]

Using the Taylor expansion this can be written as

\[ \chi^2(p_1, \ldots, p_p) = \chi^2(p_1^0, \ldots, p_p^0) + 1 \]

Ex: legendre polynomial fitting

Experimentalists have cross sections which they expand in legendre polynomials

\[ \sigma(\theta) = \sum_{\Lambda \geq 0} a_{\Lambda} P_{\Lambda}(\cos \theta) \]

We know more about the coefficients from reaction theory:

\[ \sigma(\theta) = \left| \frac{1}{k} \sum_{L=0}^{\infty} (2L+1) P_L(\cos \theta) T_L \right|^2 \]

\[ = \frac{1}{k^2} \sum_{LL'} (2L+1)(2L'+1) P_L(\cos \theta) P_{L'}(\cos \theta) T_L^* T_{L'} \]

\[ a_{\Lambda} = \frac{1}{k^2} \sum_{LL'} (2L+1)(2L'+1) \langle L0, L'0 | \Lambda 0 \rangle^2 T_L^* T_{L'} \]
Ex: optical potential fits (optical model)

- Strongly non linear (fitting is done by iteration only)
- Need data at large scattering angles
- Spin orbit affect T11 and not so much elastic cross sections
  - Ambiguities:
    - Low energy (phase equivalent potentials)
    - Medium energy (volume integral $V_{ws} = R_{ws}^2$)
      \[ \mathcal{J} = \int V(r) \, dr = 4\pi \int_0^\infty V(r) r^2 \, dr \]
    - Heavy nuclei (governed by tail of $V$)
      \[ V(R) \approx -V_{ws} e^{-\frac{(R-R_{ws})}{\alpha_{ws}}} = -V_{ws} e^{\frac{R}{\alpha_{ws}}} e^{-\frac{R}{\alpha_{ws}}} \]

Ex: multichannel fits

- Elastic: bare potential versus the optical potential
  - Can ignore dynamic polarization
  - Redo entire fitting in coupled channels
  - Switch off the backward coupling
- Inelastic scattering
  - First use first order theory
  - Then detail adjustment of optical potential
  - Plus non-linearities in deformation
  - Plus higher order effects
- Transfer
  - First 1 step dwba (SF can be cleanly extracted)
  - Higher orders (other inelastic channels CCBA or other reaction channels CRC)
Strategies for chi2 fitting

• Start with simplest data and simplest reaction model
  (for example elastic and optical model)

• Restart from any intermediate stage

• If there are ambiguities, do grid searches and look at correlations in errors

• Artificially reduce error in data points if theory is having a hard time to get close in some region

• If minimum is found near the end of the range of a parameter, this is spurious – repeat with wider range

• Constrain with other experiments

• Two correlated variables: combine into one

**Progressive improvement policy**