Analysis of optimization and numerical approaches to solve the linear least square problem

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***Abstract*—The linear least square problem can be tackled using a wide range of optimization or numerical methods. The L-BFGS method of the class of limited-memory quasi-Newton algorithms has been chosen for the former, whilst the thin QR factorization with Householder reflectors for the latter. Both these algorithms have been implemented from scratch using Python language, to finally experiment over their performances in terms of precision, stability and speed. The accordance of the implementations with the underlying theoretical models is also studied and discussed.**

Introduction

Given a dataset composed by a matrix $\hat{X} \in \mathbb{R}^{m \times n}$ with $m \geq n$ and a vector $y \in \mathbb{R}^m$, the solution of the linear least square (LLS) problem is the vector $w \in \mathbb{R}^n$ that fits best the data assuming a linear function between $\hat{X}$ and y. (Nocedal and Wright 2006, 50) This can be formalized as the following minimization problem:

$$w_* = \min_w \|\hat{X}w - y\|_2^2$$

The matrix $\hat{X}$ is actually composed in the following way:

$$\hat{X} = \begin{bmatrix} X^T \\ I \end{bmatrix}$$

Where $X \in \mathbb{R}^{n \times k}$ is a tall thin matrix, thus $m = k + n$. The LLS problem can be dealt both with iterative methods or with direct numerical methods. One algorithm has been chosen for each of these fields to finally discuss their experimental results.

L-BFGS

The L-BFGS is an iterative method of the quasi-Newton limited-memory class. This method is actually a variation of the BFGS method, with which it shares the update rule; at the $i+1$-th iteration the point is updated as follows:

$$w_{i+1} = w_i - \alpha_i H_i \nabla f_i$$

L-BFGS has an inferior space complexity due to the fact that the Hessian approximation H_i is stored implicitly, and built over a fixed number of vector pairs $\{s_j, y_j\}$ of the previous t iterations and an initial matrix H_i^0. Where

$$s_i = w_{i+1} - w_i, \quad y_i = \nabla f_{i+1} - \nabla f_i$$
$$V_i = I - \rho_i y_i s_i^T, \quad \rho_i = \frac{1}{y_k^T s_k}$$

so H_i satisfies the following:

$$\begin{aligned} H_i = {} & (V_{i-1}^T \dots V_{i-t}^T) H_i^0 (V_{i-t} \dots V_{i-1}) \\ & + \rho_{i-t}(V_{i-1}^T \dots V_{i-t}^T + 1) s_{i-t} s_{i-m}^T (V_{i-t+1} \dots V_{i-1}) \\ & + \rho_{i-t+1}(V_{i-1}^T \dots V_{i-t}^T + 2) s_{i-t+1} s_{i-t+1}^T (V_{i-t+2} \dots V_{i-1}) \\ & + \dots \\ & + \rho_{i-1} s_{i-1} s_{i-1}^T \end{aligned}$$

Different strategies to initialize the H_i^0 matrix are proposed in the literature, and so they will be tested experimentally. Finally, the step size α_i is found by performing an inexact line search based on the Armijo-Wolfe conditions.

Thin QR factorization

For the numerical counterpart, the thin QR factorization with Householder reflectors has been implemented as described in (Trefethen and Bau 1997).

By using the Householder QR factorization, the matrix R is constructed in place of $\hat{X}$ and the n reflection vectors $v_1, \dots, v_n$ are stored. The reduced matrix $\hat{R}$ is trivially obtainable by slicing as in $\hat{R} = R_{1:n,1:n}$. In fact, given that $\hat{X}$ is already stored in memory and fully needed, there would be no advantage in directly constructing the reduced matrix.

By using the Householder vectors it is also possible to implicitly compute $\hat{Q}^T b$ to finally obtain w_* by back substitution over the upper-triangular system $\hat{R}w = \hat{Q}^T b$.

Algorithmic analysis

Convergence of L-BFGS

Liu and Nocedal (1989) define three necessary assumptions to prove a theorem stating that the L-BFGS algorithm

globally converges and moreover that there exists a constant $0 \leq r < 1$ such that

$$f(w_i) - f(w_*) \leq r^i(f(w_0) - f(w_*)) = \sigma_i$$

so that the sequence w_i converges R-linearly.

The first assumption required is on the objective function f, that should be twice continuously differentiable. This is in fact true and we can define the gradient and the Hessian of the objective function as in:

$$\nabla f(w) = \hat{X}^T(\hat{X}w - y)$$

$$\nabla^2 f(w) = \hat{X}^T\hat{X}$$

Moreover the Hessian is positive definite since it can be rearranged in the following way:

$$\begin{aligned}\nabla^2 f(w) &= \hat{X}^T\hat{X} \\ &= \left|XI\right| \begin{vmatrix} X^T \\ I \end{vmatrix} \\ &= XX^T + I\end{aligned}$$

Being the Hessian positive definite, the objective function f is a convex function. This comes in handy for the second assumption requiring the sublevel set $D = \{w \in \mathbb{R}^n | f(w) \leq f(w_0)\}$ must be convex, it can be easily proved that if a function is convex all of its sublevel sets are convex sets.

$$\begin{aligned}&\forall x, y \in D,\ \lambda \in [0,1] \\ &\qquad \text{f convex} \\ &\qquad \implies f(\lambda x + (1-\lambda)y) \\ &\qquad \leq \lambda f(x) + (1-\lambda)f(y) \\ &\qquad \leq \lambda f(w_0) + (1-\lambda)f(w_0) \\ &\qquad = f(w_0) \\ &\qquad \implies \lambda x + (1-\lambda y) \in D\end{aligned}$$

The third and last assumption requires the existence of two positive constants M_1 and M_2 such that $\forall z \in \mathbb{R}^n, w \in D$:

$$M_1\|z\|^2 \leq z^T\nabla^2 f(w) \leq M_2\|z\|^2$$

or equivalently

$$M_1 I \preceq \nabla^2 f(w) \preceq M_2 I$$

The first part of the equation is surely satisfied by $M_1 = 1$, keeping in mind the previous decomposition $\nabla^2 f(w) = XX^T + I$. Considering also that all the eigenvalues in a positive definite matrix are real and positive, it is possible to use the largest eigenvalue as in $M_2 = \lambda_{max}$.

Other then these assumptions, the theorem requires for the sequence of Hessian substitutes H_i to be bounded. This obviously depends on the initialization technique used to generate H_i^0, various techniques are suggested in the literature and so they will be empirically tested.

Finally the convergence requires to perform a line search respectful of the Armijo-Wolfe conditions. The algorithm described in Al-Baali and Fletcher (1986) to perform an inexact line search is ensured to converge under the assumption that $\sigma > \rho$ where $\rho \in (0, \frac{1}{2}), \sigma \in (0,1)$, respectively the constant for the Armijo condition and for the Wolfe one.

Analysis of standard and modified thin QR

Ignoring constants, we know from theory that the standard QR factorization algorithm applied on the matrix $\hat{X}$ yields a time complexity of $O(mn^2)$. Actually, given that we are generally dealing with a very tall and thin matrix X, the resulting $\hat{X}$ is going to be squarish ($m \approx n$). This means that we can consider the complexity to be cubic in n.

From now on, we show a way to bring down the time complexity of the algorithm from $O(mn^2)$ to $O(kn^2)$, with $k = m - n$. The resulting modified QR factorization algorithm will become useful when k is much smaller than m, as in our case.
In the standard algorithm, at each step we focus on a single column of the input matrix, constructing a householder vector to zero out all the entries below the diagonal. Following the geometric reasoning in (Trefethen and Bau 1997), this brings the algorithm to depend on m. While this cannot be avoided in general, in our particular case we can be a little bit smarter.

Since the block matrix $\hat{X}$ contains the identity as its lower block, at each step of the algorithm we can just focus on zeroing out the $k = m - n$ entries below the diagonal up to the 1s of the identity. In the modified algorithm then, to obtain R, the matrix $\hat{X}$ is multiplied on the left side by a sequence of matrices $L_i \in \mathbb{R}^{m \times m}$ of the form ($i = 1, \ldots, n$):

$$L_i = \begin{bmatrix} I_{i-1} & 0 & 0 \\ 0 & H_i & 0 \\ 0 & 0 & I_{n-i} \end{bmatrix}$$

where $H_i \in \mathbb{R}^{(k+1)\times(k+1)}$ are all householder reflectors that zero out the k entries in the i-th column of the matrix which is being multiplied by L_i.
To derive the time complexity of this phase we can reason as follows. The right side matrix can be divided in three blocks as in $\left[\begin{smallmatrix} A \\ B \\ C \end{smallmatrix}\right]$. When we multiply this matrix by L_i the only relevant operation is the matrix multiplication H_iB, which costs $O(kn)$. Since the total number of multiplications is n, the total complexity is $O(kn^2)$.
Since each L_i is orthogonal and symmetric it is then possible to reconstruct Q and the reduced $\hat{Q}$ in the following way:

$$Q = L_1 L_2 \dots L_n$$
$$\hat{Q} = L_1 L_2 \dots L_n \begin{bmatrix} I_n \\ 0 \end{bmatrix}$$

Applying again the reasoning above, the time complexity of these reconstructions is $O(kn^2)$. It follows that the overall time complexity of the modified QR factorization is $O(kn^2)$.

Input data

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