# Fitting a Gaussian Function to Binned Data

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# Motivation

- Commonly encountered situation in spectroscopy: an emission or absorption line on a continuum
  - Example: estimating redshift errors on faint targets
- Commonly encountered situation in astronomy: a star or galaxy atop a diffuse background
  - Example: estimating star tracker photon jitter
- Often need an estimate of the likely errors in the fitted intensity, position, breadth derived from a real observation or hypothetical observation
- Lots of standard fitting routines are out there!
- Here I apply one approach based on the minimum chisquared maximum likelihood Fisher matrix formalism.
- Although these examples are one dimensional, the methods can be extended to two or more dimensions.

# Model the Gaussian + Background

- **Four parameters model**
  - Level background to be fitted
  - Integral of the Gaussian
  - centroid of the Gaussian
  - Width of the Gaussian
- **Data “d”are binned into NBINS**
  - The data have known measurement errors
- **Find the best-fit model parameters**
  - Requires the data
  - Requires the measurement errors
- **Find the uncertainty in the parameters**
  - Requires the model (best-fit or hypothetical)
  - Requires the errors (observed or hypothetical)
  - Hypothetical allows prediction of future experiments
  - Therefore becomes powerful tool in planning

# General least squares

**Model f(i,p); data bin “i”; parameter vector p; sigma=measurement error per bin**

$$\chi^2 \equiv \sum_{i=1}^{NDAT} \frac{[f(i,p) - d_i]^2}{\sigma_i^{\,2}}$$

$$\text{Jacobian matrix } \mathrm{J}_{\mathrm{i,j}} \equiv \frac{\partial f(i,p)}{\partial p_j}$$

$$\text{Fisher matrix } \mathrm{F}_{\mathrm{j,k}} = \frac{1}{2}\frac{\partial^2 \chi^2}{\partial p_j \partial p_k} = \sum_{\mathrm{i=1}}^{\mathrm{NDAT}} \frac{1}{\sigma_{\mathrm{i}}^2} \cdot \frac{\partial f}{\partial p_j} \cdot \frac{\partial f}{\partial p_k}$$

$$\text{Covariance matrix } \mathrm{C} = \mathrm{F}^{\mathrm{inverse}}$$

$$\text{RMS error on parameter } \mathrm{p_j} \text{ is } \sqrt{\mathrm{C_{jj}}}$$

# Make this specific

- Where does the fitting model come in?
  - It is the f(i,p) for each data point "i" and parameter set "p"
  - Create a callable function that models the expected bin content for any reasonable "p" vector
- Where do the data come in?
  - Directly into the sum-of-squares; they are the "d" values.
  - Create a function that loads these data into an array.
- And the measurement errors?
  - Those are the sigma values in the s-o-s.
  - Create a function that loads the error values into an array.
- How to navigate to the best-fit parameters?
  - Use Levenberg-Marquardt.
- Where to start the parameter adjustment sequence?
  - Somewhere close to the right answer!

# Example calculation of single fit

**filename GausSingle.java**

```
public class GausSingle
{
    final static int NPARMS     = 4;
    final static int NPTS       = 200;
    static double parms[]       = new double[NPARMS];
    static double errors[]      = new double[NPTS];
    static double data[]        = new double[NPTS];

    public static void main (String args[])
    {
        setInitParms(parms);
        showParms(parms);
        getData(data);
        setErrors(data, errors);
        solve(parms, data, errors);
        showParms(parms);
    }


///
/// further functions follow…
///
```

# The method solve() – what is that?

```
static void solve(double parms[], double data[], double errors[])
// Starts with given parms, exits with best fit parms.
{
    LM myLM = new LM(NPTS, NPARMS, data, errors, parms);
    myLM.lmfit();
    myLM.getparms(parms);
}
```

- Class LM is a Levenberg-Marquardt nonlinear least-squares solver
- To begin, solve() calls constructor to create object “myLM” to communicate all the necessary startup information
- Then solve() calls object’s lmfit() method to begin the iterative fitting; solve() waits peacefully while the fitting iterates.
- When lmfit() is done, solve() grabs the iterated parms and returns.

# What's in the LM class?

- Constructor LM()
  - Receive startup data, constructs object with working arrays
- lmfit()
  - Performs the iterative improvement in the fit
  - Uses the s.o.s. gradient vector and curvature matrix
  - Method is combination of steepest descent and full Newton
  - Strategy is how/when to combine these for best progress
- getsos(parms[ ])
  - For any parm vector, returns sum-of-squares
- getparms(p[ ])
  - Allows client to claim iterated parm vector
- dpdf()
  - Two sided derivative of fitting function
- gaussj()
  - A reasonably efficient real matrix inverter.

# Multiple fits to rerandomized data

**filename GausMulti.java**

- Like GausSingle but gathers statistics on successive fits to data that have been rerandomized.
- Can be used to simulate experiments whose data are not yet available.

```
public class GausMulti
{
    final static int NPARMS     = 4;
    final static int NPTS       = 200;
    final static int NITER      = 100;
    static double trueparms[]   = new double[NPARMS];
    static double fittedparms[] = new double[NPARMS];
    static double cleandata[]   = new double[NPTS];
    static double errors[]      = new double[NPTS];
    static double noisydata[]   = new double[NPTS];
    static double stats[][]     = new double[2][NPARMS];
    static double parmerrors[]  = new double[NPARMS];

    public static void main (String args[])
    {
        setTrueParms(trueparms);
        setCleanData(trueparms, cleandata);
        setErrors(cleandata, errors);
        zeroStats(stats);
        for (int n=0; n<NITER; n++)
        {
            setNoisyData(cleandata, errors, noisydata);
            initParms(trueparms, fittedparms);
            solve(fittedparms, noisydata, errors);
            showParms(fittedparms);
            addStats(fittedparms, stats);
        }
        finishStats(stats);
        showParms(stats[0]);   // the parameter means.
        showParms(stats[1]);   // the rms parm errors.
    }
```

# A model where the Gaussian function is just one sample at the center of the bin: OK when width >> 1 bin

```
class F
{
    static double func(int i, double p[])
    // samples one point at x=i
    // OK if funcx() varies only mildly over the bin.
    {
        double x = (double) i;
        return funcx(x, p);
    }

    static double funcx(double x, double p[])
    //  p[0] = background level
    //  p[1] = integral of the Gaussian
    //  p[2] = centroid of the Gaussian
    //  p[3] = rms breadth of Gaussian distribution
    {
        double numer = (x-p[2])*(x-p[2]);
        double denom = p[3]*p[3];
        double ratio = numer/denom;
        if (ratio < 30.0)
          return p[0] + (0.39894*p[1]/p[3])*Math.exp(-0.5*ratio);
        return p[0];
    }
}
```

# A model where each bin is an integrated Gaussian: needed when Gaussian width ~ 1 bin

```
class F
{
    static double func(int i, double p[])
    // samples uniformly within bin "i"
    {
        int NSAMP = 20;
        double dx = 1.0/NSAMP;
        double sum = 0.0;
        for (double x=-0.5+0.5*dx; x<0.5; x+=dx)
         sum += dx*funcx(i+x, p);
        return sum;
    }

    static double funcx(double x, double p[])
    //  p[0] = background level
    //  p[1] = integral of the Gaussian
    //  p[2] = centroid of the Gaussian
    //  p[3] = rms breadth of Gaussian distribution
    {
        double numer = (x-p[2])*(x-p[2]);
        double denom = p[3]*p[3];
        double ratio = numer/denom;
        if (ratio < 30.0)
          return p[0] + (0.39894*p[1]/p[3])*Math.exp(-0.5*ratio);
        return p[0];
    }
}
```

# How to evaluate numerical derivatives?

- **Double sided finite difference works well**
- **Step size deserves some care in choosing**
- **Roughly |paramSize| *cubeRoot(MACHEPS)**
- **Often 1E-6 works well.**

```
double dfdp(int i, int j, double parms[])
// Two sided derivative of F.func(i,p) w.r.t. any given parm[j]
// Gives one jacobian matrix element dfi/dpj at given parmvector.
{
    double pminus[] = new double[NPARMS];
    double pplus[]  = new double[NPARMS];
    for (int k=0; k<NPARMS; k++)
      pminus[k] = pplus[k] = parms[k];
    pminus[j] -= DELTAP;
    pplus[j] += DELTAP;
    return (F.func(i,pplus) - F.func(i,pminus))/(2.0*DELTAP);
}
```

# But I don't have real data yet! I just want to predict errors for a hypothetical experiment!

- **Follow the formalism of chart 4.**
  - **The parameter errors don't depend on any of the data!**
  - **They depend only on the model and the expected measurement errors "sigma".**
- **So, do this…**
  - **Write your model f(i,p) function for some nominal data concept**
    - **May involve observation time, nominal background, instrument**
  - **Compute its derivatives w.r.t each parameter at given parm set**
    - This is your Jacobian matrix
  - **Combine Jacobian with sigma, get Fisher information matrix.**
  - **Invert that, getting the covariance matrix.**
  - **Evaluate the square roots of its diagonal elements.**

# Estimating parm errors, single parm vector

filename GausErr.java

```
public class GausErr
{
    final static int NPARMS    = 4;
    final static int NPTS      = 200;
    static double data[]       = new double[NPTS];
    static double erro[]       = new double[NPTS];
    static double jacobian[][] = new double[NPTS][NPARMS];
    static double fisher[][]   = new double[NPARMS][NPARMS];
    static double covar[][]    = new double[NPARMS][NPARMS];
    static double parms[]      = new double[NPARMS];
    static double rmsparms[]   = new double[NPARMS];

    public static void main (String args[])
    {
        setParms(parms);
        showParms(parms);
        setData(parms, data);
        setErro(data, erro);
        getJacobian(parms, jacobian);
        getFisher(erro, jacobian, fisher);
        getCovar(fisher, covar);
        getRMSparms(covar, rmsparms);
        showRMS(rmsparms);
    }
……
……code continues with detail methods….
```

To explore a grid of parm values, put this sequence into a loop that steps through the grid wanted.

# Implementation details

- **Where to find a Java Levenberg-Marquardt nonlinear least squares routine to use in getting best-fit parameter set?**
  - **"Levenberg-Marquardt Demo" at MikeLampton.com**
- **Where to find a Java matrix inverter, to convert my Fisher matrix to a covariance matrix?**
  - **Use gaussj() from "Levenberg-Marquardt Demo" at MikeLampton.com**
- **How to best illustrate my Gaussian fitting results?**
  - **It's all about how errors propagate from the data world into the parameters. For that, a useful approach is to make plots of how the parameter errors depend on the broad model characteristics. Expect that a big Gaussian on top of a feeble background will have photometric error ~ sqrt(Area), so that relative photometric error will vary as 1/sqrt(Area). Expect error in breadth to be proportional to breadth/sqrt(Area). Expect rising background will increase the fitting errors especially with fainter targets.**

# Other code snippets too trivial to publish

```
static void setParms(double p[])
 {
     p[0] = 1;      // background level
     p[1] = 1E4;    // integral of Gaussian
     p[2] = 100.5;  // centroid of Gaussian
     p[3] = 1.0;    // RMS width of Gaussian
 }

 static void setData(double p[], double d[])
 {
     for (int i=0; i<NPTS; i++)
       d[i] = F.func(i, p);
 }

 static void setErro(double d[], double e[])
 // Installs Poisson errors based on model data
 {
     for (int i=0; i<NPTS; i++)
       e[i] = Math.sqrt(d[i]);
 }

 static void showParms(double p[])
 {
     for (int i=0; i<NPARMS; i++)
       System.out.print(U.fwd(p[i], 16,4));
     System.out.println();
 }

 static void showRMS(double r[])
 {
     for (int i=0; i<NPARMS; i++)
       System.out.print(U.fwd(r[i], 16,4));
     System.out.println();
 }
```

```
static void getJacobian(double p[], double jac[][])
{
    for (int i=0; i<NPTS; i++)
      for (int j=0; j<NPARMS; j++)
        jac[i][j] = dfdp(i, j, p);
}

static void getFish(double e[], double jac[][], double f[][])
{
    for (int j=0; j<NPARMS; j++)
      for (int k=0; k<NPARMS; k++)
      {
          f[j][k] = 0.0;
          for (int i=0; i<NPTS; i++)
            f[j][k] += jac[i][j]*jac[i][k]/(e[i]*e[i]);
      }
}

static double getCovar(double fish[][], double cov[][])
{
    for (int j=0; j<NPARMS; j++)
      for (int k=0; k<NPARMS; k++)
        cov[j][k] = fish[j][k];
    double det = gaussj(cov, NPARMS);
    return det;
}

static void getRMSparms(double cov[][], double rms[])
{
    for (int j=0; j<NPARMS; j++)
      rms[j] = Math.sqrt(cov[j][j]);
}
```

# Alternative method: Monte Carlo

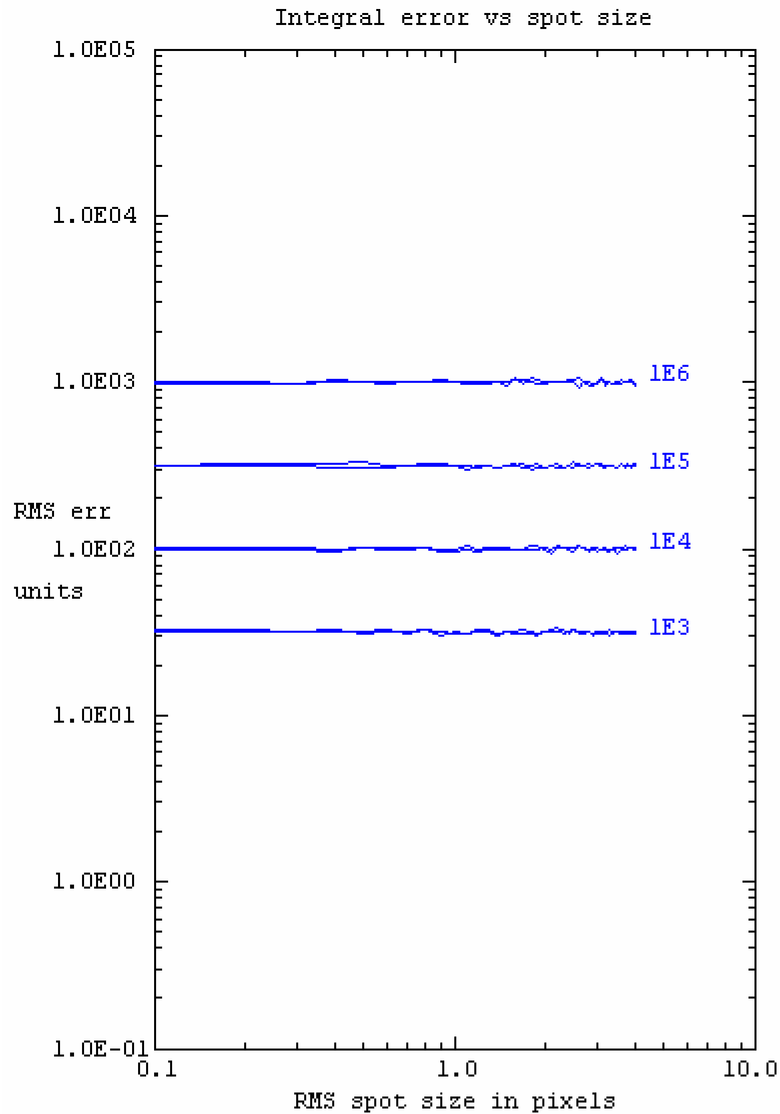
- Start with a hypothetical “true” model
- Use it to evaluate a model data pattern
- Repeat 1000 times:
  - Add Gaussian random errors to the model data pattern
  - Fit this data vector, getting parameter vector
  - Accumulate mean & variance statistics on each parameter
- Are the means close to the initial true values?
- Are the variances in agreement with the diagonal values of the covariance matrix obtained via Fisher formalism?

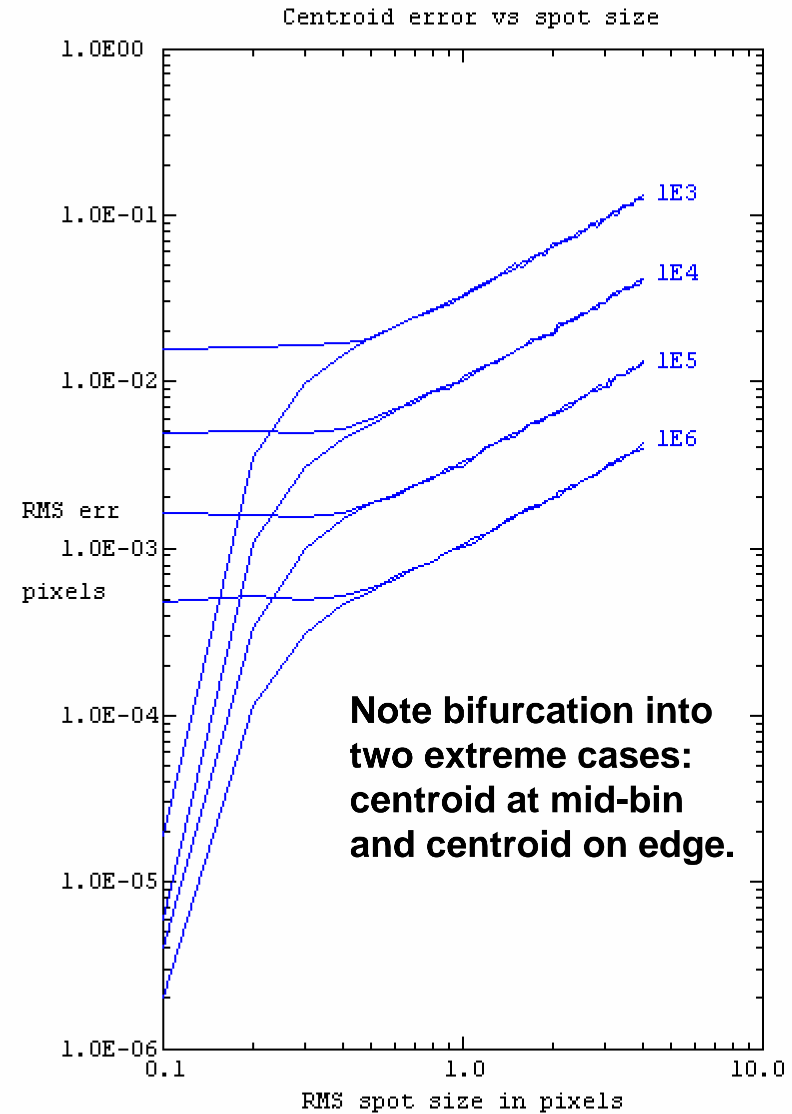
# Simple estimate of Gaussian moments

- Zero background
- Step through a grid of Totals and Widths
- At each point, run 1000 iterations
  - Produce random data
  - Calculate zeroth moment   tot=sum(di)
    - **Not optimum if background is present!**
  - Calculate first moment   xbar=sum(x*di)
    - **Not optimum especially if background is present!**
  - Build statistics on these
- Make a plot of rms errors in tot and xbar
- Notice that there are two extreme cases for xbar estimate
  - True centroid at center of bin
  - True centroid at a bin edge

# Simple Check: results

**filename Pachinko.java**




**Note bifurcation into two extreme cases: centroid at mid-bin and centroid on edge.**

References:

Press et al “Numerical Recipes” Chapter 14.

Lampton, Computers in Phys., v.11#1, pp.110-115, 1997.

Tegmark et al Ap.J. 480  pp.22-35, 1997.