Solving Non-negative Least Squares Problems by Damped Dynamcial Systems and Reflection

The non-negative least squares problem (NNLSQ) looks like

$$\min_{u \geq 0} \frac{1}{2}\|Au - b\|_2^2, \quad A \in \mathbb{R}^{m \times n},\ b \in \mathbb{R}^m,\ m \geq n. \tag{1}$$

It can be solved numerically with standard iterative methods, see [1] for a method used in Matlab.

Ignoring the constraints in (1) we know from linear algebra that the solution of the linear least squares problem is given by the normal equations $A^T(Au - b) = 0$. Using this fact, and with some additional assumptions the solution of (1) is also given by the stationary solution u^* of the second order damped dynamical system

$$\ddot{u}(t) + \eta\dot{u}(t) = -A^T(Au - b),\ \eta > 0, u \geq 0. \tag{2}$$

An intuitive argument for the convergence is that the damping η will decrease the velocity $\dot{u}(t)$ and acceleration $\ddot{u}(t)$ to zero giving $0 = -A^T(Au^* - b)$, i.e., $u(t)$ will tend to the solution of the normal equations. However, because of the non-negativity contraints, solving (2) numerically is non-trivial. Recently in [2] new methods for (2) have been developed using the idea of reflecting the iterates in the numerical solution whenever a component falls outside any boundary. An physical analogy of the approach is imagining the elements of u as particles trapped in an open box with boundaries given by the planes $u_i = 0$. Whenever one component hits a boundary it is reflected back into the domain with the condition that the total energy in the open box is perserved.

We suggest a mix of numerical tests and analysis as the following.

1. Formulate the unconstrained system (2) as a first order system in a stable way, implement symplectic Euler, and verify the known numerical properties of the method.
2. Given a violation of one or more constraints find the reflection(s) that conserves the total energy and implement the method using symplectic Euler.
3. Evaluate the methods on very large sparse problems comparing with Matlabs solver lsqnonneg.
4. Find locally optimal parameters using a projection on the subspace of active constraints at the solution.
5. Analyse the connection between these kind of methods and the conjugate gradient method (numerically and analytically).

The first part 1 is a straightforward exercise. The main first challange is 2 that is not trivial. Task 3 should be straight forward given the implementations. Task 4 should be quite easy with some linear algebra. The last part is difficult and may be omitted.

References

[1] Lawson, C. L. and R. J. Hanson. Solving Least-Squares Problems. Upper Saddle River, NJ: Prentice Hall. 1974. Chapter 23, p. 161.

[2] Kaufman, D.M. and Pai, D.K., Geometric Numerical Integration of Inequality Constrained, Nonsmooth Hamiltonian Systems, ArXiv e-prints, arXiv, eprint = 1007.2233,2010

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