Refreshing Your Linear Algebra Knowledge with NumPy, Part II

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[SL (11/10/2018): This is the notebook as produced live from my talk today. Note: "Part I" was my presentation of similar material at the 7/12/2018 PyMNtos meeting. It consisted essentially of the same material below but ended just before the "LU Decomposition" section.]

Example

System of 3 linear equations in 3 unknowns (variables):

$$2x + 2y + 4z = 0$$
$$y - 5z = 13$$
$$3y + 4z = 1$$

Goal is to find the values of x, y, and z that make all three equations true simultaneously.

One way to solve is to manipulate the equations directly:

(1) Subtract 3 times the second equation from the third to eliminate y and solve for z:

$$\begin{array}{rcrcr}
3y & + & 4z & = & 1 \\
-3y & + & 15z & = & -39 \\
\hline
& & 19z & = & -38 \\
z & = & -2
\end{array}$$

(2) Plug z=-2 back into the second equation to solve for y:

$$y - 5(-2) = 13$$

 $y + 10 = 13$
 $y = 3$

(3) Plug y=3 and z=-2 into the first equation to solve for x:

$$2x + 2(3) + 4(-2) = 0$$

 $2x = 2$
 $x = 1$

Disadvantage

Above approach is much more difficult with larger systems of equations:

$$2v + 7w - x + 3y + 6z = 24$$
 $3v + 3w + x - y + 5z = -1$
 $v - w - 2x - 3y - 8z = -16$
 $4v + 5w - 3x + 7y + 10z = 52$
 $-5v + 3w - 9x - 9y + z = 25$

Power of matrix notation

TIX **notation**

$$\begin{bmatrix} 2 & 7 & -1 & 3 & 6 \\ 3 & 3 & 1 & -1 & 5 \\ 1 & -1 & -2 & -3 & -8 \\ 4 & 5 & -3 & 7 & 10 \\ -5 & 3 & -9 & -9 & 1 \end{bmatrix} \times \begin{bmatrix} v \\ w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 24 \\ -1 \\ -16 \\ 52 \\ 25 \end{bmatrix}$$

$$A \times t = d$$

Using Matrix Techniques to Solve a Linear System

First, let's first return to the original system:

$$2x + 2y + 4z = 0$$
$$y - 5z = 13$$
$$3y + 4z = 1$$

or

$$\begin{bmatrix} 2 & 2 & 4 \\ 0 & 1 & -5 \\ 0 & 3 & 4 \end{bmatrix} \quad \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad = \quad \begin{bmatrix} 0 \\ 13 \\ 1 \end{bmatrix}$$

Step 0

Form the augmented matrix:

$$\left[\begin{array}{ccc|ccc} 2 & 2 & 4 & 0 \\ 0 & 1 & -5 & 13 \\ 0 & 3 & 4 & 1 \end{array}\right]$$

Enter data into Python

In [8]: M

Goal

Given the augmented matrix

$$\left[\begin{array}{ccc|ccc} 2 & 2 & 4 & 0 \\ 0 & 1 & -5 & 13 \\ 0 & 3 & 4 & 1 \end{array}\right]$$

we want to perform elementary row operations (Gaussian elimination) to transform the above into an equivalent matrix of the the following form, from which the solution can be read:

$$\left[\begin{array}{ccc|c} 1 & 0 & 0 & ? \\ 0 & 1 & 0 & ? \\ 0 & 0 & 1 & ? \end{array}\right]$$

or

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} ? \\ ? \\ ? \end{bmatrix}$$

or

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} ? \\ ? \\ ? \end{bmatrix}$$

Elementary row operations (Gaussian elimination)

- · multiply a row by a non-zero scalar
- add to one row a scalar multiple of another row
- · interchange of two rows

Step 1

First step is multiply the first row by
$$\frac{1}{2}$$
 to get a 1 in the first column:
$$\begin{bmatrix} 2 & 2 & 4 & 0 \\ 0 & 1 & -5 & 13 \\ 0 & 3 & 4 & 1 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 1 & 2 & 0 \\ 0 & 1 & -5 & 13 \\ 0 & 3 & 4 & 1 \end{bmatrix}$$

Step 1 as a matrix multiplication

The idea of "multiply the first row by ½" can be expressed as a matrix multiplication:

$$\begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 2 & 4 & 0 \\ 0 & 1 & -5 & 13 \\ 0 & 3 & 4 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 2 & 0 \\ 0 & 1 & -5 & 13 \\ 0 & 3 & 4 & 1 \end{bmatrix}$$

Matrix on the left, an identity matrix with a small adjustment, is a **elementary matrix**.

Create a Python function to return the elementary matrix:

```
def scalerow(r, \alpha, n=3):
 In [9]:
             """Elementary matrix to multiply row r by the scalar \alpha,
         when multiplied on the left of a target matrix of n rows."""
             E = np.asmatrix(np.eye(n))
             E[r,r] = \alpha
              return E
In [12]: E1 = scalerow(0, .5); E1
Out[12]: matrix([[0.5, 0. , 0. ],
                  [0., 1., 0.],
                  [0., 0., 1.]
         E1*M
In [13]:
Out[13]: matrix([[ 1.,
                         1., 2.,
                                   0.1,
                  [0., 1., -5., 13.],
                        3., 4., 1.]])
                  [ 0.,
In [ ]:
```

[SL (11/10/2018): The following was in response to a question during the talk. This confirms that np.matrix() can be used in place of np.asmatrix() to convert a data array to a matrix.]

Step 2

Next, subtract 3 times row 1 from row 2.

$$\begin{bmatrix} 1 & ? & ? \\ ? & 1 & ? \\ ? & ? & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 2 & 0 \\ 0 & 1 & -5 & 13 \\ 0 & 3 & 4 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 2 & 0 \\ 0 & 1 & -5 & 13 \\ 0 & 0 & 19 & -38 \end{bmatrix}$$

```
In [14]: def addtorow(r, \alpha, j, n=3):
             """Elementary matrix to add \alpha times row j to row r,
         when multiplied on the left of a target matrix of n rows."""
             E = np.asmatrix(np.eye(n))
             E[r,j] = \alpha
             return E
In [15]: |E2| = addtorow(2, -3, 1); E2
Out[15]: matrix([[ 1., 0.,
                 [ 0., 1., 0.],
                 [0., -3., 1.]
In [16]: E2*E1*M
                                2., 0.],
Out[16]: matrix([[ 1., 1.,
                 [ 0., 1., -5., 13.],
                        0., 19., -38.]])
                    0.,
```

Remaining row operation steps

```
In [17]: E3 = addtorow(0, -1, 1); E3*E2*E1*M
                        0., 7., -13.],
Out[17]: matrix([[ 1.,
                  0., 1., -5., 13.],
                        0., 19., -38.]])
                   0.,
In [18]: E4 = scalerow(2, 1/19); E4*E3*E2*E1*M
Out[18]: matrix([[ 1.,
                        0., 7., -13.],
                [ 0., 1., -5., 13.],
                [0., 0., 1., -2.]
In [19]: E5 = addtorow(1, 5, 2); E5*E4*E3*E2*E1*M
Out[19]: matrix([[ 1.00000000e+00,
                                  0.00000000e+00, 7.0000000e+00,
                 -1.3000000e+01],
                [ 0.00000000e+00, 1.00000000e+00, -2.22044605e-16,
                  3.00000000e+001,
                [ 0.00000000e+00, 0.0000000e+00, 1.00000000e+00,
                 -2.00000000e+0011)
```

Summary

We have transformed the original augmented matrix

$$\left[egin{array}{ccccc} 2 & 2 & 4 & 0 \ 0 & 1 & -5 & 13 \ 0 & 3 & 4 & 1 \end{array}
ight]$$

to the equivalent augmented matrix

$$\left[\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & -2 \end{array}\right].$$

In other words,

$$egin{bmatrix} 1 & 0 & 0 \ 0 & 1 & 0 \ 0 & 0 & 1 \end{bmatrix} egin{bmatrix} x \ y \ z \end{bmatrix} = egin{bmatrix} 1 \ 3 \ -2 \end{bmatrix}$$

Or

$$\left[egin{array}{c} x \ y \ z \end{array}
ight] = \left[egin{array}{c} 1 \ 3 \ -2 \end{array}
ight]$$

Thus, x = 1, y = 3, and z = -2 is the solution to the original system of equations.

The point (1, 3, -2) in xyz-space is the intersection of the planes given by the three equations.

```
In [ ]:
```

Revisiting the elementary matrices

```
In [22]: np.round( (E6*E5*E4*E3*E2*E1) * A ,9)
Out[22]: array([[ 1., -0., 0.],
                [ 0., 1., -0.],
                [ 0., 0., 1.]])
In [23]: A
Out[23]: matrix([[ 2, 2, 4],
                 [0, 1, -5],
                 [0, 3, 4]
In [24]: E6*E5*E4*E3*E2*E1
Out[24]: matrix([[ 0.5
                               0.10526316, -0.36842105],
                 [ 0.
                               0.21052632, 0.26315789],
                             , -0.15789474, 0.05263158]])
                 [ 0.
In [25]: A.I
Out[25]: matrix([[ 0.5
                               0.10526316, -0.36842105],
                 [ 0.
                            , 0.21052632, 0.26315789],
                 [-0.
                            , -0.15789474, 0.05263158]])
```

Answer (version 2)

General Solution

The original matrix equation:

$$\begin{bmatrix} 2 & 2 & 4 \\ 0 & 1 & -5 \\ 0 & 3 & 4 \end{bmatrix} \quad \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad = \quad \begin{bmatrix} 0 \\ 13 \\ 1 \end{bmatrix}$$

$$A \qquad \qquad t \qquad \qquad d$$

The general solution to such a matrix equation is

$$At = d$$
 $A^{-1}At = A^{-1}d$
 $I \ t = A^{-1}d$
 $t = A^{-1}d$

Example 2

$$\begin{bmatrix} 2 & 7 & -1 & 3 & 6 \\ 3 & 3 & 1 & -1 & 5 \\ 1 & -1 & -2 & -3 & -8 \\ 4 & 5 & -3 & 7 & 10 \\ -5 & 3 & -9 & -9 & 1 \end{bmatrix} \begin{bmatrix} v \\ w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 24 \\ -1 \\ -16 \\ 52 \\ 25 \end{bmatrix}$$

Check:

```
In [33]: A2*t2
Out[33]: matrix([[ 24.],
                  [-1.],
                  [-16.],
                  [ 52.],
                  [ 25.]])
In [34]: A2*t2-d2
Out[34]: matrix([[-2.13162821e-14],
                  [-8.88178420e-15],
                  [ 7.10542736e-15],
                  [-2.13162821e-14],
                  [-7.10542736e-15]])
In [35]: np.round( A2*t2-d2 ,9)
Out[35]: array([[-0.],
                 [-0.],
                 [ 0.],
                 [-0.],
                 [-0.]])
```

Example 3

$$egin{bmatrix} 1 & 0 & -5 & 6 \ 1 & 1 & 1 & 1 \ 3 & 0 & -5 & 8 \ 1 & -1 & -1 & 1 \end{bmatrix} egin{bmatrix} w \ x \ y \ z \end{bmatrix} = egin{bmatrix} -1 \ 7 \ 7 \ 1 \end{bmatrix}$$

```
In [36]: A3 = np.mat("1 0 -5 6; 1 1 1 1; 3 0 -5 8; 1 -1 -1 1")
In [37]:
         A3
Out[37]: matrix([[ 1,
                       0, -5,
                                6],
                 [ 1, 1, 1,
                               11,
                  [3, 0, -5,
                               81,
                  [1, -1, -1,
                               1]])
In [38]: d3 = np.mat([-1, 7, 7, 1]).T; d3
Out[38]: matrix([[-1],
                  [7],
                  [7],
                  [ 1]])
In [39]:
         t3 = A3.I*d3; t3
Out[39]: matrix([[-32.],
                 [ 0.],
                  [ 16.],
                  [ 16.]])
In [40]: A3*t3
Out[40]: matrix([[-16.],
                 [ 0.],
                  [-48.],
                  [-32.11)
In [41]: A3.I
Out[41]: matrix([[-1.35107989e+16, -1.35107989e+16, 1.35107989e+16,
                  -1.35107989e+16],
                  [-1.35107989e+16, -1.35107989e+16, 1.35107989e+16,
                  -1.35107989e+16],
                  [ 1.35107989e+16, 1.35107989e+16, -1.35107989e+16,
                   1.35107989e+161,
                  [ 1.35107989e+16, 1.35107989e+16, -1.35107989e+16,
                   1.35107989e+1611)
```

Singular (Noninvertible) Matrices

Test 1: Determinants

A square matrix is invertible (nonsingular) if and only if its **determinant** is nonzero.

```
In [42]: import numpy.linalg
```

Test 2: Matrix rank

A square matrix is invertible (nonsingular) if and only if it is of **full rank**.

```
In [45]: np.linalg.matrix rank(A3)
Out[45]: 3
In [46]: A3.shape
Out[46]: (4, 4)
In [47]: np.linalg.matrix rank(A2)
Out[47]: 5
In [48]: A2.shape
Out[48]: (5, 5)
In [49]: np.rank(A3)
         /home/sl/anaconda3/lib/python3.7/site-packages/ipykernel_launcher.py:
         1: VisibleDeprecationWarning: `rank` is deprecated; use the `ndim` at
         tribute or function instead. To find the rank of a matrix see `numpy.
         linalg.matrix rank`.
           """Entry point for launching an IPython kernel.
Out[49]: 2
In [50]: A3.shape
Out[50]: (4, 4)
In [ ]:
```

LU Decomposition

Getting back to Example 3, how do we deal with fact that A is singular?

```
In [51]: import scipy.linalg
In [52]: P, L, U = scipy.linalg.lu(A3)
In [53]:
Out[53]: array([[0., 0., 1., 0.],
                 [0., 1., 0., 0.],
                 [1., 0., 0., 0.],
                 [0., 0., 0., 1.]]
In [54]: L
Out[54]: array([[ 1.
                                               0.
                                                            0.
                                                                       ],
                 [ 0.33333333,
                                 1.
                                               0.
                                                            0.
                                                                       ],
                                              1.
                 [ 0.33333333,
                                 0.
                                                            0.
                                                                       ],
                 [ 0.33333333, -1.
                                             -1.
                                                            1.
                                                                       ]])
In [55]: np.round( U ,9)
Out[55]: array([[ 3.
                                 0.
                                                            8.
                                               2.66666667, -1.66666667],
                 [ 0.
                                 1.
                                             -3.33333333, 3.33333333],
                 [ 0.
                                 0.
                 [ 0.
                                                            0.
                                 0.
                                               0.
                                                                       ]])
In [56]: | np.asmatrix(P)*L*U
                         0., -5.,
Out[56]: matrix([[ 1.,
                                    6.],
                  [ 1., 1., 1.,
                                    1.],
                  [ 3., 0., -5.,
                                    8.],
                  [ 1., -1., -1.,
                                    1.]])
 In [ ]:
In [57]: P
Out[57]: array([[0., 0., 1., 0.],
                 [0., 1., 0., 0.],
                 [1., 0., 0., 0.],
                 [0., 0., 0., 1.]])
In [58]: | np.linalg.det(P)
Out[58]: -1.0
In [59]:
Out[59]: array([[ 1.
                                               0.
                                                            0.
                                 0.
                                                                       ],
                 [ 0.33333333,
                                 1.
                                               0.
                                                            0.
                                                                       ],
                 [ 0.33333333,
                                 0.
                                               1.
                                                            0.
                                                                       ],
                 [0.33333333, -1.
                                              -1.
                                                            1.
                                                                       ]])
```

```
In [60]: np.linalg.det(L)
Out[60]: 1.0
In [61]: np.round(U ,9)
Out[61]: array([[ 3.
                               0.
                                         , -5.
                                                , 8.
                                         , 2.66666667, -1.66666667],
                [ 0.
                              1.
                [ 0.
                                           -3.33333333, 3.33333333],
                               0.
                [ 0.
                               0.
                                            0.
                                                , 0.
                                                                   ]])
In [62]: | np.linalg.det(U)
Out[62]: -7.401486830834343e-16
In [63]: | np.linalg.matrix rank(U)
Out[63]: 3
In [64]: PL = np.asmatrix(P)*L
In [65]: PL
Out[65]: matrix([[ 0.33333333,
                                          , 1.
                                0.
                                                          0.
                                                                    ],
                                          , 0.
                 [ 0.33333333, 1.
                                                          0.
                                                                    ],
                 [ 1.
                                             0.
                                0.
                                                          0.
                                                                    ],
                 [ 0.33333333, -1.
                                            -1.
                                                          1.
                                                                    ]])
In [66]: PL*U
Out[66]: matrix([[ 1., 0., -5.,
                                  6.1,
                 [ 1., 1., 1., 1.],
                 [3., 0., -5., 8.],
                 [1., -1., -1., 1.]
In [67]: | np.linalg.det(PL)
Out[67]: -1.0
In [68]: PL.I
Out[68]: matrix([[-0.
                                0.
                                            1.
                                                                    ],
                                          , -0.33333333, -0.
                 [-0.
                                1.
                                                                    ],
                 [ 1.
                                          , -0.33333333, -0.
                                0.
                                                                    ],
                 [ 1.
                                1.
                                          , -1.
                                                      , 1.
                                                                    ]])
In [ ]:
```

This suggests we can do the following:

$$egin{aligned} At &= d \ PLUt &= d \ Ut &= (PL)^{-1}d \end{aligned}$$

```
In [69]: np.round( U ,9)
Out[69]: array([[ 3.
                                0.
                                           , -5.
                                                         , 8.
                 [ 0.
                                1.
                                              2.66666667, -1.66666667],
                 [ 0.
                                0.
                                             -3.33333333,
                                                           3.3333333],
                 [ 0.
                                0.
                                              0.
                                                           0.
                                                                      ]])
In [70]: PL.I*d3
Out[70]: matrix([[ 7.
                  [ 4.6666667],
                  [-3.33333333],
                  [ 0.
                              ]])
In [71]: np.round( 3*U ,9)
Out[71]: array([[
                    9.,
                          0., -15.,
                                     24.],
                              8.,
                    0.,
                          3.,
                                     -5.],
                    0.,
                          0., -10.,
                                     10.],
                    0.,
                                0.,
                                      0.]])
                          0.,
In [72]: | 3*PL.I*d3
Out[72]: matrix([[ 21.],
                  [ 14.],
                  [-10.],
                  [0.]
```

Recap

$$egin{aligned} At &= d \ PLUt &= d \ Ut &= (PL)^{-1}d \end{aligned}$$

And in this case (optionally), we multiplied both sides by $\boldsymbol{3}$ to make the numbers nicer:

$$3Ut = 3(PL)^{-1}d$$

Or:

$$egin{bmatrix} 9 & 0 & -15 & 24 \ 0 & 3 & 8 & -5 \ 0 & 0 & -10 & 10 \ 0 & 0 & 0 & 0 \end{bmatrix} egin{bmatrix} w \ x \ y \ z \end{bmatrix} = egin{bmatrix} 21 \ 14 \ -10 \ 0 \end{bmatrix}$$

```
In [ ]:
```

Solution to Example 3

Let z be anything and backsolve (easy because U is upper triangular):

$$-10y + 10z = -10 \ -y + z = -1 \ y = z + 1$$

$$3x + 8y - 5z = 14$$
 $3x + 8(z + 1) - 5z = 14$
 $3x = 6 - 3z$
 $x = 2 - z$

$$9w - 15y + 24z = 21$$
 $9w - 15(z + 1) + 24z = 21$
 $9w - 15z - 15 + 24z = 21$
 $9w = 36 - 9z$
 $w = 4 - z$

Thus, for any number z,

$$t = egin{bmatrix} w \ x \ y \ z \end{bmatrix} \ = \ egin{bmatrix} 4-z \ 2-z \ z+1 \ z \end{bmatrix}$$

is a solution.

Underdetermined Systems of Equations

The last equation in the system

$$egin{bmatrix} 9 & 0 & -15 & 24 \ 0 & 3 & 8 & -5 \ 0 & 0 & -10 & 10 \ 0 & 0 & 0 & 0 \end{bmatrix} egin{bmatrix} w \ x \ y \ z \end{bmatrix} = egin{bmatrix} 21 \ 14 \ -10 \ 0 \end{bmatrix}$$

can be eliminated since it doesn't convey any information (it is always true):

$$egin{bmatrix} 9 & 0 & -15 & 24 \ 0 & 3 & 8 & -5 \ 0 & 0 & -10 & 10 \end{bmatrix} egin{bmatrix} w \ x \ y \ z \end{bmatrix} = egin{bmatrix} 21 \ 14 \ -10 \end{bmatrix}$$

This (and the original system) is an **underdetermined** system of linear equations. It has infinitely many solutions because there are more variables (degrees of freedom) than equations (constraints).

Inconsistent Systems of Equations

Conversely, a system of linear equations with no solutions is inconsistent or overdetermined.

Example 4

For example, here is an overdetermined system of three equations in two unknowns:

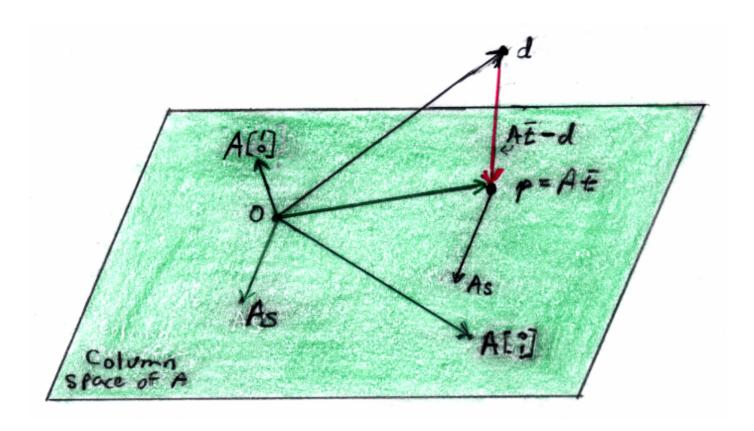
$$3x - 4y = 7$$
$$2x + 6y = 5$$
$$5x + 2y = 9$$

How do you "solve" such a system of equations?

In matrix notation,

Geometric Point of View

Goal: Find the projection $p=A\bar{t}$ of d onto the column space of A. It will follow that $t=\bar{t}$ minimizes the distance $\|At-d\|$ and is the **least squares** solution to the linear system At=d.



For all possible values of s, the vector As must be perpendicular (orthogonal) to the vector $A\bar{t}-d$:

$$egin{aligned} (As) \cdot (Aar{t} - d) &= 0 \ (As)^T (Aar{t} - d) &= 0 \ s^T A^T (Aar{t} - d) &= 0 \ s^T (A^T Aar{t} - A^T d) &= 0 \end{aligned}$$

This can only be true for *all* values of s if $A^TA\bar{t}-A^Td=0$, or $A^TA\bar{t}=A^Td.$

If A^TA is invertible, then the unique solution is

$$\bar{t} = (A^T A)^{-1} A^T d.$$

Is $A_4^T A_4$ is invertible? Check the determinant:

Summary of Solution to Example 4

Thus, the least squares solution is

$$ar{t} = \left[egin{matrix} 2 \ 0 \end{matrix}
ight].$$

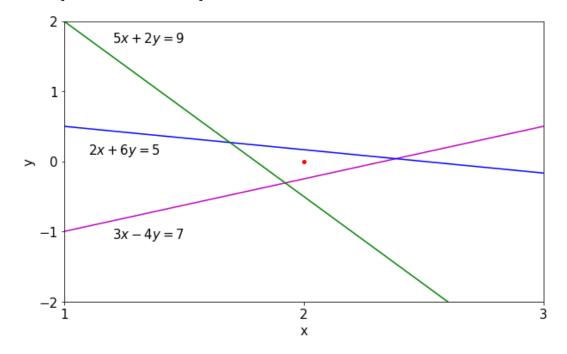
The projection of d onto the column space of A (the closest we could get) is

$$p=Aar{t}=egin{bmatrix} 3 & -4 \ 2 & 6 \ 5 & 2 \end{bmatrix}egin{bmatrix} 2 \ 0 \end{bmatrix}=egin{bmatrix} 6 \ 4 \ 10 \end{bmatrix}pproxegin{bmatrix} 7 \ 5 \ 9 \end{bmatrix}=d.$$

Another geometric look:

```
In [85]:
         import matplotlib.pyplot as plt
         plt.figure(figsize=(10,6))
         plt.rcParams.update({'font.size': 15})
         plt.suptitle('Example 4: Least Squares Solution vs. Intersection of L
         ines', fontsize=20, fontweight='bold')
         plt.xlabel('x')
         plt.xticks(np.arange(1, 4, 1))
         plt.xlim(1,3)
         plt.yticks([-2, -1, 0, 1, 2])
         plt.ylabel('y')
         plt.ylim(-2,2)
         x = np.arange(1, 3.1, 0.1)
         plt.plot(x, 3/4*x-7/4, 'm-', x, -1/3*x+5/6, 'b-', x, -5/2*x+9/2, 'q-'
         plt.plot(2, 0, marker='.', markersize=8, color='red')
         plt.text(1.2, -1.1, r'$3x-4y=7$', color='k')
         plt.text(1.1, 0.1, r'$2x+6y=5$', color='k')
         plt.text(1.2, 1.7, r'$5x+2y=9$', color='k')
         plt.show()
```

Example 4: Least Squares Solution vs. Intersection of Lines



In general:

Least Squares Solution to a System of Equations $A \quad t = d$

The least squares solution \bar{t} to a system At=d of n linear equations in k unknowns satisfies the **normal** equations:

$$A^T A \bar{t} = A^T d.$$

If the columns of A are linearly independent, then A^TA is invertible and the unique least squares solution is $\bar{t}=(A^TA)^{-1}A^Td$.

Example 5

A system of five linear equations in one unknown:

$$x = 37$$
 $x = 22$
 $x = 70$
 $x = 16$
 $x = 84$

In matrix notation,

$$\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad \begin{bmatrix} x \end{bmatrix} = \begin{bmatrix} 37 \\ 22 \\ 70 \\ 16 \\ 84 \end{bmatrix}$$

```
In [86]: A5 = np.matrix("1; 1; 1; 1")
In [87]: d5 = np.matrix("37; 22; 70; 16; 84")
In [88]: A5.T*A5
Out[88]: matrix([[5]])
```

```
In [89]: A5.T*d5
Out[89]: matrix([[229]])
In [90]: (A5.T*A5).I * A5.T * d5
Out[90]: matrix([[45.8]])
```

Question

If you replace the equation x=70 with the equivalent equation 2x=140, does the answer change?

Linear Regression

Problem: Given n data points $(x_1,y_1),\ldots,(x_n,y_n)$, find the line y=mx+b that best fits the data.

 \boldsymbol{x} is the independent variable and \boldsymbol{y} is the dependent variable.

Here, b and m are the unknowns, and the x_i and y_i are known data points. Our goal is to find the best solution to the following overdetermined system of n linear equations in two unknowns (b and m):

$$egin{aligned} b+x_1m&=y_1\ dots\ b+x_nm&=y_n \end{aligned}$$

Or, in matrix form,

The least squares best fit values of b and m are

$$\left[egin{array}{c} b \ m \end{array}
ight] = ar{t} = (A^TA)^{-1}A^TY.$$

We know A^TA will be invertible if the columns of A are linearly independent.

A set of columns (vectors) is **linearly independent** if and only if there is no one column that can be expressed as a linear combination (sum of scalar multiples) of the other columns.

Intuitively, what must be true of the x_i for this to be true?

The columns of A are **not** linearly independent if

$$egin{bmatrix} x_1 \ dots \ x_n \end{bmatrix} = eta egin{bmatrix} 1 \ dots \ 1 \end{bmatrix} = egin{bmatrix} eta \ dots \ eta \end{bmatrix}.$$

That is, the x_i 's are all equal. It is not surprising that linear regression would not work if all of the values of the independent variable x in the data were the same value. Otherwise, linear regression works.

Example 6

```
In [94]: from sklearn import datasets
In [95]: boston = datasets.load_boston()
```

In [96]: print(boston.DESCR)

Boston House Prices dataset

Notes

Data Set Characteristics:

:Number of Instances: 506

:Number of Attributes: 13 numeric/categorical predictive

:Median Value (attribute 14) is usually the target

:Attribute Information (in order):

- CRIM per capita crime rate by town
- ZN proportion of residential land zoned for lots over 25,000 sq.ft.
 - INDUS proportion of non-retail business acres per town
- CHAS Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)
 - NOX nitric oxides concentration (parts per 10 million)
 - RM average number of rooms per dwelling
 - AGE proportion of owner-occupied units built prior to

1940

- DIS weighted distances to five Boston employment centr

es

- RAD index of accessibility to radial highways
 TAX full-value property-tax rate per \$10,000
- PTRATIO pupil-teacher ratio by town
- B 1000(Bk 0.63)^2 where Bk is the proportion of bl

acks by town

- LSTAT % lower status of the population
- MEDV Median value of owner-occupied homes in \$1000's

:Missing Attribute Values: None

:Creator: Harrison, D. and Rubinfeld, D.L.

This is a copy of UCI ML housing dataset.

http://archive.ics.uci.edu/ml/datasets/Housing

This dataset was taken from the StatLib library which is maintained a t Carnegie Mellon University.

The Boston house-price data of Harrison, D. and Rubinfeld, D.L. 'Hedo nic

prices and the demand for clean air', J. Environ. Economics & Managem ent,

vol.5, 81-102, 1978. Used in Belsley, Kuh & Welsch, 'Regression dia gnostics

...', Wiley, 1980. N.B. Various transformations are used in the table on

pages 244-261 of the latter.

The Boston house-price data has been used in many machine learning papers that address regression

problems.

References

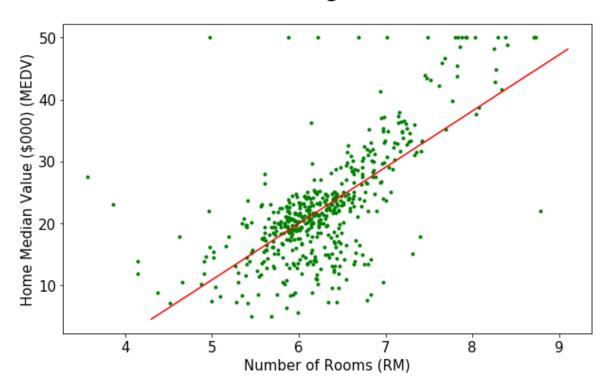
- Belsley, Kuh & Welsch, 'Regression diagnostics: Identifying Influential Data and Sources of Collinearity', Wiley, 1980. 244-261.
- Quinlan,R. (1993). Combining Instance-Based and Model-Based Learning. In Proceedings on the Tenth International Conference of Machine Learning, 236-243, University of Massachusetts, Amherst. Morgan Kaufmann.
 - many more! (see http://archive.ics.uci.edu/ml/datasets/Housing)

```
In [97]: | type(boston.data)
 Out[97]: numpy.ndarray
 In [98]: boston.data.shape
 Out[98]: (506, 13)
 In [99]: boston.feature names
 Out[99]: array(['CRIM', 'ZN', 'INDUS', 'CHAS', 'NOX', 'RM', 'AGE', 'DIS', 'RA
          D',
                  'TAX', 'PTRATIO', 'B', 'LSTAT'], dtype='<U7')
In [100]: boston.feature names[5]
Out[100]: 'RM'
In [101]: Xrm = np.asmatrix(boston.data[:,5]).T; <math>Xrm[0:10]
Out[101]: matrix([[6.575],
                   [6.421],
                   [7.185],
                   [6.998],
                   [7.147],
                   [6.43],
                   [6.012],
                   [6.172],
                   [5.631],
                   [6.004]])
In [102]: | Xrm.shape
Out[102]: (506, 1)
```

```
In [103]: A6 = np.hstack( (np.matrix(np.ones(506)).T, Xrm) ); A6
Out[103]: matrix([[1.
                         , 6.575],
                         , 6.421],
                   [1.
                   [1.
                         , 7.185],
                   . . . ,
                   [1.
                         , 6.976],
                   [1.
                         , 6.794],
                   [1.
                         , 6.03 ]])
          Y = np.asmatrix(boston.target).T; Y[0:10]
In [104]:
Out[104]: matrix([[24. ],
                   [21.6],
                   [34.7],
                   [33.4],
                   [36.2],
                   [28.7],
                   [22.9],
                   [27.1],
                   [16.5],
                   [18.9]])
           (A6.T*A6).I * A6.T * Y
In [105]:
Out[105]: matrix([[-34.67062078],
                   [ 9.10210898]])
           scipy.stats.linregress(boston.data[:,5], boston.target)
In [106]:
Out[106]: LinregressResult(slope=9.102108981180306, intercept=-34.6706207764385
          4, rvalue=0.695359947071539, pvalue=2.487228871008377e-74, stderr=0.4
          1902656012134054)
```

```
In [107]: import matplotlib.pyplot as plt
plt.figure(figsize=(10,6))
plt.rcParams.update({'font.size': 15})
plt.suptitle('Boston Housing Prices Data', fontsize=20, fontweight='b
old')
plt.xlabel('Number of Rooms (RM)')
plt.ylabel("Home Median Value ($000) (MEDV)")
plt.plot(Xrm, Y, 'g.')
x = np.array([4.3, 9.1])
plt.plot(x, 9.1021*x - 34.6706, 'r-')
plt.show()
```

Boston Housing Prices Data



[SL (11/10/2018): It was pointed out to me after the talk that the median house price is actually in multiples of \$10,000, not \$1,000 as indicated in the DESCR text.]

```
In [ ]:
```

Example 7—Multiple Regression

Let's add CRIM (crime rate) as a second independent variable.

```
In [108]: boston.feature_names[0]
Out[108]: 'CRIM'
```

```
In [109]: Xcrim = np.asmatrix(boston.data[:,0]).T; Xcrim[0:10]
Out[109]: matrix([[0.00632],
                   [0.02731],
                   [0.02729],
                   [0.03237],
                   [0.06905],
                   [0.02985],
                   [0.08829],
                   [0.14455],
                   [0.21124],
                   [0.17004])
In [110]: A7 = np.hstack( (A6,Xcrim) ); A7
Out[110]: matrix([[1.0000e+00, 6.5750e+00, 6.3200e-03],
                   [1.0000e+00, 6.4210e+00, 2.7310e-02],
                   [1.0000e+00, 7.1850e+00, 2.7290e-02],
                   [1.0000e+00, 6.9760e+00, 6.0760e-02],
                   [1.0000e+00, 6.7940e+00, 1.0959e-01],
                   [1.0000e+00, 6.0300e+00, 4.7410e-02]])
In [111]: A7.shape
Out[111]: (506, 3)
In [112]: | np.linalg.matrix rank(A7)
Out[112]: 3
In [113]: | np.linalg.det(A7.T*A7)
Out[113]: 4480321370.151303
In [114]:
          (A7.T*A7).I * A7.T * Y
Out[114]: matrix([[-29.30168135],
                    8.3975317 ],
                   [ -0.2618229 ]])
In [115]: from sklearn import linear model
In [116]: XX = np.hstack((Xrm, Xcrim)); XX
Out[116]: matrix([[6.5750e+00, 6.3200e-03],
                   [6.4210e+00, 2.7310e-02],
                   [7.1850e+00, 2.7290e-02],
                   [6.9760e+00, 6.0760e-02],
                   [6.7940e+00, 1.0959e-01],
                   [6.0300e+00, 4.7410e-02]])
```

```
In [117]: XX.shape
Out[117]: (506, 2)

In [118]: regr = linear_model.LinearRegression()

In [119]: regr.fit(XX, Y)
Out[119]: LinearRegression(copy_X=True, fit_intercept=True, n_jobs=1, normalize =False)

In [120]: regr.intercept_
Out[120]: array([-29.30168135])

In [121]: regr.coef_
Out[121]: array([[ 8.3975317, -0.2618229]])

In [ ]:
```

END

```
In [ ]:

In [ ]:
```

Appendix: Additional Material

[SL (11/10/2018): The following is some additional material we did not discuss during my talk today.]

```
In [ ]:
```

Appendix 1: Calculating Determinant of Example 1

In Example 1, we performed Gaussian elimination on the following matrix A. This essentially provided us with A^{-1} . It also provides an easy way to calculate the determinant of A.

$$A = egin{bmatrix} 2 & 2 & 4 \ 0 & 1 & -5 \ 0 & 3 & 4 \end{bmatrix}$$

First we note that the determinant respects multiplication and inverses:

$$\det A \cdot \det A^{-1} = \det(AA^{-1}) = \det I = 1 \implies \det A = \frac{1}{\det A^{-1}}.$$

The Gaussian elimination we preformed produced elementary matrices E_1 , E_2 , ..., E_6 such that $A^{-1}=E_6E_5E_4E_3E_2E_1$.

Thus,

$$\det A = \left[\det A^{-1}\right]^{-1} \ = \left[\det (E_6 E_5 E_4 E_3 E_2 E_1)\right]^{-1} \ = \left(\det E_6 \cdot \det E_5 \cdot \det E_4 \cdot \det E_3 \cdot \det E_2 \cdot \det E_1\right)^{-1}$$

In []:

We now need only figure out the determinants of the individual elementary matrices.

```
In [ ]: E1 = scalerow(0, .5); E1
In [ ]: E2 = addtorow(2, -3, 1); E2
In [ ]: E3 = addtorow(0, -1, 1); E3
In [ ]: E4 = scalerow(2, 1/19); E4
In [ ]: E5 = addtorow(1, 5, 2); E5
In [ ]: E6 = addtorow(0, -7, 2); E6
```

Therefore,

$$\det A = \left(\det E_6 \cdot \det E_5 \cdot \det E_4 \cdot \det E_3 \cdot \det E_2 \cdot \det E_1\right)^{-1}$$

$$= \left(1 \cdot 1 \cdot \frac{1}{19} \cdot 1 \cdot 1 \cdot \frac{1}{2}\right)^{-1}$$

$$= \left(\frac{1}{38}\right)^{-1}$$

$$= 38.$$

Appendix 2: Calculating Determinants Recursively

```
In [ ]:
        def redet(A):
             """Determinant of matrix A.
             Recursively calculates determinant, using method typically follow
         ed "by hand."
             if A.shape == (1,1):
                 return A[0,0]
             else:
                 return sum( (-1)**j * A[0,j] * redet(np.hstack((A[1:,:j], A[1
         :, j+1:])))
                            for j in range(0, A.shape[1])
In [ ]:
         redet(A)
In [ ]:
        np.linalg.det(A)
In [ ]:
         redet(A2)
In [ ]:
        np.linalg.det(A2)
In [ ]:
         redet(A3)
        np.linalg.det(A3)
In [ ]:
In [ ]:
```

Appendix 3: Deriving the Formulas for Linear Regression

Problem: Given n data points $(x_1, y_1), \ldots, (x_n, y_n)$, find the line y = mx + b that best fits the data.

As noted previously, the least squares best fit values of b and m are given by

$$\left[egin{array}{c} b \ m \end{array}
ight] = (A^TA)^{-1}A^TY.$$

Derivation of direct formulas of slope and intercept:

$$A^TA = egin{bmatrix} 1 & \cdots & 1 \ x_1 & \cdots & x_n \end{bmatrix} egin{bmatrix} 1 & x_1 \ dots & dots \ 1 & x_n \end{bmatrix} \ = egin{bmatrix} n & \sum_{i=1}^n x_i \ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{bmatrix}$$

$$\det(A^TA) \hspace{1cm} = \hspace{1cm} n \sum x_i^2 - (\sum x_i)^2$$

$$(A^TA)^{-1} \hspace{1cm} = \hspace{1cm} rac{1}{n\sum x_i^2-(\sum x_i)^2}egin{bmatrix} \sum x_i^2 & -\sum x_i \ -\sum x_i & n \end{bmatrix}$$

$$egin{array}{lll} A^TY & & & = & \left[egin{array}{ccc} 1 & \cdots & 1 \ x_1 & \cdots & x_n \end{array}
ight] \left[egin{array}{c} y_1 \ dots \ y_n \end{array}
ight] \ & & = & \left[\sum\limits_{\sum x_i y_i} y_i \end{array}
ight] \end{array}$$

$$\left[egin{array}{c} b \ m \end{array}
ight] = (A^TA)^{-1}A^TY \quad = \quad rac{1}{n\sum x_i^2 - (\sum x_i)^2} \left[egin{array}{c} \left(\sum x_i^2
ight)\left(\sum y_i
ight) - \left(\sum x_i
ight)\left(\sum x_iy_i
ight)
ight] \ n\left(\sum x_iy_i
ight) - \left(\sum x_i
ight)\left(\sum y_i
ight)
ight] \end{array}
ight]$$

Thus, the intercept and slope are given by the following formulas

$$egin{array}{lll} ext{Intercept:} & b & = & rac{(\sum x_i^2)(\sum y_i) - (\sum x_i)(\sum x_i y_i)}{n\sum x_i^2 - (\sum x_i)^2} \ ext{Slope:} & m & = & rac{n(\sum x_i y_i) - (\sum x_i)(\sum y_i)}{n\sum x_i^2 - (\sum x_i)^2} \end{array}$$

Slope:
$$m = \frac{n(\sum x_i y_i) - (\sum x_i)(\sum y_i)}{n \sum x_i^2 - (\sum x_i)^2}$$

Appendix 4: Condition Number

A square matrix is invertible (nonsingular) if and only if its **condition number** is finite.

Generally used in a numerical analysis context.

```
In [ ]: np.linalg.cond(A3)
```

Very large (albeit technically finite); suggests A3 may be singular.

```
In [ ]: np.linalg.cond(A2)
In [ ]:
```