

Applications of the Moore-Penrose Inverse of a Matrix

Karsten Schmidt, FH Schmalkalden, Germany, kschmidt@fh-sm.de

Introduction

After giving an introduction to the Moore-Penrose inverse of a matrix, and its computation in *DERIVE*, in DNL #50 (Schmidt 2003), this paper deals with two important applications of the Moore-Penrose inverse. One is a method for solving a system of linear equations, and the other is the computation of the Ordinary Least Squares estimator in linear regression. Some familiarity with matrix algebra as well as basic understanding of the Moore-Penrose inverse of a matrix (as provided in DNL #50) is required.

Computation and Properties of the Moore-Penrose Inverse

In order to facilitate working with this paper, the definition and *DERIVE* functions for the computation of the Moore-Penrose inverse of a matrix are repeated from DNL #50:

For any $m \times n$ -matrix A there exists a unique matrix with properties related to those of the inverse of a nonsingular matrix. This is the Moore-Penrose inverse, denoted by A^+ , which satisfies the four conditions (the transpose of A is denoted by A')

$$AA^+A = A \quad (1)$$

$$A^+AA^+ = A^+ \quad (2)$$

$$(A^+A)' = A^+A \quad (3)$$

$$(AA^+)' = AA^+ \quad (4)$$

Conditions (3) and (4) require both A^+A and AA^+ to be symmetric matrices. Note that A^+ is an $n \times m$ -matrix, i.e. the dimension of A^+ is equal to the dimension of A' .

The Moore-Penrose inverse of a matrix can be computed in *DERIVE* with the following two functions:

```
MPIV(a) :=
  If DIM(a') = 1
    If (a'·a)↓1↓1 = 0
      0·a'
      a'/(a'·a)↓1↓1
    "This is not a column vector!"

MPI(A, APLUS, aj, dt, c, bt, J) :=
  Prog
  APLUS := MPIV(A COL [1])
  J := 2
  Loop
    If J > DIM(A')
      RETURN APLUS
    aj := A COL [J]
    dt := aj'·APLUS'·APLUS
    c := (IDENTITY_MATRIX(DIM(A)) - A COL [1, ..., J - 1]·APLUS)·aj
    bt := MPIV(c) + (1 - MPIV(c)·c)/(1 + dt·aj)·dt
    APLUS := APPEND(APLUS - APLUS·aj·bt, bt)
    J :=+ 1
```

MPIV computes the Moore-Penrose inverse of a vector and MPI the Moore-Penrose inverse of a matrix (or vector). Note that MPIV requires a column vector passed as parameter, which has to be declared in *DERIVE* as a matrix with one column. Note also that MPIV and, therefore, MPI, via calling MPIV repeatedly, might not be able to compute the Moore-Penrose inverse since it might be impossible to determine if $\mathbf{a} = \mathbf{0}$, when \mathbf{a} has nonnumeric entries. Both functions, along with a couple more from the next section, are provided in the utility file **MP.mth**.

Among the many properties that hold for the Moore-Penrose inverse the following three will be useful later in this paper (\mathbf{I} denotes the identity matrix):

$$(\mathbf{A}'\mathbf{A})^+ \mathbf{A}' = \mathbf{A}^+ \quad (5)$$

$$\mathbf{A}'\mathbf{A}\mathbf{A}^+ = \mathbf{A}' \quad (6)$$

$$\text{rank} \begin{pmatrix} \mathbf{A} \\ m \times n \end{pmatrix} = n \Leftrightarrow \mathbf{A}^+ = (\mathbf{A}'\mathbf{A})^{-1} \mathbf{A}' \quad \text{and} \quad \mathbf{A}^+ \mathbf{A} = \mathbf{I}_{n \times n} \quad (7)$$

Application to Systems of Linear Equations

We consider a system of linear equations (SLE)

$$\begin{matrix} \mathbf{A} & \mathbf{x} & = & \mathbf{b} \\ m \times n & n \times 1 & & m \times 1 \end{matrix}$$

where \mathbf{A} is the known coefficient matrix, \mathbf{b} a vector of known constants, and \mathbf{x} a vector of unknown variables.

The Moore-Penrose inverse of \mathbf{A} can be applied to such a system

- to check if it is *consistent* or *inconsistent*, i.e. to find out if it has solutions or not, and
- if it is consistent, to provide the general solution, which may consist of either one unique or an infinite number of solutions.

A system of linear equations $\mathbf{A}\mathbf{x} = \mathbf{b}$ is consistent if and only if

$$\mathbf{A}\mathbf{A}^+ \mathbf{b} = \mathbf{b} \quad (8)$$

As an example, consider an SLE defined by

$$\begin{matrix} \mathbf{A} & \mathbf{b} \\ 2 \times 2 & 2 \times 1 \end{matrix} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}; \quad \mathbf{b} = \begin{pmatrix} 5 \\ 10 \end{pmatrix} \quad (9)$$

The Moore-Penrose inverse of \mathbf{A} is

$$\mathbf{A}^+ = \begin{pmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix}$$

Since \mathbf{A} is nonsingular ($\det(\mathbf{A}) = -\frac{1}{2} \neq 0$) we have $\mathbf{A}^+ = \mathbf{A}^{-1}$. Hence

$$\mathbf{A}\mathbf{A}^+ \mathbf{b} = \underbrace{\mathbf{A}\mathbf{A}^{-1}}_{\mathbf{I}} \mathbf{b} = \mathbf{b}$$

for any vector \mathbf{b} . System (9), like any other system with a nonsingular coefficient matrix \mathbf{A} , is therefore consistent according to (8).

As another example, consider

$$\begin{matrix} \mathbf{A} & \mathbf{b} \\ 2 \times 2 & 2 \times 1 \end{matrix} = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}; \quad \mathbf{b} = \begin{pmatrix} 5 \\ 10 \end{pmatrix} \quad (10)$$

This time \mathbf{A} is singular ($\det(\mathbf{A}) = 0$), its inverse \mathbf{A}^{-1} does not exist. Computing the Moore-Penrose inverse

$$\mathbf{A}^+ = \begin{pmatrix} \frac{1}{25} & \frac{2}{25} \\ \frac{2}{25} & \frac{4}{25} \end{pmatrix}$$

is nevertheless possible and we find that condition (8) is satisfied for system (10):

$$AA^+b = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix} \begin{pmatrix} \frac{1}{25} & \frac{2}{25} \\ \frac{2}{25} & \frac{4}{25} \end{pmatrix} \begin{pmatrix} 5 \\ 10 \end{pmatrix} = \begin{pmatrix} \frac{1}{5} & \frac{2}{5} \\ \frac{2}{5} & \frac{4}{5} \end{pmatrix} \begin{pmatrix} 5 \\ 10 \end{pmatrix} = \begin{pmatrix} 5 \\ 10 \end{pmatrix} = b$$

As a third example, look at

$$A = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}_{2 \times 2}; b = \begin{pmatrix} 5 \\ 15 \end{pmatrix}_{2 \times 1} \quad (11)$$

This time we find that condition (8) is not satisfied:

$$AA^+b = \begin{pmatrix} \frac{1}{5} & \frac{2}{5} \\ \frac{2}{5} & \frac{4}{5} \end{pmatrix} \begin{pmatrix} 5 \\ 15 \end{pmatrix} = \begin{pmatrix} 7 \\ 14 \end{pmatrix} \neq b$$

System (11) is therefore inconsistent.

```

CHECKSLE(A, b) :=
  If A.MPI(A).b = b
#1:    "consistent"
      "NO SOLUTIONS!"

#2:  A := [ 1  2 ]
        [ 3  4 ]

#3:  b := [ 5 ]
        [ 10 ]

#4:                                CHECKSLE(A, b) = consistent

#5:  A := [ 1  2 ]
        [ 2  4 ]

#6:                                CHECKSLE(A, b) = consistent

#7:  b := [ 5 ]
        [ 15 ]

#8:                                CHECKSLE(A, b) = NO SOLUTIONS!

#9:  b := [ 5 ]
        [ λ ]

#10:  CHECKSLE(A, b) = IF(λ = 10, consistent, NO SOLUTIONS!)

```

The function CHECKSLE in the above screenshot checks if a system of linear equations is consistent or not, and prints the result on the screen. Since there is no *unknown* clause in the IF-expression, the entire (simplified) IF-expression is returned, which can obviously be fairly informative in cases such as the last SLE (consisting of matrix A in #5 and vector b in #9).

If a system of linear equations $Ax = b$ is consistent, its general solution is given by

$$x = A^+b + \begin{pmatrix} I - A^+A \\ n \times n \end{pmatrix} z \quad (12)$$

where z is an arbitrary vector.

Note that since the vector $z \in \mathbb{R}^n$ in (12) is arbitrary, we might simply choose $z = \mathbf{0}$. Consequently, one (possibly unique) solution of a consistent system of linear equations $Ax = b$ is always given by

$$x = A^+b$$

The following function SOLVESLE either solves a system of linear equations $Ax = b$ where the matrix A and the vector b have been passed as parameters, or displays a message if the system is inconsistent.

```

z := VECTOR(VECTOR(APPEND(z, J), i, 1), J, 1, DIM(A'))

SOLVESLE(A, b) :=
  If A • MPI(A) • b = b
    MPI(A) • b + (IDENTITY_MATRIX(DIMENSION(A'))) - MPI(A) • A • z
    "No solution(s)!"

```

We now want to compute the solution(s) of the above three systems. We start with system (9). Since A is a nonsingular matrix, we have $A^+ = A^{-1}$, and (12) simplifies to

$$\begin{aligned}
 x &= A^+ b + (I - A^+ A) z \\
 &= A^{-1} b + \left(I - \underbrace{A^{-1} A}_I \right) z \\
 &= A^{-1} b
 \end{aligned}$$

for any choice of z . Obviously, the general solution (12) simplifies to a unique solution if A is nonsingular. Hence

$$x = A^{-1} b = \begin{pmatrix} -2 & 1 \\ \frac{3}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} 5 \\ 10 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{5}{2} \end{pmatrix}$$

For system (10) we get

$$x = A^+ b + (I - A^+ A) z = \begin{pmatrix} \frac{4}{5} z_1 - \frac{2}{5} z_2 + 1 \\ -\frac{2}{5} z_1 + \frac{1}{5} z_2 + 2 \end{pmatrix}$$

In this case there is an infinite number of solutions. For example, by choosing $z = \mathbf{0}$ we get

$$x = A^+ b = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

```

#1:  A := [ 1  2 ]
        [ 3  4 ]

#2:  b := [ 5 ]
        [10 ]

#3:  SOLVESLE(A, b) = [ 0 ]
                      [ 5 ]
                      [ 2 ]

#4:  A := [ 1  2 ]
        [ 2  4 ]

#5:  SOLVESLE(A, b) = [ 4·z1 - 2·z2 + 1 ]
                      [ - 2·z1 + z2 + 2 ]

#6:  [ 1 ]
        [ 2 ]

#7:  b := [ 5 ]
        [15 ]

#8:  SOLVESLE(A, b) = No solution(s)!

```

The above screenshot shows the capability of the function SOLVESLE to handle all three possible scenarios in considering a system of linear equations: a unique solution, an infinite number of solutions, and the case that no solution exists.

Linear Regression and the Moore-Penrose Inverse

We consider the (multiple) linear regression model

$$\underset{N \times 1}{\mathbf{y}} = \underset{N \times K}{\mathbf{X}} \underset{K \times 1}{\boldsymbol{\beta}} + \underset{N \times 1}{\mathbf{u}} \quad (13)$$

where \mathbf{y} is the vector of observations on the dependent variable, \mathbf{X} the regressor matrix, $\boldsymbol{\beta}$ a vector of parameters, and \mathbf{u} a vector of disturbances.

Denoting an estimator of the unknown parameter vector $\boldsymbol{\beta}$ by $\tilde{\boldsymbol{\beta}}$, we have

$$\begin{aligned} \tilde{\mathbf{y}} &= \mathbf{X} \tilde{\boldsymbol{\beta}} \\ \tilde{\mathbf{u}} &= \mathbf{y} - \tilde{\mathbf{y}} \end{aligned}$$

where $\tilde{\mathbf{y}}$ is the estimate of \mathbf{y} using $\tilde{\boldsymbol{\beta}}$, and $\tilde{\mathbf{u}}$ is the vector of residuals.

The most popular estimator for $\boldsymbol{\beta}$ is the (Ordinary) Least Squares estimator which minimizes the sum of squared residuals

$$\begin{aligned} \phi(\tilde{\boldsymbol{\beta}}) &= \sum_{i=1}^N \tilde{u}_i^2 \\ &= \tilde{\mathbf{u}}' \tilde{\mathbf{u}} \\ &= (\mathbf{y} - \mathbf{X} \tilde{\boldsymbol{\beta}})' (\mathbf{y} - \mathbf{X} \tilde{\boldsymbol{\beta}}) \rightarrow \min_{\tilde{\boldsymbol{\beta}}} \end{aligned}$$

Note that

$$\begin{aligned} \phi(\tilde{\boldsymbol{\beta}}) &= (\mathbf{y} - \mathbf{X} \tilde{\boldsymbol{\beta}})' (\mathbf{y} - \mathbf{X} \tilde{\boldsymbol{\beta}}) \\ &= \mathbf{y}' \mathbf{y} - \mathbf{y}' \mathbf{X} \tilde{\boldsymbol{\beta}} - \tilde{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{y} + \tilde{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{X} \tilde{\boldsymbol{\beta}} \\ &= \tilde{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{X} \tilde{\boldsymbol{\beta}} - 2 \mathbf{y}' \mathbf{X} \tilde{\boldsymbol{\beta}} + \mathbf{y}' \mathbf{y} \end{aligned}$$

is a convex function since $\mathbf{X}' \mathbf{X}$ is a nonnegative definite matrix. Therefore, finding its first derivative

$$\begin{aligned} \frac{\partial \phi(\tilde{\boldsymbol{\beta}})}{\partial \tilde{\boldsymbol{\beta}}} &= \tilde{\boldsymbol{\beta}}' (\mathbf{X}' \mathbf{X} + (\mathbf{X}' \mathbf{X})') - 2 \mathbf{y}' \mathbf{X} \\ &= 2 \tilde{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{X} - 2 \mathbf{y}' \mathbf{X} \end{aligned}$$

and setting it equal to $\mathbf{0}$ is necessary and sufficient to determine the minimum of $\phi(\tilde{\boldsymbol{\beta}})$:

$$2 \tilde{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{X} - 2 \mathbf{y}' \mathbf{X} = \underset{1 \times K}{\mathbf{0}} \Leftrightarrow \mathbf{X}' \mathbf{X} \tilde{\boldsymbol{\beta}} - \mathbf{X}' \mathbf{y} = \underset{K \times 1}{\mathbf{0}} \Leftrightarrow \mathbf{X}' \mathbf{X} \tilde{\boldsymbol{\beta}} = \mathbf{X}' \mathbf{y}$$

The last equation constitutes the so-called *system of normal equations*.

Under the (usual) assumption that $\text{rank}(\mathbf{X}) = K$, which assures that $\mathbf{X}' \mathbf{X}$ is nonsingular, we can easily derive the Least Squares estimator from the normal equations

$$\mathbf{X}' \mathbf{X} \tilde{\boldsymbol{\beta}} = \mathbf{X}' \mathbf{y} \Leftrightarrow \underbrace{(\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}' \mathbf{X}}_{\mathbf{I}} \tilde{\boldsymbol{\beta}} = (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}' \mathbf{y} \Leftrightarrow \tilde{\boldsymbol{\beta}} = (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}' \mathbf{y}$$

One might think that the system of normal equations is inconsistent if $\text{rank}(\mathbf{X}) < K$. However, this is not true.

Observe that the system of normal equations is essentially a system of linear equations in the notation of the previous section:

$$\underbrace{\mathbf{X}' \mathbf{X}}_{\mathbf{A}} \underbrace{\tilde{\boldsymbol{\beta}}}_{\mathbf{x}} = \underbrace{\mathbf{X}' \mathbf{y}}_{\mathbf{b}}$$

Using properties (5) and (6) of the Moore-Penrose inverse, it can be shown that the system of normal equations is consistent without any rank assumption on \mathbf{X} :

$$\begin{aligned} \mathbf{A} \mathbf{A}^+ \mathbf{b} &= \mathbf{b} \Rightarrow \\ \mathbf{X}' \mathbf{X} \underbrace{(\mathbf{X}' \mathbf{X})^+}_{\mathbf{X}^+} \mathbf{X}' \mathbf{y} &= \underbrace{\mathbf{X}' \mathbf{X} \mathbf{X}^+}_{\mathbf{X}'} \mathbf{y} = \mathbf{X}' \mathbf{y} \end{aligned}$$

Hence, its general solution is given by

$$\begin{aligned} \mathbf{x} &= \mathbf{A}^+ \mathbf{b} + (\mathbf{I} - \mathbf{A}^+ \mathbf{A}) \mathbf{z} \Rightarrow \\ \tilde{\beta} &= \underbrace{(\mathbf{X}'\mathbf{X})^+ \mathbf{X}'}_{\mathbf{X}^+} \mathbf{y} + \left(\mathbf{I} - \underbrace{(\mathbf{X}'\mathbf{X})^+ \mathbf{X}'\mathbf{X}}_{\mathbf{X}^+} \right) \mathbf{z} \\ &= \mathbf{X}^+ \mathbf{y} + (\mathbf{I} - \mathbf{X}^+ \mathbf{X}) \mathbf{z} \end{aligned}$$

where $\mathbf{z} \in \mathbb{R}^K$ is an arbitrary vector.

The number of solutions, however, depends on the rank of the regressor matrix. If $\text{rank}(\mathbf{X}) = K$, it follows from (7) that $\mathbf{X}^+ \mathbf{X} = \mathbf{I}$, and the general solution simplifies to the unique solution

$$\begin{aligned} \tilde{\beta} &= \mathbf{X}^+ \mathbf{y} + \left(\mathbf{I} - \underbrace{\mathbf{X}^+ \mathbf{X}}_{\mathbf{I}} \right) \mathbf{z} \\ &= \mathbf{X}^+ \mathbf{y} \end{aligned}$$

i.e. the Least Squares estimator is simply the product of the Moore-Penrose inverse of the regressor matrix and the vector of the observations on the dependent variable.

If, however, $\text{rank}(\mathbf{X}) < K$, we have an infinite number of solutions. Therefore, it is not the consistency of the system of normal equations that is guaranteed by assuming \mathbf{X} to be of full column rank, but the uniqueness of its solution.

Finally, this straightforward method of computing the Least Squares estimator is demonstrated by means of an example. We want to apply linear regression analysis to predict the number of O-ring failures to be expected when the space shuttle *Challenger* was launched on January 28, 1986.

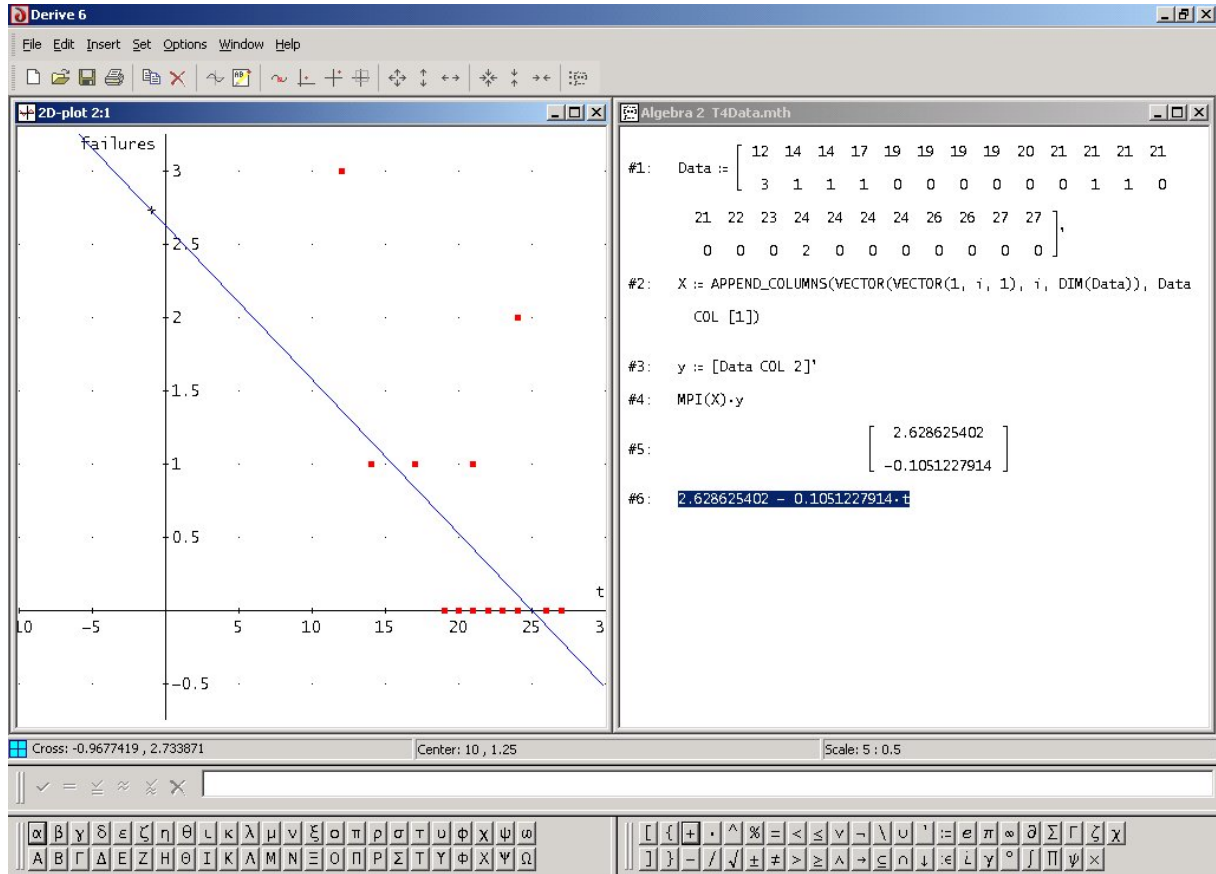
O-ring failure is when an O-ring, which seals the gaps between the parts of the solid fuel rocket motors, leaks. There had been 24 previous space shuttle launches. During 17 of them no O-ring failure occurred, while during the remaining 7 launches there were between one and three O-ring failures. The table below provides the number of failures and the ambient temperatures before launch, sorted according to temperature.

<i>failures</i>	<i>t [temp. in °C]</i>	<i>temp. in °F</i>	<i>failures</i>	<i>t [temp. in °C]</i>	<i>temp. in °F</i>
3	12	53	0	21	70
1	14	57	0	21	70
1	14	58	0	22	72
1	17	63	0	23	73
0	19	66	2	24	75
0	19	67	0	24	75
0	19	67	0	24	76
0	19	67	0	24	76
0	20	68	0	26	78
0	21	69	0	26	79
1	21	70	0	27	80
1	21	70	0	27	81

The following screenshot shows an algebra window and a 2D-plot window. The first three expressions in the algebra window are the contents of the file **T4Data.mth**. Expression #1 defines a 24×2 -matrix **Data**, which was entered in transposed form to save space (unfortunately, this requires simplification of **Data** prior to plotting the points in the 2D-plot window). In expressions #2 and #3 the data are rear-

ranged according to the definition of the linear regression model (13). X denotes the regressor matrix, containing a column of ones (for the y -intercept), and a column with the observations on the independent variable (temperature in Celsius), y denotes the vector of observations on the dependent variable (number of failures).

Expression #4 is the formula for the computation of the Least Squares estimator using the Moore-Penrose inverse. Approximating #4 yields #5, which is in turn used to define and finally plot the straight line which is the result of the Least Squares estimation.



Considering the relatively high coefficient of determination ($R^2 = 0.3$), and the fact that the slope parameter is statistically significant (at the 1%-level; both values not shown in the screenshot), the above result is fairly reliable.

Since the pre-launch ambient temperature on January 28, 1986, was -1°C (31°F), the prediction from the above regression would have been

$$\text{failures} = 2.629 - 0.105(-1) = 2.734$$

i.e. 2 or 3 O-ring failures were to be expected according to our regression result. Nevertheless, the space shuttle was launched. Less than two minutes into the flight, due to O-ring failure, leaking fuel was ignited by a rocket engine, and *Challenger* exploded.

Reference

Schmidt, K. (2003), An Introduction to the Moore-Penrose Inverse of a Matrix, *The DERIVE-Newsletter* #50 (June 2003), 12 – 18.