In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from scipy.linalg import solve_triangular
from sklearn.linear_model import Ridge
```

Problem 1

Derive/show how to compute linear regression coefficients (for general choice of y and X) using the following four methods: naive linear algebra; QR decomposition; SVD; and Cholesky decomposition.

Optionally, look up the computational (time) complexity of each of these methods as a function of p (number of predictors/columns of X) and n (number of observations/length of y/rows of X)

Pick three of the four algorithms and implement them in the language of your choice. Benchmark your algorithms for a range of magnitudes of p and n covering at least one order of magnitude in p and at least two orders of magnitude in n. Plot your results on a log-log scale. Fit a log-log model to the average times (you can leave out some points if they mess up the scaling relationship).

1. Naive linear algebra

The residual sum-of-squares can be written as

$$\begin{aligned}
\text{RSS}(\beta) &= (\mathbf{y} - \mathbf{X}\beta)^T(\mathbf{y} - \mathbf{X}\beta) && (1)\\
&= (\mathbf{y}^T - \beta^T\mathbf{X}^T)(\mathbf{y} - \mathbf{X}\beta) && (2)\\
&= \mathbf{y}^T\mathbf{y} - \mathbf{y}^T\mathbf{X}\beta - \beta^T\mathbf{X}^T\mathbf{y} + \beta^T\mathbf{X}^T\mathbf{X}\beta && (3)\\
&= \mathbf{y}^T\mathbf{y} - 2\beta^T\mathbf{X}^T\mathbf{y} + \beta^T\mathbf{X}^T\mathbf{X}\beta && (4)
\end{aligned}$$

where the last equality is due to the special case that $\mathbf{y}$ and β are vectors, such that $\mathbf{y}^T\mathbf{X}\beta$ and $\beta^T\mathbf{X}^T\mathbf{y}$ are scalars and therefore symmetric.

Differentiating w.r.t. β:

$$\begin{aligned}
\frac{\partial \text{RSS}}{\partial \beta} &= -2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\beta && (5)\\
&= -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta) && (6)
\end{aligned}$$

Setting the derivative to zero gives

$$\begin{aligned}
\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta) &= 0 && (7)\\
\mathbf{X}^T\mathbf{X}\beta &= \mathbf{X}^T\mathbf{y} && (8)\\
\beta &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} && (9)
\end{aligned}$$

Resources:
http://www.gatsby.ucl.ac.uk/teaching/courses/sntn/sntn-2017/resources/Matrix_derivatives_cribsheet.pdf
https://math.stackexchange.com/questions/2753210/when-can-we-say-that-a-mathrm-t-b-b-mathrm-t-a

In [9]:
```
def ls_naive(X,y):
    return np.matmul(np.matmul(np.linalg.inv(np.matmul(X.T, X)), X.T), y)
```

2. QR decomposition

Given the factorization $\mathbf{X} = \mathbf{QR}$ where $\mathbf{Q}$ is an orthogonal matrix ($\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$) and $\mathbf{R}$ is an upper triangular matrix, the equation for β simplifies to:

$$
\begin{align}
\beta &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \tag{10}\\
&= (\mathbf{R}^T\mathbf{Q}^T\mathbf{QR})^{-1}\mathbf{R}^T\mathbf{Q}^T\mathbf{y} \tag{11}\\
&= (\mathbf{R}^T\mathbf{R})^{-1}\mathbf{R}^T\mathbf{Q}^T\mathbf{y} \tag{12}\\
&= \mathbf{R}^{-1}\mathbf{Q}^T\mathbf{y} \tag{13}
\end{align}
$$

As $\mathbf{R}$ is an upper triangular matrix, the equation

$$\mathbf{R}\beta = \mathbf{Q}^T\mathbf{y}$$

can be solved by back substitution.

QR decomposition can be computed using e.g. the Gram-Schmidt method

Resources:
For realizing that $\beta = \mathbf{R}^{-1}\mathbf{Q}^T\mathbf{y}$ should be re-arranged to $\mathbf{R}\beta = \mathbf{Q}^T\mathbf{y}$ and solved using backward substitution:
https://stats.stackexchange.com/questions/160007/understanding-qr-decomposition
Implementation of Gram-Schmidt for QR decomposition:
https://en.wikipedia.org/wiki/QR_decomposition

In [10]:
```
def GramSchmidt_QR(X):
    U = np.zeros(X.shape)
    U[:,0] = X[:,0]
    for col_i in range(1,X.shape[1]):
        a_i = X[:,col_i]
        U[:,col_i] = a_i
        for i in range(col_i):
            u = U[:,i]
            U[:,col_i] -= np.dot(u, a_i)/np.dot(u,u) * u
    Q = np.divide(U, np.linalg.norm(U, axis=0))
    R = np.matmul(Q.T, X)
    return Q, R

def ls_QR(X,y):
```

```
#     Q, R = GramSchmidt_QR(X)
    Q, R = np.linalg.qr(X)
    beta = solve_triangular(R, np.matmul(Q.T, y))
    return beta
```

3. SVD

SVD can be used to decompose $\mathbf{X}$ into the product of $\mathbf{USV}^T$ where $\mathbf{U}$ and $\mathbf{V}$ are unitary matrices. The equation for β can then be simplified:

$$\begin{aligned}
\beta &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} && (14)\\
&= (\mathbf{VS}^T\mathbf{U}^T\mathbf{USV}^T)^{-1}\mathbf{VS}^T\mathbf{U}^T\mathbf{y} && (15)\\
&= (\mathbf{VS}^T\mathbf{SV}^T)^{-1}\mathbf{VS}^T\mathbf{U}^T\mathbf{y} && (16)\\
&= \mathbf{VS}^{-1}(\mathbf{S}^T)^{-1}\mathbf{V}^T\mathbf{VS}^T\mathbf{U}^T\mathbf{y} && (17)\\
&= \mathbf{VS}^{-1}\mathbf{U}^T\mathbf{y} && (18)
\end{aligned}$$

Resources used:
https://en.wikipedia.org/wiki/Moore%E2%80%93Penrose_inverse

In [11]:
```
def ls_SVD(X,y):
    u, s, vh = np.linalg.svd(X)
    s_pseudoinv = np.zeros([u.shape[1],vh.shape[0]])
    s_pseudoinv[:len(s),:len(s)] = np.diag(1/s)
    s_pseudoinv = s_pseudoinv.T
    X_pseudoinv = np.matmul(np.matmul(vh.T, s_pseudoinv),u.T)

    return np.matmul(X_pseudoinv,y)
```

4. Cholesky decomposition

Alternatively, we can solve $\mathbf{X}^T\mathbf{X}\beta = \mathbf{X}^T\mathbf{y}$ by applying a Cholesky decomposition to $\mathbf{X}^T\mathbf{X}$, i.e. $\mathbf{X}^T\mathbf{X} = \mathbf{LL}^T$, where $\mathbf{L}$ is lower triangular. We solve for β by first solving

$$\mathbf{Lb} = \mathbf{X}^T\mathbf{y}$$

by forward substitution, then

$$\mathbf{L}^T\beta = \mathbf{b}$$

by backward substitution

Resources used:
https://en.wikipedia.org/wiki/Cholesky_decomposition
https://numpy.org/doc/stable/reference/generated/numpy.linalg.cholesky.html

In [12]:
```
def ls_cholesky(X,y):
    L = np.linalg.cholesky(np.matmul(X.T, X))
    b1 = solve_triangular(L, np.matmul(X.T,y), lower=True)
```

```
    beta = solve_triangular(L.T, b1)
    return beta
```

Run time analysis:

Somehow the naive linear algebra is faster than the QR decomposition and SVD methods (not shown because it crashed the kernel for some of the test cases). Not sure what I am doing wrong.

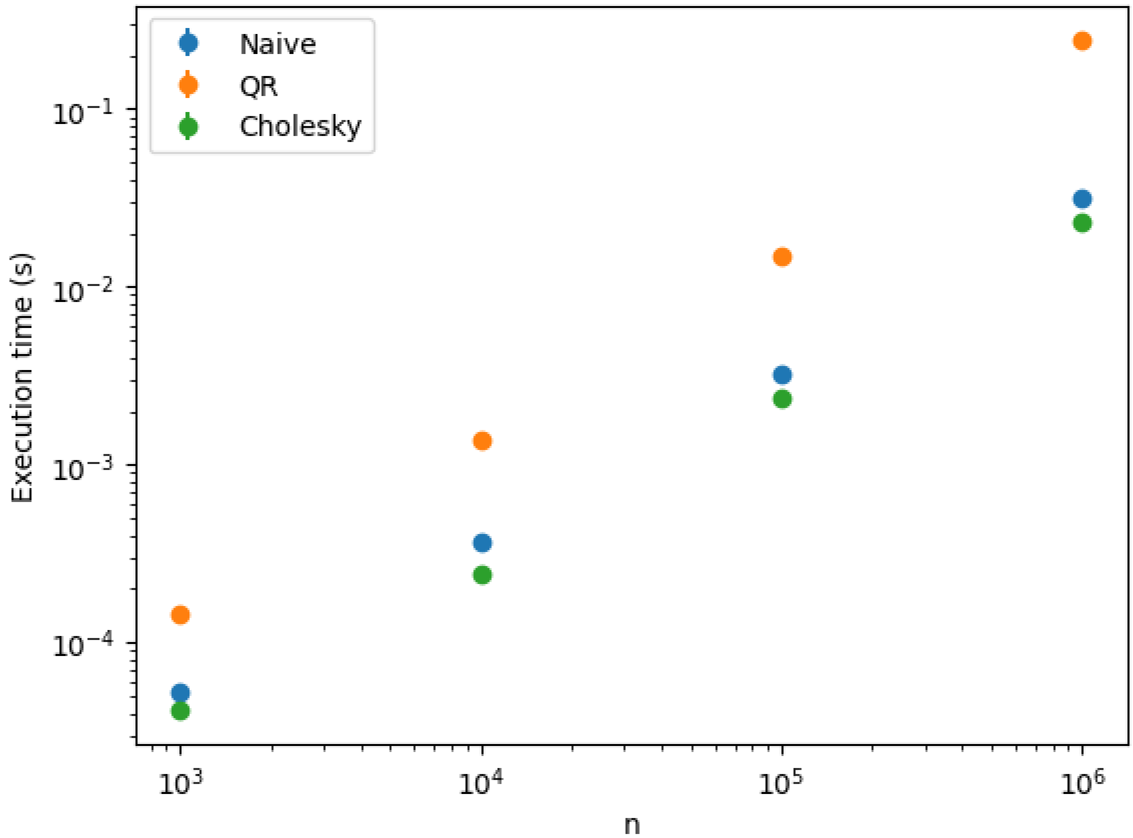
In [13]:
```
def generate_data(n, p):
    means = np.random.normal(loc=0, scale=10, size=p)
    stds = np.abs(np.random.normal(loc=5, scale=1, size=p))
    betas = np.random.normal(loc=0, scale=20, size=p+1)
    X = np.ones([n, p+1])
    for i in range(p):
        X[:,i] = np.random.normal(loc=means[i], scale=stds[i], size=n)
    y = np.matmul(X, betas)
    y += np.random.normal(loc=0, scale=2, size=y.shape)
    return X, y
```

In [14]:
```
n = np.logspace(3, 6, 4, dtype=int)
naive_times = np.zeros([len(n),2])
QR_times = np.zeros([len(n),2])
SVD_times = np.zeros([len(n),2])
cholesky_times = np.zeros([len(n),2])

for i in range(len(n)):
    X, Y = generate_data(n[i], 10)
    naive = %timeit -o ls_naive(X, Y)
    naive_times[i] = [np.mean(naive.timings), np.std(naive.timings)]
    QR = %timeit -o ls_QR(X, Y)
    QR_times[i] = [np.mean(QR.timings), np.std(QR.timings)]
#     SVD = %timeit -o ls_SVD(X, Y)
#     SVD_times[i] = [np.mean(SVD.timings), np.std(SVD.timings)]
    cholesky = %timeit -o ls_cholesky(X, Y)
    cholesky_times[i] = [np.mean(cholesky.timings), np.std(cholesky.timings)
```

```
52.6 µs ± 4.61 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
145 µs ± 4.13 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
41.7 µs ± 395 ns per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
370 µs ± 33.1 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
1.36 ms ± 19.4 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
245 µs ± 271 ns per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
3.24 ms ± 221 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
14.8 ms ± 193 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
2.39 ms ± 8.94 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
31.8 ms ± 1.65 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
246 ms ± 2.02 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
23.4 ms ± 15.5 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

In [21]:
```
plt.errorbar(n, naive_times[:,0], yerr=naive_times[:,1], fmt='o', label="Nai
plt.errorbar(n, QR_times[:,0], yerr=QR_times[:,1], fmt='o', label="QR")
plt.errorbar(n, cholesky_times[:,0], yerr=cholesky_times[:,1], fmt='o', labe
plt.xscale("log")
plt.yscale("log")
```

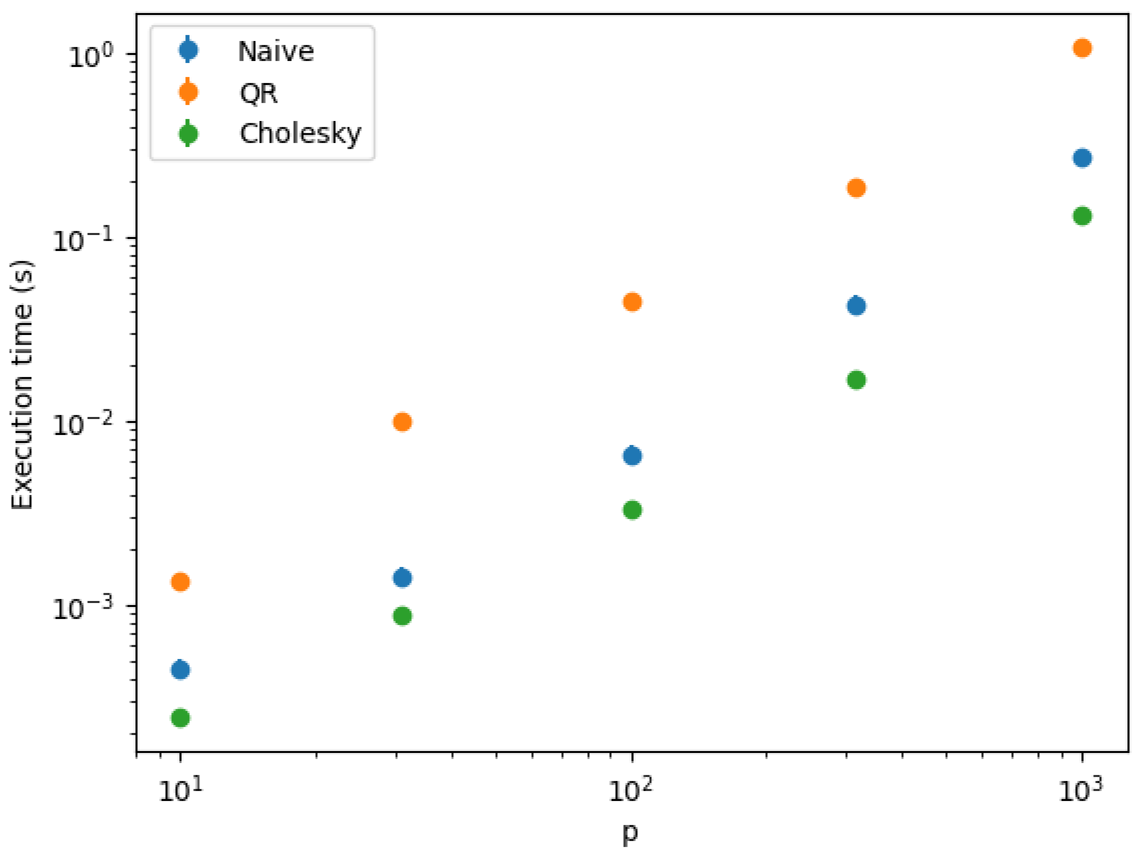
```
plt.xlabel("n")
plt.ylabel("Execution time (s)")
plt.legend(loc="best")
plt.show()
```



In [22]:
```
p = np.logspace(1, 3, 5, dtype=int)
naive_times_p = np.zeros([len(p),2])
QR_times_p = np.zeros([len(p),2])
cholesky_times_p = np.zeros([len(p),2])

for i in range(len(p)):
    X, Y = generate_data(10000, p[i])
    naive = %timeit -o ls_naive(X, Y)
    naive_times_p[i] = [np.mean(naive.timings), np.std(naive.timings)]
    QR = %timeit -o ls_QR(X, Y)
    QR_times_p[i] = [np.mean(QR.timings), np.std(QR.timings)]
#     SVD = %timeit -o ls_SVD(X, Y)
#     SVD_times[i] = [np.mean(SVD.timings), np.std(SVD.timings)]
    cholesky = %timeit -o ls_cholesky(X, Y)
    cholesky_times_p[i] = [np.mean(cholesky.timings), np.std(cholesky.timing
```

```
451 µs ± 59.2 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
1.34 ms ± 11 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
245 µs ± 452 ns per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
1.44 ms ± 167 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
10 ms ± 723 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
873 µs ± 35 µs per loop (mean ± std. dev. of 7 runs, 1,000 loops each)
6.57 ms ± 775 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
44.8 ms ± 3.73 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
3.32 ms ± 370 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
43.3 ms ± 5.56 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
188 ms ± 17.5 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
17.1 ms ± 410 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
273 ms ± 15.3 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
1.07 s ± 28.2 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
132 ms ± 8.04 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

In [23]:
```
plt.errorbar(p, naive_times_p[:,0], yerr=naive_times_p[:,1], fmt='o', label=
plt.errorbar(p, QR_times_p[:,0], yerr=QR_times_p[:,1], fmt='o', label="QR")
plt.errorbar(p, cholesky_times_p[:,0], yerr=cholesky_times_p[:,1], fmt='o',
plt.xscale("log")
plt.yscale("log")
plt.xlabel("p")
plt.ylabel("Execution time (s)")
plt.legend(loc="best")
plt.show()
```



Problem 2

Implement ridge regression by data augmentation in the language of your choice. Compare results and timing with a native implementation of ridge regression.

1. Data augmentation

From the notes, using the augmented data matrix

$$\mathbf{B} = \begin{bmatrix} \mathbf{X} \\ \sqrt{\lambda}\mathbf{I} \end{bmatrix}$$

and augmented observations $\mathbf{y}^* = (\mathbf{y} \quad 0)$, we have

$$(\mathbf{B}^T\mathbf{B})\beta = \mathbf{B}^T\mathbf{y}^*$$

Applying QR decomposition: $\mathbf{B} = \mathbf{QR}$

$$(\mathbf{R}^T\mathbf{Q}^T\mathbf{QR})\beta = \mathbf{R}^T\mathbf{Q}^T\mathbf{y}^* \tag{19}$$
$$\mathbf{R}^T\mathbf{R}\beta = \mathbf{R}^T\mathbf{Q}^T\mathbf{y}^* \tag{20}$$

which can be solved by first solving

$$\mathbf{R}^T\mathbf{A} = \mathbf{R}^T\mathbf{Q}^T\mathbf{y}^*$$

then solving

$$\mathbf{R}\beta = \mathbf{A}$$

In [2]:
```
def ridge_augmentation(X,y,lamb):
    B = np.zeros([X.shape[0]+X.shape[1], X.shape[1]])
    B[:X.shape[0],:] = X
    B[X.shape[0]:,:] = np.diag(lamb**0.5 * np.ones(X.shape[1]))

    y_star = np.zeros(len(y)+X.shape[1])
    y_star[:len(y)] = y

    Q, R = np.linalg.qr(B)
    A = solve_triangular(R.T, np.matmul(np.matmul(R.T,Q.T),y_star), lower=Tr
    beta = solve_triangular(R, A)
    return beta
```

In [14]:
```
def compute_RSS(X, y, beta):
    residuals = y - np.matmul(X,beta)
    return np.matmul(residuals.T, residuals)

def normalize_columns(A):
    """scale to have mean zero and variance 96 like in ESL"""
    A -= np.mean(A, axis=0)
    std = np.std(A, axis=0)
    A /= std
    A *= 96**0.5
    return A
```

In [5]:
```
prostate_data = pd.read_csv("prostate_cancer.txt", index_col=0, delimiter='\
prostate_data["train"].astype("category")
prostate_data.head()
```

Out[5]:

	lcavol	lweight	age	lbph	svi	lcp	gleason	pgg45	lpsa	train
1	-0.579818	2.769459	50	-1.386294	0	-1.386294	6	0	-0.430783	T
2	-0.994252	3.319626	58	-1.386294	0	-1.386294	6	0	-0.162519	T
3	-0.510826	2.691243	74	-1.386294	0	-1.386294	7	20	-0.162519	T
4	-1.203973	3.282789	58	-1.386294	0	-1.386294	6	0	-0.162519	T
5	0.751416	3.432373	62	-1.386294	0	-1.386294	6	0	0.371564	T

In [6]:
```
train_set = prostate_data[prostate_data["train"]=="T"]
test_set = prostate_data[prostate_data["train"]=="F"]

train_X = train_set[["lcavol", "lweight", "age", "lbph", "svi", "lcp", "glea
train_X = normalize_columns(train_X)
train_Y = train_set["lpsa"].to_numpy()

test_X = test_set[["lcavol", "lweight", "age", "lbph", "svi", "lcp", "gleaso
test_X = normalize_columns(test_X)
test_Y = test_set["lpsa"].to_numpy()
```

In order to prevent shrinking the intercept, we center $\mathbf{y}$ upfront by subtracting the mean of the training set from both the training and test labels.

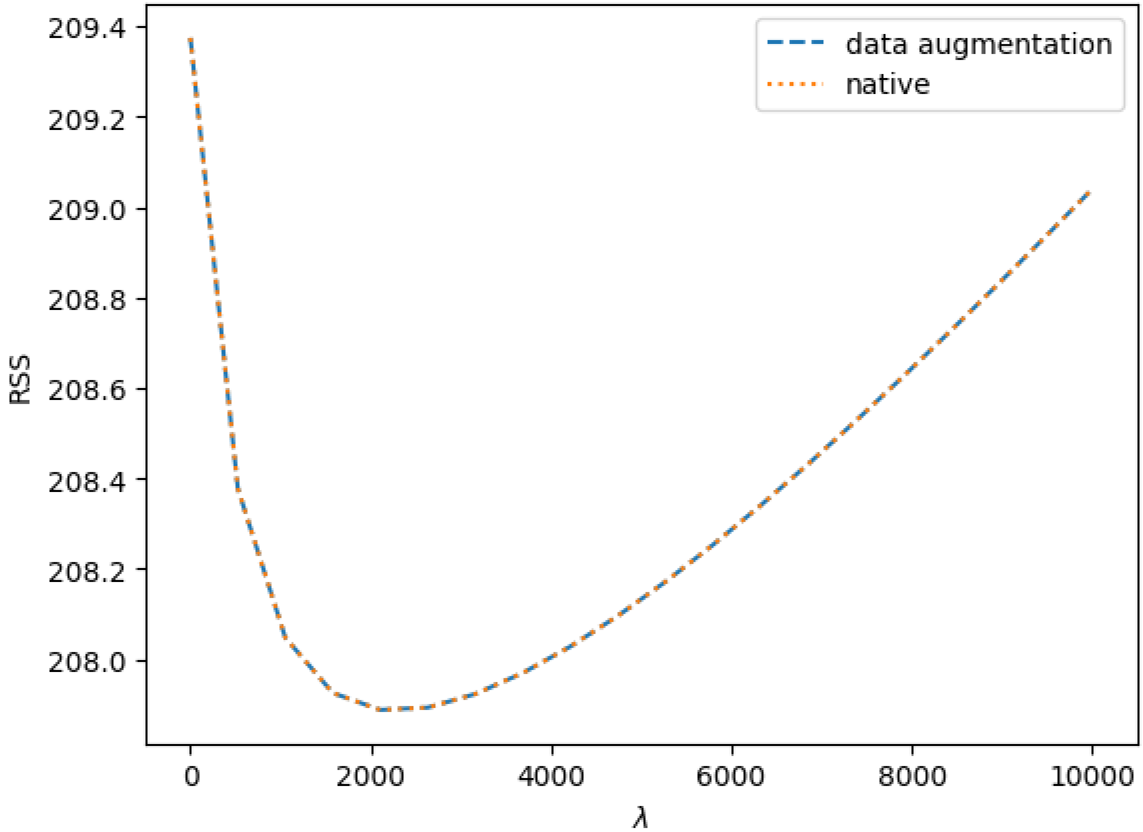
In [36]:
```
n = 20
lambdas = np.linspace(0, 10000, n)
intercept = np.mean(train_Y)

RSS_aug = np.zeros(n)
RSS_native = np.zeros(n)
for i in range(len(lambdas)):
    beta_aug = ridge_augmentation(train_X, train_Y-intercept, lambdas[i])
    RSS_aug[i] = compute_RSS(test_X, test_Y-intercept, beta_aug)

    ## native implementation using scikit-learn, automatically fits intercep
    clf = Ridge(alpha=lambdas[i])
    clf.fit(train_X, train_Y)
    y_hat = clf.predict(test_X)
    residuals = test_Y - y_hat
    RSS_native[i] = np.matmul(residuals.T, residuals)
```

Performance results:

The two approaches give essentially identical results. It is surprising to me that such a high value of λ is optimal...

In [35]:
```
plt.plot(lambdas, RSS_aug, ls='dashed', label="data augmentation")
plt.plot(lambdas, RSS_native, ls='dotted', label="native")
```

```
plt.legend(loc='best')
plt.xlabel("$\lambda$")
plt.ylabel("RSS")
plt.show()
```



Timing comparison:

Somehow the native implementation is slower. Maybe there is some overhead in the fit() method which I haven't isolated out of the timing loop.

In [22]:
```
%timeit -r 10 ridge_augmentation(train_X, train_Y, 1)
```

```
32.6 µs ± 31.1 ns per loop (mean ± std. dev. of 10 runs, 10,000 loops each)
```

In [39]:
```
clf = Ridge(alpha=1)
```

In [38]:
```
%timeit -r 10 clf.fit(train_X, train_Y)
```

```
89.9 µs ± 712 ns per loop (mean ± std. dev. of 10 runs, 10,000 loops each)
```

I'm not taking the class for credit, and have not attempted the remainder of the problem set, but would really appreciate comments/feedback on the first two problems.