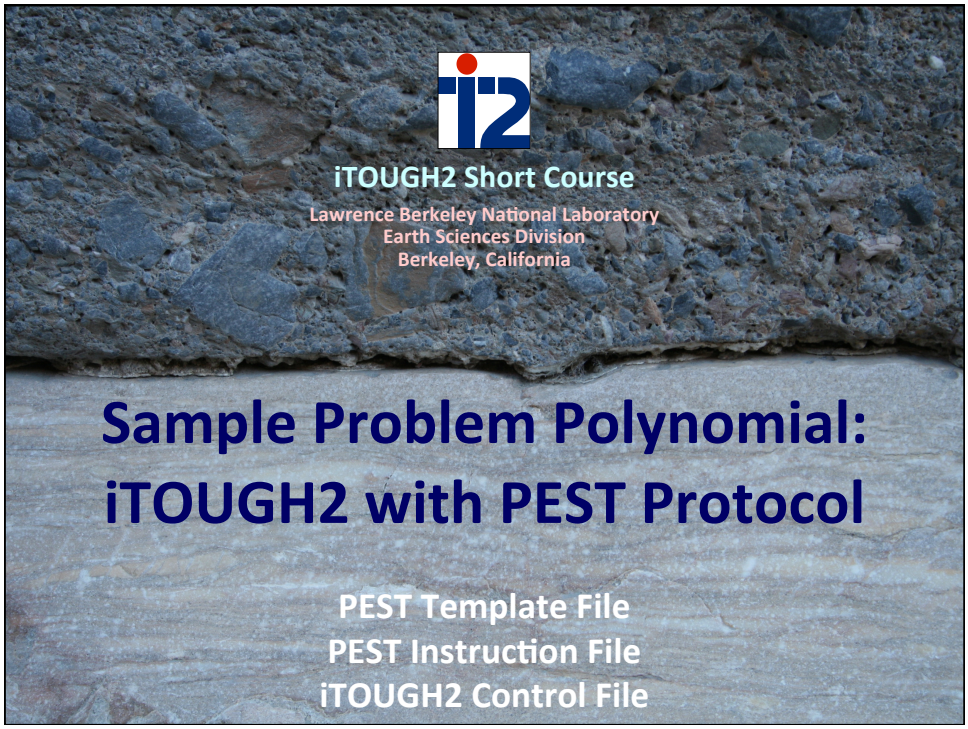

iTOUGH2 Sample Problem *Polynomial*

- Tutorial sample problem demonstrating iTOUGH2-PEST features to estimate coefficients of a polynomial.
- Directory:

`…/Polynomial`

- Files:

`pestonly`	dummy TOUGH2 input file for non-TOUGH2 inversions
`polyi`	incomplete iTOUGH2 input file (for Exercise 3)
`poly.exe`	Executable

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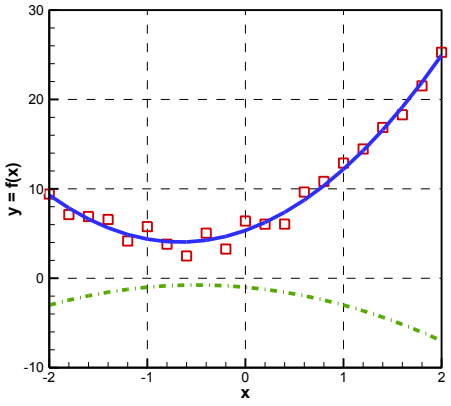
Problem Description

- Fit polynomial to data

$$y(x) = \sum_{i=0}^{n} a_i \cdot x^i$$



- *Data*:
  - $y(x)_i$, $i = 1, \ldots, 21$
- *Parameter to be estimated*:
  - a_i, $i = 0, \ldots, n$

Program *Polynomial*

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
      program polynomial
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
C
C --- Evaluates polynomial
C
      dimension c(9)
C
C --- Read degree of polynomial, coefficients, x-value range and
C     number of evaluation points
C
      write(*,*) ' Evaluate Polynomial'
      write(*,*) ' ********************'
      write(*,*)
      write(*,*) ' Degree of polynomial : ?'
      read(*,*)  n
      do i=1,n+1
         write(*,7000) i-1
 7000 format('  Coefficient a',i1,7x,': ?')
         read(*,*) c(i)
      enddo
      write(*,*) ' Range of x: Xmin     : ?'
      read(*,*)  xmin
            write(*,*) '             Xmax     : ?'
      read(*,*)  xmax
      write(*,*) ' Number of points     : ?'
      read(*,*)  m
      dx=(xmax-xmin)/(max(m,2)-1)
C
C --- Calculate and output f(x)
C
      write(*,7001) n
 7001 format(/,/,'  Polynomial of degree',i2,' with coefficients:')
      do i=1,n+1
         write(*,7002) i,c(i)
 7002 format('  a(',i1,') =',f9.5)
      enddo
      write(*,*)
      write(*,*) '               x             y(x)'
      x=xmin
      do j=1,m
         y=c(1)
         do i=2,n+1
            y=y+c(i)*x**(i-1)
         enddo
         write(*,'(2f17.10)') x,y
         x=x+dx
      enddo
      end
```

Exercise 1: Template File

- Here's a sample input file needed to run *poly.exe*:

```
 2      Degree of polynomial, n
-1.0    Coefficient a0
-1.0    Coefficient a1
-1.0    Coefficient a2
-2.0    xmin
 2.0    xmax
21      Number of points, m
```

- Write a PEST *Template File* to estimate coefficients a_0, a_1, and a_2.

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Exercise 2: Instruction File

- *poly.exe* generates the screen output on the right
- Write a PEST *Instruction File* that reads the output $y(x)_i$, i = 1, …, 21

```
Evaluate Polynomial
*******************

Degree of polynomial : ?
Coefficient a0       : ?
Coefficient a1       : ?
Coefficient a2       : ?
Range of x: Xmin     : ?
            Xmax     : ?
Number of points     : ?
Polynomial of degree 2 with coefficients:
a(0) =  5.00000
a(1) =  4.00000
a(2) =  3.00000

                x            y(x)
  -2.0000000000     9.0000000000
  -1.7999999523     7.5199995041
  -1.5999999046     6.2799992561
  -1.3999998569     5.2799992561
  -1.1999998093     4.5199995041
  -0.9999998212     3.9999997616
  -0.7999998331     3.7199997902
  -0.5999998450     3.6800000668
  -0.3999998569     3.8800001144
  -0.1999998540     4.3200006485
   0.0000001490     5.0000004768
   0.2000001520     5.9200010300
   0.4000001550     7.0800008774
   0.6000001431     8.4800014496
   0.8000001311    10.1200017929
   1.0000001192    12.0000009537
   1.2000001669    14.1200027466
   1.4000002146    16.4800014496
   1.6000002623    19.0800037384
   1.8000003099    21.9200038910
   2.0000002384    25.0000038147
```

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Exercise 3: iTOUGH2 Control File

- Edit file *polyi*, which is an (incomplete) iTOUGH2 input file (see next slides)
- Replace all question marks with input needed to run the inverse problem using iTOUGH2-PEST
- Make sure the input is consistent with the decisions you made during Exercises 1 and 2

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iTOUGH2 Input File *polyi* (1 of 3)

```
iTOUGH2 input file demonstrating parameter estimation
(polynomial fit) using external program and PEST protocol

> PARAMETER
  >> PEST
     >>> NONE
         >>>> NAME :       ?
         >>>> VALUE
         >>>> GUESS:    -1.0
         <<<<
     >>> NONE
         >>>> NAME :       ?
         >>>> VALUE
         >>>> GUESS:       ?
         <<<<
     >>> ???
         ???
         ???
         ???
     <<<
  <<
```

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iTOUGH2 Input File *polyi* (2 of 3)

```
> OBSERVATION
  >> ????
     >>> UNIVERSAL:  y=f(x)
          >>>> DATA
               y1    0.94179E+01
               y2    0.71294E+01
               y3    0.69108E+01
               y4    0.65802E+01
               y5    0.41660E+01
               y6    0.57779E+01
               y7    0.38172E+01
               y8    0.24940E+01
               y9    0.50483E+01
               y10   0.32697E+01
               y11   0.64006E+01
               y12   0.60516E+01
               y13   0.60600E+01
               y14   0.96430E+01
               y15   0.10834E+02
               y16   0.12887E+02
               y17   0.14458E+02
               y18   0.16869E+02
               y19   0.18289E+02
               y20   0.21521E+02
               y21   0.25278E+02
          >>>> DEVIATION: ?
          ???
          ???
          ???
```

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iTOUGH2 Input File *polyi* (3 of 3)

```
> COMPUTATION
  >> STOP
     >>> after: ? ITERATIONS
     <<<

  >> OPTION
     ??? LEVENBERG-MARQUARDT
     ??? GAUSS-NEWTON
     >>> PEST
         >>>> TEMPLATE file   : 1
              ???.tpl  poly.in

         >>>> INSTRUCTION file: ?
              ???.ins  ???

         >>>> EXECUTABLE      : 'poly.exe < ??? > poly.out'

         <<<<
     <<<
  <<
<
```

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Run iTOUGH2-PEST

- Two options to run iTOUGH2-PEST:
  - Double click **`it2_pest.exe`**
  - open DOS Command Prompt, change to the working directory, and type **`it2_pest`**
- Enter name of iTOUGH2 control file (**`polyi`**)
- Open **`polyi.out`** and answer the following questions:

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Exercise 3: Questions

Open the iTOUGH2 output file *polyi.out* and answer the following questions:

1. What is the degree of freedom (define and provide number)?

2. Which minimization algorithm is the most efficient, and why?

3. Which is the most sensitive parameter? Justify your answer.

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Exercise 3: Questions (cont.)

4. Which single observation (type and time) contains the most information regarding each of the parameters, and overall?

5. What is the value of the *a posteriori* error variance s_0^2?

6. Was the error analysis based on the *a priori* error variance σ_0^2 or s_0^2? Why?

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Exercise 3: Questions (cont.)

8. What is the uncertainty of the estimated parameters?

8. What does the correlation coefficient between the coefficients indicate?

9. Which of the three parameters can be estimated most independently?

10. Examine and discuss the correlation chart.

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Exercise 4: Explore!

- Change the inverse problem; comment on the changes in the results
- For example:
  - Increase or reduce the order of the polynomial and estimate additional coefficients; check uncertainty of estimated parameters
  - Change weights of individual data point
  - Change number of iterations
  - Change minimization algorithm

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