Beamline Controls & Data Acquisition

An algorithm for efficient optimization directed by noisy data

ESRF Workshop on Automatic Beamline Alignment Tim Mooney March 12, 1999

ABSTRACT

At the heart of several efficient nonlinear-optimization algorithms is a parabolic fit in which the function (or a one-dimensional "slice" of its hypersurface) is represented by three evaluations in the neighborhood of a local extremum. (The extremum of the parabola through those points is assumed to approximate the function's true extremum.) The three-point solution fails (optimization converges slowly or not at all) when function evaluations contain enough noise, granularity, etc. The algorithm presented here solves analytically for the best-fit parabola and line(s) to four or more data points, calculates the uncertainties of fit parameters, compares chi-square values of the fits, and uses various heuristic information to direct the search for an optimal value.

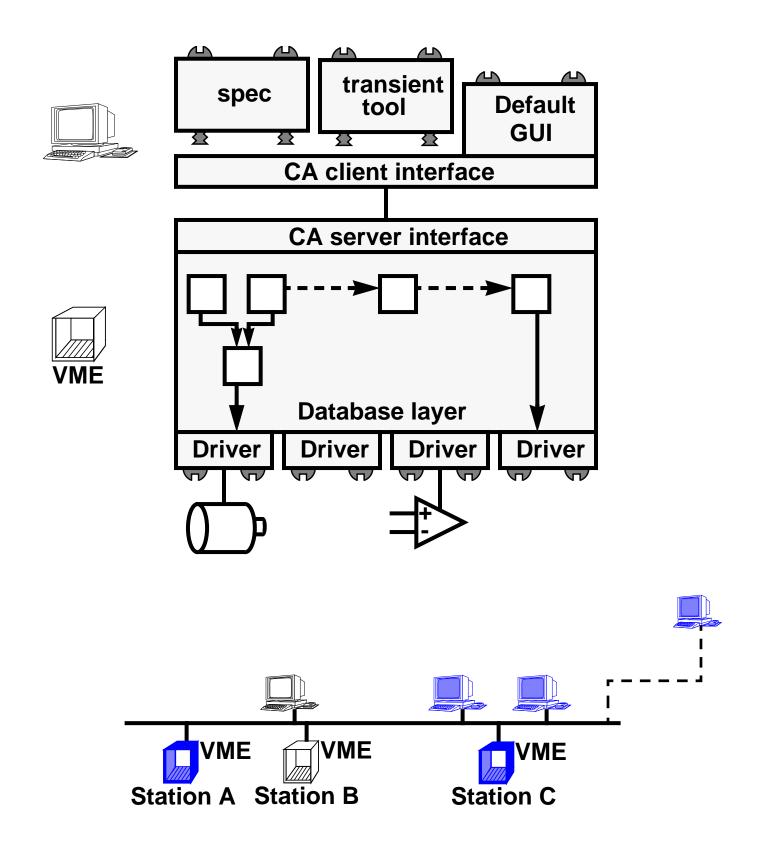
Beamline Controls & Data Acquisition

Objective: N-dimensional optimization tool for online use

- User specifies:
 - Positioners, limits, step sizes, convergence criteria
 - Detector trigger(s)
 - Signals to be acquired
 - Function to be optimized
 - (Looks pretty much like a scan specification)
- Algorithm must be efficient and robust
 - Function evaluations are many orders of magnitude more costly than in typical data-analysis applications
 - Can't waste beam time
 - Can't challenge equipment-protection system
- Noise, granularity, etc. limit algorithm options:
 - Can't use derivatives
 - Can't base any major decision on a single data point
 - Strongly correlated parameters are indistinguishable

Beamline Controls & Data Acquisition

Context: EPICS-based beamline software architecture



Beamline Controls & Data Acquisition

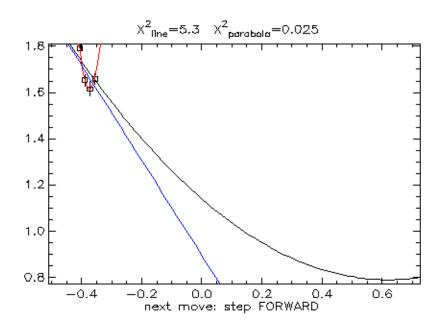
Algorithm

- Starting points
 - Powell's conjugate gradient method (e.g., Numerical Recipes)
 - Turns n-dimensional search into m 1-dimensional searches
 - nD decisions based on 1D results (i.e., several data points)
 - Analytical fit of polynomial to data (e.g., Bevington 2nd Ed.)
 - Build line and parabola fits
 - Gives error estimate for fit parameters
- Search strategy
 - Compare χ^2_{parabola} to χ^2_{line} (i.e., χ^2 per degree of freedom)
 - Require 0.5 < $\chi^2_{parabola}$ < 2 before using result to direct search. (Exact criteria depends on functional form of extremum)
 - Require roughly symmetrical distribution of >5 data points about extremum before using error estimate for $\chi^2_{parabola}$ Must have a reasonable estimate of detector noise to use χ^2 in this way. (Could use the ratio $\chi^2_{line}/\chi^2_{parabola}$ without a noise estimate.)

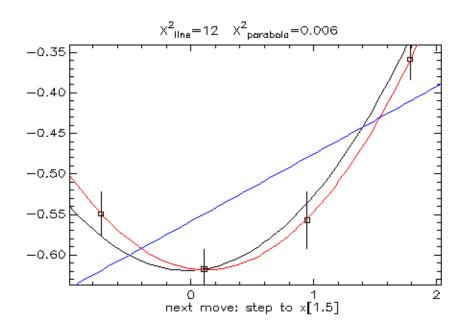
Beamline Controls & Data Acquisition

Examples

• missing the point (χ^2 too small)

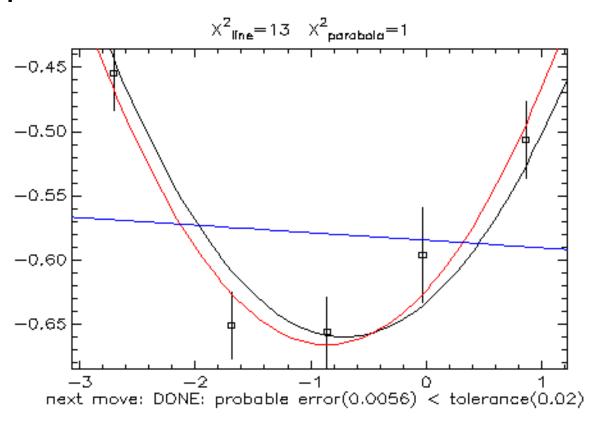


ditto

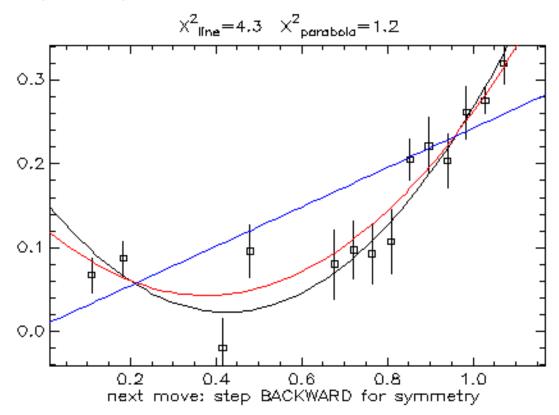


Beamline Controls & Data Acquisition

Examples: fooled

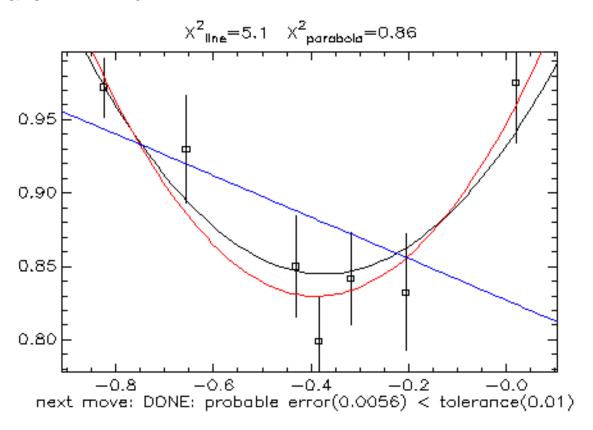


need symmetry

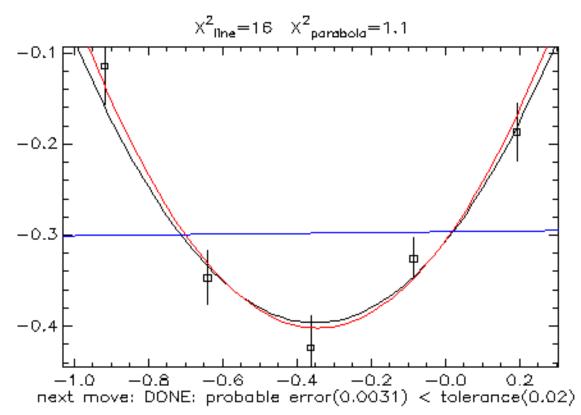


Beamline Controls & Data Acquisition

shallow minimum

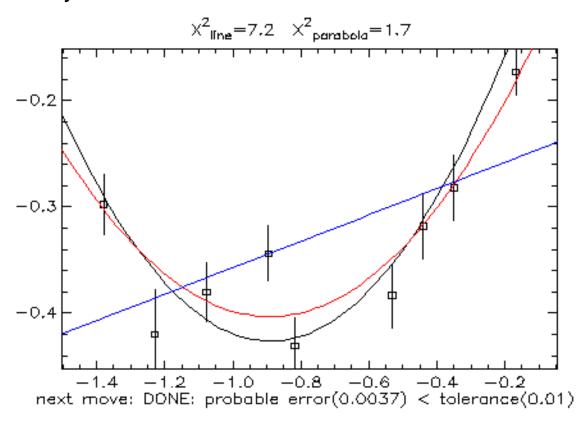


good start point and step size

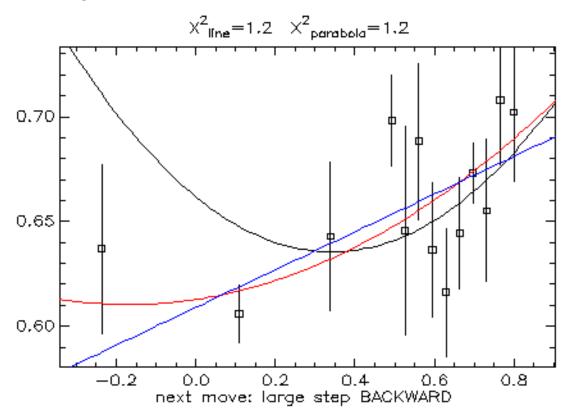


Beamline Controls & Data Acquisition

got lucky

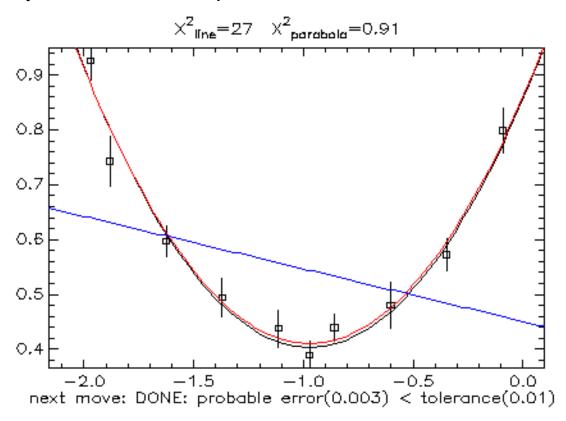


recovering from bad step size



Beamline Controls & Data Acquisition

evenly distributed data-point errors



very shallow minimum

