Exercise 1

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1 Linear Regression

1.1 (A)

Matrix form:

$$\hat{\beta} = \arg\min_{\beta \in \mathcal{R}^P} \frac{1}{2}(y - X\beta)^T W (y - X\beta).$$

Since W is symmetric and positive semidefinite, this is a convex optimization problem. Its first-order optimality condition is necessary and sufficient:

$$X^T W (y - X\beta) = \mathbf{0}.$$

1.2 (B)

1.2.1 Method 1: direct inversion

Described in the problem statement:

$$\beta = (X^T W X)^{-1} X^T W y.$$

To exploit sparsity of W, we use broadcasting in Python instead of matrix multiplication to compute operations w.r.t. W matrix. This method has a complexity of $O(np^2)$.

1.2.2 Method 2: pseudoinverse

Since the weight matrix W is diagonal, we can define $W^{\frac{1}{2}}$ to be a diagonal matrix where the i-th diagonal element equals $\sqrt{w_i}$. Now we can re-write the optimality condition:

$$\beta = [(W^{\frac{1}{2}} X)^T (W^{\frac{1}{2}} X)]^{-1} (W^{\frac{1}{2}} X)^T y,$$

which we re-write as

$$\beta = (W^{\frac{1}{2}} X)^{\dagger} W^{\frac{1}{2}} y,$$

where $(W^{\frac{1}{2}} X)^{\dagger}$ is the pseudoinverse of $W^{\frac{1}{2}} X$.

We first "preprocess" the feature matrix X and y by multiplying $W^{\frac{1}{2}}$ on the left.

We then compute the pseudoinverse through computing SVD of $W^{\frac{1}{2}} X$. This method is numerically more stable than the direct inverse method. (There could be correlation between our observations X. Therefore we care about numerical stability.)

Pseudocode for pseudoinverse of matrix A:

$(U, \Sigma, V) = \texttt{svd}(A)$
for Σ_{ii} in Σ: `#traverse through the diagonal elements`
  if $\Sigma_{ii} \neq 0$:
    $\Sigma_{ii} = 1/\Sigma_{ii}$
return $V^T \Sigma U^T$

In the Python code, we call `numpy.linalg.pinv` to perform the pseudoinverse. This method also has a complexity of $O(np^2)$.

In addition, this is the implementation of `scikit-learn`.

1.2.3 Method 3: Cholesky decomposition

We can use Cholesky decomposition on the matrix X^TWX. Now we have $LL^T\beta = D$. Then we can obtain β by solving two linear systems.

This method also has a complexity of $O(np^2)$.

Pseudocode for Cholesky-decomposition-based method:

Let $C = X^TWX$, $d = X^TWy$.
Compute Cholesky decomposition $C = LL^T$.
Solve for α in $L\alpha = d$.
Solve for β in $L^T\beta = \alpha$.

1.3 (C)

I coded the three methods in Python, using the `numpy` package. The codes can be find in my GitHub.

The results are summarized here:

Table 1: CPU Times (s) for Three Methods of Weighted Least Squares

(n, p)	Method 1	Method 2	Method 3
$(2000, 50)$	0.001	0.007	0.001
$(1000, 1000)$	0.122	0.346	0.064
$(20000, 50)$	0.012	0.034	0.005
$(50000, 50)$	0.028	0.118	0.013
$(5000, 5000)$	6.402	37.00	4.462

We can see that:

- Method 3 (Choleskey) consistently performs better than Method 1 (Direct Inverse), which is faster than Method 2 (pseudoinverse).
- When X is close to a square matrix, the performance of Method 3 is way worse than the other two methods.

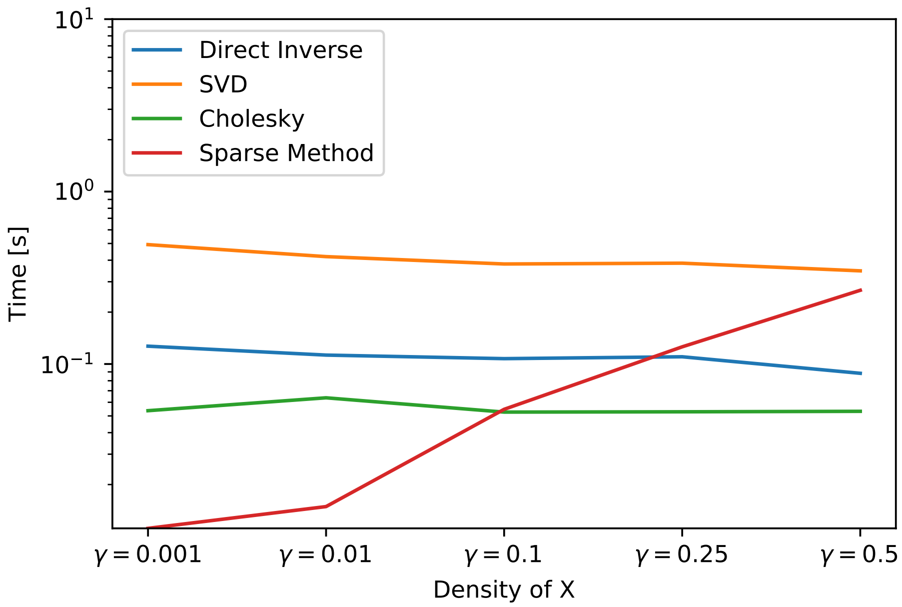
1.4 (D)

We use `scipy.sparse` in Python as our tool for sparse matrix operations. In particular, we use `scipy.sparse.linalg.lsqr` to solve the sparse least square problem:

$$\beta = (W^{\frac{1}{2}}X)^{\dagger}W^{\frac{1}{2}}y.$$

We generate random X matrices of size $(200000, 50)$, with different density. We name the sparse method as Method 4. The results are summarized as follows:

Figure 1: CPU Times (s) of Four Methods for the Sparse Matrix



We can see that:

- Method 1–3 do not exploit sparsity. Their CPU times do not change with density.
- When density is relatively small, the sparse method has an advantage over all the other three method. When density is relatively large, the sparse method is slower than Method 1 and 3, possibly due to overhead of the sparse data structure.