STATS 790

Assignment 2

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```
In [116…
import time
import timeit
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
from numpy.linalg import inv, qr, svd, cholesky
from scipy.linalg import solve_triangular

import warnings
warnings.simplefilter("ignore")
```

Q1.a

Denote by β the linear regression coefficients, by X the predictors, and by y the response variable.

Naive linear algebra derivation

$$\begin{gathered}X\beta = y\\ X^TX\beta = X^Ty\\ \beta = (X^TX)^{-1}X^Ty\end{gathered}$$

QR decomposition derivation

In this case, if X is an $n \times p$ matrix of full rank, we have $X = QR$ where Q is a $n \times p$ orthonormal matrix and R is a $p \times p$ upper triangular matrix.

Thus, we can derive

$$\begin{gathered}X\beta = y\\ X^TX\beta = X^Ty\\ (QR)^TQR\beta = (QR)^Ty\\ R^T(Q^TQ)R\beta = R^TQ^Ty\\ R^TR\beta = R^TQ^Ty\\ (R^T)^{-1}R^TR\beta = (R^T)^{-1}R^TQ^Ty\\ R\beta = Q^Ty\\ \beta = R^{-1}Q^Ty\end{gathered}$$

SVD derivation

In this case, if X is an $n \times p$ matrix of full rank, we have $X = USV^T$ where U is a $n \times n$ unitary matrix and S is an $n \times p$ matrix consisting of non-negative singular values and zeros else where, and V^T is an $p \times p$ unitary matrix.

Besides, as U, V are unitary matrices, we have

$$\begin{gathered}UU^T = U^TU = I\\ VV^T = V^TV = I\end{gathered}$$

Thus, we can derive

$$\begin{gathered}X\beta = y\\ USV^T\beta = y\\ (USV^T)^{-1}USV^T\beta = (USV^T)^{-1}y\\ (V^T)^{-1}S^{-1}(U^{-1}U)SV^T\beta = (V^T)^{-1}S^{-1}U^{-1}y\\ V(S^{-1}S)V^T\beta = VS^{-1}U^Ty\\ VV^T\beta = VS^{-1}U^Ty\\ \beta = VS^{-1}U^Ty\end{gathered}$$

Cholesky decomposition derivation

In this case, if X is an $n \times p$ of full rank, we have $A = X^TX$ is positive definite. Then there exists a lower triangular matrix L such at $A = LL^T$.

Thus, we can derive

$$\begin{gathered}X\beta = y\\ X^TX\beta = X^Ty\\ LL^T\beta = X^Ty\\ L^T\beta = L^{-1}X^Ty\\ \beta = (L^T)^{-1}L^{-1}X^Ty\end{gathered}$$

Now, since L^T is an upper triangular matrix (row-echelon form), we can solve for β using back substitution.

Q1.b

The `benchmarking` function takes as input the name of the algorithm and given values of n and p. It will return the time spent on running the algorithm for solving β.

```
In [112…
def benchmarking(algorithm, n, p):

    np.random.seed(123)
    X = np.random.randn(n, p)
    y = np.random.randn(n)

    if algorithm == "Naive linear algebra":
        t = 0
        for i in range(10):
            start = time.time()
            beta = inv(np.dot(X.T, X)).dot(X.T).dot(y)
            end = time.time()
            t += end-start
    elif algorithm == "QR decomposition":
        t = 0
        for i in range(10):
            start = time.time()
            q, r = qr(X)
            beta = np.dot(inv(r), q.T).dot(y) # solve_triangular(r, np.dot(q.T, y))
            end = time.time()
            t += end-start
    elif algorithm == "SVD":
        t = 0
        for i in range(10):
            start = time.time()
            u, s, vT = svd(X)
            s_inv = np.zeros(X.shape).T
            s_inv[:p,:p] = np.diag(1/s)
            beta = np.dot(vT.T, s_inv).dot(u.T).dot(y)
            end = time.time()
            t += end-start
    elif algorithm == "Cholesky decomposition":
        t = 0
        for i in range(10):
            start = time.time()
            L = cholesky(np.dot(X.T, X))
            beta = np.dot(inv(L.T), inv(L)).dot(X.T).dot(y) # solve_triangular(L.T, np.dot(inv(L), X.T).dot(y))
            end = time.time()
            t += end-start

    return t/10
```

We use the `benchmarking` function to benchmark the four algorithms for $p = [10]$ and $n = [1000, 10000, 100000]$.

```
In [113…
algorithms = ["Naive linear algebra", "QR decomposition", "SVD", "Cholesky decomposition"]
p_values = [10]
n_values = [1000, 10000]

results = []
for algorithm in algorithms:
    for p in p_values:
        for n in n_values:
            t = benchmarking(algorithm, n, p)
            results.append(pd.Series({
                'Algorithm': algorithm,
                'P': p,
                'N': n,
                'Avg Time (ms)': t*1000
            }))


results_df = pd.concat(results, axis=1).T
results_df
```

Out[113]:

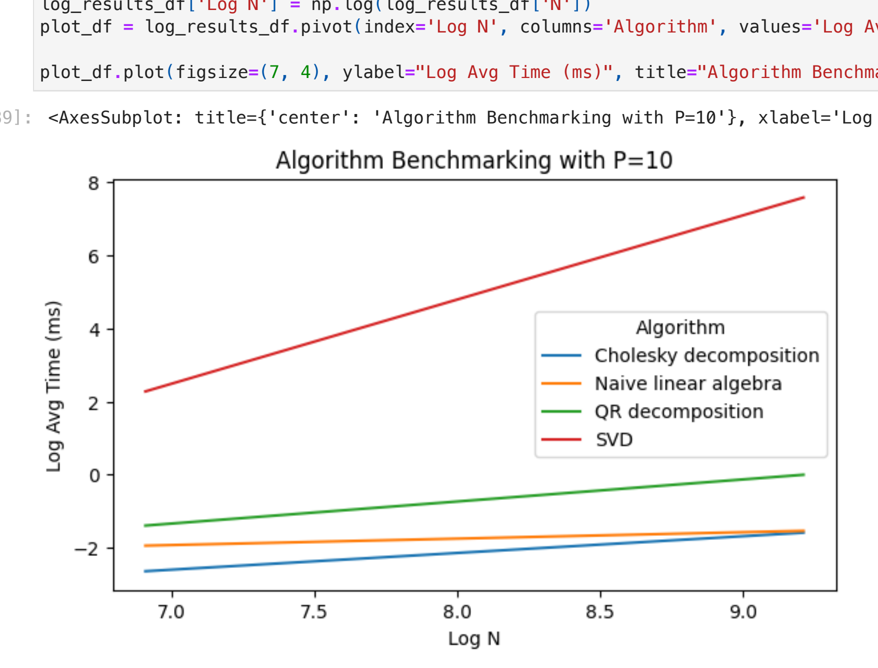
	Algorithm	P	N	Avg Time (ms)
0	Naive linear algebra	10	1000	0.143194
1	Naive linear algebra	10	10000	0.214767
2	QR decomposition	10	1000	0.248003
3	QR decomposition	10	10000	0.996351
4	SVD	10	1000	9.748769
5	SVD	10	10000	1964.84561
6	Cholesky decomposition	10	1000	0.071144
7	Cholesky decomposition	10	10000	0.204206

We plot the results dataframe on a log-log scale.

```
In [139…
log_results_df = results_df.copy()
log_results_df['Avg Time (ms)'] = log_results_df['Avg Time (ms)'].astype("float")
log_results_df['N'] = log_results_df['N'].astype("float")
log_results_df['Log Avg Time (ms)'] = np.log(log_results_df['Avg Time (ms)'])
log_results_df['Log N'] = np.log(log_results_df['N'])
plot_df = log_results_df.pivot(index='Log N', columns='Algorithm', values='Log Avg Time (ms)')

plot_df.plot(figsize=(7, 4), ylabel="Log Avg Time (ms)", title="Algorithm Benchmarking with P=10")
```

```
Out[139]: <AxesSubplot: title={'center': 'Algorithm Benchmarking with P=10'}, xlabel='Log N', ylabel='Log Avg Time (ms)'>
```



Q2

```
In [2]:
import pandas as pd

df = pd.read_csv("https://hastie.su.domains/ElemStatLearn/datasets/prostate.data", sep="\t", index_col=0)
df.reset_index(drop=True, inplace=True)
df.head()
```

Out[2]:

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

Train test split

```
In [38]:
X_train = df[df.train=="T"].iloc[:,:7]
y_train = df[df.train=="T"].iloc[:,8]
X_test = df[df.train=="F"].iloc[:,:7]
y_test = df[df.train=="F"].iloc[:,8]

X_train.shape, y_train.shape, X_test.shape, y_test.shape
```

```
Out[38]: ((67, 7), (67,), (30, 7), (30,))
```

Feature scaling

We scale the features so that they have mean 0 and standard deviation $\sqrt{96} \approx 9.8$.

```
In [39]:
mean = X_train.mean()
std = X_train.std()

X_train = (X_train - mean) / std
X_train = X_train * np.sqrt(96) + 0

X_test = (X_test - mean) / std
X_test = X_test * np.sqrt(96) + 0
```

Let's check that `X_train` and `X_test` are scaled correctly.

```
In [40]: X_train.describe()
```

Out[40]:

	lcavol	lweight	age	lbph	svi	lcp	gleason
count	6.700000e+01	6.700000e+01	6.700000e+01	6.700000e+01	6.700000e+01	6.700000e+01	6.700000e+01
mean	-5.832814e-16	-1.818777e-14	-7.980349e-15	5.302558e-16	-1.166563e-15	2.200561e-15	3.141765e-15
std	9.797959e+00	9.797959e+00	9.797959e+00	9.797959e+00	9.797959e+00	9.797959e+00	9.797959e+00
min	-2.097884e+01	-2.572221e+01	-3.101286e+01	-9.758325e+00	-5.222929e+00	-8.198625e+00	-1.010868e+01
25%	-6.506891e+00	-6.079992e+00	-4.892664e+00	-9.758325e+00	-5.222929e+00	-8.198625e+00	-1.010868e+01
50%	1.217325e+00	-5.638379e-01	3.313757e-01	-8.215973e-01	-5.222929e+00	-4.087135e+00	3.713391e+00
75%	8.165610e+00	5.293733e+00	5.555416e+00	9.881041e+00	-5.222929e+00	8.456766e+00	3.713391e+00
max	1.977200e+01	2.372959e+01	1.861552e+01	1.509443e+01	1.810615e+01	2.008199e+01	3.135752e+01

```
In [41]: X_test.describe()
```

Out[41]:

	lcavol	lweight	age	lbph	svi	lcp	gleason
count	30.000000	30.000000	30.000000	30.000000	30.000000	30.000000	30.000000
mean	0.931034	0.188443	-3.717255	0.625866	-0.557112	0.787909	0.948978
std	8.174025	6.186211	9.198831	9.668280	9.491160	9.886349	10.520312
min	-16.480036	-15.645743	-28.400844	-9.758325	-5.222929	-8.198625	-10.108675
25%	-4.076432	-3.011001	-6.198674	-9.758325	-5.222929	-8.198625	-10.108675
50%	1.033493	0.501776	-0.974634	2.455523	-5.222929	-1.514948	3.713391
75%	5.831936	4.352737	3.922903	10.050141	-5.222929	9.099812	3.713391
max	17.019807	10.183721	6.861426	14.057073	18.106155	21.812575	31.357523

Data augmentation

We create new training data by adding Gaussian noises `X_noise` and `y_noise` to `X_train` and `y_train` respectively. We append the new data `X_new` and `y_new` to `X_train` and `y_train` respectively. By doing so, we obtain the augmented training data `y_train_aug` and `y_train_aug`.

```
In [70]:
np.random.seed(123)

# augmenting X_train
X_noise = np.random.normal(size=X_train.shape)
X_new = pd.DataFrame(X_train.values + X_noise, columns = X_train.columns)
X_train_aug = pd.concat([X_train, X_new])
X_train_aug.reset_index(drop=True, inplace=True)

# augmenting y_train
y_noise = np.random.normal(size=y_train.shape)
y_new = pd.Series(y_train.values + y_noise) #y_aug = pd.DataFrame(y_train.values + y_noise, columns = ["lpsa"])
y_train_aug = pd.concat([y_train, y_new])
y_train_aug.reset_index(drop=True, inplace=True)

X_train_aug.shape, y_train_aug.shape
```

```
Out[70]: ((134, 7), (134,))
```

Let's look at our augmented training data `X_train_aug` and `y_train_aug`.

```
In [71]: X_train_aug.head()
```

Out[71]:

	lcavol	lweight	age	lbph	svi	lcp	gleason
0	-14.928954	-17.610985	-19.258774	-9.758325	-5.222929	-8.198625	-10.108675
1	-18.196809	-6.300651	-8.810694	-9.758325	-5.222929	-8.198625	-10.108675
2	-14.384937	-19.218949	12.085466	-9.758325	-5.222929	-8.198625	3.713391
3	-19.850478	-7.057946	-8.810694	-9.758325	-5.222929	-8.198625	-10.108675
4	-4.432026	-3.982798	-3.586654	-9.758325	-5.222929	-8.198625	-10.108675

```
In [72]: y_train_aug.head()
```

```
Out[72]:
0   -0.430783
1   -0.162519
2   -0.162519
3   -0.162519
4    0.371564
dtype: float64
```

Implement and compare two Ridge Regressions

```
In [92]:
from sklearn.linear_model import LinearRegression, Ridge


def ridge_benchmarking(method, X, y, alpha=1.0):

    if method == "Data augmentation":
        t = 0
        for i in range(100):
            start = time.time()
            model = LinearRegression()
            model.fit(X, y)
            end = time.time()
            t += end-start

    elif method == "Naive ridge":
        t = 0
        for i in range(100):
            start = time.time()
            model = Ridge(alpha=1.0)
            model.fit(X, y)
            end = time.time()
            t += end-start

    return model, t/100

# ridge regression by data augmentation
rrda, t1 = ridge_benchmarking("Data augmentation", X_train_aug, y_train_aug)

# naive ridge regression
nrr, t2 = ridge_benchmarking("Naive ridge", X_train, y_train)
```

Compare their timing:

```
In [115…
print(f"Ridge regression by data augmentation on average took {round(t1,5)} seconds for fitting the training data.")
print(f"Naive ridge regression on average took {round(t2,5)} seconds for fitting the training data.")
```

```
Ridge regression by data augmentation on average took 0.00139 seconds for fitting the training data.
Naive ridge regression on average took 0.00094 seconds for fitting the training data.
```

Compare the test results:

```
In [96]:
from sklearn.metrics import mean_squared_error

# ridge regression by data augmentation
y_pred = rrda.predict(X_test)
rmse_rrda = np.sqrt(mean_squared_error(y_pred, y_test))
print(f"Ridge regression by data augmentation has Root Mean Squared Error of {round(rmse_rrda,3)} on the test data.")

# naive ridge regression
y_pred = nrr.predict(X_test)
rmse_nrr = np.sqrt(mean_squared_error(y_pred, y_test))
print(f"Naive ridge regression has Root Mean Squared Error of {round(rmse_nrr,3)} on the test data.")
```

```
Ridge regression by data augmentation has Root Mean Squared Error of 0.712 on the test data.
Naive ridge regression has Root Mean Squared Error of 0.671 on the test data.
```

Therefore, for the `prostate cancer` dataset, Naive ridge regression on average is faster than Ridge regression by data augmentation, and it also produces smaller root mean squared error value.

THE END

Ex. 3.6 Show that the ridge regression estimate is the mean (and mode) of the posterior distribution, under a Gaussian prior $\beta \sim N(0, \tau\mathbf{I})$, and Gaussian sampling model $\mathbf{y} \sim N(\mathbf{X}\beta, \sigma^2\mathbf{I})$. Find the relationship between the regularization parameter λ in the ridge formula, and the variances τ and σ^2.

$p(\beta|y,X) = \dfrac{p(y|\beta,X)\,p(\beta)}{p(y,X)}$ where $\beta \sim N(0,\tau I)$ and $y \sim N(X\beta, \sigma^2 I)$.

$\because$ $p(y,X)$ is independent of β

$\therefore$ $p(\beta|y,X) \propto p(y|\beta,X)\,p(\beta)$.

$$= \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y-X\beta)'(y-X\beta)}{2\sigma^2}\right) \cdot \frac{1}{\sqrt{2\pi\tau}} \exp\left(-\frac{\beta'\beta}{2\tau}\right)$$

$$\therefore \log(p(\beta|y,X)) = C - \frac{(y-X\beta)'(y-X\beta)}{2\sigma^2} - \frac{\beta'\beta}{2\tau}$$

By letting $\dfrac{\partial \log(p(\hat\beta|y,X))}{\partial\hat\beta} = -\dfrac{2X'y + 2X'X\hat\beta}{2\sigma^2} - \dfrac{2\hat\beta}{2\tau} = 0$

we obtain $\hat\beta = (X^TX + \frac{\sigma^2}{\tau}I)^{-1}X'y$. $*$

$\therefore$ By comparing $*$ to ESL 3.44, we know $\lambda = \frac{\sigma^2}{\tau}$.

Also, since $p(\beta|y,X) \propto \frac{1}{2\pi\sigma\sqrt{\tau}} \exp\left(-\frac{(y-X\beta)'(y-X\beta)}{2\sigma^2} - \frac{\beta'\beta}{2\tau}\right)$, which implies that the posterior distribution is Gaussian. $\Rightarrow$ mean = mode.

If we rearrange the posterior, we can arrive at $\Sigma^{-1} = \frac{1}{\sigma^2}(X'X + \frac{\sigma^2}{\tau}I)$ and $\mu = \frac{1}{\sigma^2}\Sigma X'y = (X'X + \frac{\sigma^2}{\tau}I)X'y = \hat\beta$.

Thus, we proved that the ridge regression estimate is the mean (mode) of the posterior.

Ex. 3.19 Show that $\|\hat\beta^{\text{ridge}}\|$ increases as its tuning parameter $\lambda \to 0$. Does the same property hold for the lasso and partial least squares estimates? For the latter, consider the "tuning parameter" to be the successive steps in the algorithm.

$$
\begin{aligned}
\hat\beta_{ridge} &= (X^TX + \lambda I)^{-1} X^Ty \\
&= (VD^2T^T + \lambda I)^{-1} VDU^Ty \\
&= (V(D^2+\lambda I)V^T)^{-1} VDU^Ty \\
&= V(D^2+\lambda I)^{-1} DU^Ty.
\end{aligned}
$$

$X = UDV^T$ by SVD.

$$
\begin{aligned}
X^TX &= (UDV^T)^T UDV^T \\
&= VDU^TUDV^T = VD^2V^T
\end{aligned}
$$

$$
\begin{aligned}
\therefore \|\hat\beta_{ridge}\|^2 &= \hat\beta_{ridge}^T \hat\beta_{ridge} \\
&= y^TUD(D^2+\lambda I)^{-1}V^T V(D^2+\lambda I)^{-1} DU^Ty \\
&= y^TUD(D^2+\lambda I)^{-2} DU^Ty \\
&= (U^Ty)^T [D(D^2+\lambda I)^{-2} D] (U^Ty) \\
&= \sum_{j=1}^{p} \frac{d_j^2 (U^Ty)_j^2}{(d_j^2+\lambda)^2}
\end{aligned}
$$

$\therefore$ As $\lambda \to 0$, $\|\hat\beta_{ridge}\|^2$ increases.

For Lasso, there is no closed form solution for $\hat\beta_{Lasso}$.
If X has orthogonal columns, $\hat\beta_{Lasso} = \text{sign}(\hat\beta_{Lasso})(|\hat\beta_{Lasso}| - \lambda)_+$, then $\|\hat\beta_{Lasso}\|^2$ increases as $\lambda \to 0$.
In general, from ESL 3.51 and 3.52, we know that λ and t have an inverse relationship. Thus, if $\lambda \to 0$, t increases and so does $\|\hat\beta_{Lasso}\|^2$.

Ex. 3.28 Suppose for a given t in (3.51), the fitted lasso coefficient for variable X_j is $\hat{\beta}_j = a$. Suppose we augment our set of variables with an identical copy $X_j^* = X_j$. Characterize the effect of this exact collinearity by describing the set of solutions for $\hat{\beta}_j$ and $\hat{\beta}_j^*$, using the same value of t.

After the data augmentation, our $X^{new} = [X, X^*]$, $\beta^{new} = [\beta, \beta^*]$.

$X^{new}\beta^{new} = X(\beta + \beta^*)$.

$$\mathcal{L} = \|y - X^{new}\beta^{new}\|^2 + \lambda \sum_{j=1}^{p} |\beta_j| + |\beta_j^*|$$

$$= \|y - X^{new}\beta^{new}\|^2 + \lambda \sum_{j=1}^{p} |\beta_j + \beta_j^*| + \underbrace{|\beta_j| + |\beta_j^*| - |\beta_j + \beta_j^*|}_{\geqslant 0}$$

$\therefore$ $\hat{\beta}^{new} = \operatorname{argmin}_{\beta^{new}} \|y - X^{new}\beta^{new}\|^2$

subject to $\underbrace{|\beta_j + \beta_j^*|}_{①} + \underbrace{\left(|\beta_j| + |\beta_j^*| - |\beta_j + \beta_j^*|\right)}_{②} \leq t$

$\because$ ② is minimized when $|\beta_j| + |\beta_j^*| = |\beta_j + \beta_j^*|$.

$\therefore$ It requires that the $\hat{\beta}_j$ and $\hat{\beta}_j^*$ have the same sign.

$\because$ $\hat{\beta}_j = a$ before the data augmentation,

$\therefore$ The optimal solution after data augmentation is $\hat{\beta}_j + \hat{\beta}_j^* = a$

$\forall j = 1, 2, \cdots p$.

Ex. 3.30 Consider the elastic-net optimization problem:

$$\min_{\beta} ||\mathbf{y} - \mathbf{X}\beta||^2 + \lambda\big[\alpha||\beta||_2^2 + (1-\alpha)||\beta||_1\big]. \tag{3.91}$$

Show how one can turn this into a lasso problem, using an augmented version of $\mathbf{X}$ and $\mathbf{y}$.

Suppose X is $n\times p$, y is $n\times 1$, we augment X by aI $(p\times p)$, y by $p\times 1$ zeros,

s.t $X^{new} = \begin{bmatrix} X \\ aI \end{bmatrix}$, $y^{new} = \begin{bmatrix} y \\ 0 \end{bmatrix}$

$\therefore \|y^{new} - X^{new}\beta\|_2^2 = \left\| \begin{bmatrix} y - X\beta \\ a\beta \end{bmatrix} \right\|_2^2 = \|y - X\beta\|_2^2 + a^2\|\beta\|_2^2$

$\therefore$ The Lasso problem for β is: $\hat{\beta} = \underset{\beta}{\operatorname{argmin}}\left(\|y^{new} - X^{new}\beta\|_2^2 + \lambda\|\beta\|_1\right)$

$\therefore \hat{\beta} = \underset{\beta}{\operatorname{argmin}}\left(\|y - X\hat{\beta}\|_2^2 + a^2\|\beta\|_2^2 + b\|\beta\|_1\right)$,

which will be the Lasso problem if we choose $a = \sqrt{\lambda\alpha}$ and $b = \lambda(1-\alpha)$.