Least Squares Fitting and Equation Solving with MPFIT

Craig Markwardt

University of Maryland and
NASA's Goddard Spaceflight Center

http://purl.com/net/mpfit

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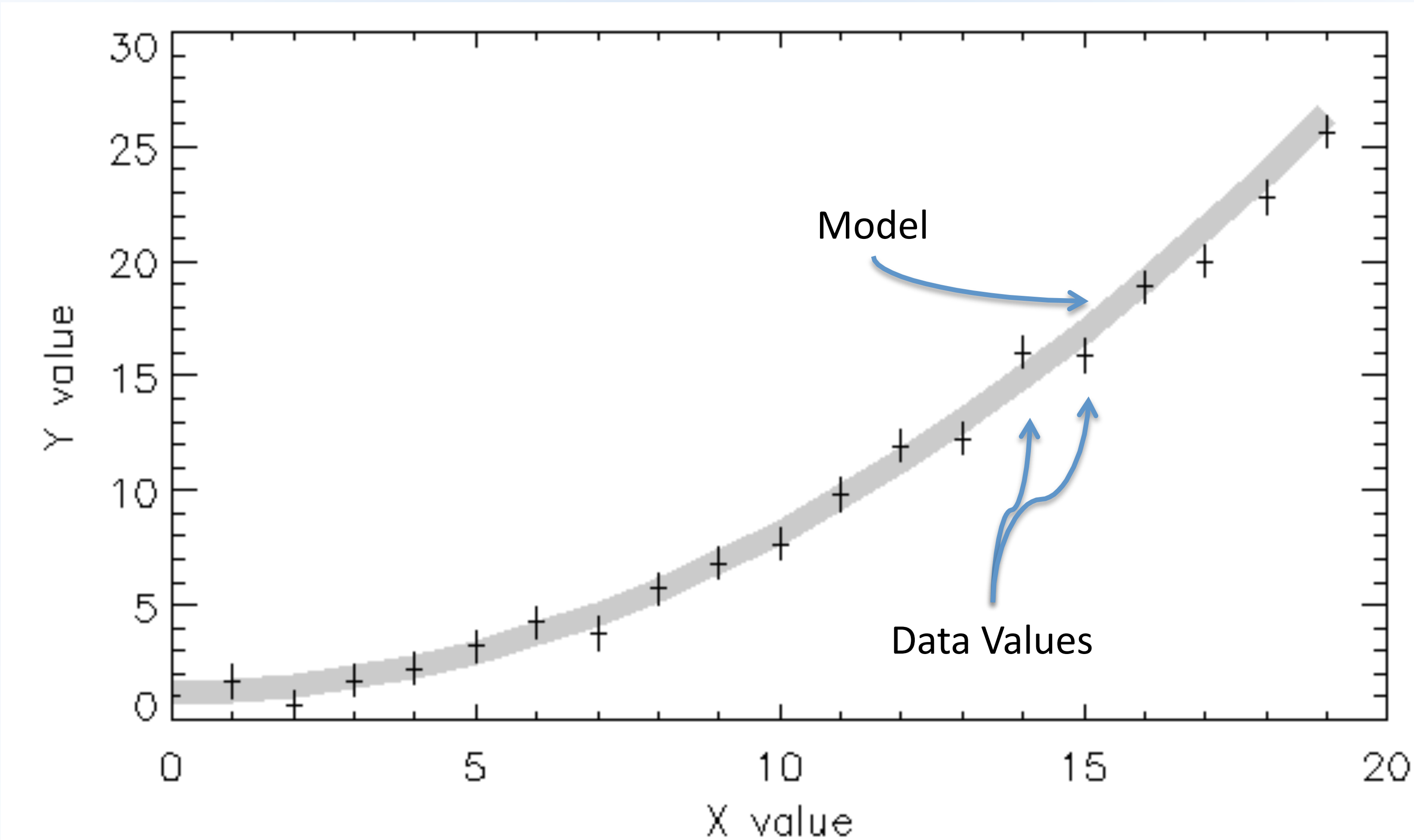
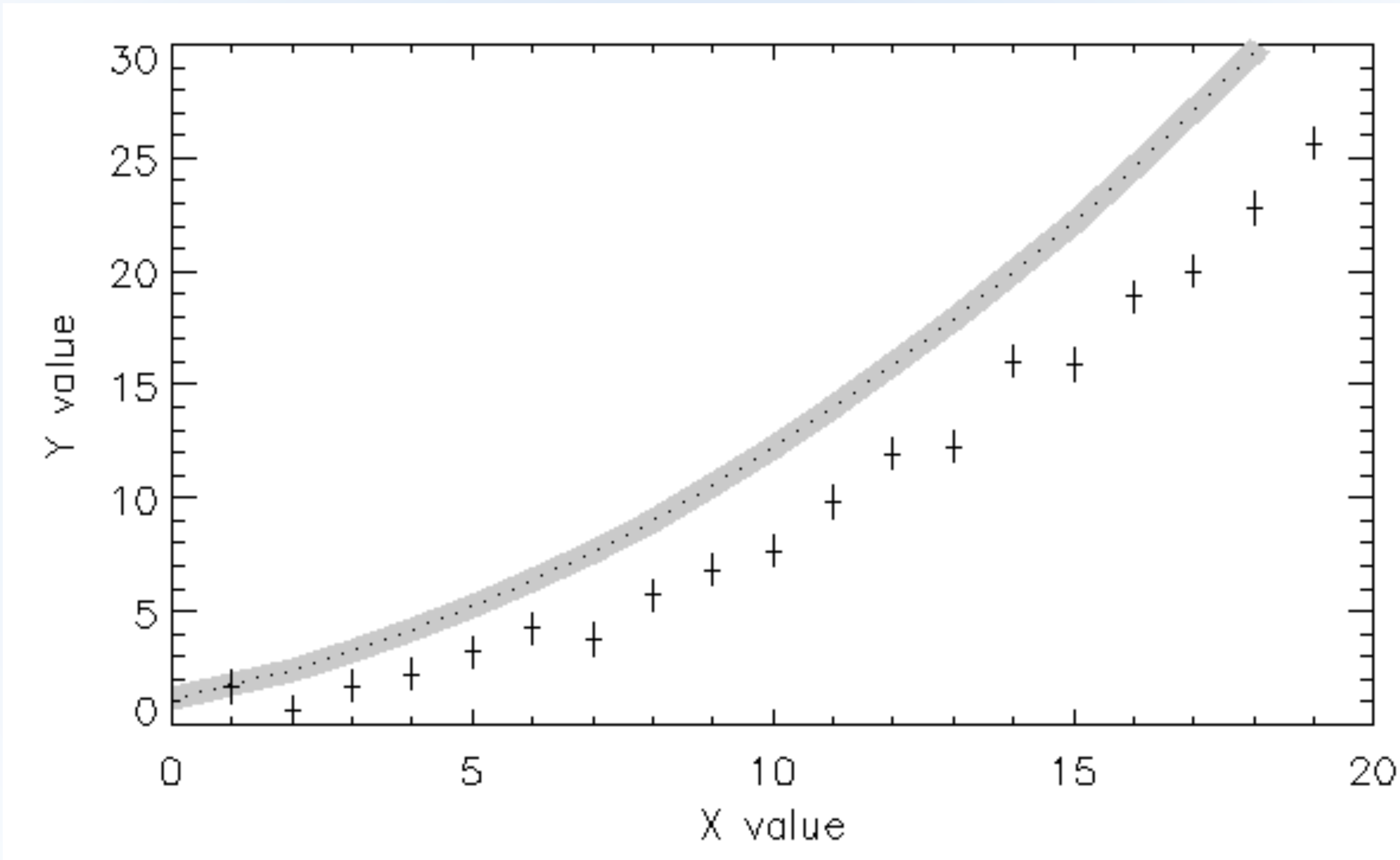
Data and Modeling

- Least squares fitting
- Act of hypothesis testing
- Simple Hypothesis:
  - data $\{x_i, y_i\}$ are consistent with model $f(x_i,p)$ to within the measurement uncertainties σ_i
  - where $\{x_i\}$ is the independent variable and $\{y_i\}$ is the dependent variable
  - $f(x_i,p)$ is the model function, which is parameterized by parameters p

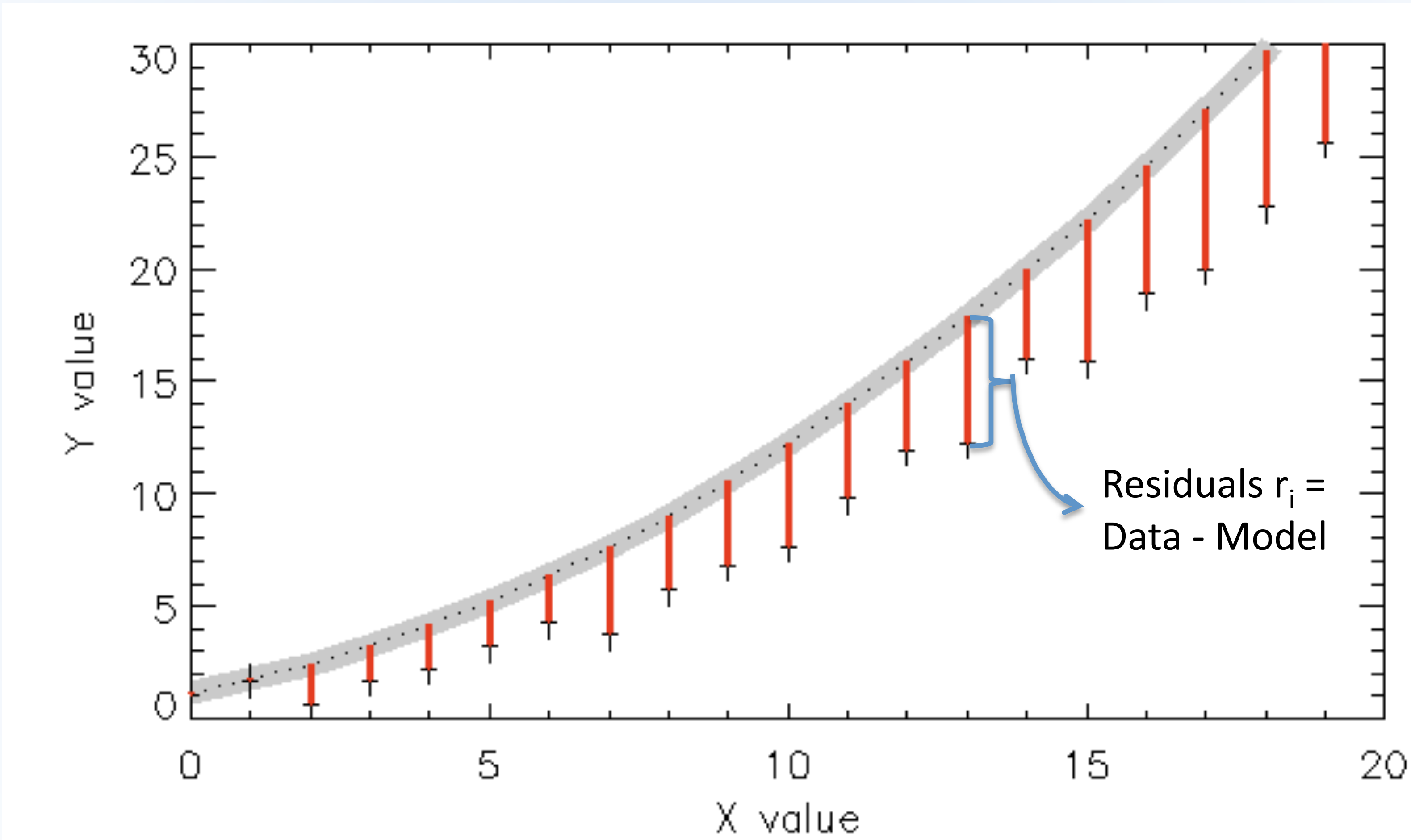
Fitting Example

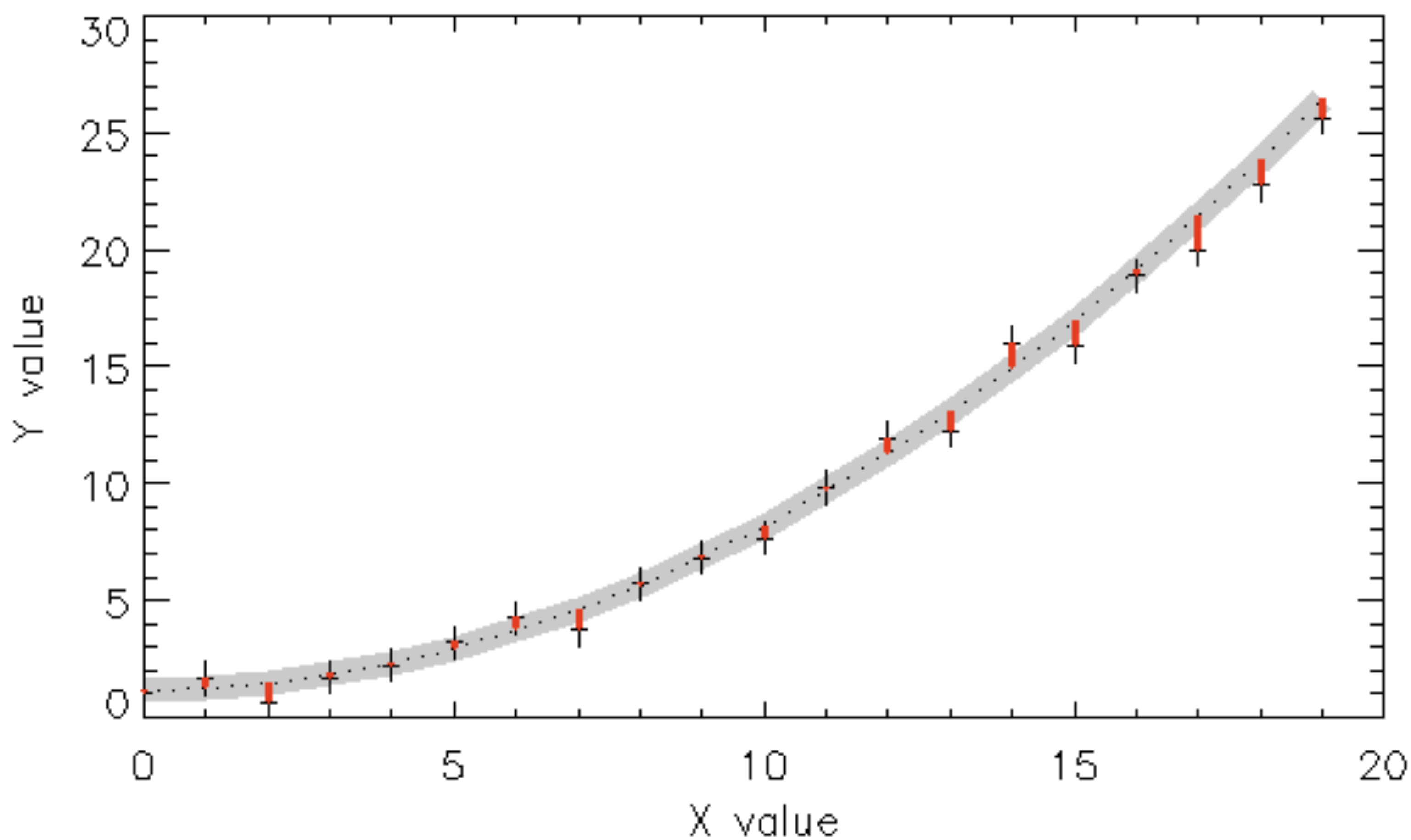


We Often "Know" When a Fit is Bad …



… because the Residuals are Large




30
25
20
15
10
5
0
Y value
0
5
10
15
20
X value

Summary

- At its basic level a "good fit" should minimize the residuals, r_i, between the data and model
- To balance the measurements with large and small uncertainty appropriately, our "scaled" residual looks like this,

"data" "model"

"residual"

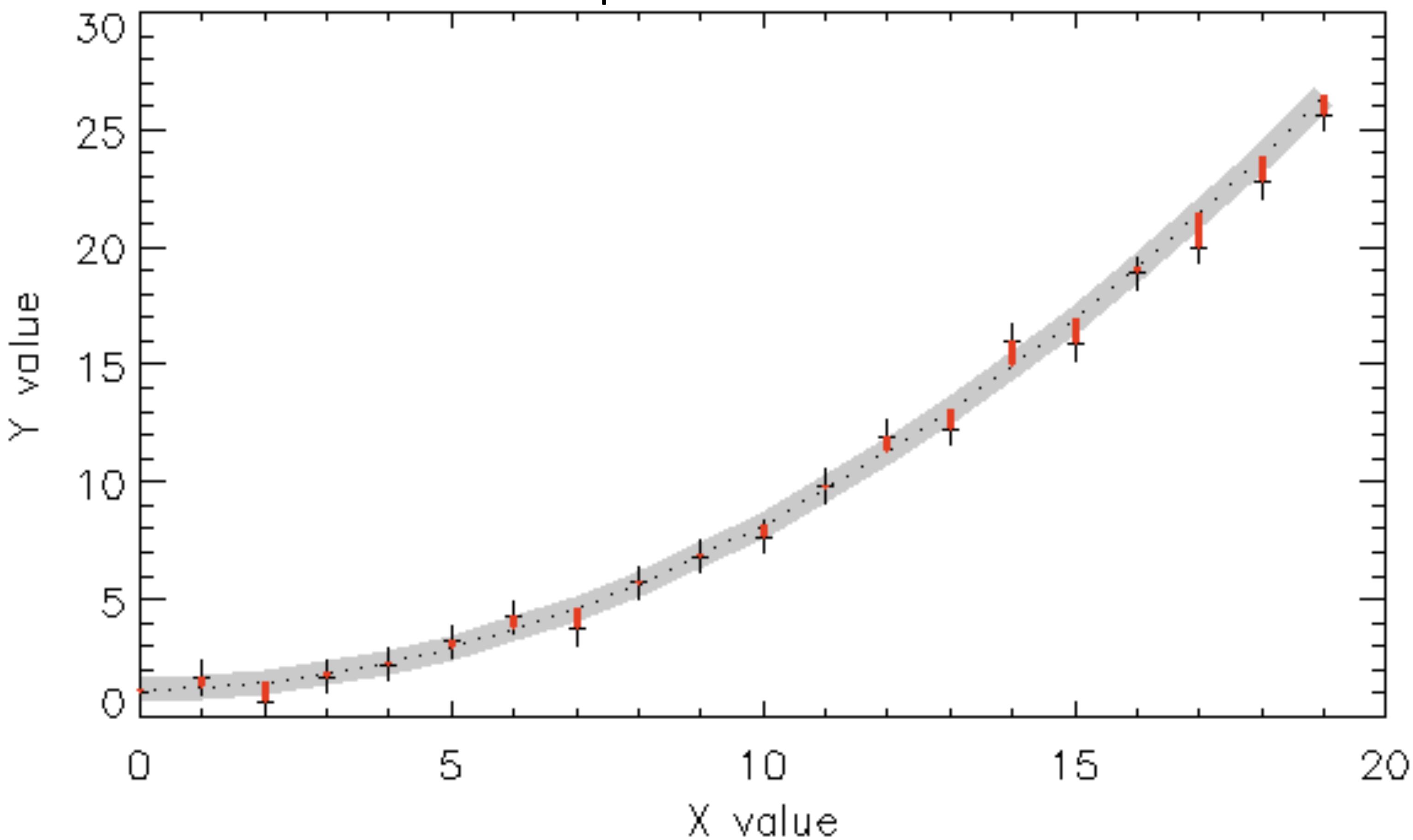
$$r_i = \frac{y_i - f(x_i, p)}{\sigma_i}$$

"measurement uncertainty"

- In an ideal world, we would want a perfect match between data and model, i.e. solve the following equations simultaneously for M data points:

$$\begin{aligned} r_0 &= 0 \\ r_1 &= 0 \\ &\vdots \\ r_M &= 0 \end{aligned}$$

In Practice this is not possible because of measurement noise…



- Instead we solve the system of equations in a "least squares" sense
- Define the chi-square statistic as the sum of the squared residuals,

$$\chi^2 = \sum_{i=1}^{M} r_i^2$$

and minimize this statistic.

Statistical Background

- The chi-square statistic is important and well known
- For gaussian statistics, chi-square minimization should be equivalent to the maximum likelihood parameter estimate
- In the real world, an optimal chi-square value

$$\chi^2 \sim M$$

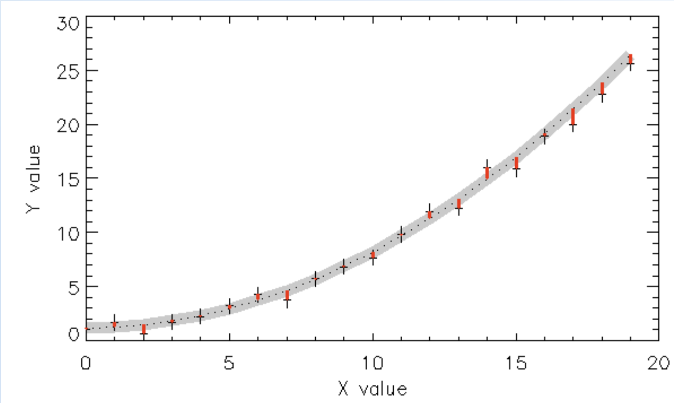
each data point contributes one degree of freedom.

Chi-Square Test

- Good fit:

$$\chi^2 \sim 19.9$$

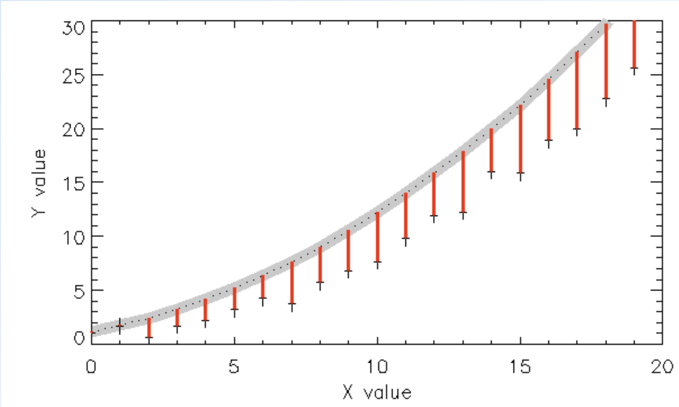
for 20 data points



- Bad fit:

$$\chi^2 \sim 756$$

for 20 data points



Existing Fitting Tools in IDL

- General non-linear:
  - CURVEFIT – Bevington algorithm (vectorized)
  - LMFIT – Numerical recipes (not vectorized)
- Specialized:
  - LINFIT – linear (y = ax + b)
  - POLY_FIT – polynomial
  - SVDFIT – linear combinations
  - GAUSSFIT – peak fitting

Introducing MPFIT

- Powerful fitting engine based on MINPACK-1 (Moré and collaborators; http://netlib.org/minpack/)
- Robust factorization and stepping algorithms
- Innovations:
  - Private data to user functions (FUNCTARGS)
  - Parameter upper and lower bounds (PARINFO)
  - User chooses who computes derivatives
  - Control over iteration, console output, stopping tolerances

- MPFIT is the main fitting engine, can solve any chi-square minimization problem expressable as

$$\min_p \sum_{i=1}^{M} r_i(p)^2$$

- Classic least squares fitting looks like this,

$$r_i(p) \quad = \quad \frac{y_i - f(x_i, p)}{\sigma_i}$$

but we will warp this to other uses later. Dimensionality of x or y are not important!

The MPFIT Family of Routines

- Core fitting engine: MPFIT
- 1D Convenience routines:
  - MPFITFUN
  - MPFITEXPR – command line fitting
  - MPFITPEAK – peak fitting
  - MPCURVEFIT – drop-in replacement for CURVEFIT
- 2D Convenience routines:
  - MPFIT2DFUN
  - MPFIT2DPEAK – peak fitting

Simple Example: MPFITEXPR

- Basic command line fitting, great for diagnosing data on the fly
- You supply a model function expression
  - `expr = 'P[0] + X*P[1] + X^2*P[2]'`
- And then call MPFITEXPR

  "x" "y" "errors" "start values"

  - `p = mpfitexpr(expr, xx, ys,  ye,  [1,1,1d], …)`
- Demo (mpfit_expr.pro)

MPFITFUN, MPFIT2DFUN

- For general fitting of a known model function, you will probably graduate to MPFITFUN or MPFIT2DFUN quickly
  - ```
    FUNCTION PARABOLA, X, P
          F = P[0] + X*P[1] + X^2*P[2]
          RETURN, F
    END
    ```
    ```

For More on the Basics

- Setting parameter boundaries (PARINFO)
- Passing private information (FUNCTARGS)
- Retrieving best-fit model function and chi-square value (YFIT and BESTNORM)

➔ See my website

More Advanced Topics

- Multi-dimensional data
- Complicated constraints
- Equation solving

Example: Line Fit, Errors in X and Y

- Numerical Recipes technique of modified chi-square value:

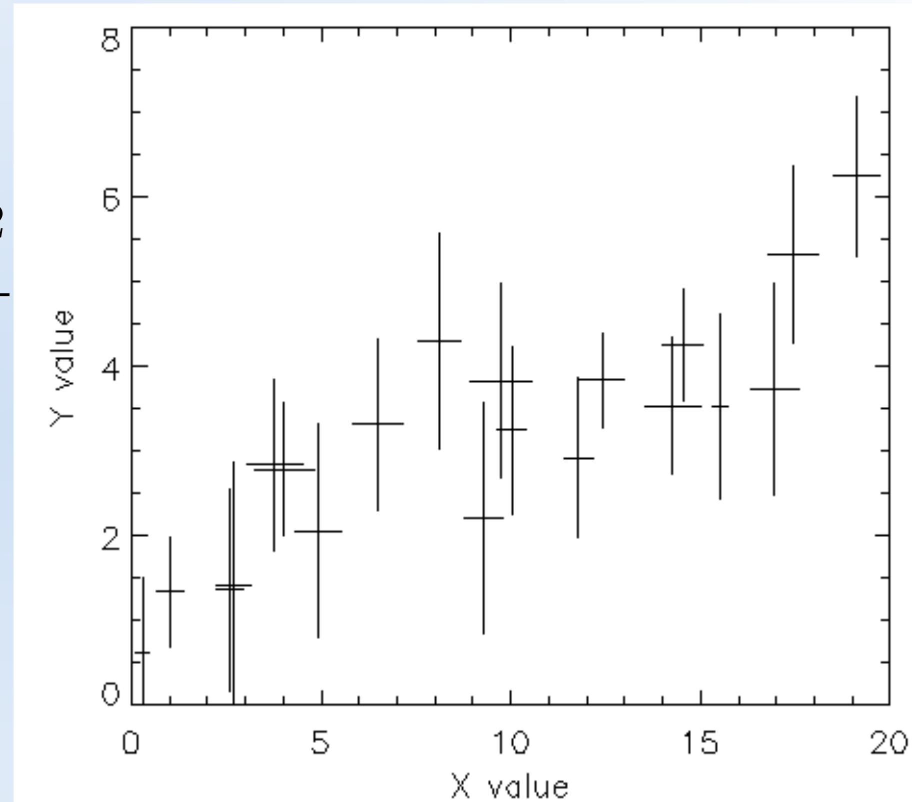
$$\chi^2 = \sum \frac{(y_i - a - bx_i)^2}{\sigma_{yi}^2 + b^2\sigma_{xi}^2}$$

- This looks exactly like an equation MPFIT will solve:

$$\chi^2 = \sum_{i=1}^{M} r_i^2$$

- If we set

$$r_i = \frac{y_i - a - bx_i}{\sqrt{\sigma_{yi}^2 + b^2\sigma_{xi}^2}}$$



Fitting with X and Y Errors

- LINFITEX: a user function which implements this technique

```
resid = (y - f)/sqrt(sigma_y^2 + (b*sigma_x)^2)
```

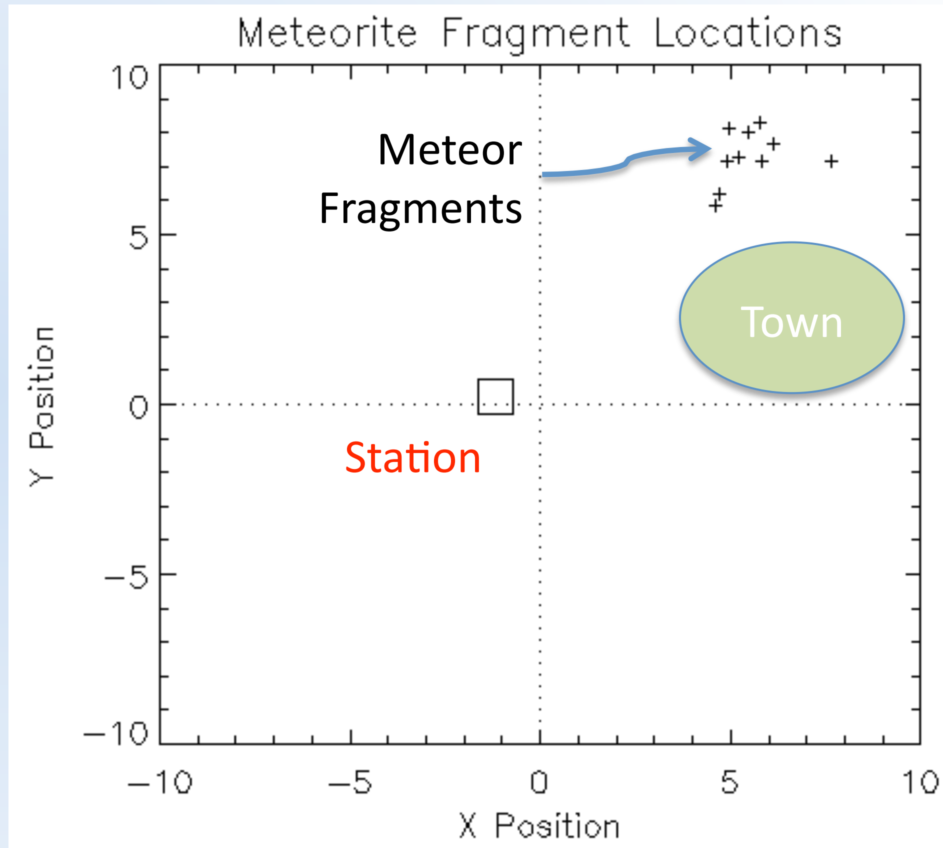
- We call MPFIT with this user function

```
p = mpfit('LINFITEX', [1d, 1d], $
             FUNCTARGS={X: XS, Y: YS, $
             SIGMA_X: XE, SIGMA_Y: YE}, …)
```

- Demo (MPFIT_LINFITEX)

Fitting In Two Dimensions

- Example problem:
  - A meteor appeared and exploded near a remote Alaskan town
  - The townspeople located several meteorite fragments and reports to us at local observing station
- Goal: determine point of meteor explosion from fragment locations



Centroid Point

- We approximate the explosion point as the centroid, (x_c, y_c), the point which has the smallest joint distance from all fragments

$$\min(\mathrm{dist}^2) = \sum_{i=1}^{M} (x_i - x_c)^2 + (y_i - y_c)^2$$

- Again, this looks exactly like a problem MPFIT can solve, except with **twice** as many residuals

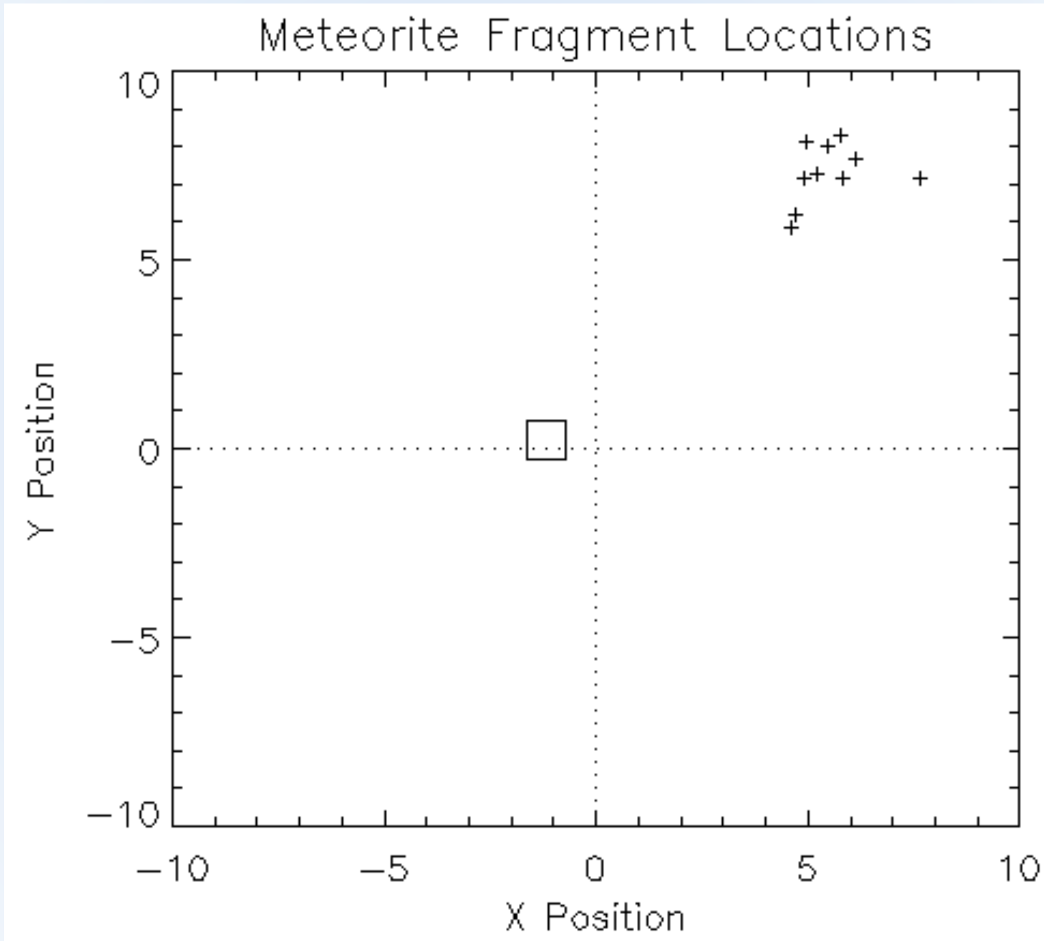
$$\chi^2 = \sum_{i=1}^{M} r_{xi}^2 + r_{yi}^2$$

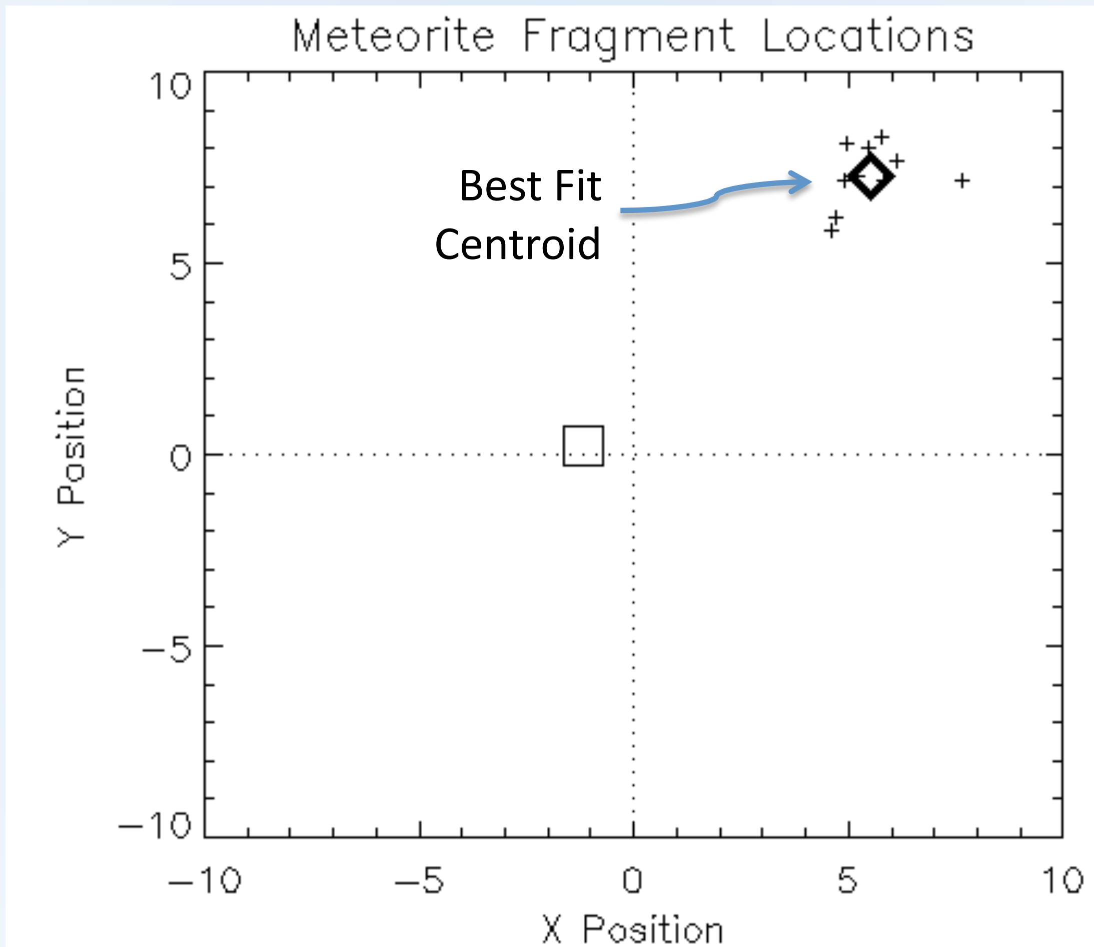
MPFIT Model

- MPFIT will understand this if the two sets of residuals are appended:

```
FUNCTION MPFIT_CENT, P, X=X, Y=Y
     resid_x = (x-p[0])
     resid_y = (y-p[1])
     resid = [resid_x, resid_y]
     return, resid
END
```

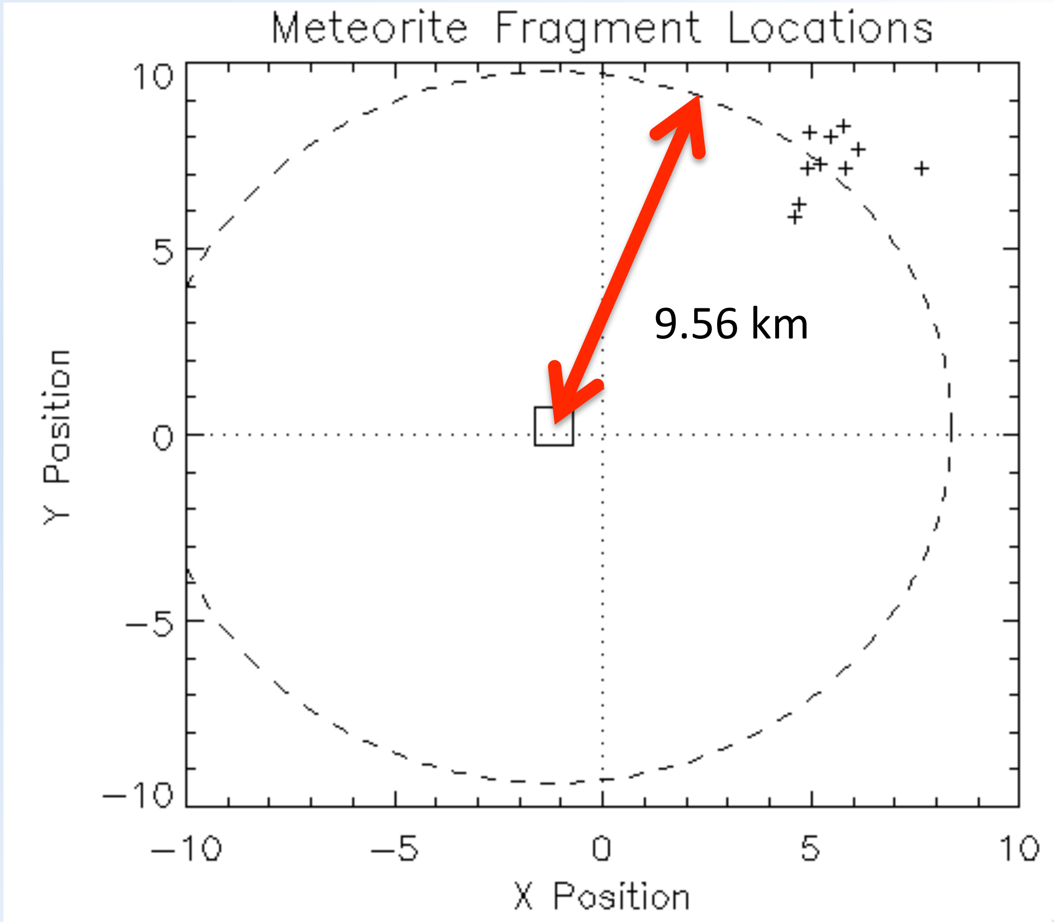
- Demonstration (MPFIT_METEORITE)


Meteorite Fragment Locations
10
5
0
−5
−10
Y Position
−10
−5
0
5
10
X Position


Meteorite Fragment Locations
Best Fit
Centroid
Y Position
X Position
10
5
0
−5
−10
−10
−5
0
5
10

Adding Complex Constraints

- New Meteorite Information!
  - Station sensors detected a light flash and sonic boom, allowing range to be determined to 9.56 km
- We now know the explosion point lies somewhere on the circle
- How can we add this new information?



MPFIT Model

- Express this new parameter constraint as,

$$(x_c - x_s)^2 + (y_c - y_s)^2 = R^2 = (9.56\mathrm{km})^2$$

- But how can we force MPFIT to honor this constraint?
- Trick: re-write the constraint to be another “residual”, which should equal 0, and MPFIT will solve it along with all the other residuals

$$
\begin{aligned}
r_0 &= 0 \\
r_1 &= 0 \\
&\vdots \\
r_M &= 0 \\
(x_c - x_s)^2 + (y_c - y_s)^2 - R^2 &= 0
\end{aligned}
$$

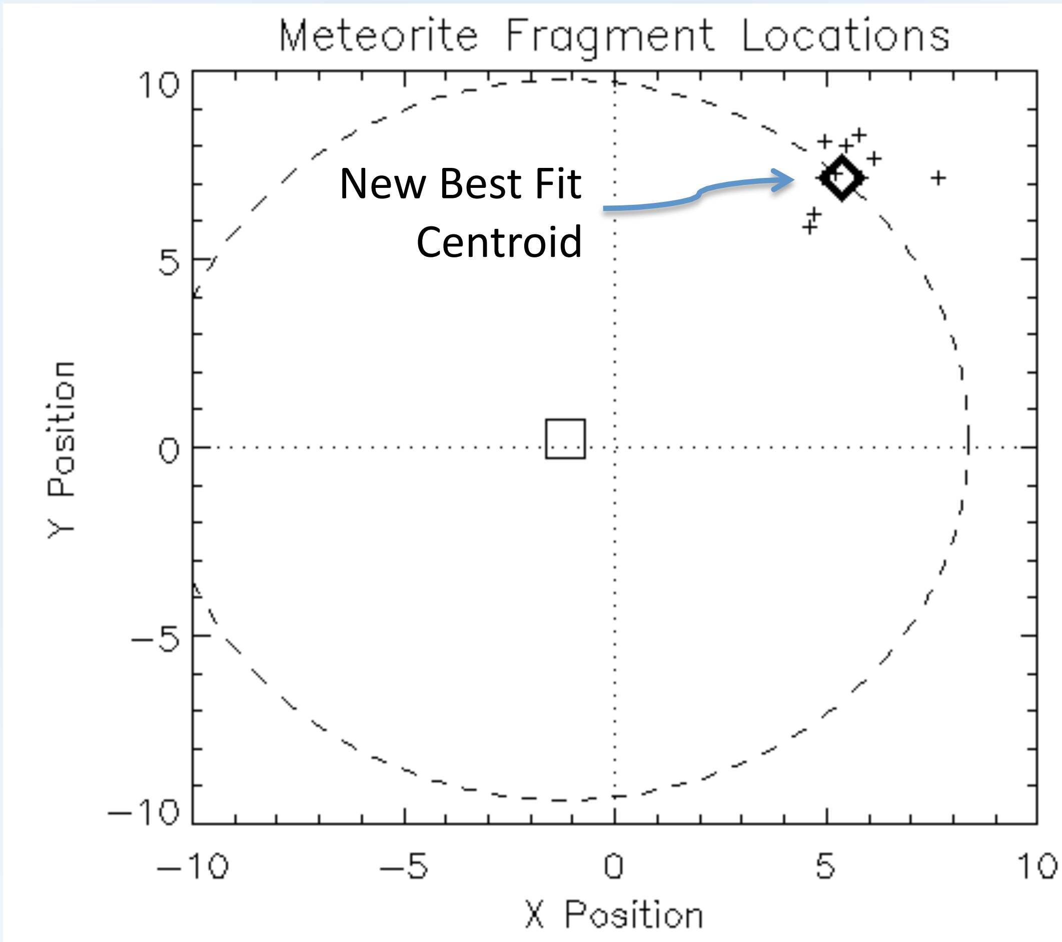
New Constraint!

MPFIT Model

- MPFIT will understand this we now append **three** sets of residuals:

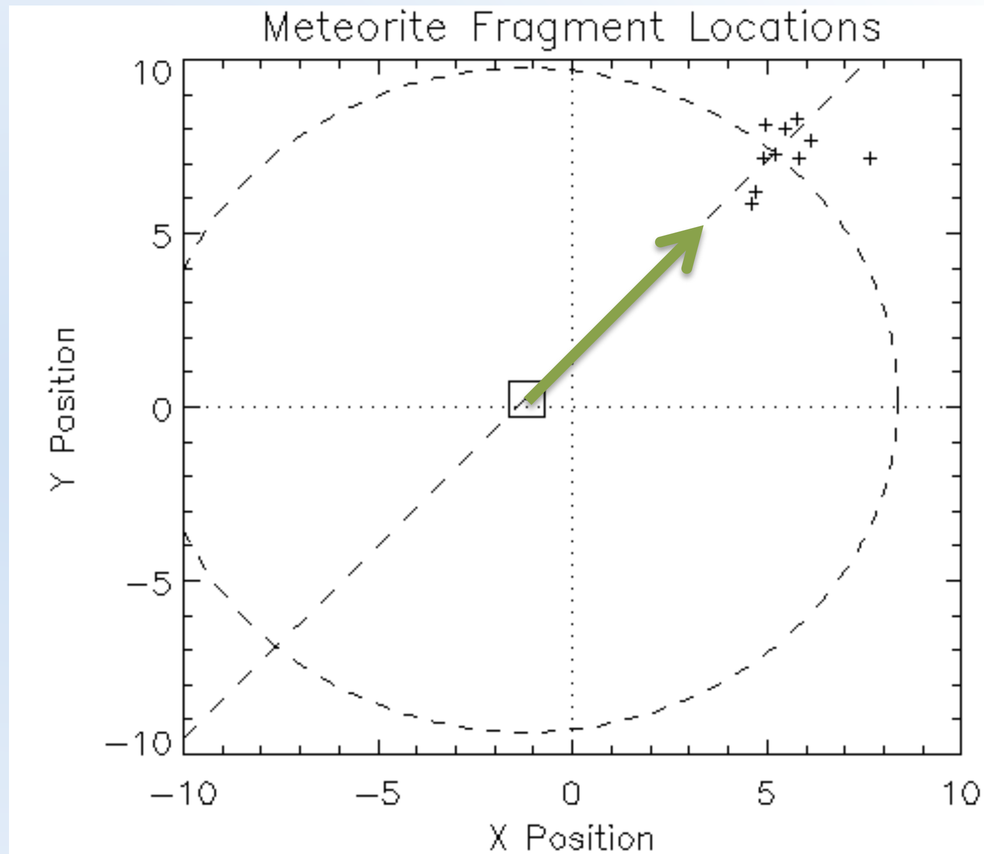
```
resid_x = (x-p[0])
resid_y = (y-p[1])
resid_r = (p[0]-xs)^2 + (p[1]-ys)^2 - radius^2
resid = [resid_x, resid_y, resid_r/tolerance]
```

- Demonstration (MPFIT_METEORITE)


Meteorite Fragment Locations
New Best Fit
Centroid
10
5
0
−5
−10
Y Position
−10
−5
0
5
10
X Position

Two Constraints!

- Even Newer Meteorite Information!
  - A station staffer observed the flash visually and obtained a sight line of 48 deg north of east
- We now know a second line of constraint
- How can we add this new information?



$$y_c = \tan(\theta)(x_c - x_s) + y_s$$

Another Constraint!

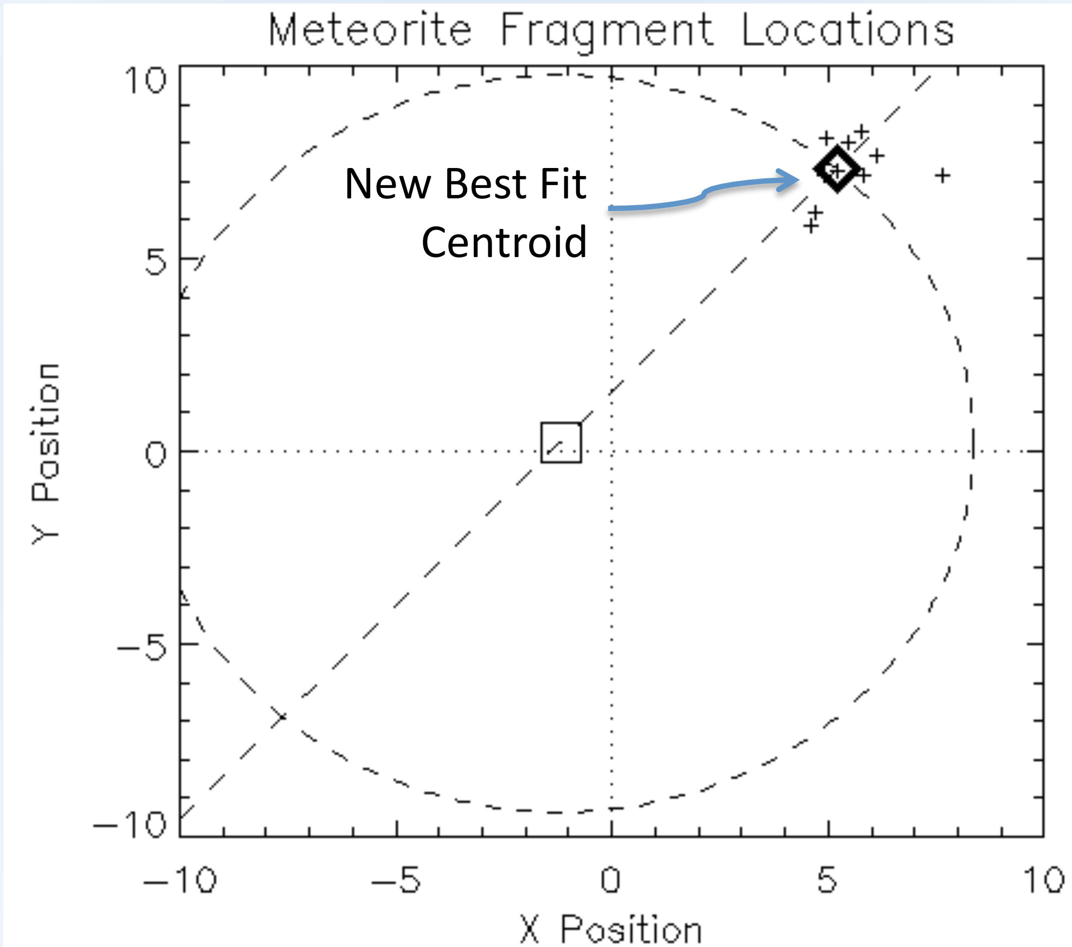
$$\begin{aligned} r_0 &= 0 \\ r_1 &= 0 \\ &\vdots \\ r_M &= 0 \\ (x_c - x_s)^2 + (y_c - y_s)^2 - R^2 &= 0 \\ \tan(\theta)(x_c - x_s) + y_s - y_c &= 0 \end{aligned}$$

MPFIT Model

- MPFIT will understand this if we now append a **fourth** residual function:

```
 …
resid_s = tan(sight_angle*!dtor)*(p[0]-xs) + ys - p[1]
resid = […, resid_s / sight_pos_tolerance]
```

- Demonstration (MPFIT_METEORITE)


Meteorite Fragment Locations
New Best Fit
Centroid
Y Position
X Position
10
5
0
−5
−10
−10
−5
0
5
10

Equation Solving

- The two last constraints in this problem are alone enough completely specify the explosion point

$$
\begin{aligned}
(x_c - x_s)^2 + (y_c - y_s)^2 - R^2 &= 0 \\
\tan(\theta)(x_c - x_s) + y_s - y_c &= 0
\end{aligned}
$$

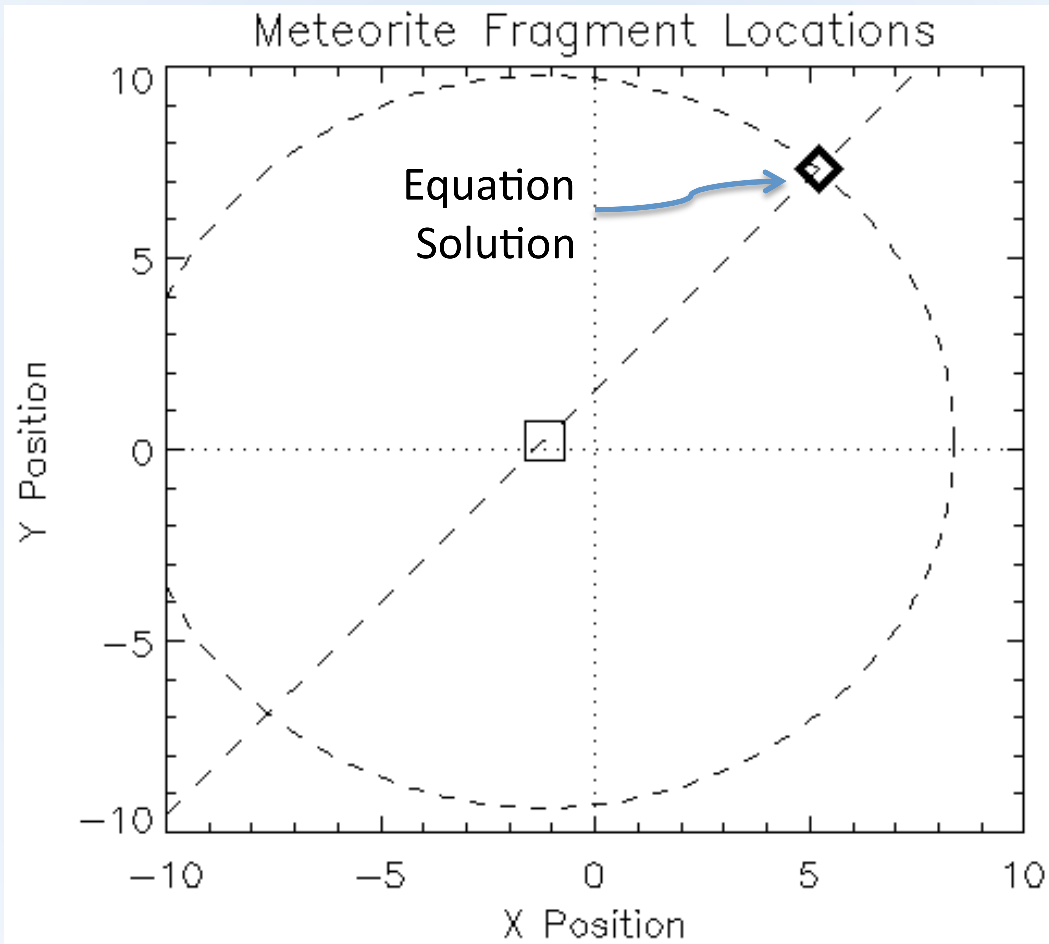
- We don’t even need data!

MPFIT Model

- MPFIT will understand this if we keep only the last two constraint equations:

```
resid_r = (p[0]-xs)^2 + (p[1]-ys)^2 - radius^2
resid_s = tan(sight_angle*!dtor)*(p[0]-xs) + ys - p[1]
resid = [resid_r/tol, resid_s / sight_pos_tolerance]
```

- Demonstration (MPFIT_METEORITE)


Meteorite Fragment Locations
Equation
Solution
Y Position
X Position
10
5
0
−5
−10
−10
−5
0
5
10

Caveats

- This technique depends on using MPFIT, not the other more "convenient" routines
- If MPFIT finds a solution, that does not prove it is unique (could be multiple solutions!)
  - Depends on initial conditions
- If equations are poorly behaved, MPFIT may get stuck
  - Need to adjust derivatives parameters via PARINFO

Take Away Messages

- MPFIT is a power equation solver
- Fitting M points is just solving M equations
- Adding new constraints is straightforward, just add new "residual" equations
  - i.e. re-express constraint as
    (*function) / (tolerance)* = 0
- Other estimators like "least absolute deviation" (LAD) and Poisson likelihood can be solved by warping their equations to look like a sum of squared residuals

Getting MPFIT

- IDL version: http://purl.com/net/mpfit
- C version at same site