Fitting Data

- We get experimental/observational data as a sequence of times (or positions) and associate values
  - N points: (x_i, y_i)
  - Often we have errors in our measurements at each of these values: σ_i for each y_i
- To understand the trends represented in our data, we want to find a simple functional form that best represents the data—this is the fitting problem
  - We'll follow the discussion in Garcia to get a basic feel for the problem (the discussion in Numerical Recipes is quite similar too)
- This is a big topic—we'll just look at the basics here
  - We'll see that our previous work on linear algebra and root finding comes back into play...

Fitting Data

- We want to fit our data to a function: $Y(x, \{a_j\})$
  - Here, the a_j are a set of parameters that we can adjust
  - We want to find the optimal set of a_j that make Y best represent our data
- The distance between a point and the representative curve is

$$\Delta_i = Y(x_i, \{a_j\}) - y_i$$

  - Least squares fit minimizes the sum of the squares of all these errors
  - With error bars, we weight each distance error by the uncertainty in that measurement, giving:

$$\chi^2(\{a_j\}) = \sum_{i=1}^{N} \left(\frac{\Delta_i}{\sigma_i}\right)^2$$

This is what we minimize

Linear Regression

- Minimization: derivative of χ^2 with respect to all parameters is zero:

$$\frac{\partial \chi^2}{\partial a_1} = 2 \sum_{i=1}^{N} \frac{a_1 + a_2 x_i - y_i}{\sigma_i^2} = 0$$

$$\frac{\partial \chi^2}{\partial a_2} = 2 \sum_{i=1}^{N} \frac{a_1 + a_2 x_i - y_i}{\sigma_i^2} x_i = 0$$

  - Define: $S = \sum_{i=1}^{N} \frac{1}{\sigma_i^2}$ $\quad \xi_1 = \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2}$ $\quad \xi_2 = \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2}$

$$\eta = \sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} \qquad \mu = \sum_{i=1}^{N} \frac{x_i y_i}{\sigma_i^2}$$

Linear Regression

- We then have a linear system: 2 equations + 2 unknowns

$$a_1 S + a_2 \xi_1 - \eta = 0$$

$$a_1 \xi_1 + a_2 \xi_2 - \mu = 0$$

  - We can solve this analytically

$$a_1 = \frac{\eta \xi_2 - \mu \xi_1}{\xi_2 S - \xi_1^2} \qquad a_2 = \frac{S\mu - \xi_1 \eta}{\xi_2 S - \xi_1^2}$$

Goodness of the Fit

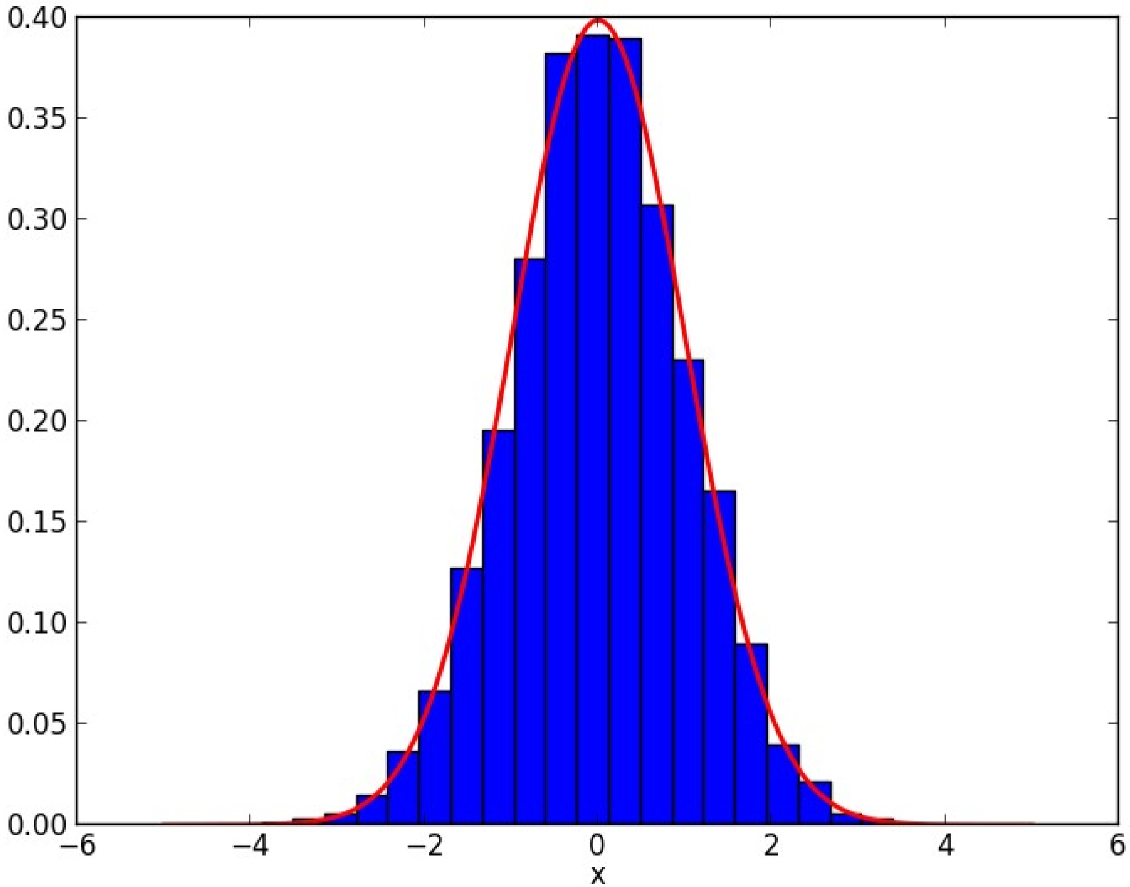
- Typically, if M is the number of parameters (2 for linear), then $N \gg M$
  - Average pointwise error should be $|y_i - Y(x_i)| \sim \sigma_i$
  - Number of degrees of freedom is $N - M$
    - i.e. larger M makes it easier to fit all the points
    - See discussion in Numerical Recipes for more details and limitations
  - Putting these ideas into the χ^2 expression suggests that we consider

$$\frac{\chi^2}{N - M}$$

    - If this is < 1, then the fit is good
    - But watch out, $\ll 1$ may also mean our errors were too large to begin with, we used too many parameters, ...

Generating Our Experimental Data

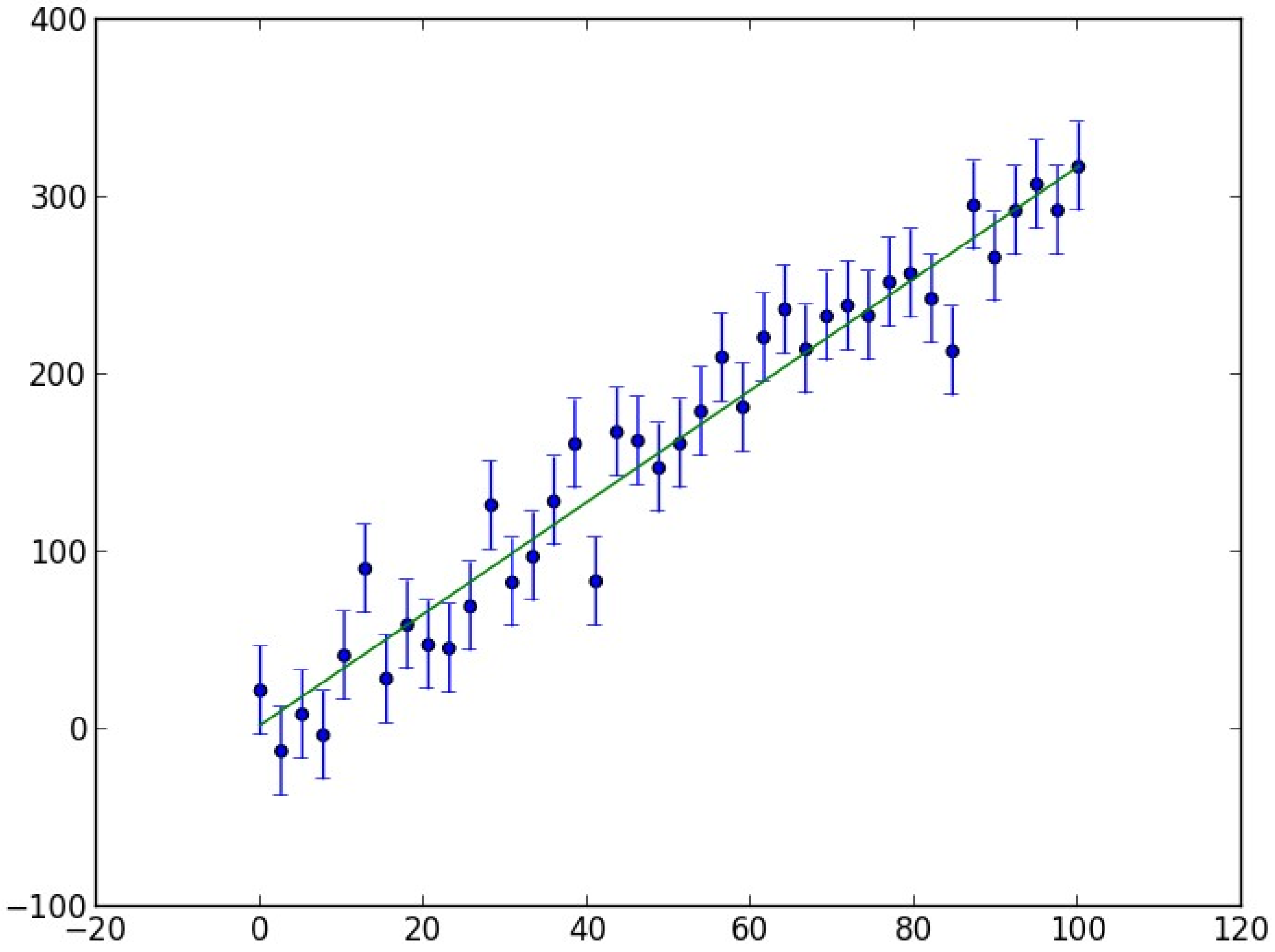
- We perturb a desired functional form with random number
  - The random numbers sample a Gaussian-normalized distribution
    - `numpy.random.randn()` in python



$$y(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/(2\sigma^2)}$$

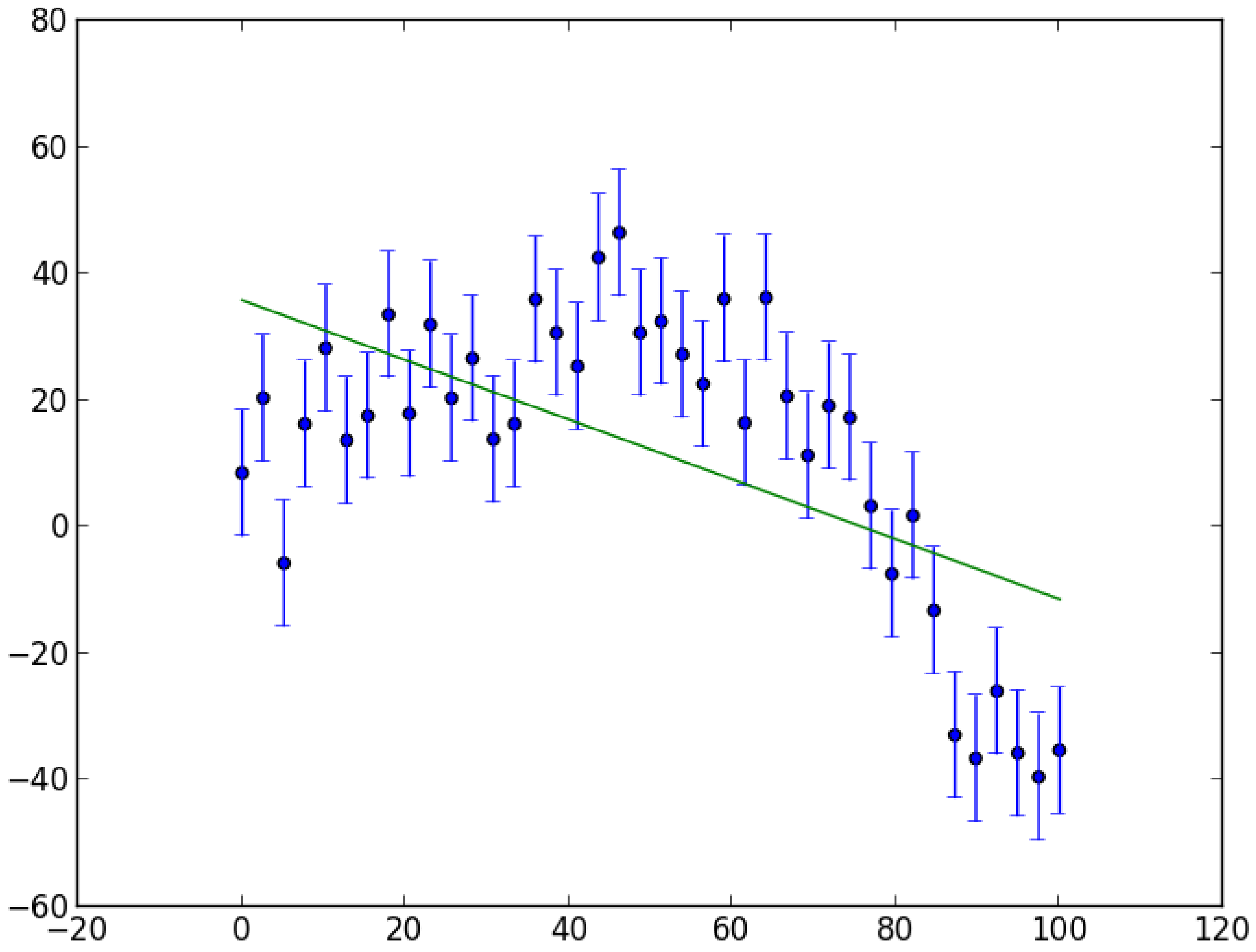
Gaussian-normalized distribution matches our expectation of the behavior of experimental error

Ex: Linear Fit



Started with $y(x) = 10 + 3x$
This has a $\chi^2/(N–2) = 0.85$

Ex: Linear Fit



Started with $y(x) = 2 + 1.5x - 0.02\,x^2$
This has a $\chi^2/(N\!-\!2) = 3.7$

Let's look at the code and see how the χ^2 varies as we play with the σ s

Extending Utility of Linear Fitting

- Sometimes a simple transform can make the data look linear
  - E.g. for fitting to $Z(t) = \alpha\, t^{\beta}$, take
  - $Y = \ln Z, x = \ln t, a_1 = \ln \alpha, a_2 = \beta$
  - See NR and Garcia for more examples

General Linear Least Squares

- The general linear least squares problem does not have a general analytic solution
  - But our linear algebra techniques come into play to save the day
  - Again, Garcia and Numerical Recipes provide a good discussion here
- We want to fit to

$$Y(x; \{a_j\}) = \sum_{j=1}^{M} a_j Y_j(x)$$

  - Note that the Ys may be nonlinear but we are still linear in the as
  - Here, Y_j are our basis set—they can be x^j in which case we fit to a general polynomial

General Linear Least Squares

- Again, we minimize our χ^2

$$\frac{\partial \chi^2}{\partial a_j} = \frac{\partial}{\partial a_j} \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \left\{ \sum_{k=1}^{M} a_k Y_k(x_i) - y_i \right\}^2 = 0$$

  - Bringing the derivative inside the sums and simplifying, we have:

$$\sum_{i=1}^{N} \sum_{k=1}^{M} \frac{Y_j(x_i)}{\sigma_i} \frac{Y_k(x_i)}{\sigma_i} a_k = \sum_{i=1}^{N} \frac{Y_j(x_i)}{\sigma_i} \frac{y_i}{\sigma_i}$$

    - Note that the only index not summed is j
    - This is M equations to solve

General Linear Least Squares

- We introduce the design matrix (N×M):

$$A_{ij} = \frac{Y_j(x_i)}{\sigma_i}$$

  - Our system then becomes (see NR or Garcia):

$$\sum_{i=1}^{N} \sum_{k=1}^{M} A_{ij} A_{ik} a_k = \sum_{i=1}^{N} A_{ij} \frac{y_i}{\sigma_i}$$

  - Looking a which indices contract, we have:

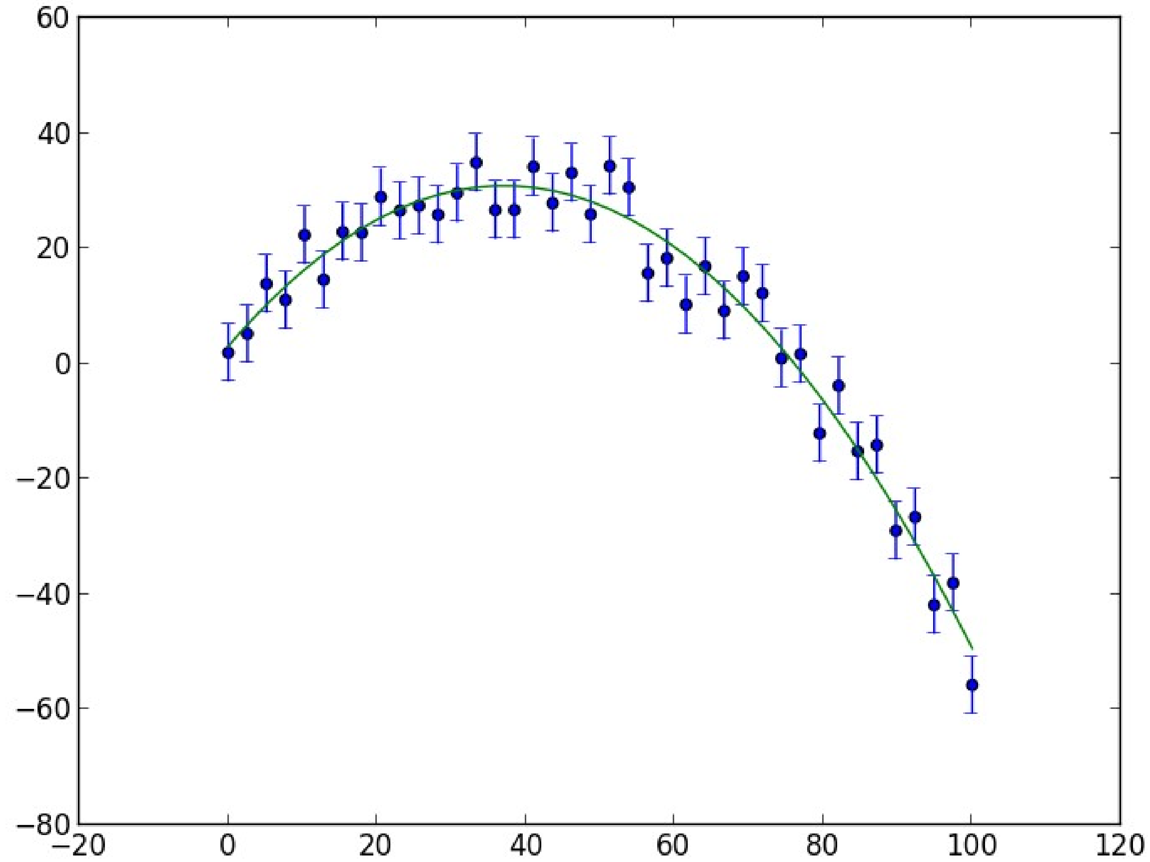
$$(\mathbf{A}^T \mathbf{A})\mathbf{a} = \mathbf{A}^T \mathbf{b}$$

    - This is a linear system, consisting of an M×M matrix
    - We can solve for the fitting parameters using Gaussian elimination

General Linear Least Squares

- M=3 (quadratic) fit to data
  - Data generated from $y(x) = 2 + 1.5\,x - 0.02\,x^2$ with Gaussian normal errors
  - $\chi^2/(N\text{–}M) = 0.81$
  - Coefficients:

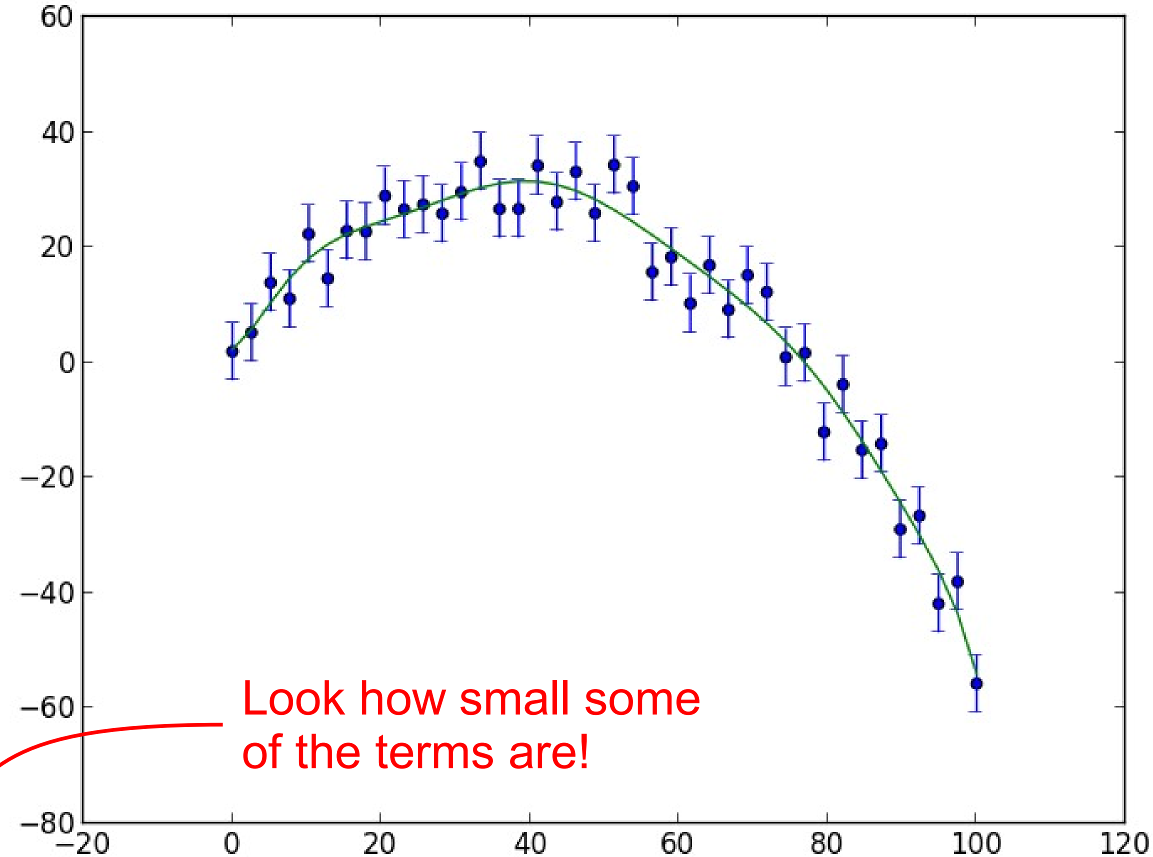
```
a =
[ 3.0835124
  1.50175118
 -0.02026005]
```



General Linear Least Squares

- M=10 (quadratic) fit to data
  - Same data (generated from $y(x) = 2 + 1.5\,x - 0.02\,x^2$ with Gaussian normal errors)
  - $\chi^2/(N\text{–}M) = 0.91$
  - Coefficients:

```
a =
[  2.27488631e+00
   8.29616711e-01
   2.89014125e-01
  -3.65205170e-02
   1.97413575e-03
  -5.80360431e-05
   9.88242216e-07
  -9.74442949e-09
   5.16759888e-11
  -1.41212120e-13]
```

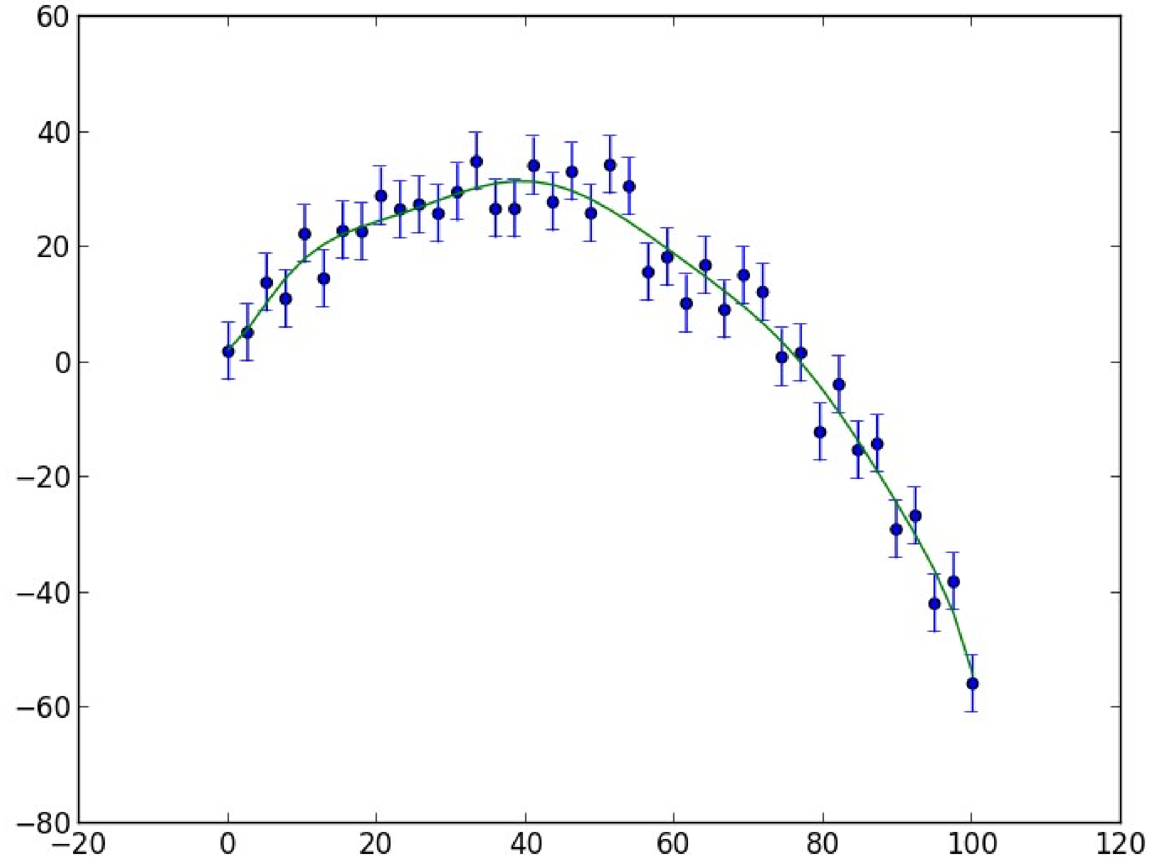


Look how small some of the terms are!

Other Basis Functions

- Instead of using $1, x, x^2, x^3, \ldots$
  - Use Legendre Polynomials
  - M-degree fit should be identical to what we already did, but coefficients will differ
  - Coefficients:

```
a =
[  2.37164216e+00
   8.07646029e-01
   1.93810011e-01
  -1.46343131e-02
   4.51547675e-04
  -7.37178812e-06
   6.84575548e-08
  -3.63443852e-10
   1.02791589e-12
  -1.20179031e-15]
```



Same polynomial, but what did that get us?

Condition Number

- The matrix $A^T A$ is notoriously ill-conditioned
  - For our examples above
  - M=3 fit: $\mathrm{cond}(\mathbf{A}^T\mathbf{A}) = 1.70 \times 10^8$
  - M=10 fit: $\mathrm{cond}(\mathbf{A}^T\mathbf{A}) = 1.93 \times 10^{33}$
  - M=10 fit w/ Legendre polynomials: $\mathrm{cond}(\mathbf{A}^T\mathbf{A}) = 9.29 \times 10^{37}$
- These are large condition numbers—in fact Gaussian elimination would have trouble with these
  - `numpy.linalg.solve()` uses singular-value decomposition
- Legendre polynomials made things worse!
  - But recall, the special thing about Legendre polynomials is that they are orthogonal in [-1, 1]

Condition Number

- On [-1,1], using the simple x^j and Legendre polynomials will again give the same resulting polynomal, but:
  - M=10, simple polynomials: $\mathrm{cond}(\mathbf{A}^T\mathbf{A}) = 1.45 \times 10^6$
  - M=10, Legendre polynomials: $\mathrm{cond}(\mathbf{A}^T\mathbf{A}) = 17.8$
- Generally speaking: using orthogonal basis functions in your interval makes the problem better posed (condition number is much smaller)
  - You can create polynomial basis function on any interval by doing the inner products in your code (see Yakowitz & Szidarovszky, for example)

Errors in Both x and y

- Depending on the experiment, you may have errors in the dependent variable
  - For linear regression, our function to minimize becomes:

$$\chi^2(a_1, a_2) = \sum_{i=1}^{N} \frac{(a_1 + a_2 x_i - y_i)^2}{\sigma_{y,i}^2 + a_2^2 \sigma_{x,i}^2}$$

    - Denominator is the total variance of the linear combination we are minimizing:

$$\begin{aligned} \mathrm{Var}(a_1 + a_2 x_i - y_i) &= \mathrm{Var}(a_2 x_i - y_i) \\ &= a_2^2 \mathrm{Var}(x_i) + \mathrm{Var}(y_i) = a_2^2 \sigma_{x,i}^2 + \sigma_{y,i}^2 \end{aligned}$$

(think about propagation of errors)

- We cannot solve analytically for the parameters, but we can use our root finding techniques on this.
  - See NR and references therein for more details

Estimating Errors in the Fit Parameters

- We can use propagation of errors to estimate the uncertainty in our fit parameters

$$\sigma_{a_j}^2 = \sum_{i=1}^{N} \left(\frac{\partial a_j}{\partial y_i} \right)^2 \sigma_i^2$$

  - For linear regression, this gives:

$$\sigma_{a_1}^2 = \frac{\xi_2}{S\xi_2 - \xi_1^2} \qquad \sigma_{a_2}^2 = \frac{S}{S\xi_2 - \xi_1^2}$$

  (blackboard derivation...)

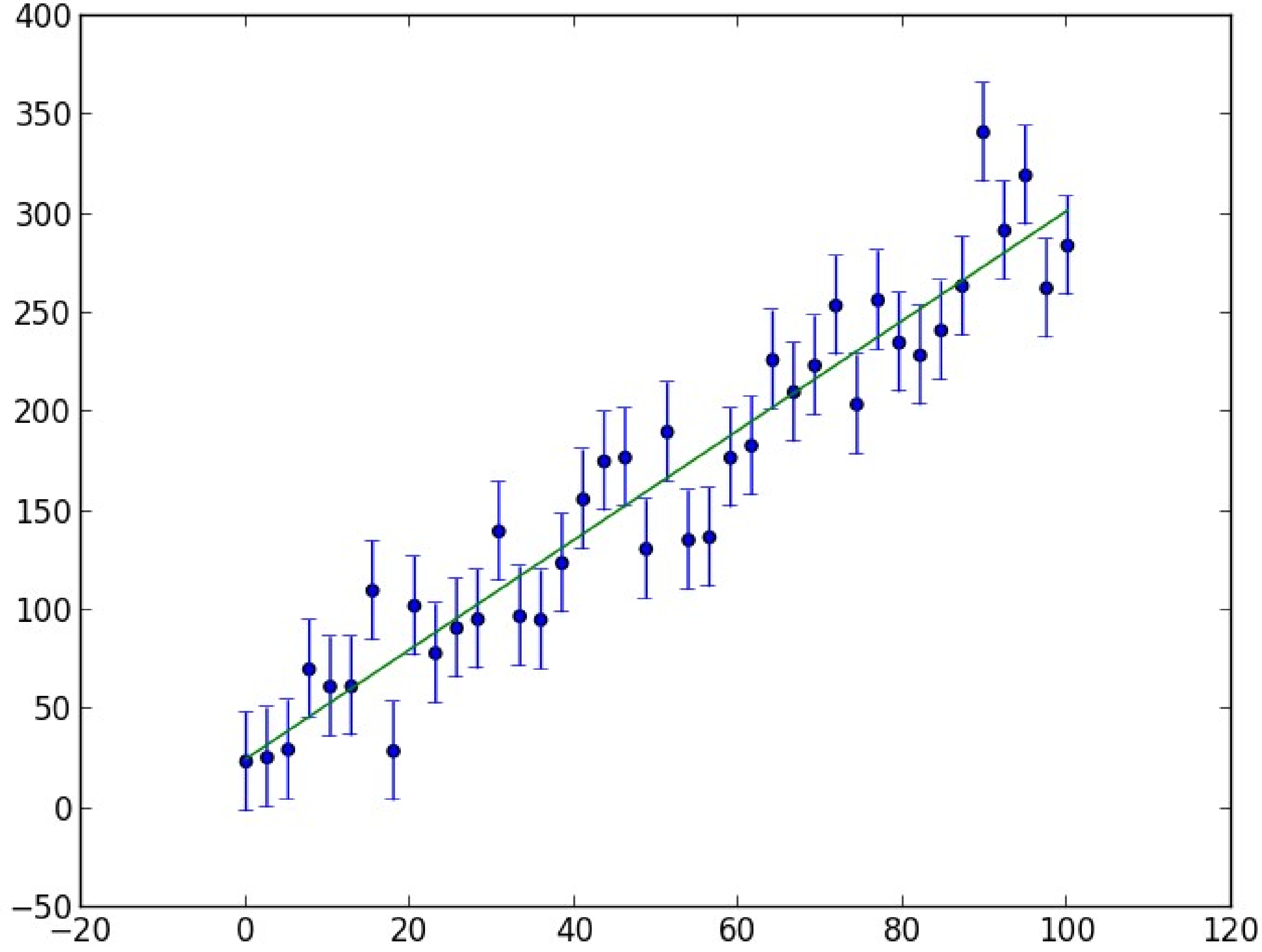
  - For the general linear least squares problem, we find:

$$\sigma_{a_j} = \sqrt{C_{jj}} \qquad \mathbf{C} = (\mathbf{A}^T \mathbf{A})^{-1}$$

  (see Numerical Recipes for a good derivation)

Estimating Errors in the Fit Parameters

- Linear fit with associate parameter errors:




```
reduced chisq =  1.05378308895
 a1 = 25.161505 +/- 7.759730
 a2 = 2.768434 +/- 0.133549
```

General Non-linear Fitting

(Yakowitz and Szidarovszky)

- Consider fitting directly to a function where the parameters enter nonlinearly:

$$f(a_0, a_1) = a_0 e^{a_1 x}$$

  - We want to minimize

$$Q \equiv \sum_{i=1}^{N} (y_i - a_0 e^{a_1 x_i})^2$$

  - Set the derivatives to zero:

$$f_0 \equiv \frac{\partial Q}{\partial a_0} = \sum_{i=1}^{N} e^{a_1 x_i} \left(a_0 e^{a_1 x_i} - y_i\right) = 0$$

$$f_1 \equiv \frac{\partial Q}{\partial a_1} = \sum_{i=1}^{N} x_i e^{a_1 x_i} \left(a_0 e^{a_1 x_i} - y_i\right) = 0$$

General Non-linear Fitting

(Yakowitz and Szidarovszky)

- This is a nonlinear system—we can use the multivariate root-finding techniques we learned earlier
  - Compute the Jacobian
  - Take an initial guess: $\mathbf{a}^{(0)}$
  - Use Newton-Raphson techniques to compute the correction:

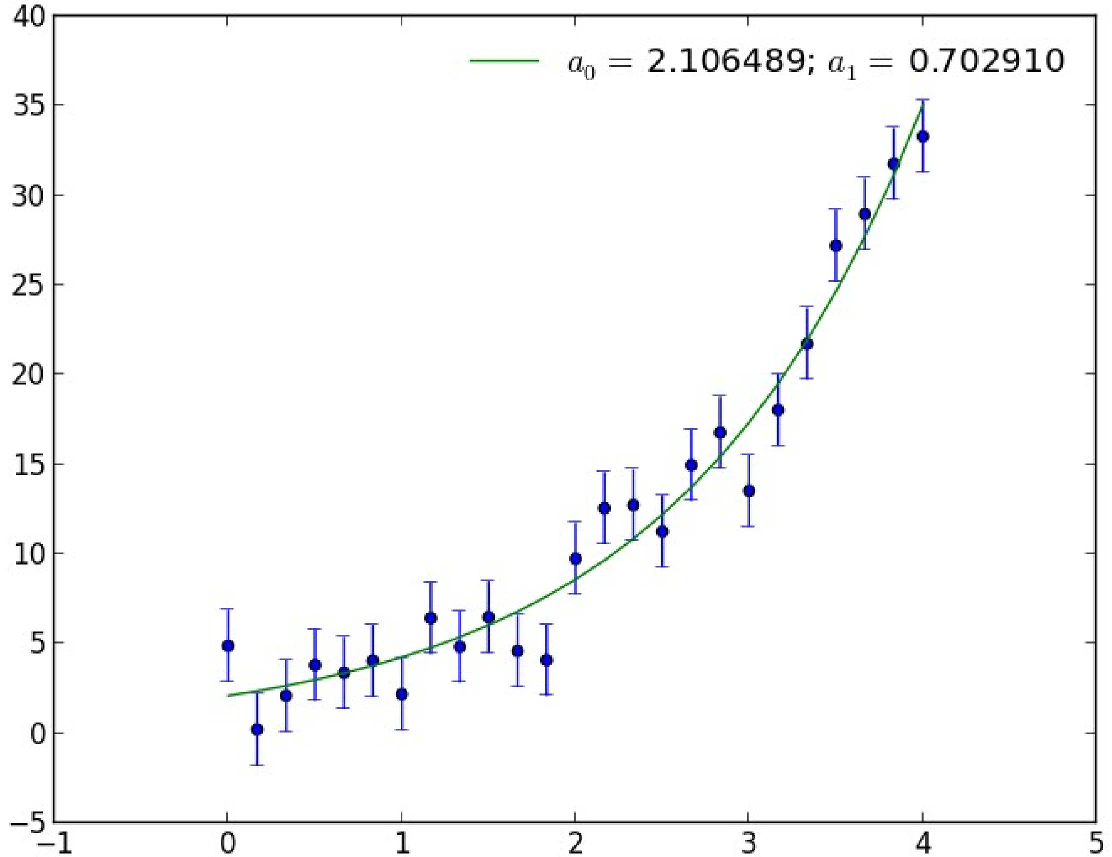
$$\delta\mathbf{a} = -\mathbf{J}^{-1}\mathbf{f}$$

  - Iterate
- Note: this can be very sensitive to your initial guess.

General Non-linear Fitting

(Yakowitz and Szidarovszky)

- Data from $f(a_0, a_1) = a_0 e^{a_1 x}$
  - With $a_0 = 2.5, a_1 = 2/3$ with a Gaussian-sampled error
  - Initial guess is very sensitive—sometimes it diverges



Gotyas

- Sometimes parameters can be redundant, leading to a singular matrix
  - NR example: $y(x) = ae^{-bx+d}$
  - Here there is functionally no difference between a and d
  - The resulting matrix will be singular

Standard Packages

- Fitting is a very sensitive procedure—especially for nonlinear cases
- Lots of minimization packages exist that offer robust fitting procedures—use them!
  - MINUIT: the standard package in high-energy physics (and yes, there is a python version: PyMinuit)
  - MINPACK: Fortran library for solving least squares problems—this is what is used under the hood for the built in SciPy least squares routine
  - These packages often allow you to impose constraints on parameters, bounds, etc...
- SciPy optimize example...

On to PDEs...

- Next up: PDEs
  - PDEs are at the heart of many physical systems
  - We will study three classes of PDEs, represented by the wave/advection equation, the Poisson equation, and the diffusion equation
- Where do we stand?
- Differentiation:
  - We saw how Taylor expansions give rise to difference formula with varying orders of accuracy
  - These ideas will be at the heart of the spatial discretization we use with PDEs
- Interpolation:
  - We will see the interpolation ideas again as we reconstruct our discretized data to find values at interfaces in our PDE discretizations

On to PDEs...

- ODEs:
  - A common procedure is to spatially discretize a PDE and then solve the result initial value ODE system using ODE methods—this is called the method of lines approach
- Linear algebra:
  - We will have a choice of discretizing explicitly or implicitly. Implicit discretizations often result in a linear system to solve, using our linear algebra techniques
  - We will see the iterative methods come into play when we consider the Poisson equation
- FFTs:
  - As already motivated, FFTs can be used to transform a PDE into an algebraic equation in Fourier-space, enabling its easy solution. (Some restrictions apply)