Phys 512
Modelling of Data

Model Fitting

- Sometime we have data. Sometimes we'd like to model it.
- Variety of techniques used, depending on what noise, model look like.
- Nearly all of these techniques require linear algebra, so we will start with numpy linear algebra.

Matrices vs. Arrays

- Unlike say Matlab, arrays and matrices are different in numpy.
- However, you can treat arrays like matrices and matrices like arrays. This can be confusing.
- * overloaded for matrices to be matrix multiply, but not for arrays. As of python3, @ is overloaded for arrays to be matrix multiply.
- I suggest you pick one and sick with it. People usually use arrays (and we will do so in this course).

Linear Algebra Operations

- Several matrix operations/factorizations built into numpy
- numpy.dot(a,b) does matrix multiplication if a,b are matrices.
- numpy.linalg.inv inverts a square matrix. pinv may help if (nearly) singular
- numpy.linalg.eig takes eigenvalues/eigenvectors. use eigh if symmetric/Hermitian
- numpy.linalg.svd takes sigular value decomposition $A=USV^T$ where S diagonal, U,V columns orthogonal
- numpy.linalg.qr takes QR decomposition A=QR where Q is orthogonal, R triangular
- numpy.linalg.chol takes Cholesky decomposition of a positive-definite matrix A=LLT.

χ^2

- The PDF of a Gaussian is $\exp(-0.5(x-\mu)^2/\sigma^2)/\mathrm{sqrt}(2\pi\sigma^2)$ with mean μ and standard deviation σ.

- If we have a bunch of data points, which may have different means and standard deviations, then the joint PDF is the product of the PDFs.

- It is often more convenient to work with the log. For many points, $\log(PDF)=\sum -0.5(x_i-\mu_i)^2/\sigma_i^2 - 0.5*\log(2\pi\sigma_i^2)$

- Usually, we know the variance of our data, and want our model to predict the expected value of x_i, which is μ_i. When we compare models, the second part is constant, so we ditch it. log likelihood becomes: $-0.5\sum(x_i-\mu_i)^2/\sigma_i^2$.

- $\sum(x_i-\mu_i)^2/\sigma_i^2$. is χ^2. We can find the maximum likelihood model by minimizing χ^2.

Linear least-squares

- Rewrite $\chi 2$ with matrices: $(x-\mu)^T N^{-1}(x-\mu)$ for noise covariance matrix N. If N has diagonal elements σ^2, this is identical to previous.

- Let's take simple case that our model depends linearly on a small number of parameters: $\mu_i=\sum A_{ij}m_j$ for model parameters m and matrix A that transforms to predicted values. In matricese: $\mu=Am$

- One example: $x(t)$ is a polynomial in time. Then $\mu_i=\sum t_i^j c_j$.

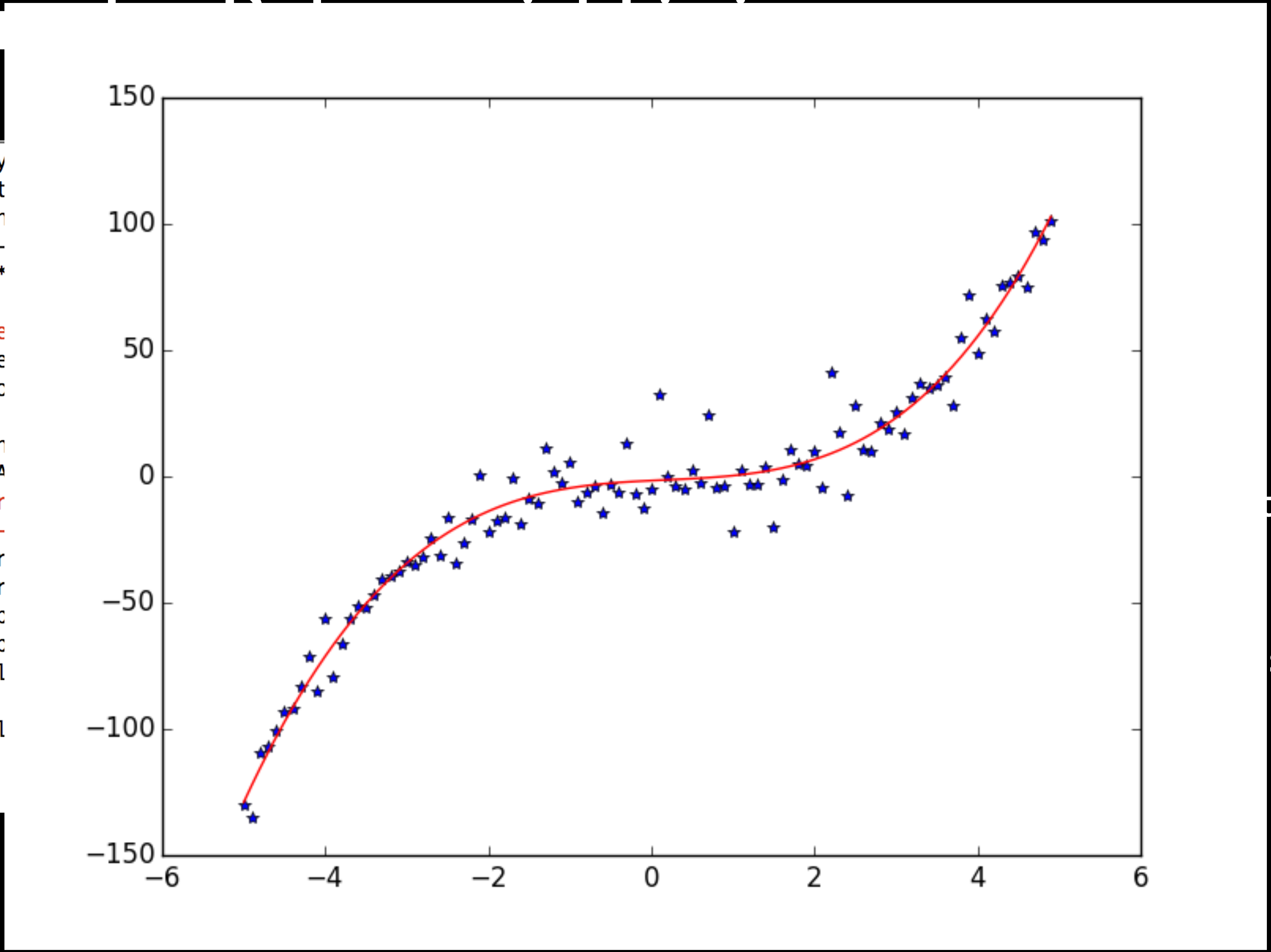
- With this parameterization, $\chi^2=(x-Am)^T N^{-1}(x-Am)$

Least Squares: $\chi^2=(x-Am)^T N^{-1}(x-Am)$

- To find best-fitting model, minimize χ^2. Calculus on matrices works like regular calculus, as long as no orders get swapped.
- $\partial\chi^2/\partial m = -A^T N^{-1}(x-Am)+\ldots=0$ (at minimum)
- We can solve for m: $A^T N^{-1} A m = A^T N^{-1} x$. Or, $m=(A^T N^{-1} A)^{-1} A^T N^{-1} x$

Exa

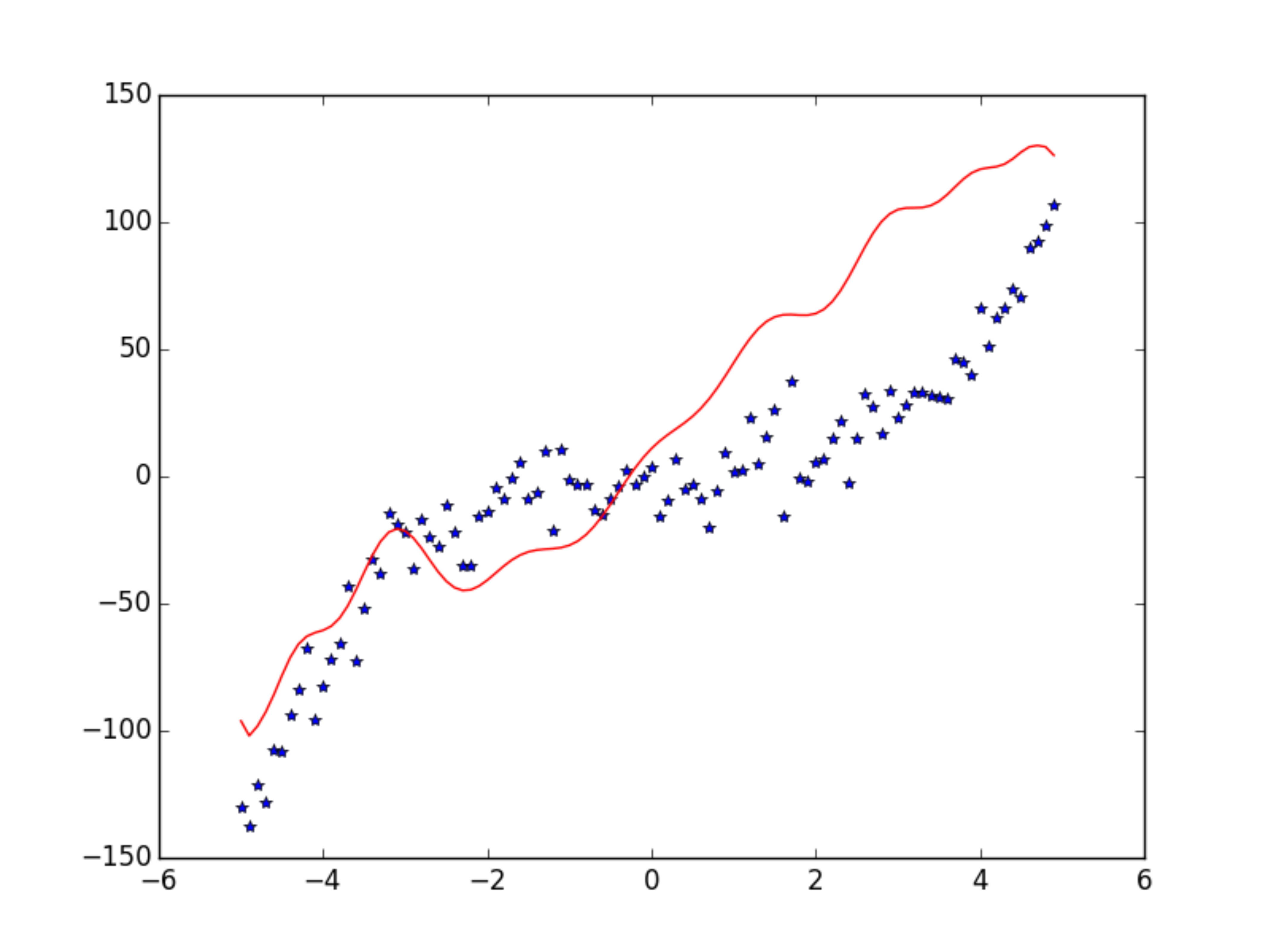
```
import numpy
from matplot
t=numpy.aran
x_true=t**3-
x=x_true+10*

npoly=5  #le
ndata=t.size
A=numpy.zerc
A[:,0]=1.0
for i in ran
    A[:,i]=A
#Let's ignor
#m=(A^TA)^{-
A=numpy.matr
d=numpy.matr
lhs=A.transp
rhs=A.transp
fitp=numpy.l
pred=A*fitp
plt.clf();pl
plt.draw()
```



tc. as matrices rather

s live in numpy.linalg,

Higher Order




```
import numpy
from matplotlib import pyplot as plt
t=numpy.arange(-5,5,0.1)
x_true=t**3-0.5*t**2
x=x_true+10*numpy.random.randn(t.size)

npoly=25 #let's fit 4th order polynomial
ndata=t.size
A=numpy.zeros([ndata,npoly])
A[:,0]=1.0
for i in range(1,npoly):
    A[:,i]=A[:,i-1]*t
#Let's ignore noise for now.  New equations are:
#m=(A^TA)^{-1}*(A^Td)
A=numpy.matrix(A)
d=numpy.matrix(x).transpose()
lhs=A.transpose()*A
rhs=A.transpose()*d
fitp=numpy.linalg.inv(lhs)*rhs
pred=A*fitp
plt.clf();plt.plot(t,x,'*');plt.plot(t,pred,'r');
plt.draw()
plt.savefig('polyfit_example_high.png')
```

Condition # and Roundoff

- Recall that the eigenvalues of a symmetric matrix are real, and the eigenvectors are orthogonal. So, $(A^TN^{-1}A)$ can be re-written $V^T\Lambda V$, where Λ is diagonal and V is orthognal (so $V^{-1}=V^T$).

- $(ABC)^{-1}=C^{-1}B^{-1}A^{-1}$, so inverse$=V^{-1}\Lambda^{-1}(V^T)^{-1}=V^T\Lambda^{-1}V$.

- If a bunch of eigenvalues are really small, they will be huge in the inverse. Double precision numbers are good to ~16 digits, so if spread gets bigger than 10^{16}, we'll lose information in the inverse.

- Ratio of largest to smallest eigenvalue is called the condition number. If it is large, matrices are ill-conditioned, and will present problems.

Condition # of Polynomial Matrices

- Condition # quickly blows up. So, we should have expected problems.

```
import numpy
def get_poly_mat(t,npoly):
    mat=numpy.zeros([t.size,npoly])
    mat[:,0]=1.0
    for i in range(1,npoly):
        mat[:,i]=t*mat[:,i-1]
    mat=numpy.matrix(mat)
    return mat

if __name__=='__main__':
    t=numpy.arange(-5,5,0.1)
    for npoly in numpy.arange(5,30,5):
        mat=get_poly_mat(t,npoly)
        mm=mat.transpose()*mat
        mm=mm+mm.transpose() #bonus symmetrization
        e,v=numpy.linalg.eig(mm)
        eabs=numpy.abs(e)
        cond=eabs.max()/eabs.min()
        print repr(npoly) + ' order poynomial matrix has condition number ' + repr(cond)
```

```
>>> execfile('cond_example.py')
5 order poynomial matrix has condition number 158940.69399024552
10 order poynomial matrix has condition number 2366966250887.5864
15 order poynomial matrix has condition number 2.722363799692467e+19
20 order poynomial matrix has condition number 2.2708595871810382e+25
25 order poynomial matrix has condition number 7.8912167454722334e+31
>>>
```

One Possibility: SVD

- Take noiseless case. Then solving $A^TAm=A^Tx$.
- Singular value decomposition (SVD) factors matrix $A=USV^T$, where S is diagonal, and U and V are orthogonal, and V is square. For symmetric, U=V, S=eigenvalues, but SVD works for any matrix.
- Solutions: $(USV^T)^TUSV^Tm=(USV^T)^Tx$. $VSU^TUSV^Tm=VSU^Tx$
- U^TU=identity, so cancels. $VS^2V^Tm=VSU^Tx$. S^2 squares the condition number, so that was bad. We can analytically cancel left-hand V and one copy of S: $SV^Tm=U^Tx$. Then $m=VS^{-1}U^Tx$
- $VS^{-1}U^T$ is known as the (Moore-Penrose) pseudo-inverse of A, and is what numpy's pinv calculates.
- NB - this can be done even faster with QR

SVD Code

- Here's how to take singular value decompositions with numpy.
- (Alternatively, if <d>=Am, <m>=pinv(A)d)
- This will work better than before, but still won't get us to e.g. 100th order polynomials.
- Main issue is that simple polynomials are ill-conditioned: x^{20} looks a lot like x^{22}.

```
import numpy
from matplotlib import pyplot as plt
t=numpy.arange(-5,5,0.1)
x_true=t**3-0.5*t**2
x=x_true+10*numpy.random.randn(t.size)

npoly=20
ndata=t.size
A=numpy.zeros([ndata,npoly])
A[:,0]=1.0
for i in range(1,npoly):
    A[:,i]=A[:,i-1]*t

A=numpy.matrix(A)
d=numpy.matrix(x).transpose()
#Make the svd decomposition, the extra False
#is to make matrices compact
u,s,vt=numpy.linalg.svd(A,False)
#s comes back as a 1-d array, turn it into a 2-d matrix
sinv=numpy.matrix(numpy.diag(1.0/s))
fitp=vt.transpose()*sinv*(u.transpose()*d)
```

Pseudoinverse with Noise

- Factor N into LL^T. For diagonal noise, this is just sqrt(diag), but in more general case, Cholesky or eigh standard choices.
- $A^T N^{-1} A m = A^T N^{-1} d \rightarrow A^T L^{T,-1} L^{-1} A m = A^T L^{T,-1} L^{-1} d \rightarrow (L^{-1}A)^T (L^{-1}A) m = (L^{-1}A)^T L^{-1} d$
- Let $\mathscr{A} \equiv L^{-1}A$, $\mathscr{d} \equiv L^{-1}d$, and we have $\mathscr{A}^T \mathscr{A} m = \mathscr{A}^T \mathscr{d}$.
- After doing this rotation, back where we started in the noise-free case. Solve as usual.

Solution: Different Poly Basis

- There are several families of polynomials that have better properties (Legendre, Chebyshev…). Usually defined on (-1,1) through recursion relations.
- Legendre polynomials are constructed to be orthogonal on (-1,1), so condition number should be good. If our t range is different from (-1,1), rescale so that it is.
- Key relation: $(n+1)P_{n+1}(t)=(2n+1)tP_n(t)-nP_{n-1}(t)$ with $P_0=1$ and $P_1=t$.
- I pick up a power of *t* each time, so these are also polynomials, just written in linear combinations that have better condition number.
- Strongly encourage you to *never* fit regular polynomials. Always use Legendre, Chebyshev…

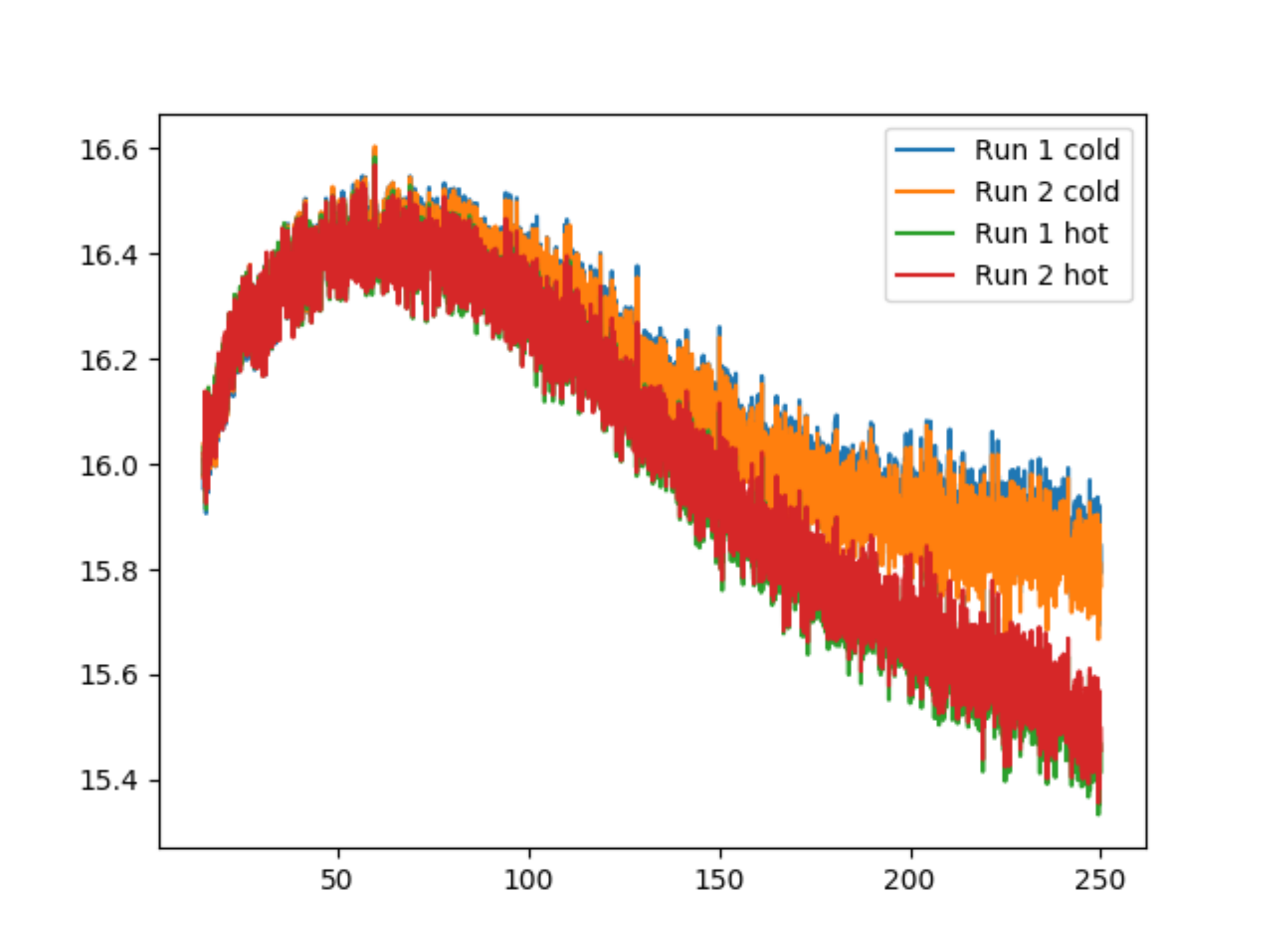
Legendre Code

```
import numpy as np
x=np.linspace(-1,1,1001)
ords=np.arange(5,101,5)
for ord in ords:
    #legvander is the numpy routine to make a matrix of legendre polynomials.
    #stands for legendre vandermond
    y=np.polynomial.legendre.legvander(x,ord)
    #the 0 argument to SVD says to keep the output in compact (rectangular)
    #form if the input matrix is rectangular
    u,s,v=np.linalg.svd(y,0)
    print('legendre condition number for order ',ord,' is ',s.max()/s.min())
```

```
legendre condition number for order  5  is  3.3004122674582725
legendre condition number for order  10  is  4.542374337123092
legendre condition number for order  15  is  5.508348566496
legendre condition number for order  20  is  6.334121283482599
legendre condition number for order  25  is  7.070257461267389
legendre condition number for order  30  is  7.74091305773132
legendre condition number for order  35  is  8.360572554145357
legendre condition number for order  40  is  8.939241298418528
legendre condition number for order  45  is  9.484316948354397
legendre condition number for order  50  is  10.001668962700121
legendre condition number for order  55  is  10.496403074691885
legendre condition number for order  60  is  10.974228862874183
legendre condition number for order  65  is  11.445362702828856
legendre condition number for order  70  is  11.942607221492095
legendre condition number for order  75  is  12.571332359572134
legendre condition number for order  80  is  13.493593404203155
legendre condition number for order  85  is  14.8728748591077
legendre condition number for order  90  is  16.932477120003394
legendre condition number for order  95  is  20.0307649803339
legendre condition number for order  100  is  24.768705279365424
```

Example: Amplifier Gain

- We have amplifiers for radio telescopes which amplify incoming signals.
- The gain varies as a function of frequency - if I want to know absolute signal level, need to correct for that.
- Plot shows two different runs for an amplifier at each of two different temperatures.
- How would I model the gain vs. frequency? vs. temperature?
- How would I decide on error bars?



Error Bars

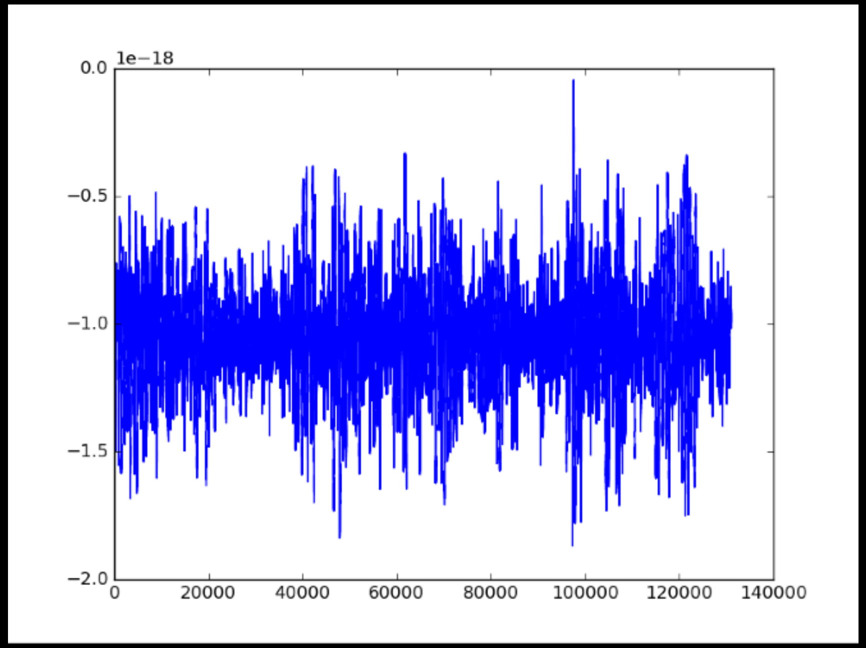
- What is the (co)variance of my model parameters?
- d_t=Am_t, where d_t=true (noiseless data), m_t=true model.
- $A^TN^{-1}Am_t=A^TN^{-1}d_t$
- $A^TN^{-1}A(m-m_t)=A^TN^{-1}(d-d_t)=A^TN^{-1}n$ where n is the actual noise I got
- $(m-m_t)=(A^TN^{-1}A)^{-1}A^TN^{-1}n$.
- $\langle(m-mt)(m-mt)T\rangle=\langle(A^TN^{-1}A)^{-1}A^TN^{-1}n((A^TN^{-1}A)^{-1}A^TN^{-1}n)T\rangle$
  $=\langle(A^TN^{-1}A)^{-1}A^TN^{-1}nnN^{-1}A^T(A^TN^{-1}A)^{-1}\rangle$
- But, $\langle nn\rangle = N$, so goes to $(A^TN^{-1}A)^{-1}A^TN^{-1}NN^{-1}A^T(A^TN^{-1}A)^{-1}=(A^TN^{-1}A)^{-1}$
- Parameter covariance is just the (inverse) of the matrix we may have already inverted!

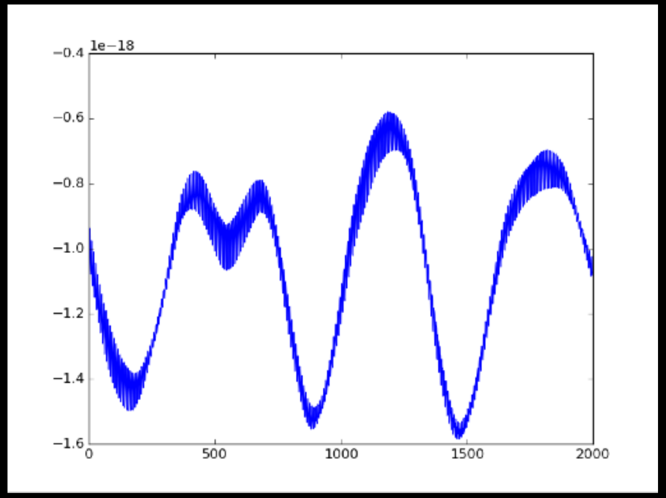
Error Bars ctd.

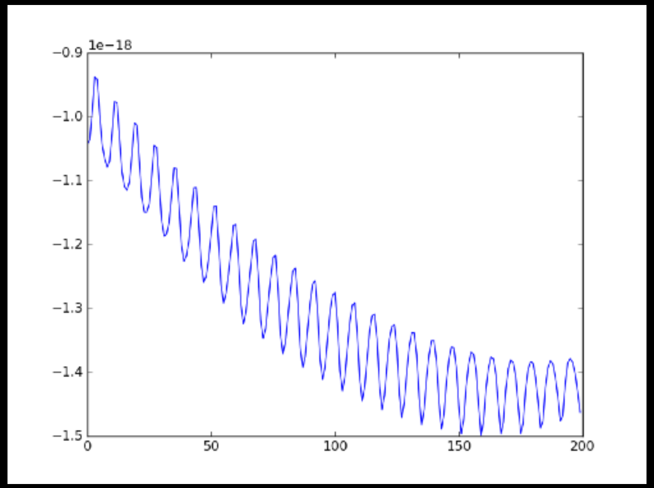
- Sometimes we want the uncertainty in our predicted data rather than model parameters.
- For this we need $<(d-Am)(d-Am)^T> = <(Am_t-Am)(Am_t-Am)T>$ $=<A(m_t-m)(m_t-m)^T A^T>$
- We already know $<(m_t-m)(m_t-m)^T>$ - it's $(A^TN^{-1}A)^{-1}$.
- Our data errors are then just $A(A^TN^{-1}A)-1A^T$.

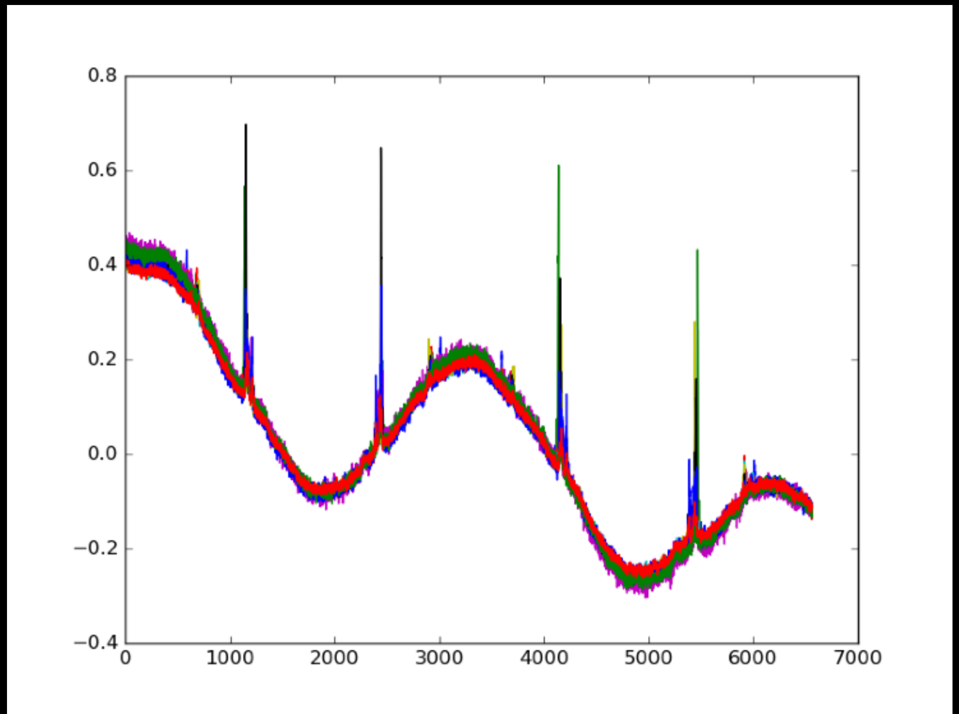
Correlated Noise

- So far, we have assumed that the noise is independent between data sets.
- Life is sometimes that kind, but very often not. We need tools to deal with this.









Right:LIGO data, with varying levels of zoom.
Left: detector timestreams from Mustang 2 camera @GBT

Fortunately…

- Linear algebra expressions for χ^2 already can handle this.
- Let V be an orthogonal matrix, so $VV^T=V^TV=I$, and $d-Am=r$ (for residual)
- $\chi2=r^TN^{-1}r = r^TV^TVN^{-1}V^TVr$. Let $r \to Vr$, $N \to VNV^T$, and $\chi2$ expression is unchanged in new, rotated space.
- Furthermore, (fairly) easy to show that $\langle N_{ij}\rangle=\langle r_ir_j\rangle$.
- So, we can work in this new, rotated space without ever referring to original coordinates. Just need to calculate noise covariances N_{ij}.

Generating Correlated Noise

- Say we have a noise matrix N and want to create realizations from it. How do we do this?

- Same trick in reverse. If $d_{new}=Vd_{old}$, then I can generate d_{old} and rotate to get d_{new}.

- We can pick any matrix that diagonalizes N, since we know how to generate uncorrelated data.

- A particularly useful one is Cholesky (LU equivalent for positive-definite): $N=LL^T$. We can generate simulated data just by taking L*g*, where *g* is a vector of zero-mean, unit-variance Gaussian random deviates.

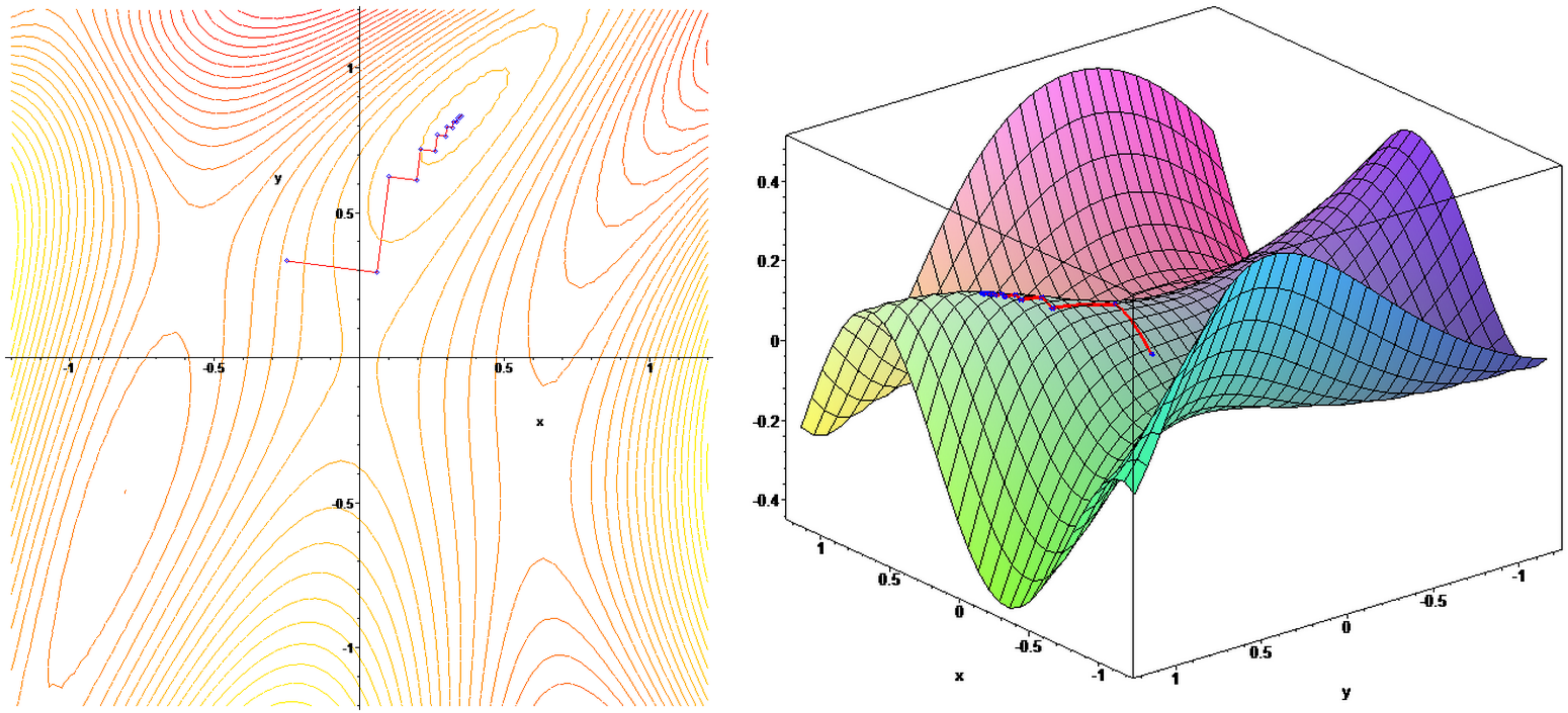
Nonlinear Fitting

- Sometimes data depend non-linearly on model parameters
- Examples are Gaussian and Lorentzian $(a/(b+(x-c)^2)$
- Often significantly more complicated - cannot reason about global behaviour from local properties. May be multiple local minima
- Many methods reduce to how to efficiently find the "nearest" minimum.
- One possibility - find steepest downhill direction, move to the bottom, repeat until we're happy. Called "steepest descent."
- How might this end badly?

Steepest Descent

e gradient descent algorithm in action. (1: contour)

The "Zig-Zagging" nature of the method is also evident below, where the gradient ascent method is applied to $F(x,y) = \sin\left(\frac{1}{2}x^2 - \frac{1}{4}y^2 + 3\right)\cos(2x + 1 - e^y)$.



From wikipedia. Zigagging is inefficient.

Better: Newton's Method

- linear: <d>=Am. Nonlinear: <d>=A(m) $\chi^2=(d-A(m))^T N^{-1}(d-A(m))$
- If we're "close" to minimum, can linearize. $A(m)=A(m_0)+\partial A/\partial m*\delta m$
- Now have $\chi^2=(d-A(m_0)-\partial A/\partial m\ \delta m)^T N^{-1}(d-A(m_0)-\partial A/\partial m\ \delta m)$
- What is the gradient?

Newton's Method ctd

- Gradient trickier - $\partial A/\partial m$ depends in general on m, so there's a second derivative
- Two terms: $\nabla\chi^2=(-\partial A/\partial m)^T N^{-1}(d-A(m_0)-\partial A/\partial m\ \delta m)-(\partial^2 A/\partial m_i \partial m_j\ \delta m)^T N^{-1}(d-A(m_0)-\partial A/\partial m\ \delta m)$
- If we are near solution $d\approx A(m_0)$ and δm is small, so first term has one small quantity, second has two. Second term in general will be smaller, so usual thing is to drop it.
- Call $\partial A/\partial m$ A_m. Call $d-A(m_0)$ r. Then $\nabla\chi^2\approx -A_m^T N^{-1}(r-A_m\delta m)$
- We know how to solve this! $A_m^T N^{-1} A_m\ \delta m = A_m^T N^{-1} r$

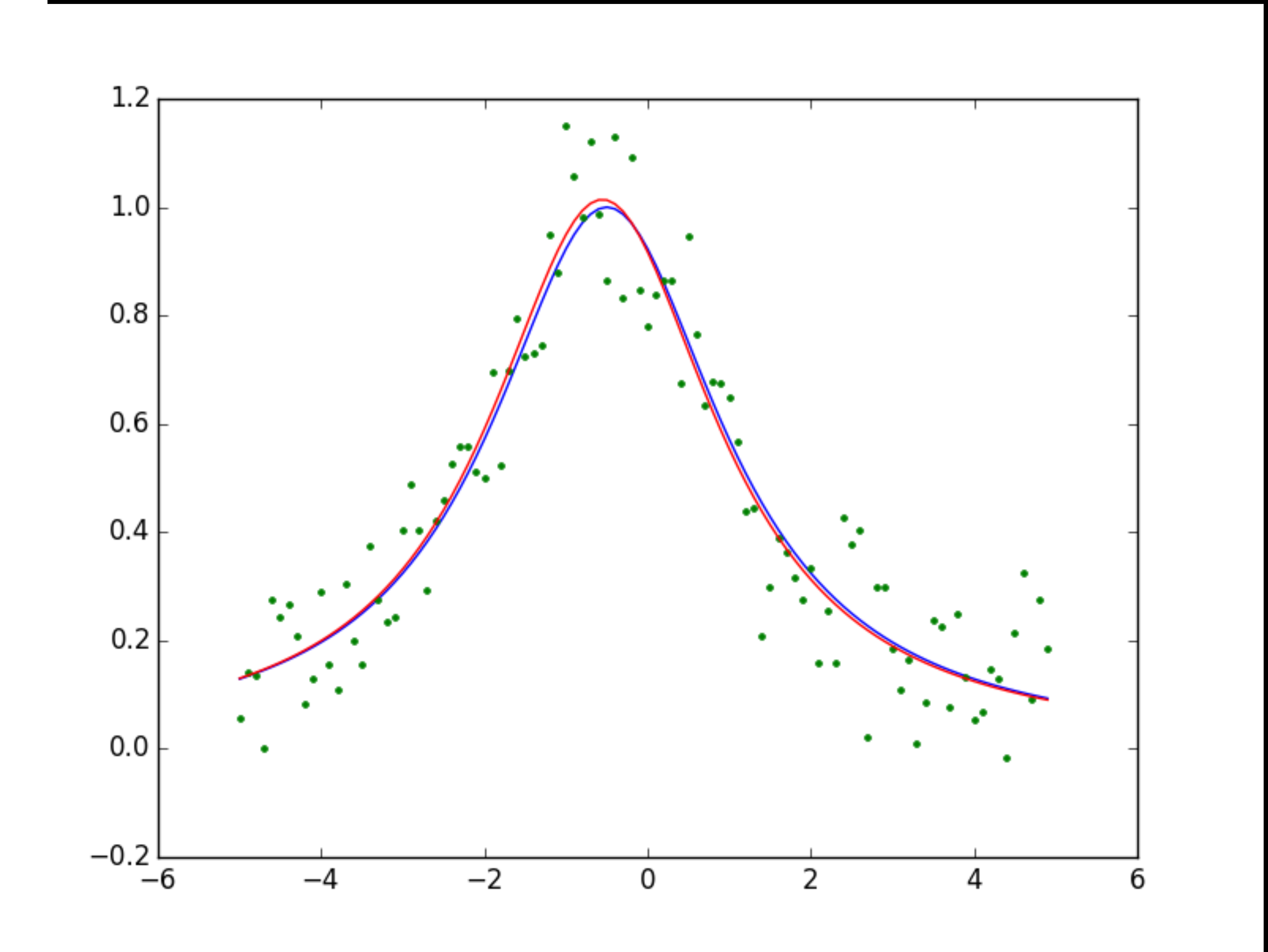
How to Implement

- Start with a guess for the parameters: m_0.
- Calculate model $A(m_0)$ and local gradient A_m.
- Solve linear system $A_m^T N^{-1} A_m \, \delta m = A_m^T N^{-1} r$
- Set $m_0 \rightarrow m_0 + \delta m$.
- Repeat until δm is "small". For χ^2, change should be << 1 (why?).

Newton's Method in Action

```
def calc_lorentz(p,t):
    y=p[0]/(p[1]+(t-p[2])**2)
    grad=numpy.zeros([t.size,p.size])
    #now differentiate w.r.t. all the parameters
    grad[:,0]=1.0/(p[1]+(t-p[2])**2)
    grad[:,1]=-p[0]/(p[1]+(t-p[2])**2)**2
    grad[:,2]=p[0]*2*(t-p[2])/(p[1]+(t-p[2])**2)**2
    return y,grad
```

```
for j in range(5):
    pred,grad=calc_lorentz(p,t)
    r=x-pred
    err=(r**2).sum()
    r=numpy.matrix(r).transpose()
    grad=numpy.matrix(grad)

    lhs=grad.transpose()*grad
    rhs=grad.transpose()*r
    dp=numpy.linalg.inv(lhs)*(rhs)
    for jj in range(p.size):
        p[jj]=p[jj]+dp[jj]
    print p,err
```



Example: Rational Function Fits

- Rational functions (ratio of polynomials) are often better behaved than equivalent degree-of-freedom polynomial fits.
- Reasons include :
  - high order polynomials shoot off steeply outside constrained region, while rational functions can behave better, even going to zero.
  - Poles lead to Taylor series non-convergence - we've already seen this cause problems. Rational functions can gracefully deal.
- Rational functions are very mildly nonlinear.

Starting Guess

- One of the hardest things in nonlinear fitting is a good enough starting guess. Rule of thumb is this takes more human time than actual fits.

- Take simple case of as many parameters as points.

- y_pred=P/Q for polynomials P and Q. Furthermore, set Q_0=1 (why can we do this?). So take Q -> 1+xQ, where the new Q is one degree lower order.

- But I can solve this! y_pred(1+xQ)=P, or y_pred=P-y_pred*x*Q. As you have seen.

- This is now a linear problem and we can use the full framework of LLS.

- Can pick a subset of points, do the exact solution and start nonlinear from there.

Newton's Method LS Ratfuns

- What is gradient of χ^2 w.r.t numerator parameters?
  - Pi/Q
- What is gradient of χ^2 w.r.t denominator parameters?
  - $-P/Q^2\ Q^i$.
- Could we take second derivatives if we wanted to?

Levenberg-Marquardt

- Sometimes Newton's method doesn't converge
- In this case maybe we should just go downhill for a bit and then try again
- One way of doing this is Levenberg-Marquardt: curve-> curve+Λ*diag(curve). For Λ=0 this is Newton, for large Λ it's downhill.
- Scheme: if fit is improving, make Λ small. If it isn't working, make Λ larger until it starts working again.
- This and many other minimizers are in scipy.optimize.

MCMC

- Nonlinear problems can be very tricky. Big problem - there can be many local minima, how do I find global minimum? Linear problem easier since there's only one minimum.
- One technique: Markov-Chain Monte Carlo (MCMC). Picture a particle bouncing around in a potential. It normally goes downhill, but sometimes goes up.
- Solution: simulate a thermal particle bouncing around, keep track of where it spends its time.
- Key theorem: such a particle traces the PDF of the model parameters, and distribution of the full likelihood is the same as particle path.
- Using this, we find not only best-fit, but confidence intervals for model parameters.

MCMC, ctd.

- Detailed balance: in steady state, probability of state going from a to b is equal to going from b to a ("detailed balance").
- Algorithm. Start a particle at a random position. Take a trial step. If trial step improves χ^2, take the step. If not, *sometimes* accept the step, with probability $\exp(-0.5\delta\chi^2)$.
- After waiting a sufficiently long time, take statistics of where particle has been. This traces out the likelihood surface.

MCMC Driver

```
def run_mcmc(data,start_pos,nstep,scale=None):
    nparam=start_pos.size
    params=numpy.zeros([nstep,nparam+1])
    params[0,0:-1]=start_pos
    cur_chisq=data.get_chisq(start_pos)
    cur_pos=start_pos.copy()
    if scale==None:
        scale=numpy.ones(nparam)
    for i in range(1,nstep):
        new_pos=cur_pos+get_trial_offset(scale)
        new_chisq=data.get_chisq(new_pos)
        if new_chisq<cur_chisq:
            accept=True
        else:
            delt=new_chisq-cur_chisq
            prob=numpy.exp(-0.5*delt)
            if numpy.random.rand()<prob:
                accept=True
            else:
                accept=False
        if accept:
            cur_pos=new_pos
            cur_chisq=new_chisq
        params[i,0:-1]=cur_pos
        params[i,-1]=cur_chisq
    return params
```

- Here's a routine to make a fixed-length chain.
- As long as our data class has a get_chisq routine associated with it, it will work.
- Big loop: take a trial step, decide if we accept or not. Add current location to chain.

Output

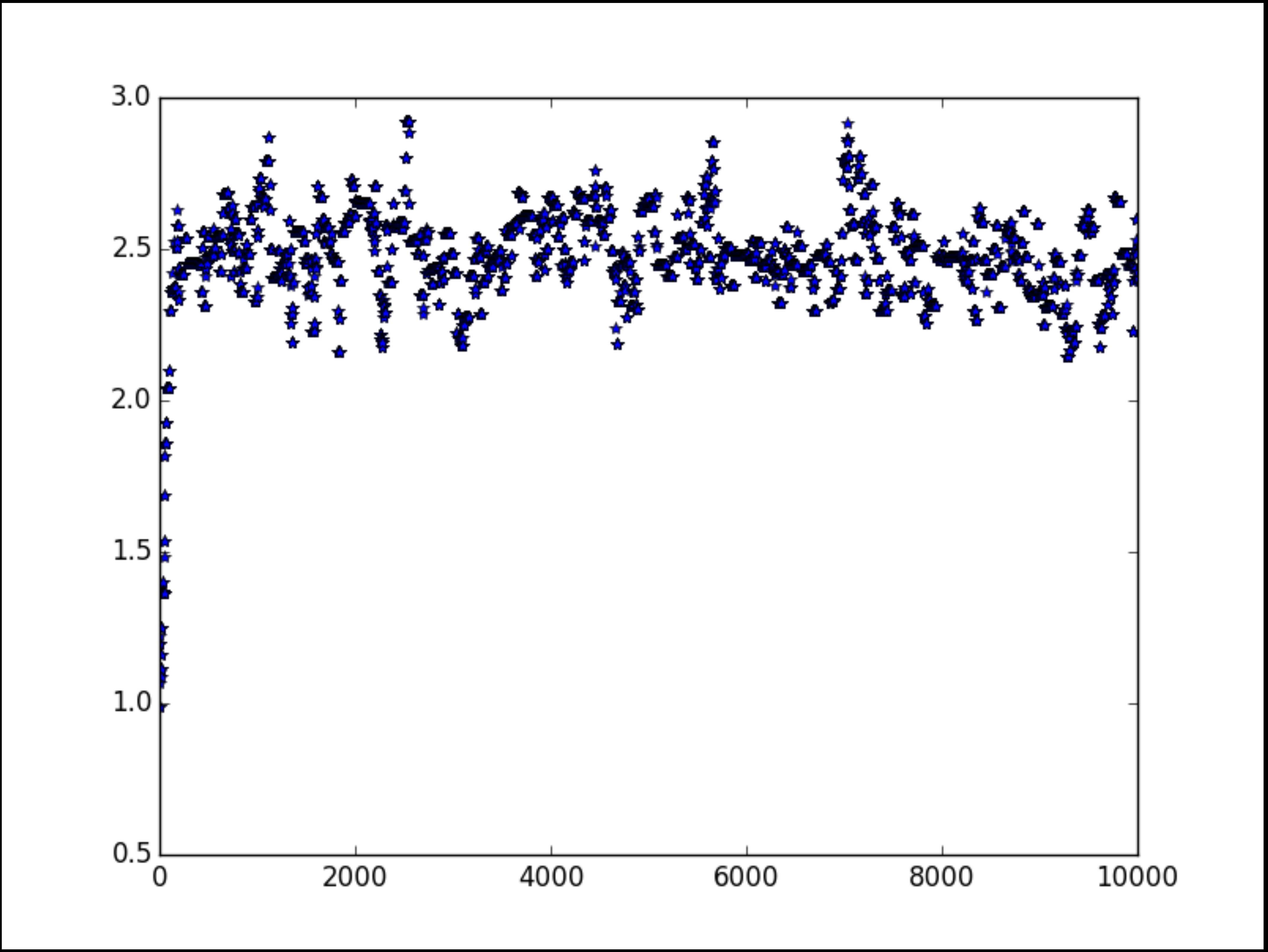
```
if __name__=='__main__':

    #get a realization of a gaussian, with noise added
    t=numpy.arange(-5,5,0.01)
    dat=Gaussian(t,amp=2.5)

    #pick a random starting position, and guess some errors
    guess=numpy.array([0.3,1.2,0.3,-0.2])
    scale=numpy.array([0.1,0.1,0.1,0.1])
    nstep=10000
    chain=run_mcmc(dat,guess,nstep,scale)
    #nn=numpy.round(0.2*nstep)
    #chain=chain[nn:,:]

    #pull true values out, compare to what we got
    param_true=numpy.array([dat.sig,dat.amp,dat.cent,dat.offset])
    for i in range(0,param_true.size):
        val=numpy.mean(chain[:,i])
        scat=numpy.std(chain[:,i])
        print [param_true[i],val,scat]
```

```
>>> execfile('fit_gaussian_mcmc.py')
[0.5, 0.48547765442013036, 0.031379203158769478]
[2.5, 2.5972175915216877, 0.16347041731916298]
[0.0, 0.039131754036757782, 0.030226015774759099]
[0.0, 0.003128115541428856, 0.039835404907011541]
```

- Main: set up data first. Then call the chain function. Finally, compare output fit to true values.

- Parameter estimates are just the mean of the chain. Parameter errors are just the standard deviation of the chain.

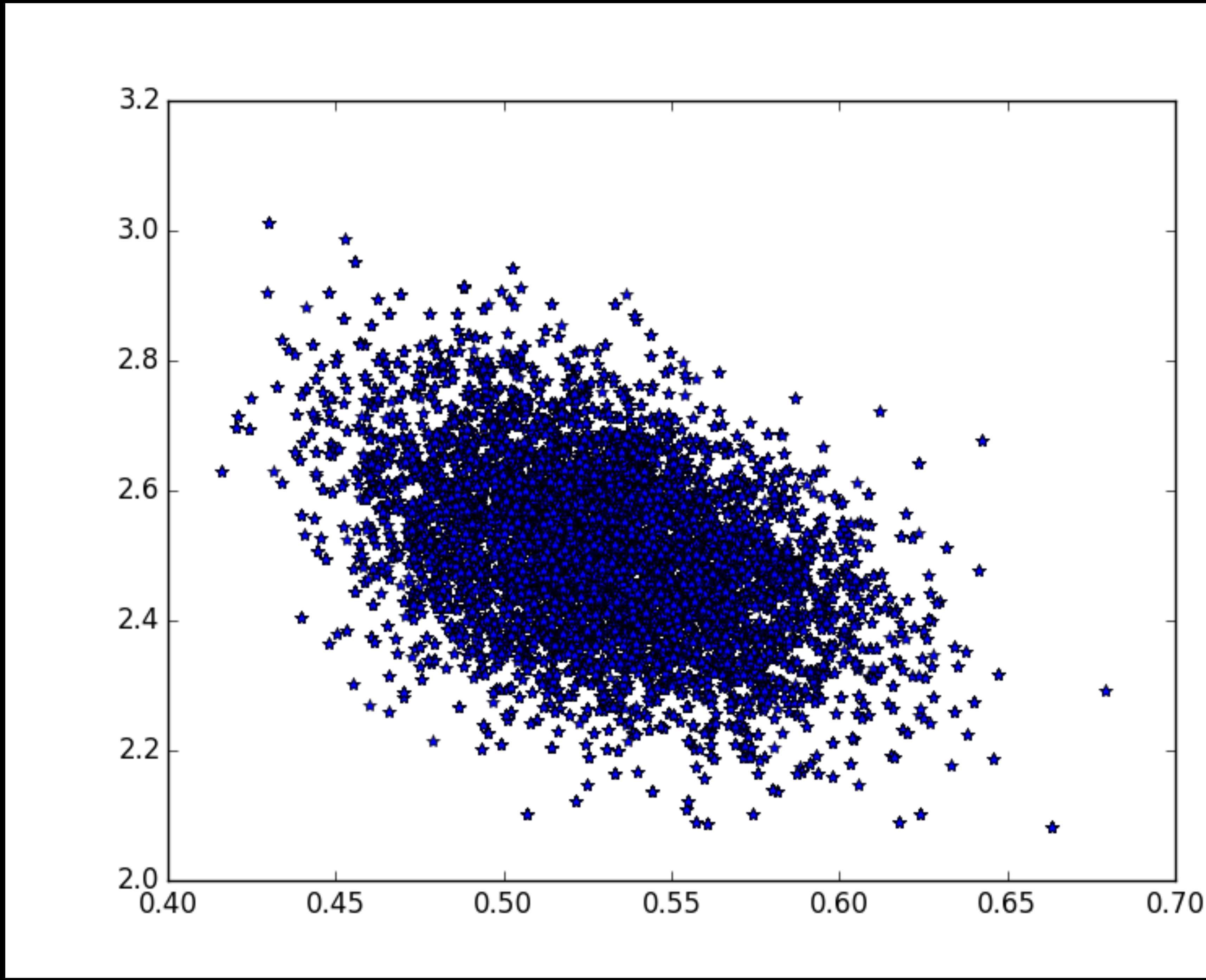
What Chain Looks Like



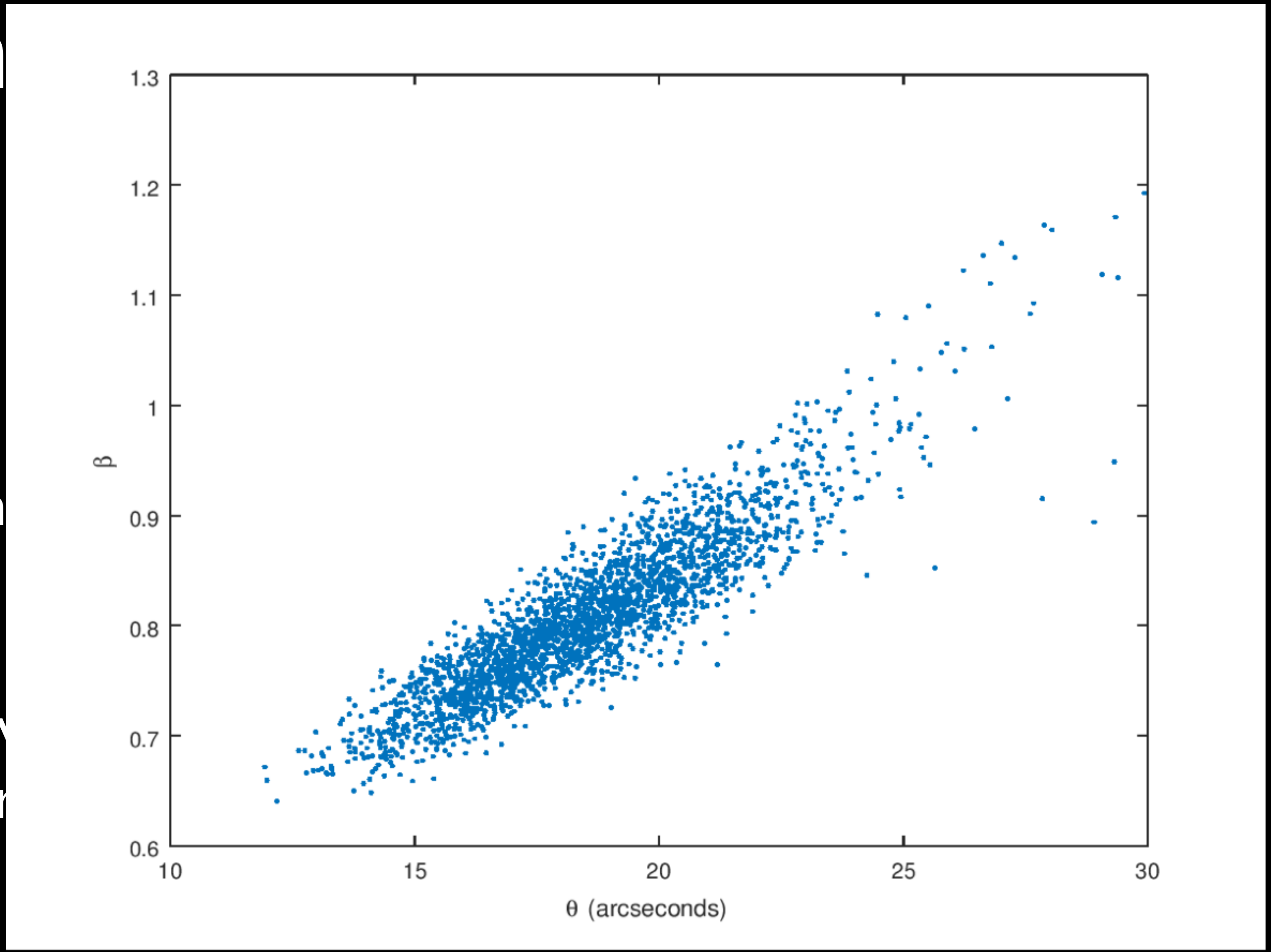
- Here's the samples for one parameter. Note big shift at beginning: we started at a wrong position, but chain quickly moved to correct value.
- Initial part is called "burn-in", and should be removed from chain.

Covariances

- Naturally get parameter covariances out of chains. Just look at covariance of samples!
- Very powerful way of tracing out complicated multi-dimensional likelihoods.



You Gotta Know Wh



- Trick in doing MCMC is knowing when to
- One standard technique is to run many ch vs. expected scatter.
- Chains *work* independent of step size. Ho step size. Too large steps, we spend all our and we only move around slowly, so takes
- If parameters are correlated, you probably want steps to know about that. (See bit on correlated variates for technical details.)
- Good rule of thumb is you want to accept ~25% of your samples. Run for a bit, then adjust step size and start new chain.

Single-Chain Convergence

- Chains eventually forget their past.
- If you plot chain samples, then eventually they should look like white noise
- FT of converged chain should be flat for large scales (low k)
- top: unconverged chain.
  bottom:converged chain.