

# In Search of a Statistically Optimal, Nonlinear Pulse-Height Estimator for TES Microcalorimeter Signals

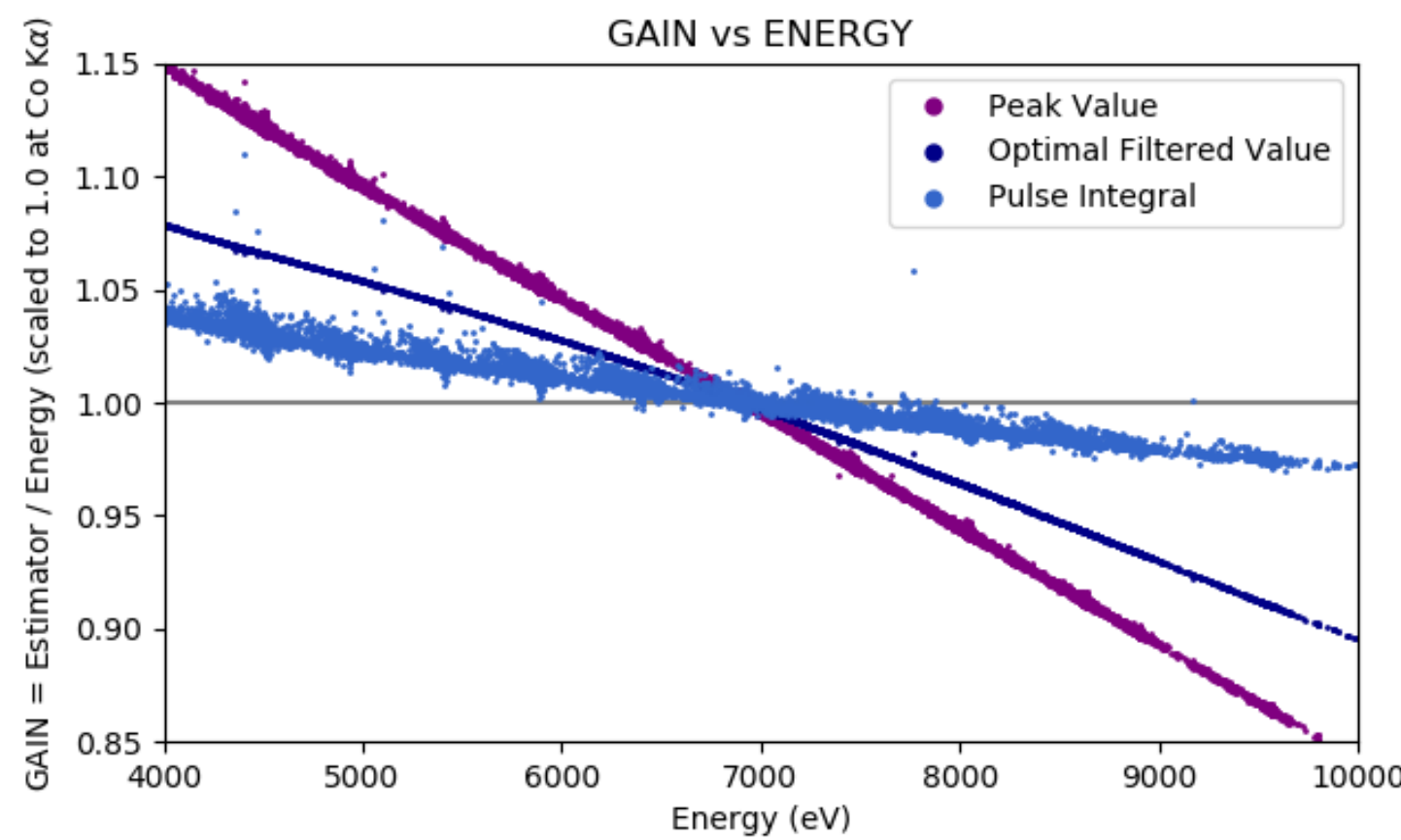
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## The Calibration and Linearity Problem

TES microcalorimeters are not strictly linear detectors: pulse sizes are not proportional to photon energy. Any well-calibrated estimator of energy must be *nonlinear* in the data. Can we somehow create a *nonlinear* estimator that nevertheless has the statistical advantages found in the *linear* procedure of optimal filtering?

## Linear Estimators are NOT Linear in $E$

Various linear estimators of pulse size are possible, including the statistically optimal one, known as *Optimal Filtering*. But when pulse sizes are not proportional to energy, and when pulse shapes change with energy, these linear estimators of pulse size make nonlinear estimators of energy.

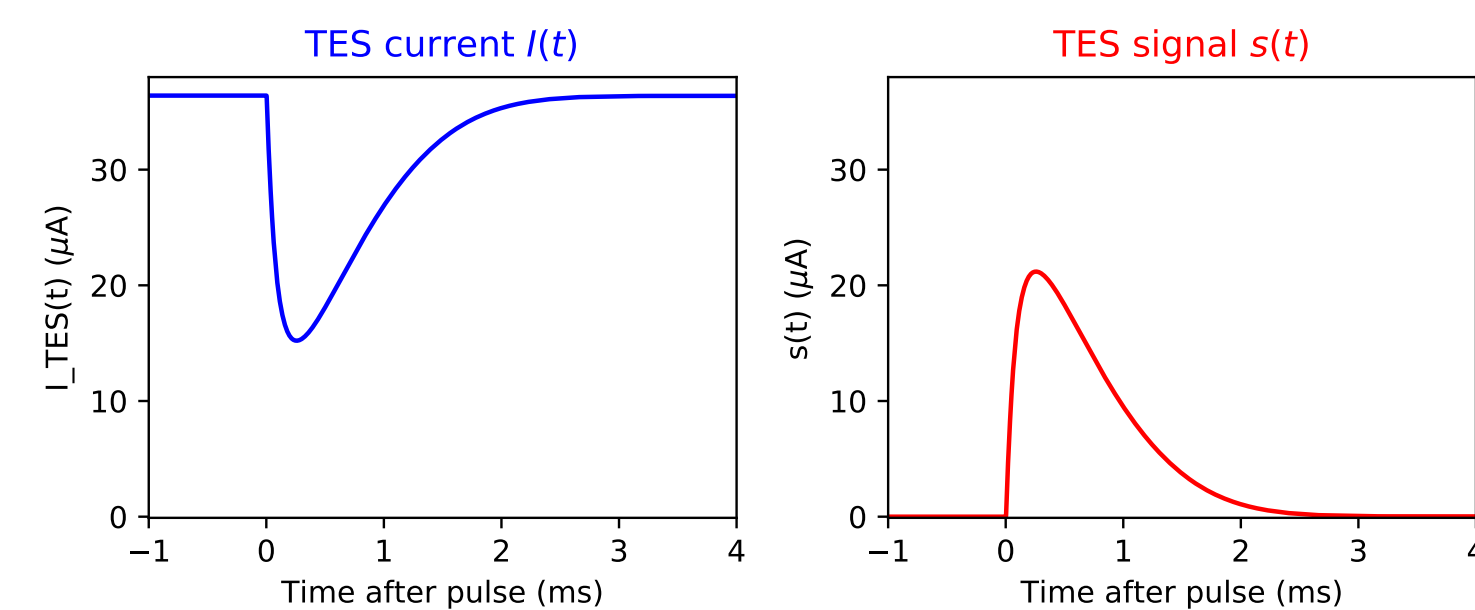


Linear TES pulse-size estimators show reduced response at high energies.

A nonlinear transformation from (linear) pulse size to energy—a “calibration curve” is needed. Absent further information about this curve, we must make smoothness assumptions. One that has worked well for us is to assume minimum curvature in the PH vs E domain, but we know this is a rather dubious principle to rely on.

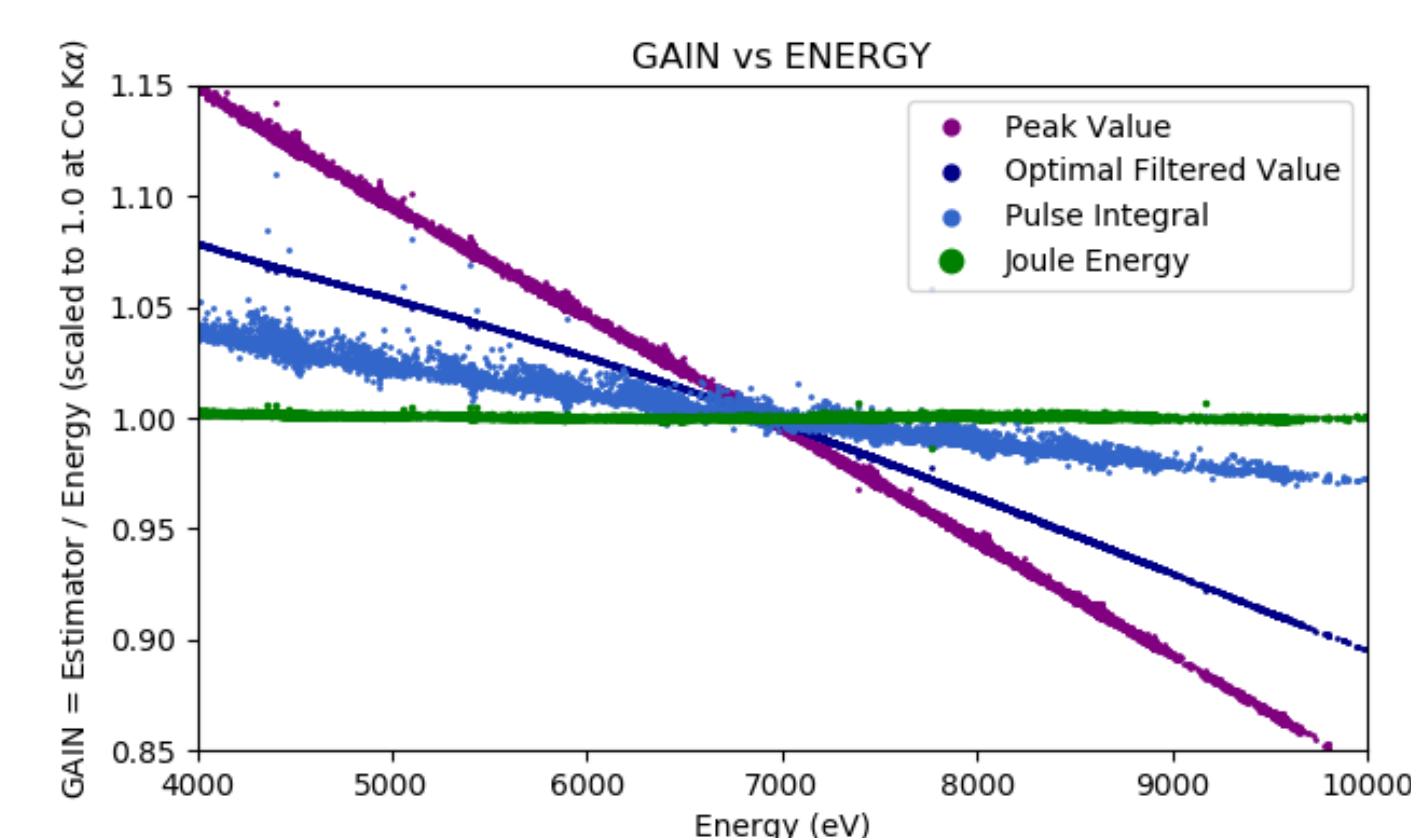
## Joule Energy Deficit $\propto$ Total Energy

A surprising and very useful fact (see talk by Christine Pappas, July 18): the TES signal represents a time-integrated deficit in Joule energy, and this *Joule energy is proportional to the deposited x-ray energy*, over a broad range of energies and TES bias and of thermal conditions.



Let  $I(t)$  and  $R(t)$  be the time-varying TES current and resistance. Let  $I_{base}$  be the baseline (quiescent) TES current and  $I_{bias}$  be the total current into the TES plus its shunt resistor. We define the positive-going signal  $s(t) \equiv I_{base} - I(t)$ . Then the Joule-energy deficit can be written:

$$E_{Joule} = \int dt R(t) [I_{base} - I(t)]^2 = R_{shunt} (I_{bias} - I_{base}) \int dt s(t) + R_{shunt} \int dt s^2(t)$$



The *Joule-energy integral* is very nearly proportional to energy.

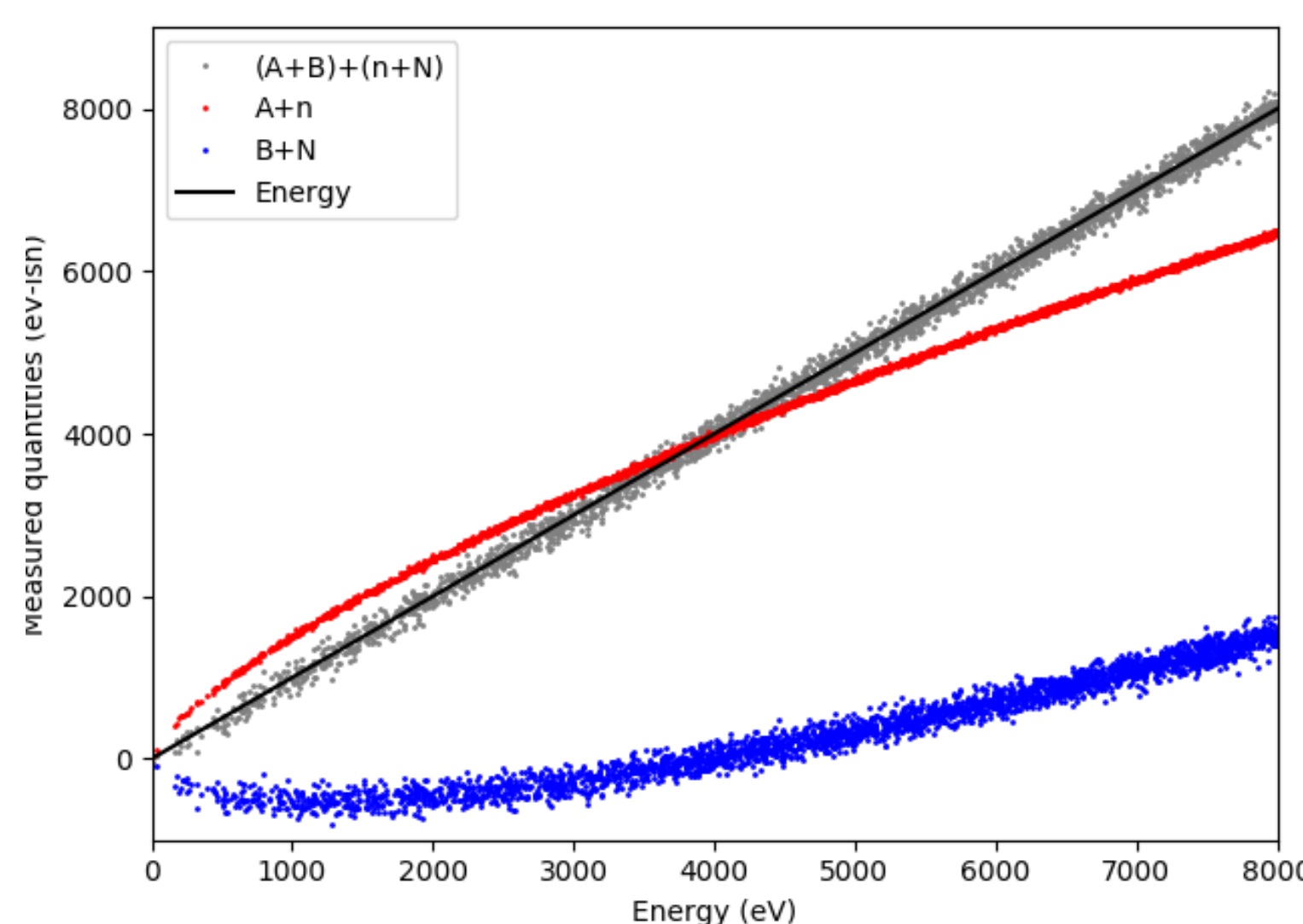
The Joule energy accounts for approximately 75% to 90% of the total deposited photon energy, depending on the exact TES design and bias voltage (the balance being dissipated by thermal conduction down the TES “legs”).

## Naïve Integrals of Noisy Signal are Noisy

We should not estimate this time-integral  $E_{Joule}$  directly on noisy pulse records; this would abandon all the advantages that optimal filtering techniques achieve by use of an appropriate noise-weighting of the data.

Imagine a simplified problem, to see why. Suppose we have measured the quantities  $A$  and  $B$  with noise levels  $n$  and  $N$ , respectively:

- $A$  is like the optimal filtering result: very low noise, but *not* linear in energy  $E$ .
- $B$  is a linearizing correction, but a noisy one. It is chosen such that...
- $(A+B)$  is an unbiased estimator of  $E$ , but also noisy because of the noise in  $B$ .



If we use the direct integrals of  $s(t)$  and  $s^2(t)$  to compute the Joule energy from noisy data, it's like the use of  $A+B$  to estimate energy in the cartoon above: it would be unbiased but noisy. What can we use in place of these integrals? More generally, how can we construct a nonlinear AND statistically optimal estimator?

## Acknowledgments

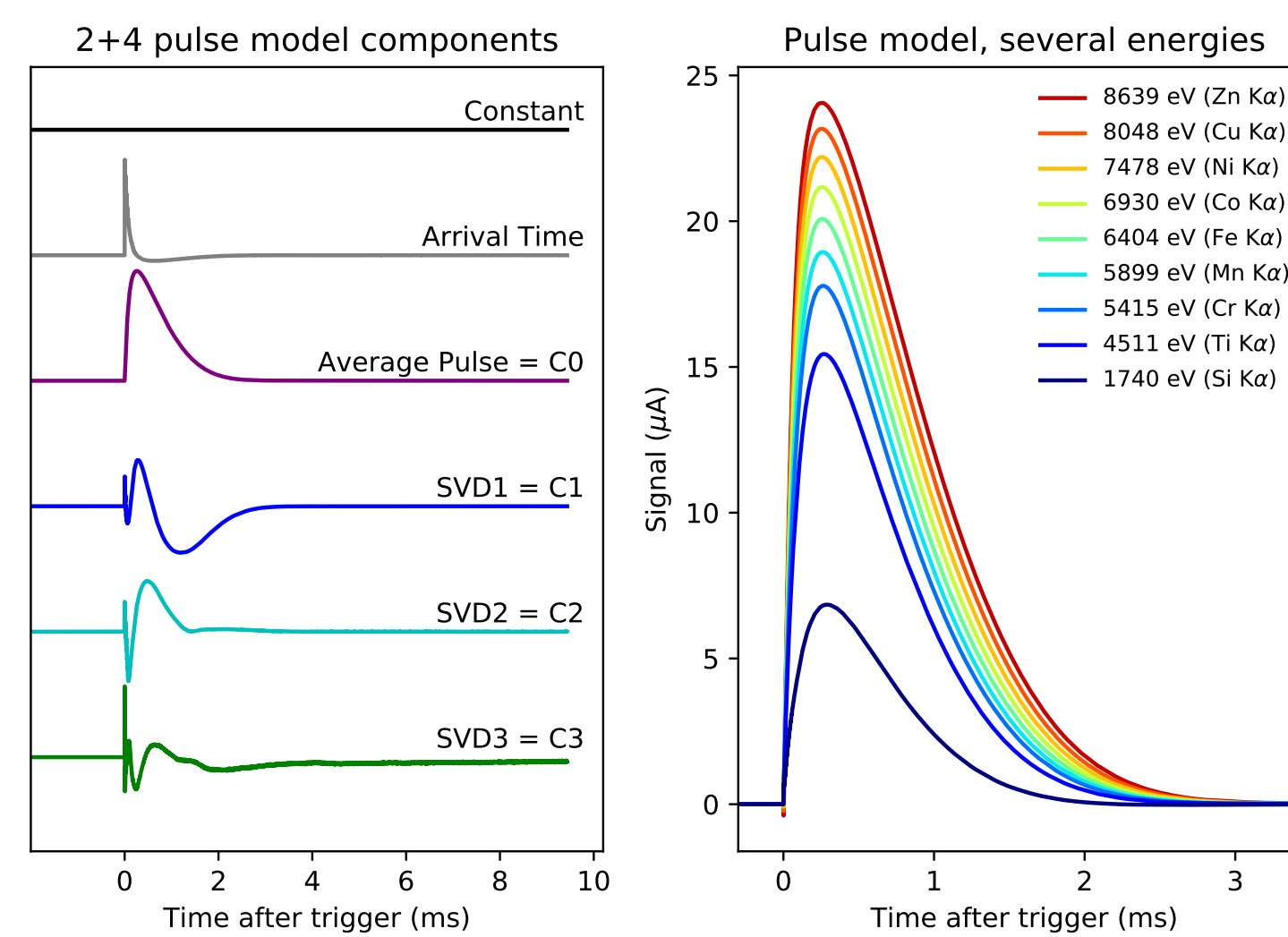
This work has been supported in part by the NIST Innovations in Measurement Science program, the NASA APRA program, the DOE BES program, and by two NRC Postdoctoral Fellowships and a NIST ARRA Senior Fellowship.

## Pulse-Height Optimal Nonlinear Estimates

We assume that pulses would lie along a 1-dimensional manifold (a curve) in higher-dimensional space, if not for noise. The curve can be parameterized by any quantity that signifies pulse size. (Ideally, it will be pulse energy, or something close.) These steps are relevant to any nonlinear analysis, not only an E-Joule estimation.

## Step 1: Approximate Pulses in a Low-Dimensional Subspace

The pulse records of length  $10^3$ – $10^4$  can be dramatically simplified by representing them as a sum of a few components. This amounts to projecting the record into a low-dimensional subspace. Here, we use 6 components: 2 are a constant baseline level and a (leading-order) arrival-time correction; the 4 of real interest are C0...C3.

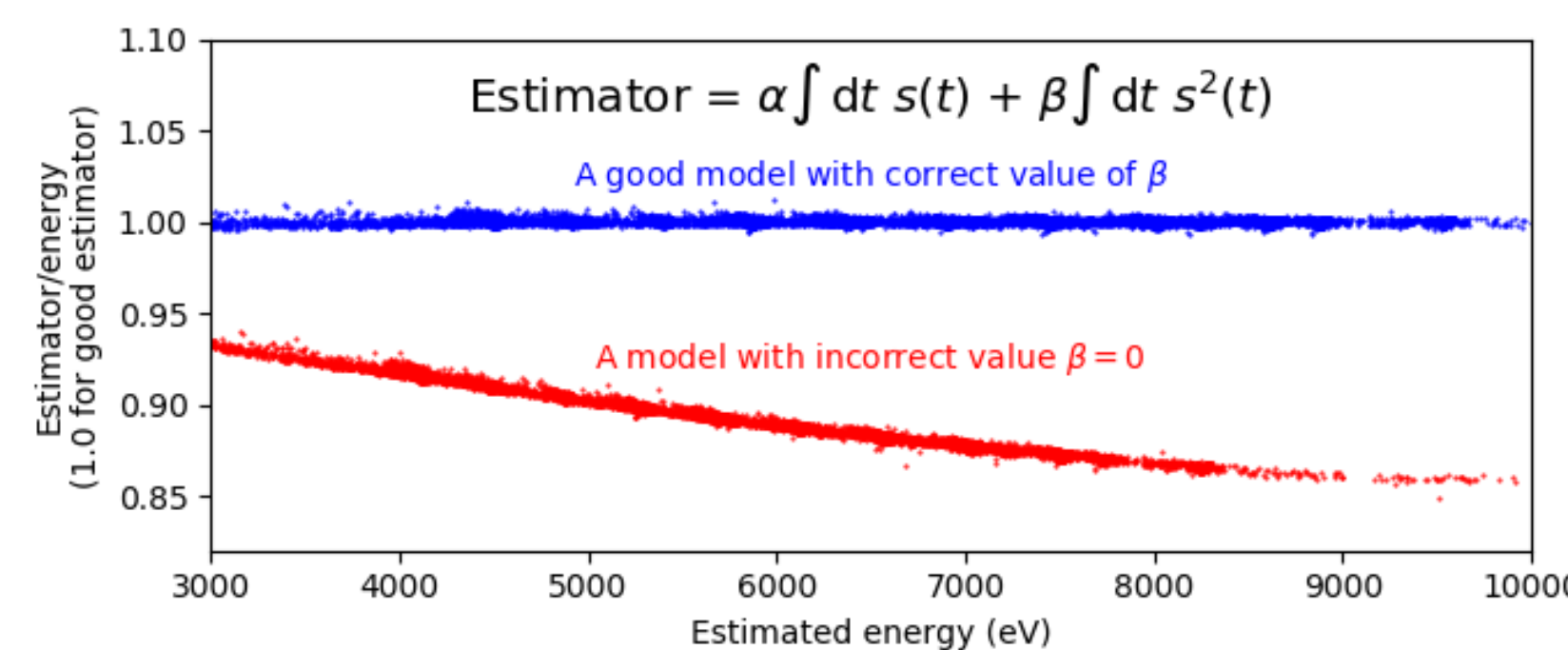


Left: pulse records are modeled as a linear combination of the 6 components shown here: 2 are “nuisance terms;” only the other 4 are used in later analysis. Right: Though important, the variation in pulse shape with energy is not readily visible from this set of typical pulses.

In this version, we choose component C0 as the average pulse shape over a broad energy range. The other components are the 3 leading singular vectors of the residual after fitting this simpler 3-component linear model. (Other choices are possible, such as a basis consisting of decaying exponentials of varying decay rates.) Projection into this subspace must be done with appropriate noise-weighting.

## Step 2: Find E-Joule's Two Weights

The formulas at left show that we know how to compute the weights for the time-integral of the first and second powers of the signal  $s(t)$ , which are needed to estimate E-Joule. However, they depend on electrical parameters that are measured only to 1%–3% uncertainty, at best. It is better to use data to estimate the weights  $\alpha$  and  $\beta$ . This requires a one-time use of external energy information, such as the identification of certain fluorescence lines.

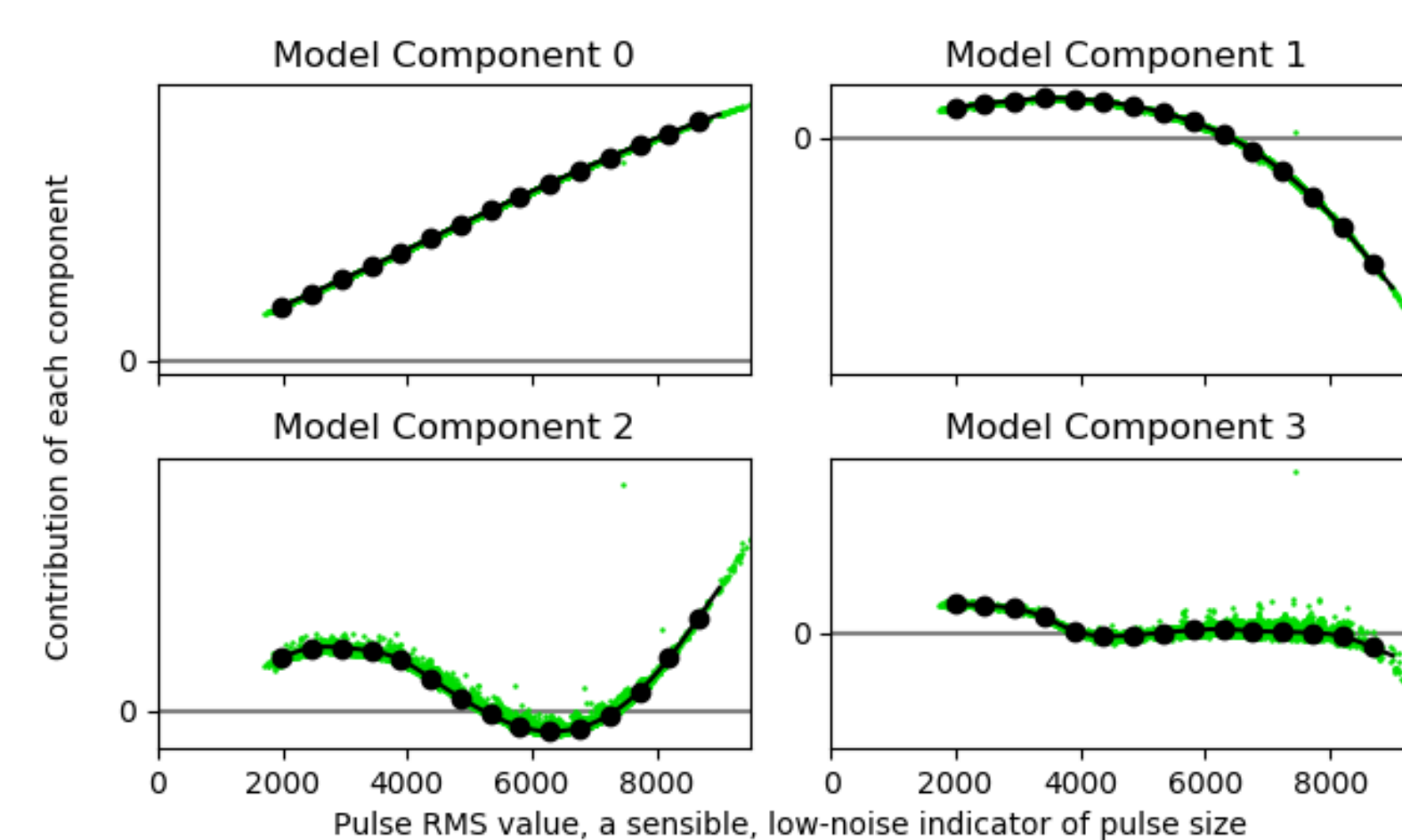


We can see that the correct value of  $\beta$  makes the estimated E-Joule proportional to photon energy. Proportionality also becomes equality with the best choice of  $\alpha$ .

## Step 3: Find the Approximate Curve

The critical noise-reduction step requires that we find and parameterize the 1-D curve within 4-D space that represents “allowed values” of C0...C3:

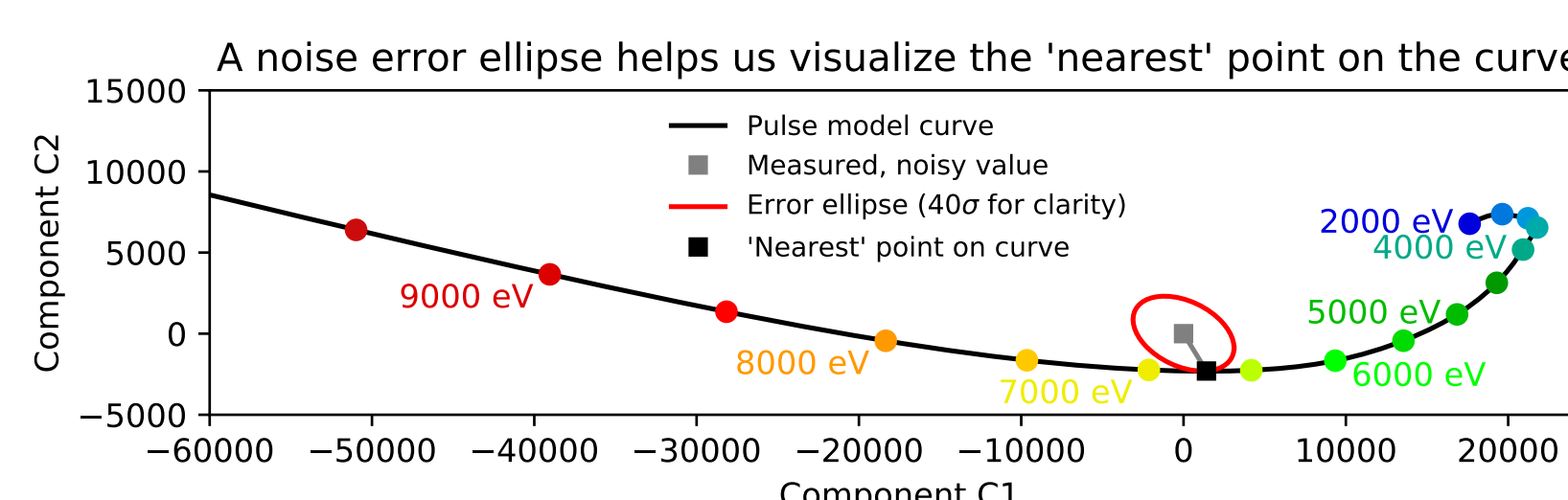
- Label each pulse by its rms deviation from the baseline. This value is simple to compute, and nearly as low in noise as an optimally filtered pulse height.
- Find 4 approximating splines for C0(rms), C1(rms), C2(rms), and C3(rms).
- This gives a model for pulse shape at any possible rms value, from which we can estimate the Joule-energy integral.



Data records (green) and spline-based model (black) for each component vs pulse rms magnitude. This same 1-D curve embedded in 4-D space can now be re-parameterized by estimated Joule energy.

## Step 4: Find the “Nearest” Point on the Curve for Each Pulse Record

To do avoid the problems shown in the “A+B” cartoon at left, we must ensure that we aren't finding components C0...C3 independently for each pulse. Instead, we have to find the point on the 1-dimensional model curve that best agrees with the data. That is, we need the (Joule-energy parameter of the) point that minimizes the Mahalanobis (signal-to-noise) distance between the noisy point and the model.



## Further Information

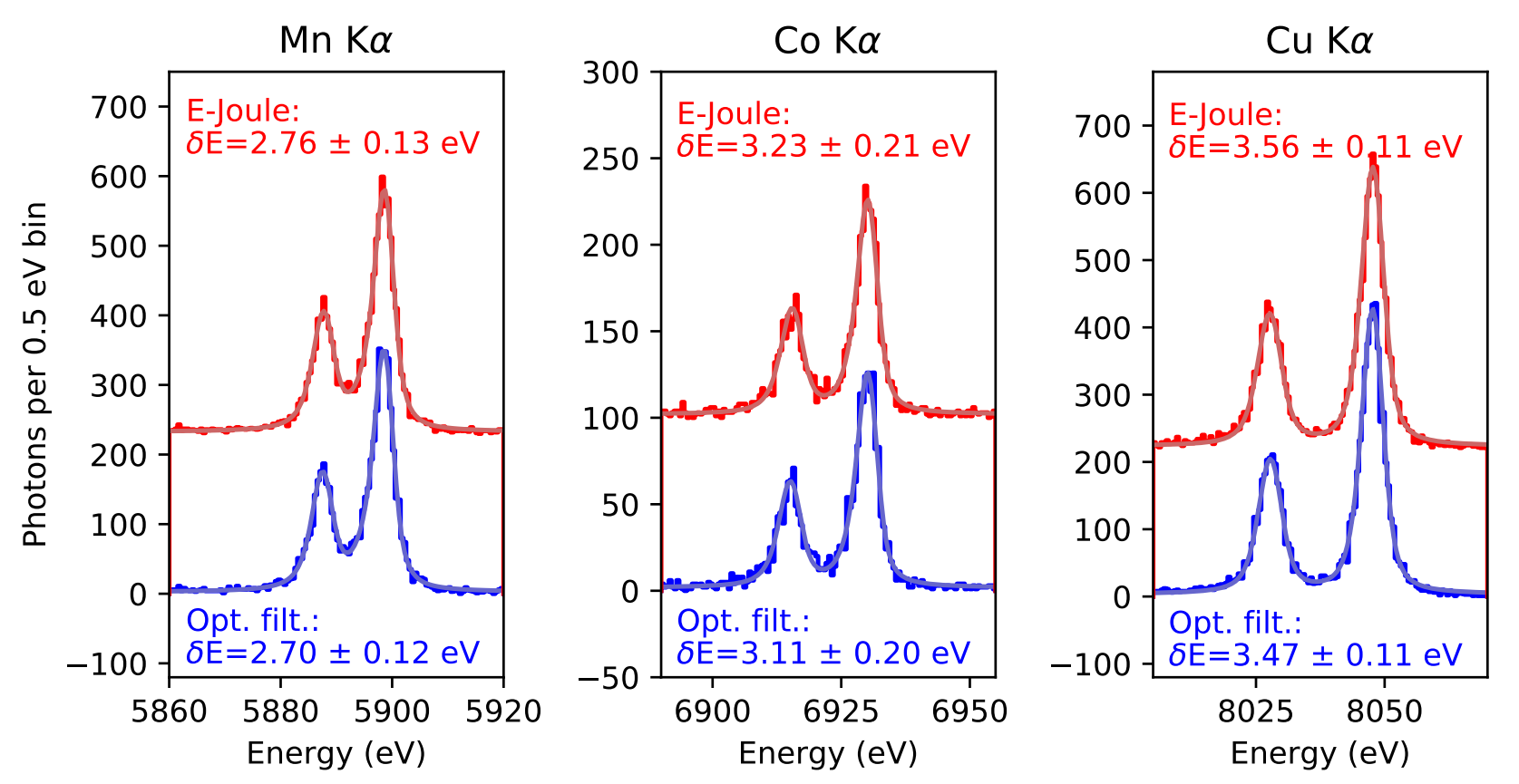
In <http://arxiv.org/abs/1611.07856>, we begin to address nonlinear pulse analysis.

## Application to Real Measurements

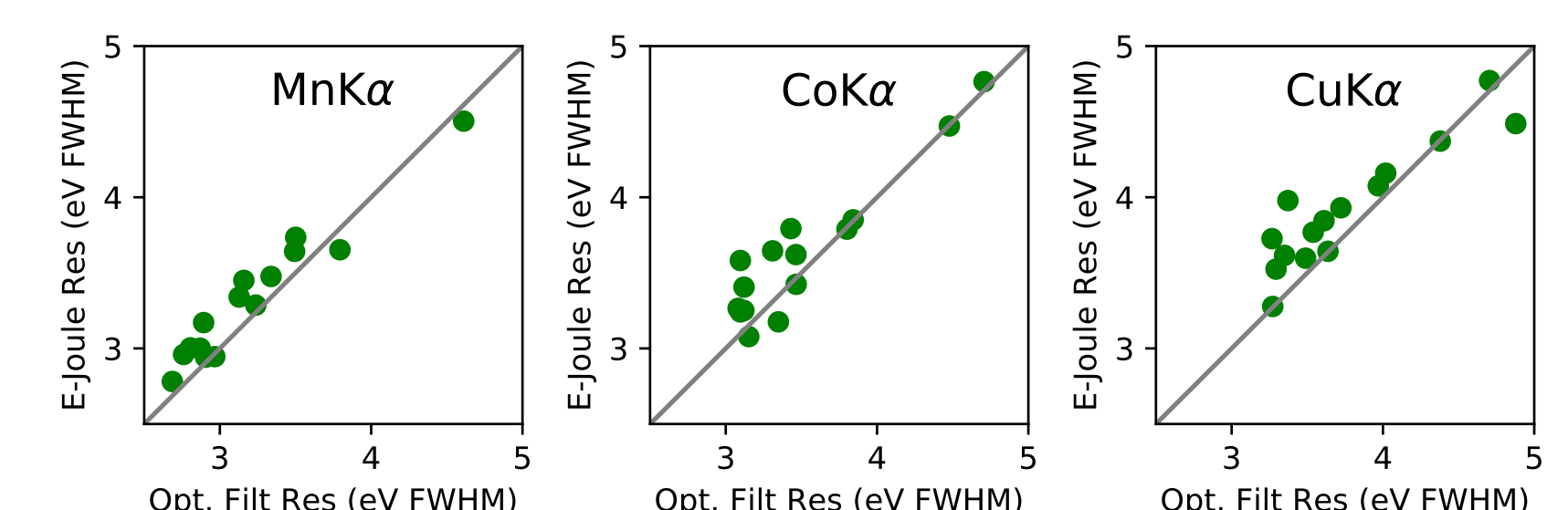
We apply this method to data taken with a  $3 \times 8$  array of TESs. The x-ray source was a fluorescence target illuminated by a broad-band commercial tube source. The target contains the 3d transition metals Ti, Cr, Mn, Fe, Co, Ni, Cu, and Zn. Their  $K\alpha$  and  $K\beta$  emission lines span the range 4.5 keV to 9.6 keV.

## Resolution: Close to Optimal Filtering

The details of this technique are still being developed, but already we find that most detectors are showing an energy resolution nearly as good as the value achieved through the standard optimal filtering technique.



The  $K\alpha$  lines of Mn, Co, and Cu for one TES, analyzed with standard optimal filtering (lower) and the Joule-energy integral (above).

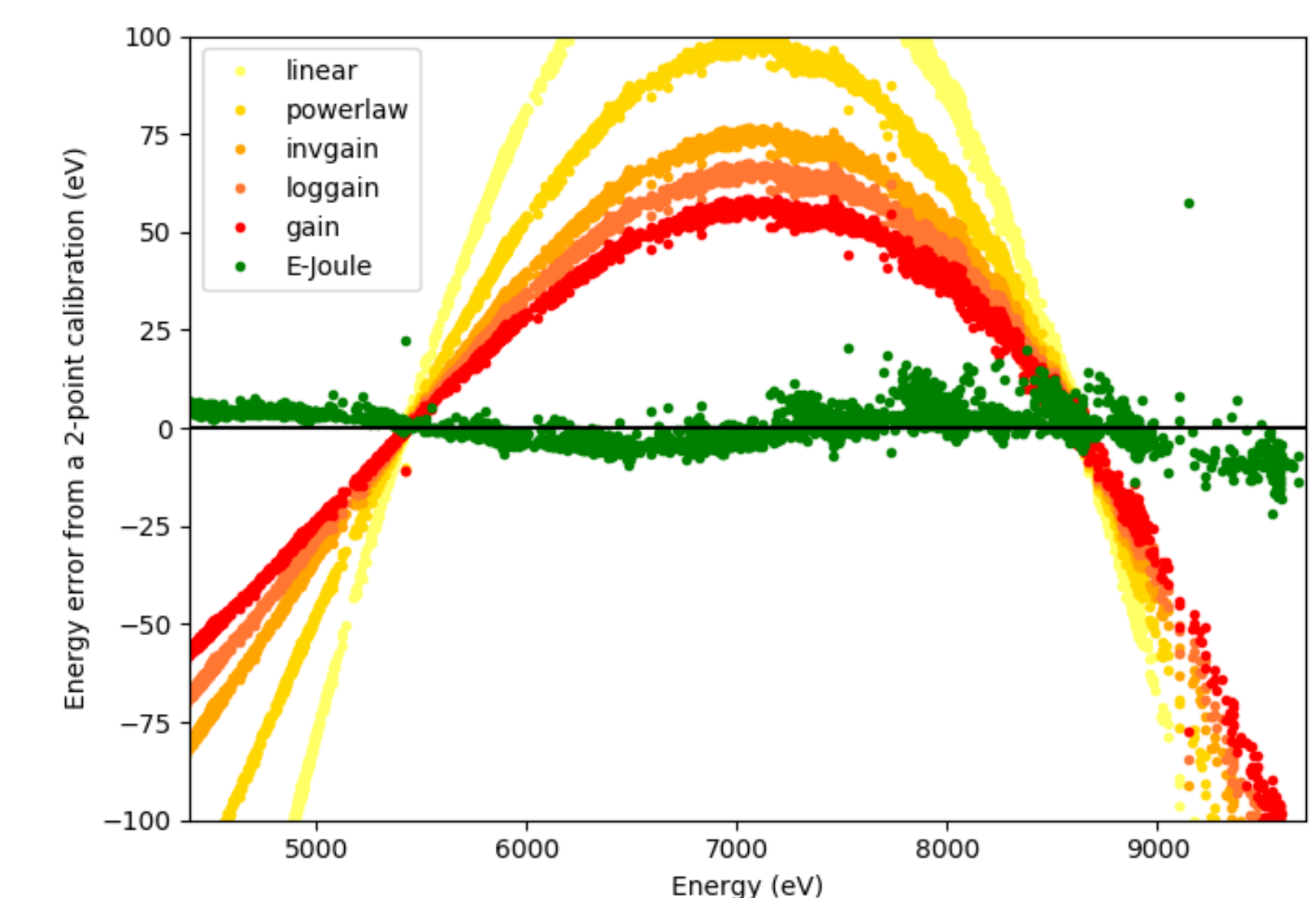


For the 15 TESs on which this method has been tried, the energy resolutions from the E-Joule technique are generally within 0.3 eV of the values found using a more traditional, optimal-filter analysis.

## E-Joule Estimator is Accurate to $\sim 5$ eV

The Joule-energy-based estimator of photon energies required us to learn only two parameters from data: the weights to give to the time-integrals of the signal current and of its square.

How far off is this energy estimator from the “true answer,” as determined through the usual painstaking multi-point calibration curve? And for comparison, how accurate would the usual optimal-filtering result be if we permitted it to be calibrated with only two free parameters?



The energy error from 2-point calibrations, for both analyses. Naturally, both would be adjusted with nonlinear “calibration curves,” but the Joule-energy analysis would require such a curve to do much less work.

Above are data calibrated with 2 free parameters per channel. For the optimal-filtered data (red, orange, yellow), we have anchored the calibration at the  $K\alpha$  energies of Cr and Zn (5.4 and 8.6 keV). The different colors reflect different choices of what is assumed to be linear in the measured pulse height: the energy, the gain, the inverse of the gain, etc. At best (gain linear in pulse height), the 2-point calibration error is off by 50 eV for the optimal filtered data over large parts of the range of interest. By contrast, the Joule energy estimator is within 5 eV over the entire range of 4 to 9 keV, an order of magnitude improvement.

## Future improvements and plans

We have developed an approach to the optimal nonlinear analysis of TES microcalorimeter pulses and applied it to the problem of making low-noise estimates of the Joule-energy deficit in a pulse. The steps include:

- Choose an appropriate low-dimensional basis in which to approximate pulse records.
- Project pulses into this basis with appropriate noise-weighting.
- Find the 1-dimensional manifold (curve) in this basis that represents the set of all “good pulses.”
- For each measured pulse, find the (noise-weighted) nearest point on the curve of good pulses, and use its “size” as the size of the chosen pulse.

These steps all present challenges and chances for future improvements:

- We have used the SVD as the “appropriate basis,” but the SVD is susceptible to capturing the noise in the training data. Can a better basis be found that is intrinsically smooth, and well-matched to the typical timescales of pulses?
- Projection is straightforward but requires a model of the noise correlation structure.
- Finding the manifold of “good pulses” is probably the biggest challenge. In full generality, it is an open research topic in machine learning! Can we restrict it to a sufficiently narrow problem?
- Computation of the (noise-weighted) nearest point on the curve needs to be made faster, or else this technique will not be competitive with optimal filtering for speed.

## Conclusions

We have attempted a fully nonlinear analysis of TES microcalorimeter pulses in order to achieve both highly accurate calibration and high signal-to-noise simultaneously. Such an analysis has not previously been made on TES data, as far as we are aware.

We expect that with further refinements, this nonlinear but statistically optimal approach can be very valuable in nearly any x-ray spectrometer measurement, particularly one in which calibration anchor points are few in number or low in intensity.