The GRETINA Signal Decomposition Algorithm

David Radford ORNL Physics Division

AGATA-GRETA Meeting ANL Dec 2016







MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

- Overview of the Algorithm
 - Signal basis
 - Signal decomposition algorithm
 - One hit segment
 - Two hit segments
 - More...
 - Adaptive Grid Search
- Strengths and weaknesses, possible improvements
- Summary



Signal Decomposition

- Digital signal processing to determine the *number, positions,* and *energies* of gamma interactions in the crystal
- Uses a "signal basis"; a set of simulated signals
- Position resolution is crucial for energy resolution, efficiency, and peak-to-total ratio in tracking
- But getting the *number* of interactions correct may be harder, and is at least as important
- Speed is critical as it determines overall gamma throughput of array





Decomposition Fits

- Shows two typical multi-segment events measured in prototype triplet cluster (red) (concatenated signals from 36 segments, 500ns time range)
- Linear combination of basis signals, as fitted by decomposition algorithm (blue)
- Includes differential cross talk from capacitive coupling between channels



Expected Distribution of Hits

GEANT simulations; 1 MeV gamma into GRETA

Most hit crystals have one or two hit segments

Most hit segments have one or two interactions





Decomposition Basis (Signal Library)

- Signal decomposition **algorithm** appears to work very well
 - Validated using simulated signals
- Most issues with the decomposition results appear to come from the fidelity of the signal basis
- Poor fidelity results in
 - Too many fitted interactions
 - Incorrect positions and energies
- We already include effects of
 - Integral cross-talk
 - Differential cross-talk
 - Preamplifier rise-time
- *Differential cross-talk* signals look like image charges, so they strongly affect position determination



GRETINA Decomposition Algorithm

Current algorithm is a *hybrid*

- Adaptive Grid Search with Linear Least-Squares (for energies)
- Non-linear Least-Squares
- Have also tried Singular Value Decomposition
 - Had slightly poorer performance than AGS
- CPU time required goes as
 - Adaptive Grid Search : $\sim O(n)$
 - Singular Value Decomp : $\sim O(n)$
 - Nonlinear Least-Squares : $\sim O(n + \delta n^2)$

for n interactions



Why is it Hard?

- Very large parameter space to search
 - Average segment ~ 6000 mm³, so for ~ 1 mm grid search,
 - two interactions in one segment: $\sim 2 \times 10^6$ possible positions
 - two interactions in each of two segments: $\sim 4 \times 10^{12}$ positions
 - two interactions in each of three segments: $\sim 8 \times 10^{18}$ positions
 - PLUS additional dimensions; energy sharing, time-zero, ...
- Under-constrained fits, especially with > 1 interaction/segment
 - For one segment, the signals provide only ~ 6 x 40 = 240 nontrivial numbers
- Strongly-varying, nonlinear sensitivity
 - $\delta\chi^2/\delta(\theta z)$ is much larger near segment boundaries



Regular Basis Grid

 The GRETINA Signal Decomposition originally made use of a Cartesian grid

Different colors show active regions for different segments



- An irregular quasi-cylindrical grid has several important advantages:
 - The possibility to optimize the spacing of points in the grid based on separation in "Chi-squared space"
 - Reducing the number of grid points forimproved speed
 - Constructing the grid around the real segment volumes allows much better and faster constraints to be programmed into the least-squares search algorithms

Optimized Quasi-Cylindrical Grid



Fitting to Extract Cross-Talk Parameters

- 36 "superpulses": averaged signals from many single-segment events (red)
- Monte-Carlo simulations used to generate corresponding calculated signals (green)
- ~ 996 parameters fitted (integral and differential cross-talk, delays, rise times) (blue)
- Calculated response can then be applied to decomposition "basis signals"



Problems with the Basis have a Big Effect

Same data set, decomposed with old and new bases Crystal Q4P4



12 Managed by UT-Battelle for the U.S. Department of Energy

National Laborato

What Can Affect the Signals?

- Field and Weighting Potential:
 - Overall impurity concentration

(Two values (~20%) from maker, one at each end; depletion voltage)

- Longitudinal impurity gradient (Linear? Nonlinear?)
- Radial impurity gradient?
- Hole diameter; hole depth; etching cycles; lithium thickness
- Neutron damage (p-type)
- Charge carrier mobilities as a function of electric field
- Crystal axis orientation (~ 5 degrees from maker)
- Crystal temperature (Some info from RTD)
- Cross-talk (differential and integral)
- Neutron damage (trapping)
- Impulse response of 37 preamps
- Charge cloud size
- Digitizer nonlinearity



Overall Strategy: One hit segment

- 1. Start by finding approximate t_0
 - Fit a single interaction and time offset using nonlinear least-squares
 - Five parameters: \mathbf{x}_1 , \mathbf{e}_1 , \mathbf{t}_0
- 2. Then find best *two-interaction* solution
 - Adaptive grid search using ~ 10^5 pairs of grid points and best-fit energies
 - Much more detail about this later
 - Then interpolate off basis grid using nonlinear least-squares
 - Two interactions, nine parameters: \mathbf{x}_1 , \mathbf{e}_1 , \mathbf{x}_2 , \mathbf{e}_2 , \mathbf{t}_0
- 3. Try adding a third interaction (if total energy is > 400 keV and chisq is bad)
 - Insert extra interaction in middle of segment, with 1/3 of the energy
 - Re-do nonlinear least-squares \mathbf{x}_1 , \mathbf{e}_1 , \mathbf{x}_2 , \mathbf{e}_2 , \mathbf{x}_3 , \mathbf{e}_3 , \mathbf{t}_0
- 4. Try coalescing two interactions into one
 - Re-do nonlinear least-squares
- 5. Choose best overall solution, with penalty factor for extra parameters (i.e. interactions). End up with 1, 2, or 3 interactions.

x₁, **e**₁, **t**₀

14 Managed by UT-Battelle for the U.S. Department of Energ



Overall Strategy: Two hit segments

- 1. List hit segments in order of decreasing energy; $e_a > e_b$
- 2. Start by finding approximate fit, with one interaction per segment
 - Nonlinear least-squares $\mathbf{x}_{a1}, \mathbf{e}_{a1}, \mathbf{x}_{b1}, \mathbf{e}_{b1}, \mathbf{t}_{0}$
- 3. Subtract calculated signals for $(\mathbf{x}_{b1}, \mathbf{e}_{b1}, \mathbf{t}_0)$ from the measured signals.
 - Use adaptive grid search to find best *two-interaction* solution for the remainder (segment a).
- 4. Now have three interactions: \mathbf{x}_{a1} , \mathbf{e}_{a1} , \mathbf{x}_{a2} , \mathbf{e}_{a2} , \mathbf{x}_{b1} , \mathbf{e}_{b1} , \mathbf{t}_0
 - Re-fit full signal using nonlinear least-squares, 13 parameters
- 5. Use the same trick: Subtract calculated signals for $(\mathbf{x}_{a1}, \mathbf{e}_{a1}, \mathbf{x}_{a2}, \mathbf{e}_{a2}, \mathbf{t}_0)$ from the measured signals.
 - Use adaptive grid search to find best *two-interaction* solution for the remainder (segment b).
 - Re-fit full signal using nonlinear least-squares, with 4 interactions

 $\boldsymbol{x}_{a1},\, \boldsymbol{e}_{a1},\, \boldsymbol{x}_{a2},\, \boldsymbol{e}_{a2},\, \boldsymbol{x}_{b1},\, \boldsymbol{e}_{b1},\, \boldsymbol{x}_{b2},\, \boldsymbol{e}_{b2},\,\, \boldsymbol{t}_{0}$



Overall Strategy: Two hit segments

- 6. For both segments, try coalescing the pairs of interactions into one
 - Re-do nonlinear least-squares each time
- 7. Choose best overall solution, with penalty factor for extra parameters. End up with 2, 3, or 4 interactions.



Overall Strategy: Three or more hit segments

- 1. List hit segments in order of decreasing energy; $e_a > e_b > e_c$
- 2. Start by finding approximate fit, with one interaction per segment
 - Three interactions, plus t₀
- 3. Subtract calculated signals for segments b and c from the measured signals.
 - Use adaptive grid search to find best *two-interaction* solution for the remainder (segment a).
 - Re-fit full signal using nonlinear least-squares with 4 interactions
- 4. Repeat step 3 twice more, to get pairs of interactions in segments b and c.
- 5. For all segments, try coalescing the pairs of interactions into one, re-doing nonlinear least-squares each time
- 6. Choose best overall solution, with penalty factor for extra parameters. End up with 3 – 6 interactions.



Adaptive Grid Search Least-Squares

Adaptive grid search fitting:

- Critical that the signals start at $t_0 = 0$ for reliable results!
- Use for only one segment at a time
- Start on a coarse grid, every second point in each direction (2x2x2)
 - All the in-segment basis dot products are pre-calculated on this coarse grid
- Loop over all pairs of positions inside the segment,
 - Energies e_i and e_j are constrained, such that 0.1 ($e_i + e_j$) < e_i < 0.9 ($e_i + e_j$)
- Once the best pair of positions (lowest χ2) is found, then all neighbor pairs are examined on the finer (1x1x1) grid. This is 26x26 = 676 pairs. If any of them are better, the procedure is repeated.
 - Here the signal dot-products cannot be pre-calculated
- Finally, nonlinear least-squares (SQP) can be used to interpolate off the grid. This improves the fit ~ 50% of the time.



Adaptive Grid Search Least-Squares

Linear Least-Squares

For two interactions of energies e_i, e_j at locations i and j, the calculated signal is $C_{kt} = (e_i s_{ikt} + e_2 s_{jkt})$ where k is the segment and t the time step. s_{ikt} is the basis signal calculated at point i.

If the observed signal is O_{kt}

$$\chi^{2} = \sum_{kt} \frac{(O_{kt} - C_{kt})^{2}}{\sigma_{kt}^{2}} = \frac{\sum_{kt} (O_{kt} - e_{i} s_{ikt} - e_{j} s_{jkt})^{2}}{\sigma^{2}}$$
(1)

where $\sigma_{kt} = \sigma$ is the uncertainty (noise) in O_{kt} , assumed independent of k, t.

We want a minimum in χ^2 , *i.e.*

$$\frac{\partial \chi^2}{\partial e_i} = \frac{\partial \chi^2}{\partial e_j} = 0 \tag{2}$$

$$\frac{\partial \chi^2}{\partial e_i} = \frac{2\sum_{kt} (O_{kt}s_{ikt} - e_i s_{ikt}^2 - e_j s_{ikt} s_{jkt})}{\sigma^2} = 0 \tag{3}$$

19 Managed by UT-Battelle for the U.S. Department of Energy

Adaptive Grid Search Least-Squares

Thus we get two equations in two unknowns:

$$\sum_{kt} O_{kt} s_{ikt} - e_i \sum_{kt} s_{ikt}^2 - e_j \sum_{kt} s_{ikt} s_{jkt} = 0$$

$$\sum_{kt} O_{kt} s_{jkt} - e_j \sum_{kt} s_{jkt}^2 - e_i \sum_{kt} s_{ikt} s_{jkt} = 0$$
(4)
(5)

kt

kt

$$\sum_{kt} s_{ikt}^2$$

and

$$\sum_{kt} s_{ikt} s_{jkt}$$

once for all events, and

$$\sum_{kt} O_{kt} s_{jkt}$$

once per event.

20 Managed by UT-Battelle



Adaptive Grid Search: Some Numbers

(Cartesian grid for illustration purposes):

- ~35000 grid points in 1/6 crystal (one column, 1x1x1 mm)
- 2x2x2 mm (slices 1-3) or 3x3x3 mm (slices 4-6) coarse grid gives N ≤ 600 course grid points per segment.
- For two interactions in one segment, have N(N-1)/2 ≤ 1.8 x 10⁵ pairs of points for grid search. This takes < 3 ms/cpu to run through.
- Two segments:
 - (N(N-1)/2)² ~ 3.2 x 10¹⁰ combinations for two interactions in each of 2 segments; unfeasible!
 - Limit N to only 4³ = 64 points; then (N(N-1)/2)² ~ 4 x 10⁶
 This may be possible? But is it worthwhile?
- Three segments:
 - But (N(N-1)/2)³ ~ 8 x 10⁹ combinations for two interactions; impossible even for N = 64.



Adaptive Grid Search: Some Numbers

- What about 1-interaction x 1-interaction in two segments, on the coarse grid?
 - Requires a very large number of pre-calculated dot-products
 - We now calculate ~ 2e5 sums for each of 36 segments
 - For all pairs of segments, would need ~ 4e5 for 630 pairs
 - 35 times the storage is required
 - But still only \sim 1.5 GB, roughly the same as the basis signals
 - Entirely feasible today
- But would this be useful?
- Remember that the grid search relies on knowing t₀ accurately...



Strengths and Weaknesses

- Able to identify up to 2 interactions per segment (three for a single segment)
- Finds correct solution in simulation tests
- Fast
- Modest memory requirements
- Optimized, irregular grid makes a very significant difference
 - Took some serious coding and a lot of time on the part of K. Lagergren

- Poor determination of number of interactions!
- Strong covariance between reported interaction positions and t₀
 - t_0 distribution is wider than normal CFT distribution \otimes



- Extra timing information to constrain t₀
 - External fast detectors or RF signal
 - Ge-Ge coincidences
 - Requires event building prior to decomposition; hard!
- Tuning of crystal-by-crystal penalty factors for extra interactions
- Further improvements in basis fidelity
 - Preamplifier impulse response function
 - Include charge cloud size and charge-sharing in signal generation
 - Especially important at small radius, near segment boundaries
 - But energy-dependent?
 - ²⁴¹Am surface-scan "superpulse" fitting for field, WP, electron drift, and preamp parameters
 - Better field determination
 - Segment capacitance measurements as a function of bias



- Preamplifier impulse response function
- Ben Shanks (UNC) for point-contact detector



Use pulser T.F. constants as a starting point, but allow them to float in a fit to physics data — very good agreement in the electronics-dominated section

- Preamplifier impulse response function
- Ben Shanks (UNC) for point-contact detector



26 Managed by UT-Battelle for the U.S. Department of

- Preamplifier impulse response function
- Ben Shanks (UNC) for point-contact detector
 - Fitted parameters include:



۲



Summary

- The algorithm is very complex
- Desired result is computationally under-determined
- But the method works reliably when the basis is known perfectly
- Fast, relatively modest memory requirements
- Basis fidelity is crucial
- Can tend to overestimate the number of interactions
 - Requires penalty factors



Acknowledgements

Karin Lagergren (ORNL / UTK)

- Signal calculation code in C
- Optimized pseudo-cylindrical grid

I-Yang Lee

- Original signal calculation code
- C. Campbell, H. Crawford, M. Cromaz, M. Descovich, P. Fallon, A. Machiavelli, ...
 - Basis calculations, cross-talk fits, in-beam data analysis, simulations, electric field calculations, and much more

Tech-X Corp, especially Isidoros Doxas

• SVD development



Backup



Calculated Signals: Sensitivity to Position





Singular Value Decomposition

Very roughly:

- The full signal -vs.- grid position matrix can be decomposed into the product of three matrices, one of which contains the correlations (eigenvalues)
- By neglecting the small eigenvalues, the length of the signal vectors (and hence computation with them) can be greatly reduced
- The more eigenvalues kept, the higher the quality of the fit



32 Managed by UT-Battelle for the U.S. Department of Energy



Singular Value Decomposition

Very roughly:

- The full signal -vs.- grid position matrix can be decomposed into the product of three matrices, one of which contains the correlations (eigenvalues)
- By neglecting the small eigenvalues, the length of the signal vectors (and hence computation with them) can be greatly reduced
- The more eigenvalues kept, the higher the quality of the fit
- Measured signals can be compressed the same way as, and then compared to, the calculated library signals
- Different similarity measures can be used to emphasize different aspects

Dot Product
$$x.y = \sum_{i=1}^{N} x_i y_i$$

Cosine $\cos(\theta_{xy}) = \frac{x.y}{|x||y|}$
Euclidean Distance $euclid(x, y) = \sqrt{\sum_{i=1}^{N} (x_i - y_i)^2}$



Problems with the Basis have a Big Effect

Distribution of decomposed interaction positions throughout the crystal

93 48

 24



34