# assignment2

July 22, 2021

## 1 Inverse Theory Assignment 2

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I'll start with some general code that'll be used all over.

[11]:
```
using SparseArrays
using Distributions
using Krylov
using LinearAlgebra
using Plots
using LaTeXStrings
using BenchmarkTools
```

[12]:
```
"""
Generate some synthetic data by applying gaussian noise to model

Parameters
    G::Matrix - Model kernel
    m::Vector - True parameters
    mean::Number - Mean of gaussian noise
    std::Number - Standard deviation of gaussian noise
"""
function FakeNormalData(G::Union{Matrix, SparseMatrixCSC}, m::Vector, mean::
 ↪Number, std::Number)::Vector
    N = size(G)[1] # get num. of data elements
    gaussian = Normal(mean, std)
    n = rand(gaussian, N) # N gaussian random numbers
    d = G * m + n
end

"""
Find cov(m) given kernel G and standard deviation of data. Not efficent for␣
 ↪large G.
"""
function Covariance(G::Union{Matrix,SparseMatrixCSC}, std::Number)::Matrix
    G = Matrix(G)
    std^2 * inv(transpose(G) * G)
```

```
end;
```

## 2 Q1 | Problem 3.1

Start with Eq 3.6

$$\frac{\partial E}{\partial m_1} = 2Nm_1 + 2m_2\sum_{i=1}^{N} z_i - 2\sum_{i=1}^{N} d_i = 0$$

$$\frac{\partial E}{\partial m_2} = 2m_1\sum_{i=1}^{N} z_i + 2m_2\sum_{i=1}^{N} z_i^2 - 2\sum_{i=1}^{N} z_i d_i = 0$$

Divide by two

$$Nm_1 + m_2\sum_{i=1}^{N} z_i - \sum_{i=1}^{N} d_i = 0$$

$$m_1\sum_{i=1}^{N} z_i + m_2\sum_{i=1}^{N} z_i^2 - \sum_{i=1}^{N} z_i d_i = 0$$

Shift last term

$$Nm_1 + m_2\sum_{i=1}^{N} z_i = \sum_{i=1}^{N} d_i$$

$$m_1\sum_{i=1}^{N} z_i + m_2\sum_{i=1}^{N} z_i^2 = \sum_{i=1}^{N} z_i d_i$$

Turn into a matrix

$$\begin{bmatrix} \sum_{i=1}^{N} d_i \\ \sum_{i=1} N z_i d_i \end{bmatrix} = \begin{bmatrix} Nm_1 & m_2\sum_{i=1}^{N} z_i \\ m_1\sum_{i=1}^{N} z_i & m_2\sum_{i=1}^{N} z_i^2 \end{bmatrix}$$

Split out **m**

$$\begin{bmatrix} \sum_{i=1}^{N} d_i \\ \sum_{i=1} N z_i d_i \end{bmatrix} = \begin{bmatrix} N & \sum_{i=1}^{N} z_i \\ \sum_{i=1}^{N} z_i & \sum_{i=1}^{N} z_i^2 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix}$$

Solve for **m**

$$\begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} N & \sum_{i=1}^{N} z_i \\ \sum_{i=1}^{N} z_i & \sum_{i=1}^{N} z_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum_{i=1}^{N} d_i \\ \sum_{i=1} N z_i d_i \end{bmatrix}$$

Which is Eq 3.18, showing it is a valid solution

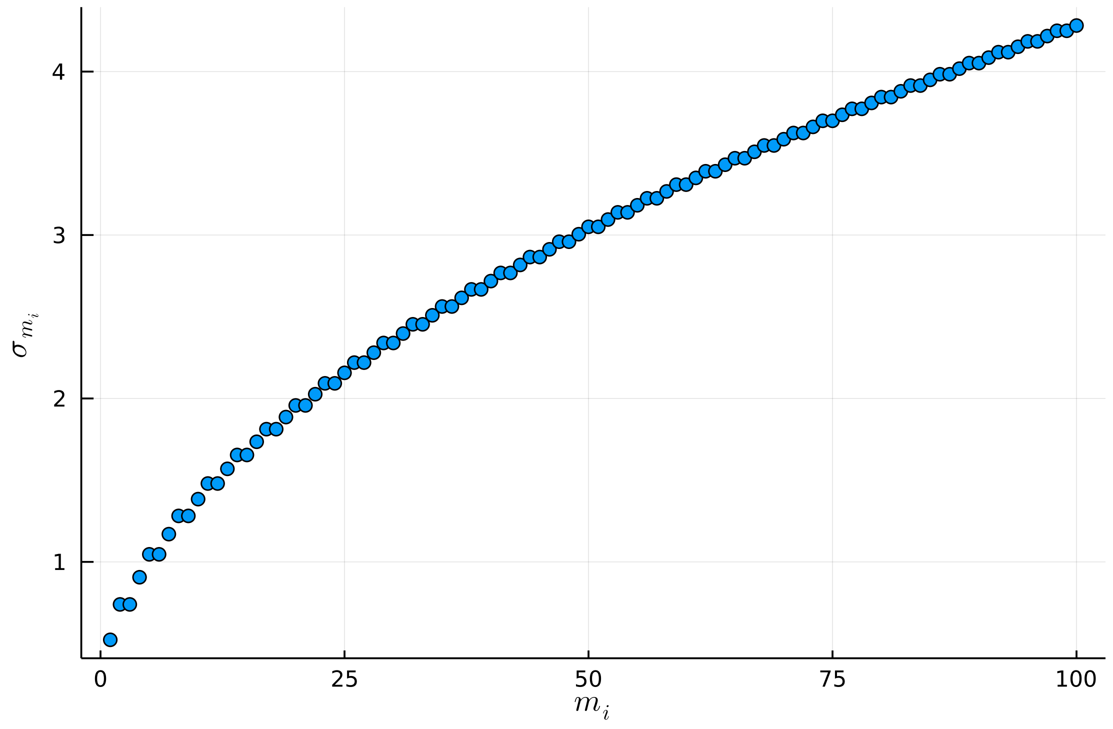
## 3 Q2 | Problem 3.2

[13]:
```
# Function taken from Assignment 1
"""Make NxN square matrix and fill it with triplets of a coefficent a.
In a row with index r, the cells [r, r], [r, r-1], [r, r-2] are filled.
Argument a multipes the entire matrix by scalar a.
For example TripletsMatrix(5, 1) produces the sparse matrix
    [1 0 0 0 0;
     1 1 0 0 0;
     1 1 1 0 0;
     0 1 1 1 0;
     0 0 1 1 1]"""
function TripletsMatrix(N::Int, a=1::Number)::SparseMatrixCSC  # a is probably␣
↪unneccessary (vs hardcoding a=1) except in some odd cases, but including it␣
↪is trivial.
     #= We are creating a matrix with COO, a coordinate list.
     For some k, row[k] gives row index, col[k] gives col index and val[k]␣
↪gives the value for that coordinate pair.
     We create the matrices in advance then increment over vector coordiantes␣
↪with k because it is reportedly faster than appending to matrices. =#

     if N < 2 error("N should be at least 2.") end

     col = Vector{Int64}(undef, 3*(N-1)) # 3*(N-1) should be the amount of␣
↪nonzero values <- 3 from the first two rows and 3*(N-2) from the rest.
     row = Vector{Int64}(undef, 3*(N-1))
     val = Vector{Float64}(undef, 3*(N-1))
     k = 1 # This tracks our location in the COO vectors
     for i = 1:N # Row index.
         for j in i-2:i # Column index, for non-zero values. We don't write to␣
↪any columns higher than i so this doesn't do anything weird in the last row.
            if j > 0 # To handle first two rows.
                col[k] = j
                row[k] = i
                val[k] = a
                k += 1
            end
         end
     end
     sparse(row, col, val) # Takes our vectors and turns them into a sparse␣
↪matrix
end


function WithinTwoSTD(actual::Vector, est::Vector, std::Vector)::Int
     diff = abs.(actual .- est)
     twosigma = diff[diff .< (2*std)]
     length(twosigma)
end;
```

[14]:
```
N = 100 # number of objects

# (A) Randomly assign true masses (0,1] to N objects
mTrue = 1 .- rand(Float64, N) # note subtraction from 1 to convert from [0,1)

# (B) create data kernal G
```

```
G = TripletsMatrix(N)

# (C) Synthesise some data
d = FakeNormalData(G, mTrue, 0, 0.01)

# (D) Least squares solution for m.
# This lovely function, implemented by Krylov.jl, uses a conjugate gradient␣
↪method to solve least squares quickly (~ 0.17 ms for this).
# See https://juliasmoothoptimizers.github.io/Krylov.jl/stable/solvers/ls/
↪#Krylov.cgls
# I looked at the BiCG method suggested in Menke, but had some problems with␣
↪the Julia equivilant (doesn't like a function argument).
# I also tried straight up solving the matrix eq:
#   m = inv(transpose(T) * G) * (transpose(G) * d)
# but that was (predicatably) slow.
(mEst, stats) = cgls(G, d)
# (E) Estimate variance of est. model params
# Slow but works for this small N
dDevEst = std(d)
mCov = Covariance(G, dDevEst)
mVar = diag(mCov) # Extract vector of variances for mEst from diagonal

# (F) Count number of model params within 2 std. of true value
mStd = mVar .^ 0.5
WithinTwoSTD(mTrue, mEst, mStd)
# (G) Plot model variance as function of index
plot(mStd, seriestype = :scatter, xlabel = L"m_i", ylabel = L"\sigma_{m_i}",␣
↪legend=false) # std increases weith i
```

[14]:



### 3.1 Design Note

```
[15]: """
An alternate function that achieves the same result as TripletsMatrix

The assignment question suggests "Try to see if you can construct G without␣
 ↪using loops over columns and rows."
For the last assignment I wrote TripletsMatrix, which uses loops and COO. That␣
 ↪isn't looping over columns and rows but it has some similarities.
TripletsMatrix does include a lot of looping, if not over rows and columns, so␣
 ↪I decided to give it a go.
I discovered the function diagm() which constructs matrices from diagonals and␣
 ↪created the short function below.
However, the benchmarks show that it is many times slower and uses much more␣
 ↪memory.
I am hence only including it here to show the attempt.
"""
function TripletsMatrixDiag(N::Int, a=1::Number)
    d1 = fill(a, N)
    dn1 = fill(a, N-1)
    dn2 = fill(a, N-2)
    diagm(0 => d1, -1 => dn1, -2 => dn2)
end
```

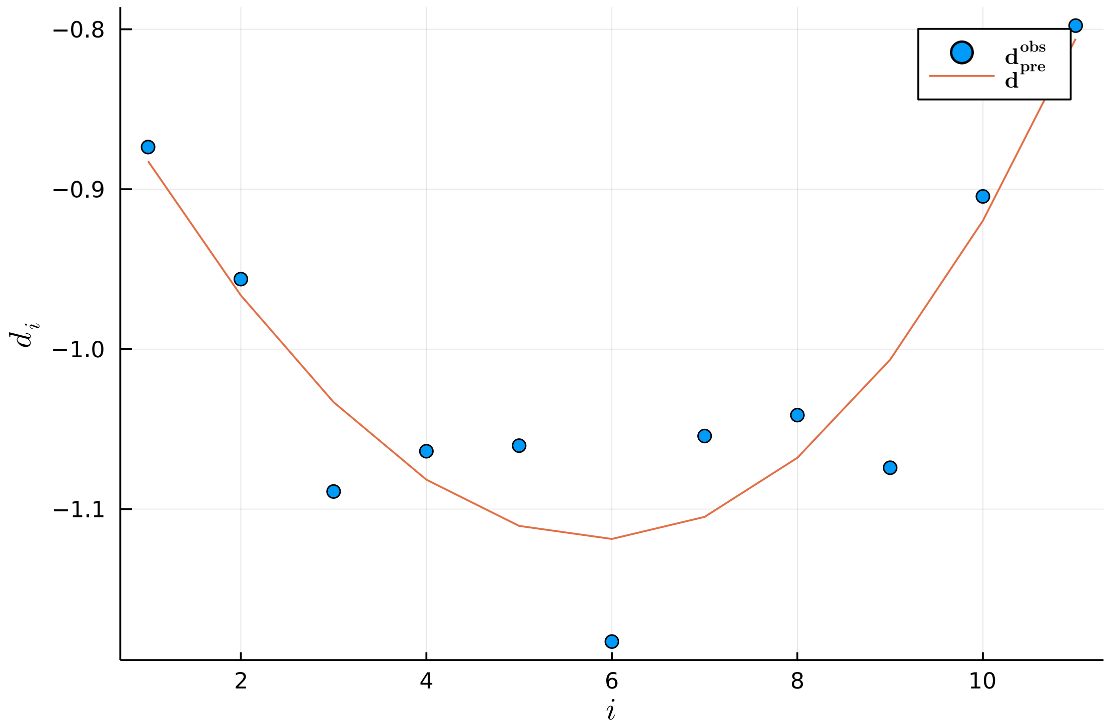
```
display(@benchmark TripletsMatrix(1000))
display(@benchmark TripletsMatrixDiag(1000))
```

```
BechmarkTools.Trial: 10000 samples with 1 evaluations.
 Range (min … max):   42.600  s …  27.628 ms   GC (min … max):  0.00% … 0.00%
 Time  (median):     118.900  s                GC (median):     0.00%
 Time  (mean ± ):   139.093  s ± 445.806  s   GC (mean ± ):  14.38% ± 6.06%



  42.6  s       Histogram: log(frequency) by time        530  s <

 Memory estimate: 188.75 KiB, allocs estimate: 20.
BechmarkTools.Trial: 1259 samples with 1 evaluations.
 Range (min … max):  2.056 ms … 36.569 ms    GC (min … max):  0.00% … 41.12%
 Time  (median):     2.990 ms                GC (median):     0.00%
 Time  (mean ± ):   3.939 ms ±  2.490 ms    GC (mean ± ):  22.54% ± 23.56%



  260 ms         Histogram: frequency by time        11.1 ms <

 Memory estimate: 7.74 MiB, allocs estimate: 6013.
```

## 4 Q3 | Problem 3.4

[16]:
```
z = Vector(LinRange(0, 1, 11)) # (A) linear spacing, start=0, stop=10, # of␣
 ↪values=11
# (B) assign true m by sampling uniform distribution
u = Uniform(-1, 1)
mTrue = rand(u, 4)
G = [ones(11) z z.^2 z.^3] # (C) Kernel
dObs = FakeNormalData(G, mTrue, 0, 0.05) # (D) synthetic data
(mEst, stats) = cgls(G, dObs) # (E) least squares
dPre = G * mEst # (F) calculate predicted data

plot(dObs, seriestype=:scatter, label=L"\mathbf{d^{obs}}", xlabel=L"i",␣
 ↪ylabel=L"d_i") # (G) plot
plot!(dPre, label=L"\mathbf{d^{pre}}")
```

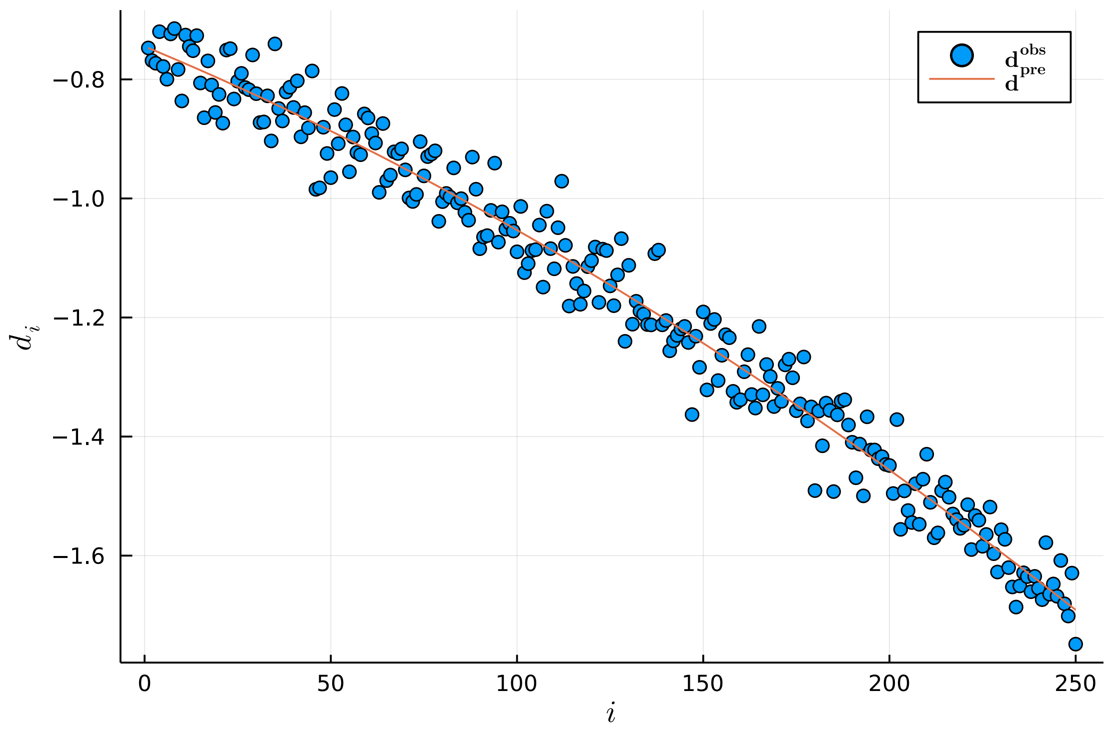
[16]:



The model matches well when the data approximately follows a trend, even if it is non-linear. However, on some interations that data is spaced wildly and the model is a terrible fit. I believe these instances are caused by high Gaussian noise in the fake data and would become less prominent with a larger number of datapoints. The plot below demonstates this by increasing data to 250 points.

[17]:
```
z = Vector(LinRange(0, 1, 250)) # (A) linear spacing, start=0, stop=10, # of␣
 ↪values=11
# (B) assign true m by sampling uniform distribution
u = Uniform(-1, 1)
mTrue = rand(u, 4)
G = [ones(250) z z.^2 z.^3] # (C) Kernel
dObs = FakeNormalData(G, mTrue, 0, 0.05) # (D) synthetic data
(mEst, stats) = cgls(G, dObs) # (E) least squares
dPre = G * mEst # (F) calculate predicted data

plot(dObs, seriestype=:scatter, label=L"\mathbf{d^{obs}}", xlabel=L"i",␣
 ↪ylabel=L"d_i") # (G) plot
plot!(dPre, label=L"\mathbf{d^{pre}}")
```

[17]:

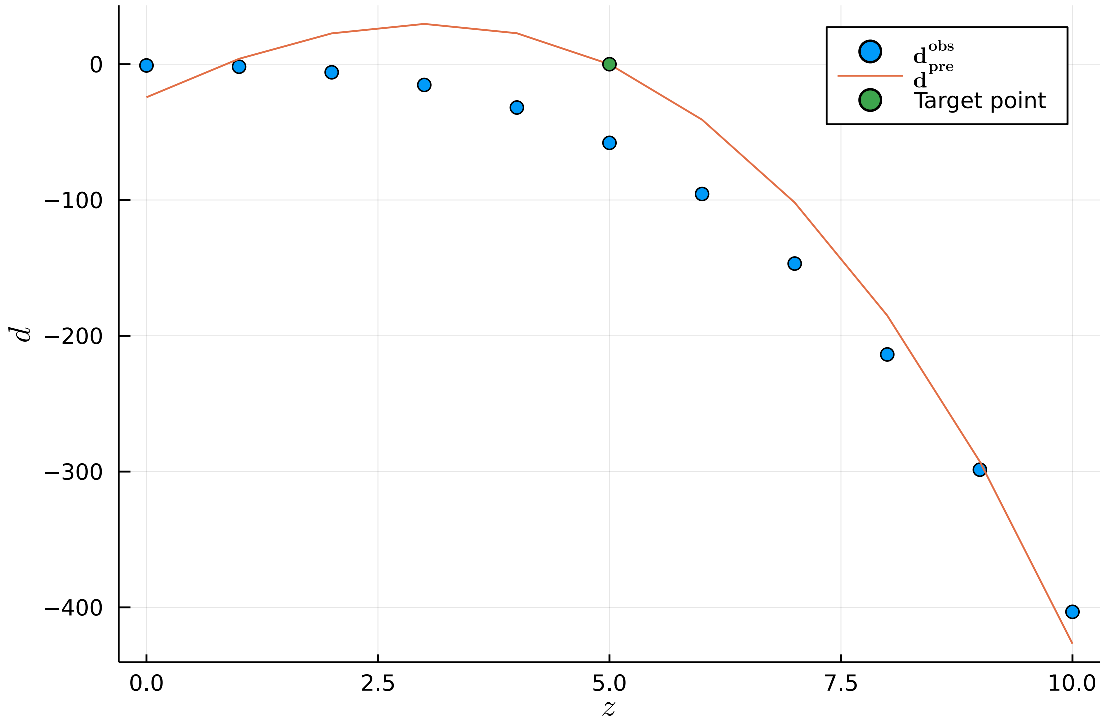


## 5 Q4 | Problem 3.5

[18]:
```
# The book asks for range 0 to 1 but if we then plot against z, fitting a point␣
↪to z=5 is not very natural. I think 1 to 10, as in Problem 1.3 works better␣
↪- feels like a book error to me.
z = Vector(LinRange(0, 10, 11)) # (A) linear spacing, start=0, stop=10, # of␣
↪values=11
# (B) assign true m by sampling uniform distribution
u = Uniform(-1, 1)
mTrue = rand(u, 4)
G = [ones(11) z z.^2 z.^3] # (C) Kernel
dObs = FakeNormalData(G, mTrue, 0, 0.05) # (D) synthetic data

function ConstrainedFit(G::Matrix, H::Matrix, h::Vector)::Vector
    lMatrix = [transpose(G)*G transpose(H); H 0]
    rMatrix = vcat(transpose(G)*dObs, h)
    inv(lMatrix)*rMatrix
end

zp = 5
dp = 0
H = [1 zp zp^2 zp^3]
```

```
h = [dp]

mEst = ConstrainedFit(G, H, h)

dPre = G * mEst[1:4] # (F) calculate predicted data

plot(z, dObs, seriestype=:scatter, label=L"\mathbf{d^{obs}}", xlabel=L"z",␣
 ↪ylabel=L"d") # (G) plot
plot!(z, dPre, label=L"\mathbf{d^{pre}}")
plot!([zp], [dp], seriestype=:scatter, label="Target point")
```

[18]:



While the model does always pass through the constraint, as desired, this doesn't do good things for the fit. The fact that the data doesn't fit this constraint suggests to me the constraint is flawed.

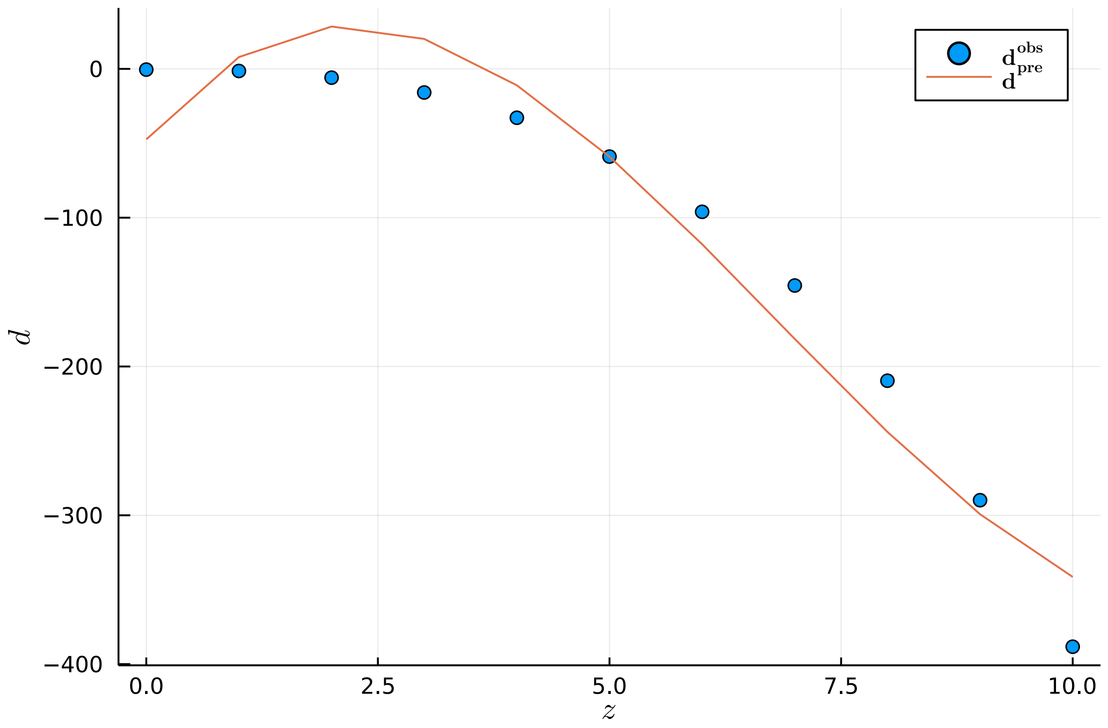
## 6 Q5

[19]:
```
# The book asks for range 0 to 1 but if we then plot against z, fitting a point␣
 ↪to z=5 is not very natural. I think 1 to 10, as in Problem 1.3 works better␣
 ↪- feels like a book error to me.
z = Vector(LinRange(0, 10, 11)) # (A) linear spacing, start=0, stop=10, # of␣
 ↪values=11
# (B) assign true m by sampling uniform distribution
u = Uniform(-1, 1)
```

```
mTrue = rand(u, 4)
G = [ones(11) z z.^2 z.^3] # (C) Kernel
dObs = FakeNormalData(G, mTrue, 0, 0.05) # (D) synthetic data

H = [0 0 0 1]
h = [1]

mEst = ConstrainedFit(G, H, h)

dPre = G * mEst[1:4] # (F) calculate predicted data

println("The fourth parameter is $(mEst[4]).")
plot(z, dObs, seriestype=:scatter, label=L"\mathbf{d^{obs}}", xlabel=L"z",␣
 ↪ylabel=L"d") # (G) plot
plot!(z, dPre, label=L"\mathbf{d^{pre}}")
```

```
The fourth parameter is 1.0.
```

[19]:



## 7 Q6

Firstly, the dead end I went down: - Trying to turn Hm into (1,1,1,1), perhaps by dividing m by its average. Can't get away with only using m once when you're doing that

The solution was rather different and appallingly simple, once it occured to me.

$$\mathbf{h} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

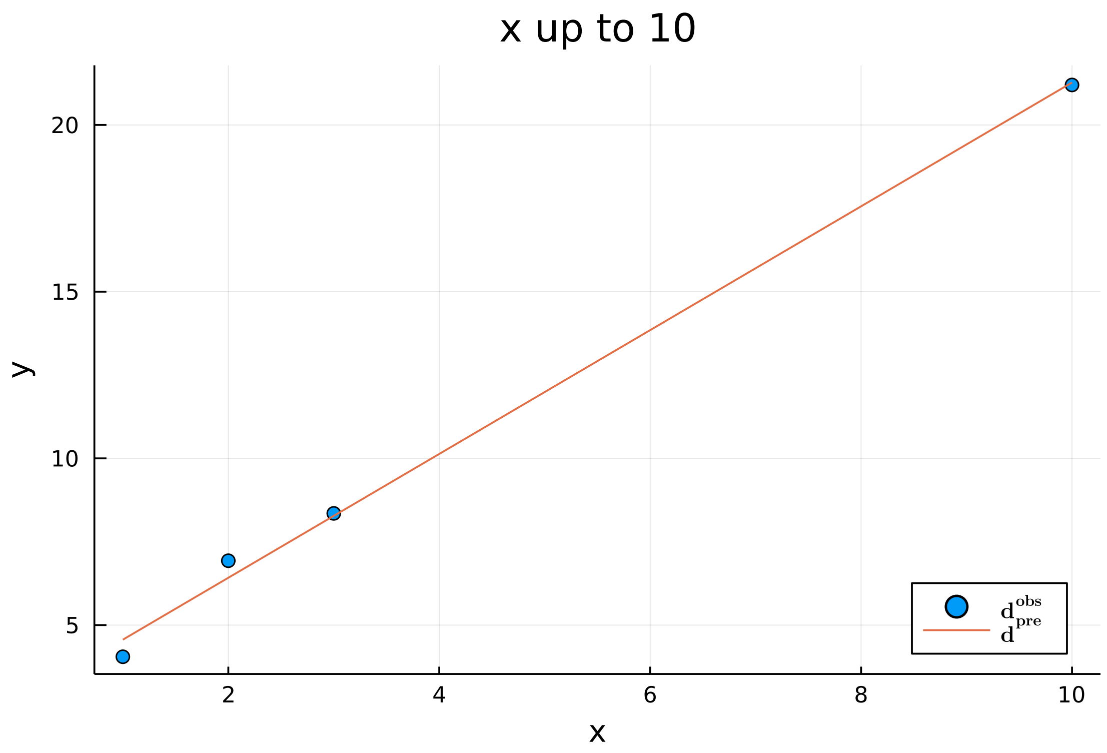
$$\mathbf{H} = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{bmatrix}$$

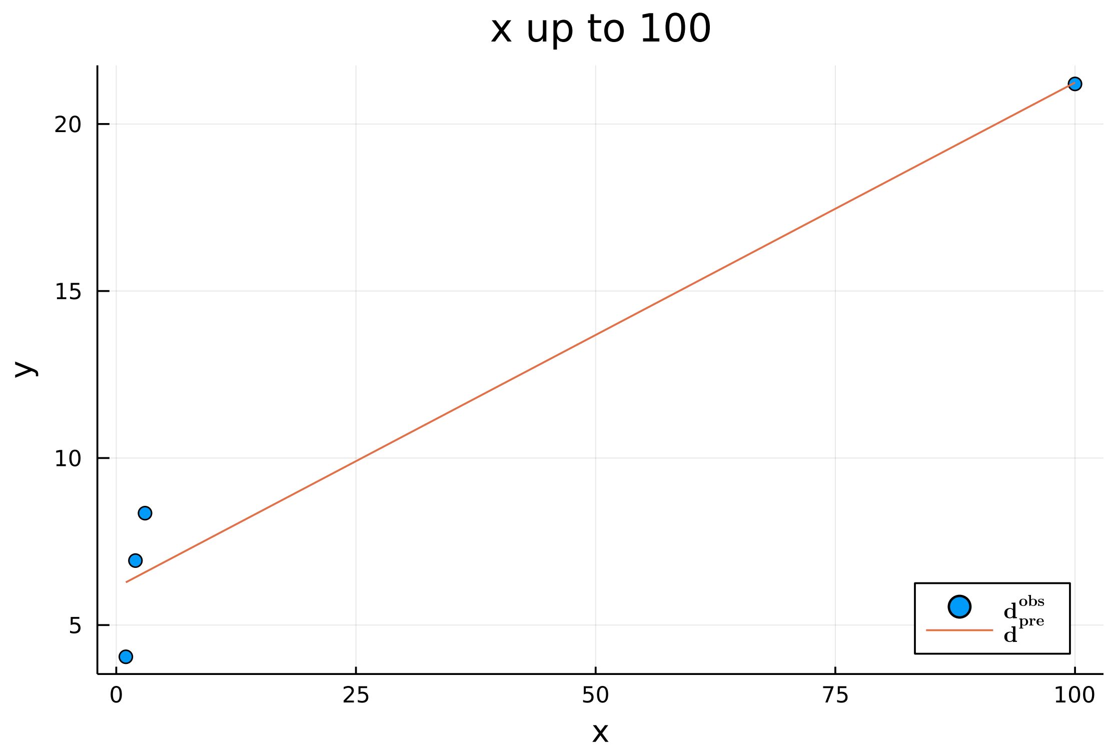
## 8 Q7

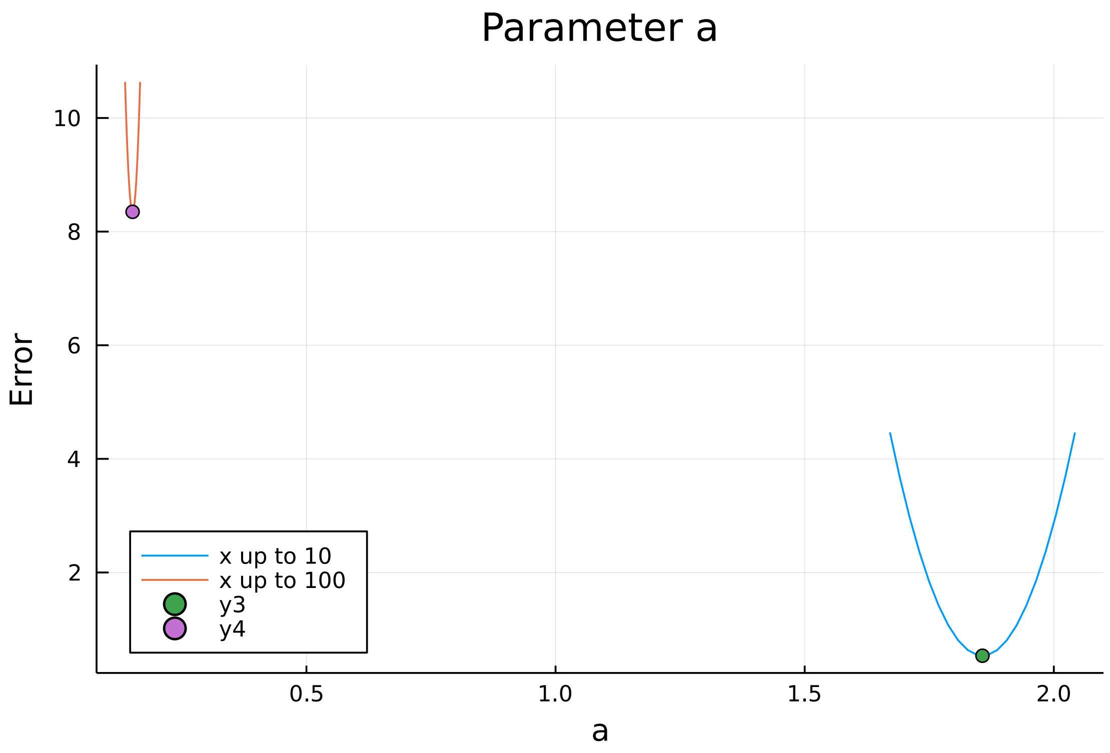
[20]:
```
"""
Finds generalised inverse of a kernel G for a least squares problems.
"""
function GeneralisedInverseLeastSq(G::Matrix)::Matrix
    Gt = transpose(G)
    inv(Gt*G)*Gt
end


"""
Find error E for least squares fit from observed data (dObs) and model data␣
 ↪(dPre).
"""
function FindErrorLeastSq(dObs::Vector, dPre::Vector)::Float64
    e = dObs - dPre
    transpose(e) * e
end


"""
Perturbs a model by a factor of ±mangitude in all parameters.

Parameters
    G::Matrix - Kernel for model
    m::Vector - Parameters of the model
    dObs::Vector - Observed data, used for evaluating FindErrorLeastSq
    iterations::Int - Number of peturbed values analysed per parameter
    magnitude::Float64 - Percentage to perturb by (as a decimal). e.g. 0.1 will␣
 ↪perturb by ±10%.

Returns a Vector of length(m) matrices.
Each matrix corresponds to one parameter from m. Order matches order of␣
 ↪parameters in m.
Each matrix has 2 columns and a row count determined by iterations.
The first column is the perturbed parameter values.
The second column is the associated error values.
```

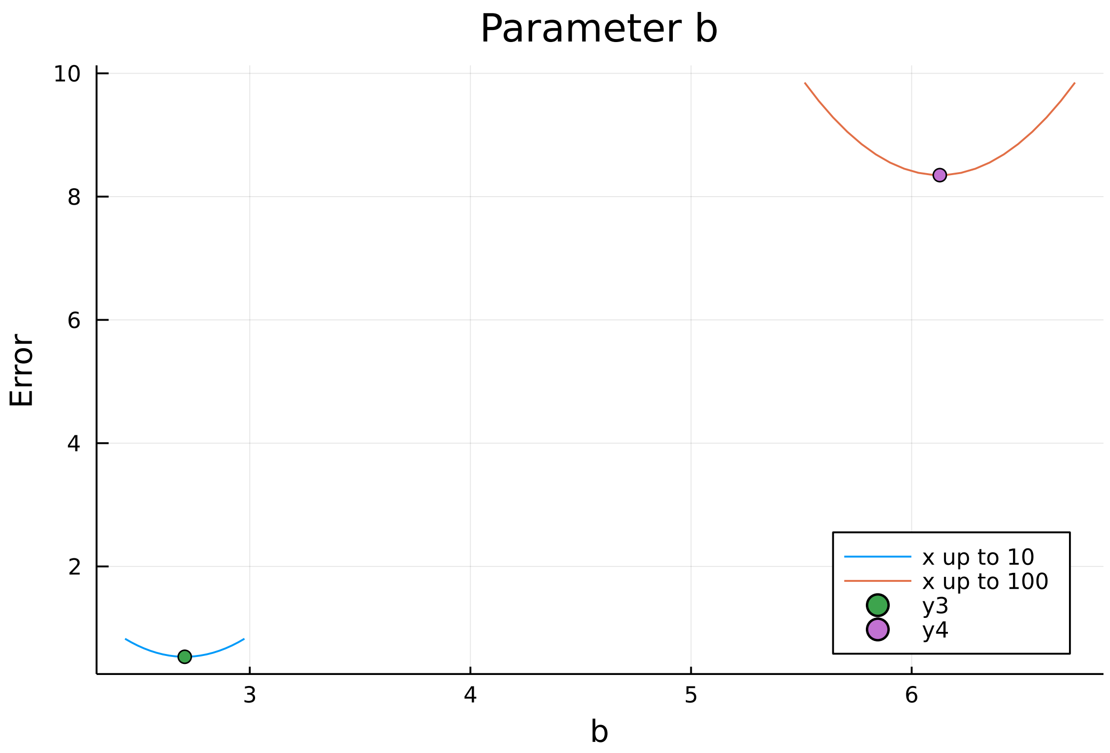
```
"""
function PeturbParameters(G::Matrix, m::Vector, dObs::Vector, iterations::
↪Int=20, magnitude::Float64=0.1)::Vector{Matrix}
    results = Vector{Matrix}(undef, length(m)) # preallocate for efficency
    mMatrix = hcat([m for i in 1:iterations]...) # create a matrix where each␣
↪column is our parameter vector
    for r in 1:length(m)
        p = m[r] # get parameter we're peturbing
        pMatrix = copy(mMatrix) # copy it so mutation doesn't affect other␣
↪iterations
        pMatrix[r,:] = LinRange((1-magnitude)*p, (1+magnitude)*p, iterations) #␣
↪replaces row of our targeted parameter with perturbed values
        E = Vector{Float64}(undef, iterations) # preallocate
        for c in 1:iterations
            E[c] = FindErrorLeastSq(dObs, G * pMatrix[:,c]) # find error for␣
↪each peturbed value
        end
        results[r] = [pMatrix[r,:] E] # creates matrix as element of results␣
↪vector as described in docstring
    end
    return results
end


"""
This function just chuckls steps a through d into a single function so I can␣
↪easily run it on multiple datasets.
Assumes y = ax + b such that x is an auxillary variable and m=[a;b] are is␣
↪parameter vector.

Parameters
    x::Vector - Auxiliary variables
    y::Vector - Data points
"""
function AnalyseStraightLine(x::Vector, y::Vector)
    G = [x ones(length(x))]

    Gg = GeneralisedInverseLeastSq(G)
    m = Gg * y # We're working with a tiny matrix so I'll do the fitting the␣
↪slow way
    dPre = G * m

    covar = Covariance(G, 1)
    mStd = diag(covar) .^ 0.5

    N = G * Gg # Data resolution matrix
    R = Gg * G # Model resolution matrix

    ptb = PeturbParameters(G, m, y)

    # output time
    println("x: $x")
    println("y: $y")
    println("Parameters [a,b] are $m")
    println("The associated covariance matrix for the model parameters is␣
 ↪$covar")
    println("The associated standard deviations are $mStd")
    println("N: $N")
    println("R: $R")
    println("-----------------------------")

    p1 = plot(x, [y dPre], seriestype=[:scatter :line],␣
 ↪label=[L"\mathbf{d^{obs}}" L"\mathbf{d^{pre}}"], xlabel="x", ylabel="y",␣
 ↪title="x up to $(x[end])", legend=:bottomright)

    display(p1)

    e = FindErrorLeastSq(y, G*m)

    return (ptb, m, e)

end


y =  [4.05; 6.93; 8.35; 21.2]
x1 = [1;    2;    3;    10]
ptb1, m1, e1 = AnalyseStraightLine(x1, y)
x2 = [1, 2, 3, 100]
ptb2, m2, e2 = AnalyseStraightLine(x2, y)

p1Am = ptb1[1][:,1]
p1Ae = ptb1[1][:,2]
p1Bm = ptb1[2][:,1]
p1Be = ptb1[2][:,2]

p2Am = ptb2[1][:,1]
p2Ae = ptb2[1][:,2]
p2Bm = ptb2[2][:,1]
p2Be = ptb2[2][:,2]

plot([p1Am p2Am], [p1Ae p2Ae], title="Parameter a", labels=["x up to 10" "x up␣
 ↪to 100"], xlabel="a", ylabel="Error", legend=:bottomleft)
display(plot!([m1[1] m2[1]], [e1 e2], seriestype=:scatter))
```

```
plot([p1Bm p2Bm], [p1Be p2Be], title="Parameter b", labels=["x up to 10" "x up␣
 ↪to 100"], xlabel="b", ylabel="Error", legend=:bottomright)
display(plot!([m1[2] m2[2]], [e1 e2], seriestype=:scatter))
```




x up to 100
y
x
0
25
50
75
100
5
10
15
20
$\mathbf{d}^{\mathrm{obs}}$
$\mathbf{d}^{\mathrm{pre}}$


Parameter a
Error
a
0.5
1.0
1.5
2.0
2
4
6
8
10
x up to 10
x up to 100
y3
y4



```
x: [1, 2, 3, 10]
y: [4.05, 6.93, 8.35, 21.2]
Parameters [a,b] are [1.8567999999999993, 2.705300000000002]
The associated covariance matrix for the model parameters is
[0.019999999999999997 -0.07999999999999999; -0.07999999999999999 0.57]
The associated standard deviations are [0.1414213562373095, 0.7549834435270749]
N: [0.43 0.37 0.30999999999999994 -0.10999999999999999; 0.37 0.32999999999999996
0.29 0.010000000000000064; 0.31000000000000005 0.29 0.26999999999999996 0.13;
-0.10999999999999988 0.010000000000000064 0.13 0.9699999999999999]
R: [0.9999999999999998 0.0; 8.881784197001252e-16 1.0]
----------------------------
x: [1, 2, 3, 100]
y: [4.05, 6.93, 8.35, 21.2]
Parameters [a,b] are [0.1511332408049965, 6.127469118667591]
The associated covariance matrix for the model parameters is
[0.00013879250520471893 -0.0036780013879250516; -0.0036780013879250516
0.34746703678001384]
The associated standard deviations are [0.01178102309668897, 0.5894633464262335]
N: [0.3402498265093684 0.33671061762664817 0.3331714087439278
-0.010131852879944492; 0.3367106176266481 0.3333102012491325 0.32990978487161693
6.939625260234811e-5; 0.33317140874392775 0.32990978487161693 0.326648160999306
0.010270645385149189; -0.010131852879944503 6.93962526023828e-5
0.010270645385149213 0.9997918112421929]
R: [0.9999999999999999 -1.734723475976807e-18; -8.881784197001252e-16 1.0]
```

----------------------------

All the parameter plots should that we have indeed minimised error. Just from a visual analysis of the first two plots we can see that the original dataset can have a straight line fit to it relatively neatly. Once we switch to the second dataset, with a x=100 point, the last point is far off the approximate line created by the earlier points. This results in a terrible fit, passing through the (approximate) right end correct but only in the vague vicinity of the points on the left. A line that fit the earlier points well would be miles off the far right point, due to the massive displacement the distance and gradient would introduce. The error would be massive and so our best fit doesn't do this, instead fitting the last point.

This is supported by the parameter variation. Parameter $a$ is more susceptible to variation in both datasets. The second dataset has much higher errors no matter the parameter value, which makes sense given how much x=100 throws off the fitting.

The parabolas for parameter b appear to show similar shapes for both datasets, just displaced in space. The results for b with x=10 could almost be a section of the parabolda for b with x=100.

For parameter a, we see that the x=100 model is far more suspectible to variation in a than the x=10 model. This makes sense, given how even a small change in gradient can cause a big increase in error over a large distance.