Course > Module 2: The computational analysis of data > Assignment: Notebook 12 due Nov 27 at 11:59 UTC > Sample solutions

Sample solutions

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part0-lsd (Score: 2.0 / 2.0)

1. Test cell (Score: 2.0 / 2.0)

Important note! Before you turn in this lab notebook, make sure everything runs as expected:

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Make sure you fill in any place that says YOUR CODE HERE or "YOUR ANSWER HERE."

Part 0: Sample dataset (LSD)

In 1968, Wagner Agahajanian, and Bing conducted a study to determine whether you could improve a student's math test scores using lysergic acid diethylamide, also known as "LSD."

Here is the original data sources. The code cell below downloads the file from an alternative location, for compatibility with the Azure Notebook or Vocareum platforms you are using.

- Raw data: http://www.stat.ufl.edu/~winner/data/lsd.dat (http://www.stat.ufl.edu/~winner/data/lsd.dat)
- Data file description: http://www.stat.ufl.edu/~winner/data/lsd.txt (<a href="http:/

```
In [1]: | from pandas import read fwf
        from IPython.display import display
        import requests
        import os
        import hashlib
        import io
        def on vocareum():
            return os.path.exists('.voc')
        if on_vocareum():
            URL_BASE = "https://cse6040.gatech.edu/datasets/"
            DATA PATH = "../resource/lib/publicdata/"
            URL BASE = "https://github.com/cse6040/labs-fa17/raw/master/datasets/"
            DATA_PATH = "'
        def download(file, local_dir="", url_base=URL_BASE, checksum=None):
            local_file = "{}{}".format(local_dir, file)
            if not os.path.exists(local file):
                url = "{}{}".format(url_base, file)
                print("Downloading: {} ...".format(url))
                r = requests.get(url)
                with open(local_file, 'wb') as f:
                    f.write(r.content)
```

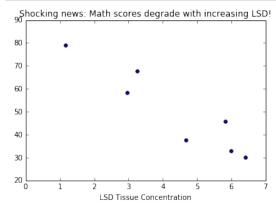
```
if checksum is not None:
        with io.open(local_file, 'rb') as f:
            body = f.read()
            body_checksum = hashlib.md5(body).hexdigest()
            assert body_checksum == checksum, \
                "Downloaded file '{}' has incorrect checksum: '{}' instead of '{}'".forma
t(local file,
body_checksum,
checksum)
    print("'{}' is ready!".format(file))
datasets = {'lsd.dat': '4c119057baf86cff8da03d825d7ce141'}
for filename, checksum in datasets.items():
    download(filename, local_dir=DATA_PATH, url_base=URL_BASE, checksum=checksum)
print("\n(All data appears to be ready.)")
Downloading: https://github.com/cse6040/labs-fa17/raw/master/datasets/lsd.dat ...
'lsd.dat' is ready!
(All data appears to be ready.)
```

Let's take a look at the data, first as a table and then using a scatter plot.

	Isd_concentration	exam_score
0	1.17	78.93
1	2.97	58.20
2	3.26	67.47
3	4.69	37.47
4	5.83	45.65
5	6.00	32.92
6	6.41	29.97

```
In [3]: from matplotlib.pyplot import scatter, xlabel, title, plot
%matplotlib inline

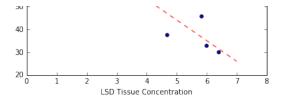
scatter(df['lsd_concentration'], df['exam_score'])
xlabel ('LSD Tissue Concentration')
title ('Shocking news: Math scores degrade with increasing LSD!');
```



Fitting a model

Exercise 0 (2 points). Complete the function below so that it computes α and β for the univariate model, $y \sim \alpha \cdot x + \beta$, given observations stored as NumPy arrays y[:] for the responses and x[:] for the predictor.

```
Use the linear regression formulas derived in class.
       In [4]:
                                                                                                          (Top)
                Student's answer
                 def linreg_fit(x, y):
                     """Returns (alpha, beta) s.t. y \sim alpha*x + beta."""
                     from numpy import ones
                     m = len(x); assert len(y) == m
                     ### BEGIN SOLUTION
                     u = ones(m)
                     alpha = x.dot(y) - u.dot(x)*u.dot(y)/m
                     alpha = x.dot(x) - (u.dot(x)**2)/m
                     beta = u.dot(y - alpha*x)/m
                     ### END SOLUTION
                     return (alpha, beta)
                 # Compute the coefficients for the LSD data:
                 x, y = df['lsd_concentration'], df['exam_score']
                 alpha, beta = linreg_fit(x, y)
                 print("alpha:", alpha)
                 print("beta:", beta)
                alpha: -9.0094664153
                beta: 89.123873768
       In [5]: | Grade cell: linreg_fit_test
                                                                                             Score: 2.0 / 2.0 (Top)
                 # Test cell: `linreg_fit_test`
                 x, y = df['lsd_concentration'], df['exam_score']
                 alpha, beta = linreg_fit(x, y)
                 r = alpha*x + beta - y
                 ssqr = r.dot(r)
                 ssqr_ex = 253.88132881
                 from numpy import isclose
                 assert isclose(ssqr, ssqr_ex, rtol=.01), "Sum-of-squared residuals is {} instead of {}.
                 ".format(ssqr, ssqr_ex)
                 print("\n(Passed!)")
                (Passed!)
       In [6]: from numpy import linspace, floor, ceil
                # Two points make a line:
                x_fit = linspace(floor(x.min()), ceil(x.max()), 2)
                y_fit = alpha*x_fit + beta
                scatter(x, y, marker='o')
                plot(x_fit, y_fit, 'r--')
                xlabel('LSD Tissue Concentration')
                title('Best-fit linear model');
                                Best-fit linear model
                 90
                 80
                 70
                 60
```



Fin! If you've gotten this far without errors, your notebook is ready to submit.

part1-gradients (Score: 2.0 / 2.0)

Test cell (Score: 1.0 / 1.0)
 Test cell (Score: 1.0 / 1.0)

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Make sure you fill in any place that says YOUR CODE HERE or "YOUR ANSWER HERE."

Part 1: Gradients example

This notebook is designed to illustrate the concept of the gradient.

Let
$$x \equiv \begin{bmatrix} x_0 \\ x_1 \end{bmatrix}$$
 be a two-dimensional vector, and let

(Passed!)

$$f(x) \equiv x^T x = x_0^2 + x_1^2.$$

Exercise 0 (1 point). Implement the Python function, f(x0, x1), so that it computes f(x).

```
In [1]: Student's answer (Top)

def f(x0, x1):
    return x0*x0 + x1*x1
```

```
In [2]: Grade cell: f_test Score: 1.0 / 1.0 (Top)

# Test cell: `f_test`

from numpy import sin, cos, vectorize, isclose
from numpy.random import randn

f_vec = vectorize(f)
theta = randn(1000)
assert all(isclose(f_vec(sin(theta), cos(theta)), 1.0))
print("\n(Passed!)")
```

The gradient

Let's create a mesh of $[x_0, x_1]$ coordinate values:

```
In [3]: | from numpy import linspace, meshgrid
       x0 = linspace(-2, 2, 11)
       x1 = linspace(-2, 2, 11)
       X0, X1 = meshgrid(x0, x1)
In [4]: print("X0:\n", X0)
       print("X1:\n", X1)
       x0:
       [[-2. -1.6 -1.2 -0.8 -0.4 0. 0.4 0.8 1.2 1.6 2.]
       [-2. \quad -1.6 \quad -1.2 \quad -0.8 \quad -0.4 \quad 0. \quad 0.4 \quad 0.8 \quad 1.2 \quad 1.6 \quad 2. ]
       [-2. -1.6 -1.2 -0.8 -0.4 0. 0.4 0.8 1.2 1.6 2.]
       [-2. -1.6 -1.2 -0.8 -0.4 0. 0.4 0.8 1.2 1.6 2.]
[-2. -1.6 -1.2 -0.8 -0.4 0. 0.4 0.8 1.2 1.6 2.]
       [-2. \quad -1.6 \quad -1.2 \quad -0.8 \quad -0.4 \quad 0. \quad 0.4 \quad 0.8 \quad 1.2 \quad 1.6 \quad 2.]
       [-2. -1.6 -1.2 -0.8 -0.4 0. 0.4 0.8 1.2 1.6 2.]
[-2. -1.6 -1.2 -0.8 -0.4 0. 0.4 0.8 1.2 1.6 2.]
       \begin{bmatrix} -2. & -1.6 & -1.2 & -0.8 & -0.4 & 0. & 0.4 & 0.8 & 1.2 & 1.6 & 2. \end{bmatrix}
       [-2. \ -1.6 \ -1.2 \ -0.8 \ -0.4 \ 0. \ 0.4 \ 0.8 \ 1.2 \ 1.6 \ 2.]
       [-2. -1.6 -1.2 -0.8 -0.4 \ 0. \ 0.4 \ 0.8 \ 1.2 \ 1.6 \ 2.]]
      X1:
       [ -0.4 \ -0.4 \ -0.4 \ -0.4 \ -0.4 \ -0.4 \ -0.4 \ -0.4 \ -0.4 \ -0.4 \ -0.4 \ ]
       2. 2.
       [ 2.
             2.
                         2.
                             2.
                                 2.
                                      2.
                                          2.
                                              2.
```

Apply f() to each of the points in the mesh:

```
In [5]: Z = f_{vec}(X0, X1)
       print("Z:\n", Z)
        [[ 8.
                6.56 5.44 4.64 4.16 4.
                                          4.16 4.64 5.44 6.56 8. ]
        [ 6.56 5.12 4. 3.2 2.72 2.56 2.72 3.2 4. 5.12 6.56]
                    2.88 2.08 1.6 1.44 1.6 2.08 2.88 4.
                                                               5.44]
        [ 5.44 4.
        [ 4.64 3.2 2.08 1.28 0.8 0.64 0.8 1.28 2.08 3.2
                                                               4.641
        [ 4.16  2.72  1.6  0.8  0.32  0.16  0.32  0.8  1.6  2.72  4.16]
        [ 4.
               2.56 1.44 0.64 0.16 0.
                                         0.16 0.64 1.44 2.56 4. ]
        [ 4.16 2.72 1.6 0.8 0.32 0.16 0.32 0.8 1.6 2.72 4.16]
        [ 4.64 3.2 2.08 1.28 0.8 0.64 0.8 1.28 2.08 3.2 4.64]
                    2.88 2.08 1.6 1.44 1.6 2.08 2.88
4. 3.2 2.72 2.56 2.72 3.2 4.
        [ 5.44 4.
                                              2.08 2.88 4.
                                                               5.441
        [ 6.56 5.12 4.
                                                         5.12 6.56]
               6.56 5.44 4.64 4.16 4.
        8.
                                         4.16 4.64 5.44 6.56 8. ]]
```

Plot z[:, :] as a three-dimensional surface:

```
In [6]: from mpl_toolkits.mplot3d import Axes3D
    from matplotlib.pyplot import figure, xlabel, ylabel
%matplotlib inline

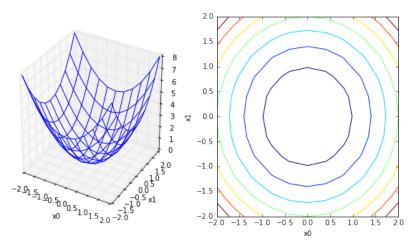
fig = figure(figsize=(10, 5))

ax3d = fig.add_subplot(121, projection='3d')
ax3d.plot_wireframe(X0, X1, Z)
xlabel('x0')
ylabel('x1')

ax2d = fig.add_subplot(122)
cp = ax2d.contour(X0, X1, Z)
```

xlabel('x0')
ylabel('x1')

Out[6]: <matplotlib.text.Text at 0x110123fd0>



The gradient of f(x) with respect to x is

$$\nabla_{x} f(x) \equiv \begin{bmatrix} \frac{\partial f}{\partial x_0} \\ \frac{\partial f}{\partial x_1} \end{bmatrix} = \begin{bmatrix} \frac{\partial}{\partial x_0} (x_0^2 + x_1^2) \\ \frac{\partial}{\partial x_1} (x_0^2 + x_1^2) \end{bmatrix} = \begin{bmatrix} 2x_0 \\ 2x_1 \end{bmatrix}.$$

Exercise 1 (1 point). Implement a function, $grad_{\pm}(x0, x1)$, that implements the gradient $\nabla_{x} f(x)$ shown above. It should return a pair of values since the gradient for this f(x) has two components.

```
In [7]: Student's answer (Top)

def grad_f(x0, x1):
    ### BEGIN SOLUTION
    return (2*x0, 2*x1)
    ### END SOLUTION
```

Visualizing the gradient

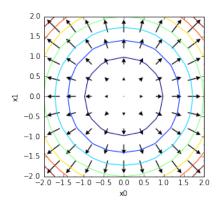
(Passed!)

Let's generate and plot $\nabla_x f(x)$:

```
In [9]: dX0, dX1 = grad_f(X0, X1)
    from matplotlib.pyplot import contour, quiver, axis
    cp = contour (X0, X1, Z)
    quiver(X0, X1, dX0, dX1, scale=40, headwidth=5)
    xlabel('x0')
```

ylabel('x1')
axis('square')

Out[9]: (-2.0, 2.0, -2.0, 2.0)



Fin! If you've gotten this far without errors, your notebook is ready to submit.

part2-algs (Score: 12.0 / 12.0)

1. Test cell (Score: 3.0 / 3.0)

2. Test cell (Score: 1.0 / 1.0)

3. Test cell (Score: 2.0 / 2.0)

4. Test cell (Score: 2.0 / 2.0)

5. Test cell (Score: 1.0 / 1.0)

6. Test cell (Score: 3.0 / 3.0)

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Part 2: Algorithms for the linear least squares problem

Recall the linear regression problem: given a data matrix, X, and responses y, we wish to determine the model parameters θ^* that minimizes $\|X\theta - y\|_2^2$. This problem is also known as the *linear least squares* problem.

Numpy has a function, np.linalg.lstsq() (https://docs.scipy.org/doc/numpy/reference/generated/numpy.linalg.lstsq.html), that will compute linear least squares solutions for you. However, the purpose of this notebook is to give you a sense of how lstsq() works. So, instead of using it as a black box, you'll study how one might implement lstsq() using two different numerical algorithms.

You may rightly ask, why bother with such details? Here are three reasons it's worth looking more closely.

- 1. It's helpful to have some deeper intuition for how one formalizes a mathematical problem and derives a computational solution, in case you ever encounter a problem that does not exactly fit what a canned library can do for you
- If you have ever used a statistical analysis package, it's likely you have encountered "strange" numerical errors or warnings. Knowing how problems are derived can help you understand what might have gone wrong. We will see an example below.
- 3. Because data analysis is quickly evolving, it's likely that new problems and new models will not exactly fit the template of existing models. Therefore, it's possible you will need to derive a new model or know how to talk to

someone who can derive one for you.

Implementation note. In this notebook, we ask that you use the following convention: any column vector should be *explicit*. That means its shape should have two dimensions where the column dimension equals one (1).

Exercise 0 (ungraded). Inspect the following code cell and make sure you understand the difference between two conventions for storing a vector, namely, as a one-dimensional array versus as a two-dimensional array (matrix) where the number of columns equals one (1). When you are asked to produce a vector, we will generally ask you to follow the second convention (z_colvec).

```
In [1]: import numpy as np
        # By default, Numpy vectors constructed from a list are 1-D
        # and have neither a row nor a column orientation.
        z_{array} = np.array([1.0, 2.0, 3.0])
        # By contrast, we want you to ensure your vectors are
        # column vectors.
        z_colvec = np.reshape(z_array, (len(z_array), 1))
        print("`z_array`:\n\n", z_array, "\n\n==> shape:", z_array.shape)
        print("\z\_colvec\:\n\n", z\_colvec, "\n\n==> shape:", z\_colvec.shape)
         `z array`:
         [ 1. 2. 3.]
        ==> shape: (3,)
        `z_colvec`:
         [[ 1.]
         [ 2.]
         [ 3.]]
        ==> shape: (3, 1)
```

Before beginning, run this code cell to load some of the key modules you'll need.

```
In [2]: # Data and computation
        import numpy as np
        import scipy as sp
        import scipy.linalg
        import pandas as pd
        # Viz
        from IPython.display import display, Math
        from matplotlib.pyplot import figure, subplot, xlim, ylim
        from matplotlib.pyplot import scatter, axis, xlabel, ylabel, title, plot
        %matplotlib inline
        # Some functions we'll use later to display results
        def show_cond_fancy(x, name, opt=''):
             ""Display a condition number in 'fancy' format (using LaTeX)."""
            def sci_to_latex(x, fmt='{:.2e}'):
                s_raw = fmt.format(x)
                s, e = s_raw.split('e')
                return s + r'\times 10^{{{{}}}}'.format(int(e))
            from IPython.display import Math
            x s = sci to latex(x)
            display(Math(r'\setminus x_s)))
        def show_2vecs_tibble(x, y, xname='x', yname='y', error=False):
            """Display two column vectors side-by-side in a tibble.""
            assert type(x) is np.ndarray and x.ndim >= 2 and x.shape[1] == 1
            assert type(y) is np.ndarray and y.ndim >= 2 and y.shape[1] == 1
            assert x.shape == y.shape
            x_df = pd.DataFrame(x, columns=[xname])
            v df = nd DataFrame(v columns=[vname])
```

```
df = pd.concat([x_df, y_df], axis=1)
       df['error'] = x - y
    display(df)
# Display (X, y) problem as a tibble
def make_data_tibble(X, y=None):
    df = pd.DataFrame(X, columns=['x_{}'.format(i) for i in range(X.shape[1])])
    if y is not None:
       y_df = pd.DataFrame(y, columns=['y'])
       df = pd.concat([y_df, df], axis=1)
    return df
# From: https://stackoverflow.com/questions/17129290/numpy-2d-and-1d-array-to-latex-bmatr
def nparray_to_bmatrix(a):
    """Returns a LaTeX bmatrix"""
   assert len(a.shape) <= 2, 'bmatrix can at most display two dimensions'</pre>
   lines = str(a).replace('[', '').replace(']', '').splitlines()
   rv = [r'\begin{bmatrix}']
    rv += [' ' + ' & '.join(1.split()) + r'\\' for 1 in lines]
    rv += [r'\end{bmatrix}']
    return '\n'.join(rv)
# Stash this function for later:
SAVE_LSTSQ = np.linalg.lstsq # You may ignore this line, which some test cells will use
```

Notation and review

Here is a quick summary of how we can formulate and approach the linear regression problem. For a more detailed derivation, see these accompanying notes (./notes-linreg.ipynb).

Your data consists of m observations and n+1 variables. One of these variables is the *response* variable, y, which you want to predict from the other n variables, $\{x_0, \ldots, x_{n-1}\}$. You wish to fit a *linear model* of the following form to these data,

$$y_i \approx x_{i,0}\theta_0 + x_{i,1}\theta_1 + \dots + x_{i,n-1}\theta_{n-1} + \theta_n$$

where $\{\theta_j | 0 \le j \le n\}$ is the set of unknown coefficients. Your modeling task is to choose values for these coefficients that "best fit" the data

If we further define a set of dummy variables, $x_{i,n} \equiv 1.0$, associated with the θ_n parameter, then the model can be written more compactly in matrix notation as

$$y \approx X\theta$$
,

where we will refer to \boldsymbol{X} as the (input) data matrix.

Visually, you can also arrange the observations into a tibble like this one:

У	x ₀	x ₁	:	x _{n-1}	x _n
У0	$x_{0,1}$	$x_{0,2}$	•••	$x_{0,n-1}$	1.0
<i>y</i> ₁	$x_{1,1}$	$x_{1,2}$	•••	$x_{1,n-1}$	1.0
у2	x _{2,1}	$x_{2,2}$	•••	$x_{2,n-1}$	1.0
:	:	:	:	:	1.0
y_{m-1}	$x_{m-1,1}$	$x_{m-1,2}$	•••	$x_{m-1,n-1}$	1.0

This tibble includes an extra column (variable), x_n , whose entries are all equal to 1.0.

Synthetic problem generator. For the exercises in this notebook, we will generate synthetic data. The function, $gen_problem(m, n)$, will return a triple, X, Y, theta, which are an $m \times (n+1)$ data matrix X, a response vector Y, and the "true" model parameters theta. We will then run two different numerical algorithms that estimate theta from Y and Y, and see how their answers compare against the true value.

Note 1. The problem generator constructs the data matrix X such that each entry (i,j) is i^j . This structure makes it an instance of a <u>Vandermonde matrix</u> (https://en.wikipedia.org/wiki/Vandermonde_matrix), which arises when fitting a polynomial to data. The "true" parameter vector θ is set to all ones, and y computed simply by summing the rows.

Note 2. Although our usual convention is to make the *last* column all ones, the Vandermonde matrix has its *first* column set to all ones. This ordering is not important in this problem, but it does mean one would interpret θ_0 as the intercept rather than θ_n , which will be our usual convention.

```
In [3]: def gen_problem(m, n):
            from numpy import arange, tile, cumprod, insert, ones
            #1 + x + x^2 + ... + x^n, x = 0:m
            X = np.empty((m, n+1))
            x_{col} = arange(m).reshape((m, 1)) # 0, 1, 2, ..., m-1
            X[:, 0] = 1.0
            X[:, 1:] = tile(x_col, reps=(1, n))
            X[:, 1:] = cumprod(X[:, 1:], axis=1)
            theta = ones((n+1, 1))
            y = np.sum(X, axis=1).reshape((m, 1))
            return X, y, theta
        print("Sample generated problem:")
        m, n = 10, 2
        X, y, theta_true = gen_problem(m, n)
        display(Math(r'X = {}), \quad y = {}) \quad implies \quad \dot x = {}'.format(nparray_to)
        bmatrix(X),
                                                                                        nparray_to
        bmatrix(y),
                                                                                         nparray_to
         _bmatrix(theta_true))))
```

Sample generated problem:

We are interested primarily in *overdetermined systems*, meaning X has more rows than columns, i.e., m > n + 1, as shown above. That's because typically we have more observations (data points, or rows) than predictors (variables or columns). For such problems, there is generally no unique solution.

Therefore, to identify some solution, we need to ask for the "best" fit and say what we mean by "best." For linear regression, the usual definition of "best" is *minimizing* the sum-of-squared residual error:

$$\theta^* = \arg\min_{\theta} ||X\theta - y||_2^2.$$

Solving this minimization problem is equivalent to solving a special system known as the normal equations,

$$X^T X \theta^* = X^T y$$
.

So, our computational task is to solve this problem.

Algorithm 1: Direct solution of the normal equations

The preceding calculation immediately suggests the following algorithm to estimate θ^* . Given X and y:

- 1. Form $C \equiv X^T X$. This object is sometimes called the <u>Gram matrix (https://en.wikipedia.org/wiki/Gramian_matrix)</u> or Gramian of X.
- 2. Form $b \equiv X^T y$.
- 3. Solve $C\theta^* = b$ for θ^* .

But, is this a "good" algorithm? There are at least three dimensions along which we might answer this question.

- 1. Is it accurate enough?
- 2. Is it fast enough?
- 3. Is it memory-efficient enough?

Let's examine these questions by experiment.

Exercise 1 (3 points). Implement a function, solve_neq(x, y) that implements Algorithm 1. It should return a Numpy vector containing the model parameter estimates.

Recall the steps of the algorithm as previously outlined:

- 1. Form the Gramian of X, $C \equiv X^T X$.
- 2. Form $b \equiv X^T y$.
- 3. Solve $C\theta^* = b$ for θ^* .

Your algorithm should carry out these steps. For the third step, use Scipy's routine, scipy.linalg.solve()

 $(\underline{\text{https://docs.scipy.org/doc/scipy/reference/tutorial/linalg.html\#solving-linear-system})}. \ \ \text{It has an option that allows you to indicate that } C \ \text{is symmetric and positive definite, which will be true of } C \ \text{for our synthetic problem.}$

The code cell will run your function to compute a set of parameter estimates. It will store these in a variable named theta neg, which we will refer to later.

Your implementation's solution versus the true solution:

	theta_neq	theta_true	error
0	1	1	-2.675637e-14
1	1	1	1.776357e-14
2	1	1	-1.887379e-15

```
In [5]:
                                                                                                 Score: 3.0 / 3.0 (Top)
          Grade cell: solve neg test
          # Test cell: `solve_neq_test`
               del np.linalg.lstsq
               solve_neq(X, y)
          except NameError as n:
               if re.findall('lstsq', n.args[0]):
                    print("*** Double-check that you did not try to use `lstsq()`. ***")
               raise n
           except AttributeError as a:
               if re.findall('lstsq', a.args[0]):
                    print("*** Double-check that you did not try to use `lstsq()`. ***")
               raise a
          finally:
               np.linalg.lstsq = SAVE LSTSQ
          assert type(theta_neq) is np.ndarray, "`theta_neq` should be a Numpy array, but isn't."

assert theta neq shape == (n+1 1) "`theta_neq shape` is A instead of A " format/the
          accort that a new chang == (n+1 1)
```

(Passed!)

```
ta_neq.shape, (n+1, 1))

assert (np.abs(theta_neq - theta_true) <= 1e-12).all(), \
    "Your `theta_neq` does not match the true solution, `theta_true`."

print("\n(Passed!)")</pre>
```

Exercise 2 (1 point). Write a function to calculate the residual norm, $||r||_2 = ||X\theta^* - y||_2$.

Although we are minimizing $||r||_2^2$, for this exercise your function should return $||r||_2$.

```
In [6]:
                                                                                                   (Top)
         Student's answer
         def calc_residual_norm(X, y, theta):
             ### BEGIN SOLUTION
             from numpy.linalg import norm
             return norm(X.dot(theta) - y, ord=2)
             ### END SOLUTION
         r_norm_neq = calc_residual_norm(X, y, theta_neq)
         print("\nThe squared residual norm:", r_norm_neq)
        The squared residual norm: 4.20692496583e-14
In [7]:
                                                                                      Score: 1.0 / 1.0 (Top)
        Grade cell: calc residual norm test
         # Test cell: `calc_residual_norm_test`
         r_norm_neq = calc_residual_norm(X, y, theta_neq)
         assert le-16 <= np.abs(r_norm_neq) <= le-12</pre>
         print ("\n(Passed.)")
```

Sources of error

(Passed.)

We said before that one question we should ask about our algorithm is whether it is "accurate enough." But what does that mean?

Exercise 3 (ungraded). For any modeling problem, there will be several sources of error. Describe at least three such sources.

Answer. Here are some possibilities.

- 1. There will be errors in the inputs. That is, the data itself may only represent measurements of a certain accuracy.
- 2. There will be errors in the model. That is, the model is only an approximation of the underlying phenomena.
- 3. There will be errors in the algorithm. That is, you may implement an algorithm that can only approximately estimate the parameters of the model.
- 4. There will be roundoff errors. Recall that floating-point arithmetic necessarily represents all values finitely, which means you may lose accuracy every time you do an arithmetic operation.

Perturbations. One way to understand error in a numerical computation is to consider how sensitive the computed solution is to perturbations to the input.

That is, suppose we change X by an amount ΔX . We can then ask by how much the computed model parameters θ^* change. If they change by a lot, then our method for computing them may be overly sensitive to perturbations. Instead, we might prefer one method over another one that is more sensitive to changes.

Let's see how Algorithm 1 fares under small perturbations. But first, we'll need a method to generate a random perturbation of a certain maximize size.

Exercise 4 (2 points). Implement a function that returns an $m \times n$ matrix whose entries are uniformly randomly distributed in the interval, $[0, \epsilon]$ for a given value of ϵ .

Hint: Check out Numpy's module for generating (pseudo)random numbers: numpy.random (https://docs.scipy.org/doc/numpy/reference/routines.random.html)

```
In [8]:
                                                                                                    (Top)
         Student's answer
         def random_mat (m, n, eps):
             ### BEGIN SOLUTION
             return np.random.random((m, n)) * eps
              ### END SOLUTION
         print(random_mat(3, 2, 1e-3))
         [[ 0.00093461  0.00012055]
          [ 0.00039101  0.00028564]
          [ 0.00041721 0.0005565 ]]
In [9]: | Grade cell: rand_eps_test
                                                                                       Score: 2.0 / 2.0 (Top)
         # Test cell: `rand_eps_test`
         Z = random_mat (5, 3, 1e-2)
         assert Z.shape == (5, 3)
         assert ((Z \ge 0) \& (Z \le 1e-2)).all()
         print("\n(Passed.)")
         (Passed.)
```

Exercise 5 (2 points). Use your $random_mat()$ function to write another function, $perturb_system(X, y, eps)$, that creates two "perturbations" to the system defined by X and y.

- 1. Let ΔX be the first perturbation. It should have the same dimensions as X, and its entries should lie in the interval $[-\epsilon, \epsilon]$. The value of ϵ is given by eps.
- 2. The second is Δy , a small perturbation to the response variable, y. Its entries should also lie in the same interval, $[-\epsilon, \epsilon]$,

Your function should return a perturbed system, $X + \Delta X$ and $y + \Delta y$, as a pair.

```
In [10]:
         Student's answer
                                                                                                 (Top)
          def perturb_system(X, y, eps):
              ### BEGIN SOLUTION
              Delta_X = random_mat(X.shape[0], X.shape[1], 2*eps) - eps
              Delta_y = random_mat(y.shape[0], y.shape[1], 2*eps) - eps
              return X + Delta_X, y + Delta_y
              ### END SOLUTION
          EPSILON = 0.1
          X_perturbed, y_perturbed = perturb_system(X, y, EPSILON)
          Delta_X = X_perturbed - X
          Delta_y = y_perturbed - y
          display(Math(r'\Delta X = {}, \quad \Delta y = {}'.format(nparray_to_bmatrix(Delta_X[:5
          , :]),
                                                                     nparray_to_bmatrix(Delta_y[:5
          1))))
```

```
\begin{bmatrix} -0.05279918 & -0.01916842 & 0.04036026 \\ 0.09870436 & 0.01551373 & -0.09303609 \end{bmatrix} \qquad \begin{bmatrix} -0.08642231 \\ 0.08198366 \end{bmatrix}
```

```
\Delta X = \begin{vmatrix} 0.04760073 & -0.0908171 & 0.0475814 \\ 0.00865634 & -0.01890514 & 0.06708056 \\ -0.01407924 & 0.03825858 & 0.07733381 \end{vmatrix}, \quad \Delta y = \begin{vmatrix} -0.05972809 \\ -0.07671632 \\ 0.06590073 \end{vmatrix}
```

Sensitivity of Algorithm 1

(Passed.)

Let's now run the following code, which uses your code from above to perform a "sensitivity experiment." In particular, the function run perturbation trials() will repeatedly perturb the system and measure the resulting change to the estimated θ^* .

All of the estimated θ^* are stored in an array, Thetas_neq. Each *column* k of Thetas_neq, or Thetas_neq[:, k], is one of the calculated estimates under a random perturbation of the system.

The size of the random perturbation is set, by default, to eps=0.01. Recall that our synthetic problem consists of numerical values that are all greater than or equal to one, so this perturbation may be regarded as fairly small.

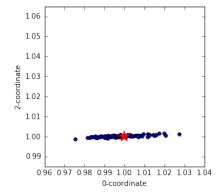
```
In [12]: def run_perturbation_trials(solver, X, y, eps=0.01, trials=100):
            Thetas = np.zeros((X.shape[1], trials)) # Store all computed thetas
            for t in range(trials):
               X_p, y_p = perturb_system(X, y, eps)
               Thetas[:, t:t+1] = solver(X_p, y_p)
            return Thetas
        Thetas_neq = run_perturbation_trials(solve_neq, X, y)
        print("Unperturbed solution:")
        print(theta_neq)
        print("First few perturbed solutions (columns):")
        print(Thetas_neq[:, :5])
        Unperturbed solution:
        [[ 1.]
         [ 1.]
         [ 1.]]
        First few perturbed solutions (columns):
        [[ 1.00579152  0.99875296  0.98559395  0.99980274  1.0044901 ]
                     1.0019043 1.00376842 1.002629
         [ 0.997179
                                                       0.99967458]
```

Here is a quick plot of the that shows two coordinates of the true parameters (red star), compared to all perturbed estimates (blue points). We would have more confidence in the algorithm's computed solutions if it did not appear to be too sensitive to changes in the input.

Since θ may have more than two coordinates, the code below shows the first two coordinates.

```
In [13]: # Makes a 2-D scatter plot of given theta values.
# If the thetas have more than two dimensions, only
# the first and last are displayed by default.
```

```
# (Override by setting ax and ay.)
def scatter_thetas(Thetas, theta_true=None, ax=0, ay=-1, xylim=None, title=None):
   import matplotlib.pyplot as plt
    assert type(Thetas) is np.ndarray and Thetas.shape[0] >= 2
   scatter(Thetas[ax, :], Thetas[ay, :])
   xlabel('{}-coordinate'.format(ax if ax >= 0 else Thetas.shape[0]+ax))
   ylabel('{}-coordinate'.format(ay if ay >= 0 else Thetas.shape[0]+ay))
   if xylim is not None:
       axis(xylim)
    else:
       axis('equal')
    if theta_true is not None:
       assert type(theta_true) is np.ndarray and theta_true.shape[0] >= 2 and theta_true
.shape[1] == 1
       scatter(theta_true[ax], theta_true[ay], marker='*', color='red', s=15**2)
    if title is not None:
       plt.title(title)
def calc_lims(x, buffer=0.1):
   xmin = x.min()
   xmax = x.max()
   dx = (xmax - xmin) * buffer
   return xmin-dx, xmax+dx
scatter_thetas(Thetas_neq, theta_true=theta_true, ax=0, ay=2)
axis('square');
```



You should observe that the change in the estimates are of the same order as the perturbation. So for this example system, the algorithm seems reliable enough.

Stress-testing Algorithm 1

This experiment suggests all is fine. But what should we expect to happen?

We've prepared another <u>notebook (./notes-cond.ipynb)</u> that walks you through an analysis of solving linear systems. It turns out you can estimate how hard it is to solve a linear system using a measure called the *condition number*. We can denote the condition number of solving a system by $\kappa(X)$ where X is the matrix. The larger this number is, the more sensitive the problem is.

In Numpy, there is a condition number estimator that will tell us approximately what the condition number is for a given matrix. Let's compare $\kappa(X)$ and $\kappa(C) = \kappa(X^TX)$:

```
In [14]: cond_X = np.linalg.cond(X)
cond_XTX = np.linalg.cond(X.T.dot(X))

assert 1. <= cond_X <= 3e3
assert 1. <= cond_XTX <= 6e6

show_cond_fancy(cond_X, 'X')
show_cond_fancy(cond_XTX, 'X^T X')
show_cond_fancy(cond_X**2, 'X', opt='^2')

\kappa(X) \approx 1.07 \times 10^2
```

$$\kappa(X^T X) \approx 1.15 \times 10^4$$

 $\kappa(X)^2 \approx 1.15 \times 10^4$

Ill-conditioning. As it happens, $\kappa(C)$ is roughly the **square** of $\kappa(X)$. So, by forming C explicitly and then trying to solve a system based on it, we make the problem *more* difficult. Indeed, if the problem is ill-conditioned enough, this algorithm based on directly constructing the normal equations will produce very different results even under small changes, and we call the algorithm *unstable*.

In this particular example, the condition numbers are not very "big." You would be more concerned if the condition numbers were close to $1/\epsilon$, where ϵ is machine epsilon. In double-precision, recall that $\epsilon_d \approx 10^{-15}$, so the values shown above is nothing to be worried about.

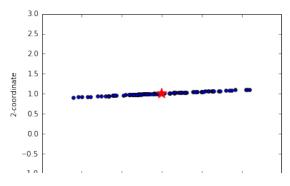
But what if we had a "hard" problem, that is, one whose condition number is large? The synthetic data generator allows us to create such a problem by making the problem bigger. Let's try that next.

```
In [15]: # Generate a "hard" problem
          m_hard, n_hard = 100, 6
          X_hard, y_hard, theta_hard_true = gen_problem(m_hard, n_hard)
          df_hard = make_data_tibble(X_hard, y_hard)
          print("First few rows of data:")
          df hard.head()
          print("True parameter estimates:\n{}".format(theta_hard_true))
          cond X hard = np.linalg.cond(X hard)
          cond_XTX_hard = np.linalg.cond(X_hard.T.dot(X_hard))
          name_X_hard = 'X h'
          show_cond_fancy(cond_X_hard, name_X_hard)
          show_cond_fancy(cond_XTX_hard, '{}^T {}'.format(name_X_hard, name_X_hard))
          First few rows of data:
          True parameter estimates:
          [[ 1.]
           [ 1.]
           [ 1.]
           [ 1.]
           [ 1.]
           [ 1.]
           [ 1.]]
          \kappa(X_h) \approx 1.72 \times 10^{12}
          \kappa(X_h^T X_h) \approx 2.91 \times 10^{23}
```

These condition numbers are much larger. So, let's run the same sensitivity experiment as before, and see how the estimate varies for the hard problem. How does it compare to the well-conditioned case?

Residual norm for one of the trials:

Out[16]: 153065336652814.84





Observe that the computed estimates can be relatively far from the true value, even getting the sign completely wrong in the case of the θ_0 .

Algorithm 2: QR decomposition

A different method for solving an overdetermined systems is to use a tool from linear algebra known as the <u>QR decomposition</u> (https://en.wikipedia.org/wiki/QR_decomposition).

Here is how we can use QR. If X has linearly independent columns, then we would first factor the $m \times n$ matrix X into the product X = QR, where Q is an $m \times n$ orthogonal matrix and R is an invertible $n \times n$ upper-triangular matrix. (These dimensions assume $m \ge n$.) That Q is orthogonal means that $Q^T Q = I$, the identity matrix; R being upper-triangular means all of its entries below the main diagonal are zero.

Next, observe that the normal equations can be transformed if we substitute X = QR:

$$X^{T}X\theta^{*} = X^{T}y$$

$$R^{T}Q^{T}QR\theta^{*} = R^{T}Q^{T}y$$

$$R\theta^{*} = Q^{T}y.$$

Lastly, because R is triangular, solving a system is "easy" using (backward) substitution. Consider the following 3×3 example (taken from http://www.purplemath.com/modules/systlin6.htm):

$$\begin{bmatrix} 5 & 4 & -1 \\ & 10 & -3 \\ & & 1 \end{bmatrix} \cdot \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 11 \\ 3 \end{bmatrix}.$$

Because it is upper-triangular, you can see right away that $1 \cdot \theta_2 = 3 \implies \theta_2 = 3$. Then, going to the equation above it, $10\theta_1 - 3\theta_2 = 10\theta_1 - 3(3) = 11 \implies \theta_1 = 2$. Lastly, $5\theta_0 + 4\theta_1 - \theta_2 = 5\theta_0 + 4(2) - 3 = 0 \implies \theta_0 = -1$.

So, to summarize, a different algorithm to solve $X\theta^* \approx y$ using QR would look like the following:

- 1. Compute X = OR.
- 2. Form the modified right-hand side, $z = Q^T y$.
- 3. Use back-substitution to solve $R\theta^* = z$.

Conditioning. What about the sensitivity of this algorithm? Given R, we only need to solve linear systems involving R. Therefore, it's $\kappa(R)$ that will determine the stability of the algorithm. So if $\kappa(R)$ is comparable to $\kappa(X)$, then the algorithm should be as stable as one can expect any algorithm to be.

Exercise 6 (1 point). Use $\underline{\text{numpy.linalg.qr}()}$ ($\underline{\text{https://docs.scipy.org/doc/numpy/reference/generated/numpy.linalg.qr,html})$ to compute the QR decomposition of X (precomputed above as the variable, X). Store the O and R factors in two variables named 0 and R.

```
[ 1. 0. 0.]
[ 1. 1. 1.]
[ 1. 2. 4.]
[ 1. 3. 9.]
```

```
[ 1. 4. 16.]]
           Q: (10, 3)
           R: (3, 3) ==
           [[ -3.16227766 -14.23024947 -90.12491331]
            [ 0.
                                9.08295106 81.74655956]
                                              22.97825059]]
            [ 0.
                                0.
In [18]: Grade cell: qr_test
                                                                                                      Score: 1.0 / 1.0 (Top)
            # Test cell: `qr test`
            assert type(Q) is np.ndarray, "`Q` is not a Numpy array but should be."
assert type(R) is np.ndarray, "`R` is not a Numpy array but should be."
assert Q.shape == (m, n+1), "`Q` has the wrong shape: it's {} rather than {}.".format(Q)
            .shape, (m, n+1))
            assert R.shape == (n+1, n+1), "R' has the wrong shape: it's {} rather than {}.".format
            (R.shape, (m, n+1))
            for i in range(R.shape[0]):
                 for j in range(i):
                      \textbf{assert np.isclose}(\texttt{R[i][j], 0.0), "R[{}][{}] == {} \texttt{ instead of 0!".format(i, j, R)} 
            [i][j])
            OTO = O.T.dot(O)
            assert np.isclose(QTQ, np.eye(Q.shape[1])).all(), "Q^T Q is not nearly the identity mat
            rix, as it should be.
            assert np.isclose(X, Q.dot(R)).all(), "QR is not sufficiently close in values to X!"
            print("\n(Passed!)")
```

```
In [19]: cond_R = np.linalg.cond(R)
    show_cond_fancy(cond_X, 'X')
    show_cond_fancy(cond_XTX, 'X^T X')
    show_cond_fancy(cond_R, 'R')
```

 $\kappa(X) \approx 1.07 \times 10^2$ $\kappa(X^T X) \approx 1.15 \times 10^4$ $\kappa(R) \approx 1.07 \times 10^2$

(Passed!)

Exercise 7 (3 points). Implement a function, solve gr(X, y), which uses the QR-based algorithm to estimate θ^* .

Condition number of R. Let's check the condition number of R empirically, to verify that it is comparable to $\kappa(X)$.

To solve the triangular system, use Scipy's specialized function, available as <a href="mailto:sp.linalg.solve_triangular.gol

```
In [20]: Student's answer

import scipy.linalg

def solve_qr(X, y):
    ### BEGIN SOLUTION
    Q, R = np.linalg.qr(X)
    b = Q.T.dot(y)
    theta = sp.linalg.solve_triangular(R, b) # Solves R u = b
    return theta
    ### END SOLUTION

theta_qr = solve_qr(X, y)
```

```
print("Comparing your QR solution to the true solution:")
show_2vecs_tibble(theta_qr, theta_true, xname='theta_qr', yname='theta_true', error=Tru
e)
print("Residual norm:")
calc_residual_norm(X, y, theta_qr)
```

Comparing your QR solution to the true solution:

	theta_qr	theta_true	error
0	1	1	-2.553513e-15
1	1	1	4.440892e-16
2	1	1	-1.110223e-16

Residual norm:

Out[20]: 1.8599135272669474e-14

(Passed!)

```
In [21]:
         Grade cell: solve_qr_test
                                                                                     Score: 3.0 / 3.0 (Top)
          # Test cell: `solve_qr_test`
          import re
          try:
              del np.linalg.lstsq
              solve_qr(X, y)
          except NameError as n:
              if re.findall('lstsq', n.args[0]):
                  print("*** Double-check that you did not try to use `lstsq()`. ***")
              raise n
          except AttributeError as a:
              if re.findall('lstsq', a.args[0]):
                  print("*** Double-check that you did not try to use `lstsq()`. ***")
              raise a
          finally:
              np.linalg.lstsq = SAVE_LSTSQ
          assert np.isclose(theta_qr, theta_true).all(), "Your QR-based solution should be closer
          to the true solution."
          print("\n(Passed!)")
```

Is QR more stable? Let's run the same perturbation experiments on the "hard" regression problem and see the result.

```
In [22]: Thetas hard qr = run perturbation trials(solve qr, X hard, y hard)
          # Plot side-by-side against normal equations method
          def compare_scatter_thetas(T0, title0, T1, title1, ax=0, ay=1, **kwargs):
              xmin, xmax = calc_lims(np.array([Thetas_hard_neq[ax, :], Thetas_hard_qr[ax, :]]))
              ymin, ymax = calc_lims(np.array([Thetas_hard_neq[ay, :], Thetas_hard_qr[ay, :]]))
              xylim = [xmin, xmax, ymin, ymax]
              figure(figsize=(12, 4))
              subplot(1, 2, 1)
              scatter thetas(T0, title=title0, ax=ax, ay=ay, xylim=xylim, **kwarqs)
              subplot(1, 2, 2)
              scatter_thetas(T1, title=title1, ax=ax, ay=ay, xylim=xylim, **kwargs)
         \label{lem:compare_scatter_thetas} $$\operatorname{Thetas\_hard\_neq, 'Normal equations', }$$ Thetas\_hard\_qr, 'QR',
                                  ax=0, ay=-1, theta_true=theta_hard_true)
          print("Sample estimate for one of the trials:")
          theta hard neq example = Thetas hard neq[:, np.random.randint(Thetas hard neq.shape[1])]
          theta_hard_qr_example = Thetas_hard_qr[:, np.random.randint(Thetas_hard_qr.shape[1])]
          msg = "- {}-based method: theta^T = \n\t{}"
          nrint/med format/"Gramian"
                                      thata hard non avamala TII
```

You should observe that the QR-based method does, indeed, produce estimates much closer to the true value despite the problem's high condition number.

Performance tradeoff. Although QR produces more reliable results, there can be a performance tradeoff, as the following quick test should show.

```
In [23]: print("=== Performance of the normal equations-based algorithm ===")
%timeit solve_neq(X_hard, y_hard)

print("\n=== Performance of the QR-based algorithm ===")
%timeit solve_qr(X_hard, y_hard)

=== Performance of the normal equations-based algorithm ===

The slowest run took 4.84 times longer than the fastest. This could mean that an intermed iate result is being cached.
1000 loops, best of 3: 102 \mu s per loop

=== Performance of the QR-based algorithm ===

1000 loops, best of 3: 181 \mu s per loop
```

Summary comment. The intent of this notebook was to help you appreciate some of the reliability and performance issues involved in the design of numerical algorithms. The key ideas are as follows.

- 1. The *conditioning* of a problem, which is a measure of how hard it is to solve. For solving linear systems, the condition number of the matrix produced by numpy.linalg.cond() is this measure.
- 2. For the specific problem of linear least squares, a method based on QR factorization is better than forming the Gram matrix, which squares the condition number. Although we did not discuss the theory of QR better, it exemplifies a common pattern or trick in linear algebraic problems: converting the original problem (or matrix) into one whose structure is easier to solve.
- 3. There is a potential tradeoff between reliability of an algorithm and speed.

Many of these algorithmic and engineering ideas have already been worked out, and are encapsulated in Numpy's built-in lstsq() solver (lstsq() solver (https://docs.scipy.org/doc/numpy/reference/generated/numpy.linalg.lstsq.html). So when you need to solve a linear system in a future notebook, you can use this function.

Fin! If you've gotten this far without errors, your notebook is ready to submit.

part3-cost--OPTIONAL (Score: 0.0 / 0.0)

1. Test cell (Score: 0.0 / 0.0)

Important note! Before you turn in this lab notebook, make sure everything runs as expected:

- First, restart the kernel -- in the menubar, select Kernel→Restart.
- Then run all cells -- in the menubar, select Cell→Run All.

Make sure you fill in any place that says YOUR CODE HERE or "YOUR ANSWER HERE."

Part 3: The cost of solving the normal equations

This notebook helps you explore the execution time cost of solving the normal equations,

$$X^T X \theta^* = X^T y.$$

This notebook only has one exercise, but it is not graded. So, you should complete it for your own edification.

```
In [1]: import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

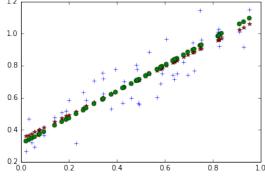
Scalability with the problem size

To start, here is some code to help generate synthetic problems of a certain size, namely, $m \times (n+1)$, where m is the number of observations and n the number of predictors. The +1 comes from our usual dummy coefficient for a non-zero intercept.

We will also implement a linear least squares solver, estimate_coeffs(), that simply calls Numpy's lstsq() routine.

```
In [2]: def generate_model (n):
             """Returns a set of (random) n+1 linear model coefficients."""
            return np.random.rand (n+1, 1)
        def generate_data (m, theta, sigma=1.0/(2**0.5)):
            Generates 'm' noisy observations for a linear model whose
            predictor (non-intercept) coefficients are given in 'theta'.
            Decrease 'sigma' to decrease the amount of noise.
            assert (type (theta) is np.ndarray) and (theta.ndim == 2) and (theta.shape[1] == 1)
            n = len (theta)
            X = np.random.rand (m, n)
            X[:, 0] = 1.0
            y = X.dot (theta) + sigma*np.random.randn (m, 1)
            return (X, y)
        def estimate_coeffs(X, y):
            Solves X*theta = y by a linear least squares method.
            result = np.linalg.lstsq (X, y)
            theta = result[0]
            return theta
```

```
In [3]: # Demo the above routines for a 2-D dataset.
        m = 50
        theta_true = generate_model (1)
        (X, y) = generate_data (m, theta_true, sigma=0.1)
        print ("Dimensions of X:", X.shape)
        print ("Dimensions of theta_true:", theta_true.shape)
        print ("Dimensions of y:", y.shape)
        print ("Condition number of X: ", np.linalg.cond (X))
        print ("True model coefficients:", theta_true.T)
        theta = estimate_coeffs (X, y)
        print ("Estimated model coefficients:", theta.T)
        fig = plt.figure()
        ax1 = fig.add_subplot(111)
        ax1.plot (X[:, 1], y, 'b+') # Noisy observations
        ax1.plot (X[:, 1], X.dot (theta), 'r*') # Fit
        ax1.plot (X[:, 1], X.dot (theta true), 'go') # True solution
        Dimensions of X: (50, 2)
        Dimensions of theta_true: (2, 1)
        Dimensions of y: (50, 1)
        Condition number of X: 4.67747186986
        True model coefficients: [[ 0.31079648  0.822169 ]]
        Estimated model coefficients: [[ 0.34339429 0.7496527 ]]
Out[3]: [<matplotlib.lines.Line2D at 0x10e380518>]
         1.2
         1.0
         0.8
```



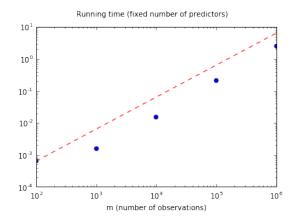
Benchmark varying m. Let's benchmark the time to compute x when the dimension n of each point is fixed but the number m of points varies. How does the running time scale with m?

```
In [4]: # Benchmark, as 'm' varies:
        n = 32 # dimension
        M = [100, 1000, 10000, 100000, 1000000]
        times = [0.] * len (M)
        for (i, m) in enumerate (M):
            theta_true = generate_model (n)
            (X, y) = generate_data (m, theta_true, sigma=0.1)
            t = %timeit -o estimate_coeffs (X, y)
            times[i] = t.best
        The slowest run took 11.63 times longer than the fastest. This could mean that an interme
        diate result is being cached.
        1000 loops, best of 3: 646 \mus per loop
        1000 loops, best of 3: 1.56 ms per loop
        100 loops, best of 3: 15 ms per loop
        1 loop, best of 3: 211 ms per loop
        1 loop, best of 3: 2.53 s per loop
```

```
In [5]: t_linear = [times[0]/M[0]*m for m in M]

fig = plt.figure()
ax1 = fig.add_subplot(111)
ax1.loglog (M, times, 'bo')
ax1.loglog (M, t_linear, 'r--')
ax1.set_xlabel ('m (number of observations)')
fig.suptitle ('Running time (fixed number of predictors)')
```

Out[5]: <matplotlib.text.Text at 0x10e50cfd0>



Exercise 0 (ungraded). Now fix the number m of observations but vary the dimension n. How does time scale with n? Complete the benchmark code below to find out. In particular, given the array N[:], compute an array, times[:], such that times[i] is the running time for a problem of size $m \times (N[i]+1)$.

Hint: You can adapt the preceding benchmark. Also, note that the code cell following the one immediately below will plot your results against O(n) and $O(n^2)$.

```
1000 loops, best of 3: 227 \mus per loop 1000 loops, best of 3: 421 \mus per loop 1000 loops, best of 3: 787 \mus per loop 100 loops, best of 3: 2.12 ms per loop 100 loops, best of 3: 7.06 ms per loop 10 loops, best of 3: 22.4 ms per loop 10 loops, best of 3: 61.2 ms per loop 10 loops, best of 3: 61.2 ms per loop 10 loops, best of 3: 133 ms per loop 1 loop, best of 3: 361 ms per loop 1 loop, best of 3: 1.39 s per loop
```

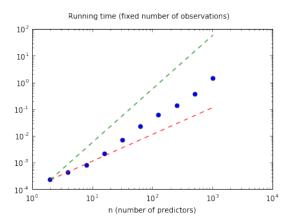
Score: 0.0 / 0.0 (Top)

In [7]: Grade cell: cell-1c7b19e5b62b895c

```
t_linear = [times[0]/N[0]*n for n in N]
t_quadratic = [times[0]/N[0]/N[0]*n*n for n in N]

fig = plt.figure()
ax1 = fig.add_subplot(111)
ax1.loglog (N, times, 'bo')
ax1.loglog (N, t_linear, 'r--')
ax1.loglog (N, t_quadratic, 'g--')
ax1.set_xlabel ('n (number of predictors)')
fig.suptitle ('Running time (fixed number of observations)')
```

Out[7]: <matplotlib.text.Text at 0x112c7eac8>



Thus, the empirical scaling appears to be pretty reasonable, being roughly linear in m. And while being quadratic in n sounds bad, one expects (or hopes!) that $n \ll \sqrt{m}$ in practical regression problems.

Fin! If you've gotten this far without errors, your notebook is ready to submit.

part4-online (Score: 5.0 / 5.0)

1. Test cell (Score: 5.0 / 5.0)

Important note! Before you turn in this lab notebook, make sure everything runs as expected:

- First, restart the kernel -- in the menubar, select Kernel \rightarrow Restart.
- Then run all cells -- in the menubar, select Cell→Run All.

Make sure you fill in any place that says YOUR CODE HERE or "YOUR ANSWER HERE."

Part 4: "Online" linear regression

When you are trying to fit a model to data and you get to see all of the data at once, we refer to the problem as an offline or batch problem,

and you would try to use certain algorithms to compute the fit that can take advantage of the fact that you a lot of available data.

But what if you only get to see one or a few data points at a time? In that case, you might want to get an initial model from whatever data you've got, and gradually improve the model as you see new data points. In this case, we refer to the problem as being an *online* problem.

The goal of this notebook is to introduce you to online algorithms. You'll start by reviewing the offline linear regression problem, and then look at its online variant. The neat thing about the online method is that you can derive it using all the tools you already have at your disposal, namely, multivariate calculus.

```
In [1]: import numpy as np
   import matplotlib.pyplot as plt
%matplotlib inline
```

Review: Offline or batch linear regression

Let's start with a quick review of the linear regression problem: given a response vector, y, and a data matrix X---whose rows are observations and columns are variables---the problem is to find the best linear model, $y \approx X\theta^*$, where θ^* is the vector of best-fit model parameters that we wish to compute. Computing it using a conventional batch linear least squares method has an asymptotic running time of $\mathcal{O}(mn^2)$.

To start, here is some code to help generate synthetic problems of a certain size, namely, $m \times (n+1)$, where m is the number of observations and n the number of predictors. The +1 comes from our usual dummy coefficient for a non-zero intercept.

```
In [2]: def generate_model (n):
              ""Returns a set of (random) n+1 linear model coefficients."""
            return np.random.rand (n+1, 1)
        def generate_data (m, theta, sigma=1.0/(2**0.5)):
            Generates \mbox{'m'} noisy observations for a linear model whose
            predictor (non-intercept) coefficients are given in 'theta'.
            Decrease 'sigma' to decrease the amount of noise.
            assert (type (theta) is np.ndarray) and (theta.ndim == 2) and (theta.shape[1] == 1)
            n = len (theta)
            X = np.random.rand (m, n)
            X[:, 0] = 1.0
            y = X.dot (theta) + sigma*np.random.randn (m, 1)
            return (X, y)
        def estimate_coeffs (X, y):
            Solves X*theta = y by a linear least squares method.
            result = np.linalg.lstsq (X, y)
            theta = result[0]
            return theta
```

An online algorithm

In [3]: def rel_diff(x, y, ord=2):

override by setting 'ord'.

The empirical scaling of linear least squares appears to be pretty good, being roughly linear in m or at worst quadratic in n. But there is still a downside in time and storage: each time there is a change in the data, you appear to need to form the data matrix all over again and recompute the solution from scratch, possibly touching the entire data set again!

return np.linalq.norm (x - y, ord=ord) / np.linalq.norm (y, ord=ord)

This begs the question, is there a way to incrementally update the model coefficients whenever a new data point, or perhaps a small batch of new data points, arrives? Such a procedure would be considered *incremental* or *online*, rather than batched or offline.

Computes ||x-y|| / ||y||. Uses 2-norm by default;

Setup: Key assumptions and main goal. In the discussion that follows, assume that you only get to see the observations *one-at-a-time*. Let (y_k, χ_k^T) denote the current observation. (Relative to our previous notation, this tuple is just element k of y and row k of X.

We will use x_k^T to denote a row k of X since we previously used x_j to denote column j of X. That is,

$$X = \begin{pmatrix} x_0 & \cdots & x_n \end{pmatrix} = \begin{pmatrix} x_0^T \\ \vdots \\ x_{m-1}^T \end{pmatrix},$$

where the first form is our previous "columns-view" representation and the second form is our "rows-view."

Additionally, assume that, at the time the k-th observation arrives, you start with a current estimate of the parameters, $\tilde{\theta(k)}$, which is a vector. If for whatever reason you need to refer to element i of that vector, use $\tilde{\theta(k)}$. You will then compute a new estimate, $\tilde{\theta(k)}$ using $\tilde{\theta(k)}$ and (y_k, x_k^T) . For the discussion below, further assume that you throw out $\tilde{\theta(k)}$ once you have $\tilde{\theta(k)}$ 1).

As for your goal, recall that in the batch setting you start with *all* the observations, (y,X). From this starting point, you may estimate the linear regression model's parameters, θ , by solving $X\theta=y$. In the online setting, you compute estimates one at a time. After seeing all m observations in X, your goal is to compute an $\tilde{\theta_{m-1}}\approx\theta$.

An intuitive (but flawed) idea. Indeed, there is a technique from the signal processing literature that we can apply to the linear regression problem, known as the *least mean square (LMS) algorithm*. Before describing it, let's start with an initial idea.

Suppose that you have a current estimate of the parameters, $\theta(k)$, when you get a new sample, (y_k, x_k^T) . The error in your prediction will be, $v_k - x_k^T \tilde{\theta(k)}$.

Ideally, this error would be zero. So, let's ask if there exists a *correction*, Δ_k , such that

$$y_k - x_k^T \left(\tilde{\theta(k)} + \Delta_k \right) = 0$$

$$\iff y_k - x_k^T \tilde{\theta(k)} = x_k^T \Delta_k$$

Then, you could compute a new estimate of the parameter by $\tilde{\theta(k+1)} = \tilde{\theta(k)} + \Delta_k$.

This idea has a major flaw, which we will discuss below. But before we do, please try the following exercise.

Mental exercise (no points). Verify that the following choice of Δ_k would make the preceding equation true.

$$\Delta_k = \frac{x_k^2}{\|x_k^2\|_2^2} \left(y_k - x_k^T \theta(\tilde{k}) \right).$$

Refining (or rather, "hacking") the basic idea: The least mean square (LMS) procedure. The basic idea sketched above has at least one major flaw: the choice of Δ_k might allow you to correctly predicts y_k from x_k and the new estimate $\tilde{\theta(k+1)} = \tilde{\theta(k)} + \Delta_k$, but there is no guarantee that this new estimate $\tilde{\theta(k+1)}$ preserves the quality of predictions made at all previous iterations!

There are a number of ways to deal with this problem, which includes carrying out an update with respect to some (or all) previous data. However, there is also a simpler "hack" that, though it might require some parameter tuning, can be made to work in practice.

That hack is as follows. Rather than using Δ_k as computed above, let's compute a different update that has a "fudge" factor, ϕ :

where
$$\begin{array}{rcl} \tilde{\theta(k+1)} & = & \tilde{\theta(k)} + \Delta_k \\ \Delta_k & = & \phi \cdot \hat{x_k} \left(y_k - x_k^T \tilde{\theta(k)} \right). \end{array}$$

A big question is how to choose ϕ . There is some analysis out there that can help. We will just state the results of this analysis without proof.

Let $\lambda_{\max}(X^TX)$ be the largest eigenvalue of X^TX . The result is that as the number of samples $m \to \infty$, any choice of ϕ that satisfies the following condition will *eventually* converge to the best least-squares estimator of $\tilde{\theta}$, that is, the estimate of $\tilde{\theta}$ you would have gotten by solving the linear least squares problem with all of the data.

$$0 < \phi < \frac{2}{\lambda_{\max}(X^T X)}.$$

This condition is not very satisfying, because you cannot really know $\lambda_{\max}(X^TX)$ until you've seen all the data, whereas we would like to apply this procedure *online* as the data arrive. Nevertheless, in practice you can imagine hybrid schemes that, given a batch of data points, use the QR fitting procedure to get a starting estimate for θ as well as to estimate a value of ϕ to use for all future updates.

Summary of the LMS algorithm. To summarize, the algorithm is as follows:

- Choose any initial guess, $\tilde{\theta(0)}$, such as $\tilde{\theta(0)} \leftarrow 0$.
- For each observation (y_k, x_k^T) , do the update:
 - $\theta(k+1) \leftarrow \theta_k + \Delta_k$,

```
where \Delta_k = \phi \cdot \hat{x_k} \left( y_k - \hat{x_k^T} \theta(k) \right).
```

Trying out the LMS idea

Now you should implement the LMS algorithm and see how it behaves.

To start, let's generate an initial 1-D problem (2 regression coefficients, a slope, and an intercept), and solve it using the batch procedure.

```
In [4]: m = 100000
    n = 1
    theta_true = generate_model(n)
    (X, y) = generate_data(m, theta_true, sigma=0.1)
    print("Condition number of the data matrix:", np.linalg.cond(X))
    theta = estimate_coeffs(X, y)
    e_rel = rel_diff(theta, theta_true)
    print("Relative error:", e_rel)
```

Condition number of the data matrix: 4.39135812542 Relative error: 5.33503083595e-05

Recall that we need a value for ϕ , for which we have an upper-bound of $\lambda_{\max}(X^TX)$. Let's cheat by computing it explicitly, even though in practice we would need to do something different.

```
In [5]: LAMBDA_MAX = max(np.linalg.eigvals(X.T.dot(X)))
    print(LAMBDA_MAX)

126906.922988
```

Exercise 1 (5 points). Implement the online LMS algorithm in the code cell below where indicated. It should produce a final parameter estimate, theta 1ms, as a column vector.

In addition, the skeleton code below uses $rel_diff()$ to record the relative difference between the estimate and the true vector, storing the k-th relative difference in $rel_diffs[k]$. Doing so will allow you to see the convergence behavior of the method.

Lastly, to help you out, we've defined a constant in terms of $\lambda_{\max}(X^TX)$ that you can use for ϕ .

In practice, you would only maintain the current estimate, or maybe just a few recent estimates, rather than all of them. Since we want to inspect these vectors later, go ahead and store them all.

```
theta_k = theta_k + delta_k
### END SOLUTION

theta_lms = theta_k
rel_diffs[m] = rel_diff(theta_lms, theta_true)
```

Let's compare the true coefficients against the estimates, both from the batch algorithm and the online algorithm.

Let's also compute the relative differences between each estimate Theta[:, k] and the true coefficients theta_true, measured in the two-norm, to see if the estimate is converging to the truth.

```
Out[8]: [<matplotlib.lines.Line2D at 0x1124cdba8>]

16
14
12
10
08
06
04
```

60000

80000

100000

You should see it converging, but not especially quickly.

1.2

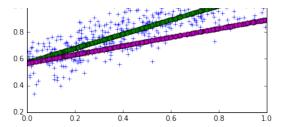
Finally, if the dimension is n=1, let's go ahead and do a sanity-check regression fit plot.

40000

20000

In [8]: plt.plot(range(len(rel_diffs)), rel_diffs)

```
In [9]: STEP = int(X.shape[0] / 500)
if n == 1:
    fig = plt.figure()
    ax1 = fig.add_subplot(111)
    ax1.plot(X[::STEP, 1], Y[::STEP], 'b+') # blue - data
    ax1.plot(X[::STEP, 1], X.dot(theta_true)[::STEP], 'r*') # red - true
    ax1.plot(X[::STEP, 1], X.dot(theta)[::STEP], 'go') # green - batch
    ax1.plot(X[::STEP, 1], X.dot(theta_lms)[::STEP], 'mo') # magenta - pure LMS
else:
    print("Plot is multidimensional; I live in Flatland, so I don't do that.")
```



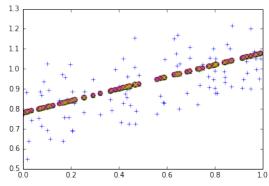
Exercise 2 (ungraded, optional). We said previously that, in practice, you would probably do some sort of hybrid scheme that mixes full batch updates (possibly only initially) and incremental updates. Implement such a scheme and describe what you observe.

In [10]: Student's answer (Top) # Setup problem and compute the batch solution m = 100000n = 1theta_true = generate_model(n) (X, y) = generate data(m, theta true, sigma=0.1) theta_batch = estimate_coeffs(X, y) # Your turn, below: Implement a hybrid batch-LMS solution # assuming you observe the first few data points all at # once, and then see the remaining points one at a time. **###** BEGIN SOLUTION def lms(X, y, theta_0=None, PHI=1e-6): """Implements the LMS algorithm for the system X theta = y.""" print(X.shape) (m, n) = X.shapeif theta_0 is None: theta_k = np.zeros((n)) else: theta_k = theta_0 theta_k = np.reshape(theta_k, (n, 1)) for k in range(m): $x_k = x[k:k+1, :].T$ $r_k = y[k] - x_k.T.dot(theta_k)$ delta_k = PHI * r_k * x_k $theta_k = theta_k + delta_k$ return theta k # Pure LMS solution START = 100lambdas = np.linalg.eigvals(X[:START, :].T.dot(X[:START, :])) lambda_max = max(lambdas) lambda min = min(lambdas) phi = 2.0 / (lambda_max + lambda_min) # See: https://en.wikipedia.org/wiki/Least_mean_s quares filter theta_lms = lms(X, y, PHI=phi) # Batch on first START observations + LMS on the rest: theta_batch_START = estimate_coeffs(X[:START, :], y[:START]) print(theta_batch_START) theta_hybrid = lms(X[START:, :], y[START:], theta_0=theta_batch_START, PHI=phi) print(theta hybrid) def calc_ssqr(theta, X, y): r = X.dot(theta) - yreturn r.T.dot(r) print("=== Sum of squared errors ===") print("True:", calc_ssqr(theta_true, X, y))
print("Batch:", calc_ssqr(theta_batch, X, y)) print("Batch-{}:".format(START), calc_ssqr(theta_batch_START, X, y)) print("LMS(phi={}):".format(phi), calc_ssqr(theta_lms, X, y)) print("Batch ($k \le d$) + LMS:" % START, calc ssqr(theta hybrid, X, y))

print("=== Relative error in the coefficients (theta) ===")

```
print("Batch:", rel_diff(theta_batch, theta_true))
print("Batch-{}:".format(START), rel_diff(theta_batch_START, theta_true))
print("LMS(phi={}):".format(phi), rel_diff(theta_lms, theta_true))
print("Batch (k <= %d) + LMS:" % START, rel_diff(theta_hybrid, theta_true))</pre>
STEP = int(X.shape[0] / 100)
if n == 1:
   fig = plt.figure()
   ax1 = fig.add_subplot(111)
   ax1.plot(X[::STEP, 1], y[::STEP], 'b+') # blue - data
   ax1.plot(X[::STEP, 1], X.dot(theta_true)[::STEP], 'r*') # red - true
   ax1.plot(X[::STEP, 1], X.dot(theta_batch)[::STEP], 'go') # green - batch
   ax1.plot(X[::STEP, 1], X.dot(theta_hybrid)[::STEP], 'yx') # yellow - hybrid
else:
   print ("Plot is multidimensional; I live in Flatland, so I don't do that.")
### END SOLUTION
```

```
(100000, 2)
[[ 0.77207733]
 [ 0.2900984 ]]
(99900, 2)
[[ 0.7816781 ]
[ 0.29958356]]
=== Sum of squared errors ===
True: [[ 1000.46946709]]
Batch: [[ 1000.43147542]]
Batch-100: [[ 1014.67895574]]
LMS(phi=0.015300595151412038): [[ 1001.19911514]]
Batch (k \le 100) + LMS: [[ 1001.19911514]]
=== Relative error in the coefficients (theta) ===
Batch: 0.00103335784341
Batch-100: 0.0134152031253
LMS(phi=0.015300595151412038): 0.00381637346062
Batch (k <= 100) + LMS: 0.00381637346062
```



Fin! If you've gotten this far without errors, your notebook is ready to submit.

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