

$$\frac{1}{2} \| \mathbf{AX} - \mathbf{B} \|^2$$

Nonnegative least squares

Suvrit Sra

ILAS (Pisa)

June 21–25, 2010

(based on joint work with D. Kim, I. Dhillon)



MAX-PLANCK-GESELLSCHAFT

(MPI für biologische Kybernetik, Tübingen)

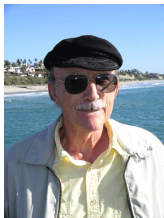


MPI FOR BIOLOGICAL CYBERNETICS

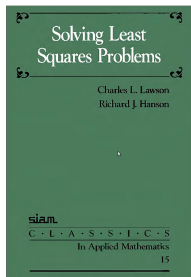
Introduction

1. Venerable history of least squares
2. Estimates optimal, but thanks to “cancellations” — so solution usually has positive and negative entries
3. Physical, modeling, or numerical reasons request nonnegative estimates

History



C. Lawson (2004)



The book

Applications

1. Astronomy [WP99, ?, ?]
2. Medicine (radio-therapy [PMB09, Gun99, MLV⁺04])
3. Drug delivery [Bur05]
4. Medical imaging (MRI [RMRG09, JVO09], PET [?], etc.)
5. Inverse problems, e.g., [ATB05, Par94, ?]
6. Image Processing, computer graphics
7. Face recognition [VMC09]
8. Neural networks [Tim08]
9. Subproblem of NMA/NMF [?, CZPiA09]
10. Anomaly detection, e.g. in remote sensing [GB08]
11. Chemometrics [Gem08]
12. Bioinformatics [SGD05]
13. Machine learning (dual of SVM)
14. Fisheries acoustics [SM05]
15. Mechanical engineering [SI99]
16. Statistics (constrained least squares)

Algorithms

1. **NNLS**, by Lawson and Hanson (1976) – Widely used; matlab impl; slow
2. **FNNLS** Bro, Jong (19??) – faster
3. take from bbsg paper, and from pqnj paper

Our approach

1. large scale problems
2. low-medium accuracy solutions acceptable
3. generic algorithmic approaches, progress in optimization
4. gradient-projection

Numerical Results

Numerical Results

Summary

Questions?

Some references I



R. C. Aster, C. H. Thurber, and B. Borchers.
Parameter estimation and inverse problems.
Academic Press, 2005.



D. J. Burgess.
Injectable dispersed systems: formulation, processing, and performance.
Informa Health Care, 2005.



Andrzej Cichocki, Rafal Zdunek, Anh Huy Phan, and Shun ichi Amari.
Nonnegative Matrix and Tensor Factorizations: Applications to Exploratory Multi-Way Data Analysis and Blind Source Separation.
John Wiley and Sons, 2009.



D. Gillis and J. H. Bowles.
Parallel implementation of the ORASIS algorithm for remote sensing data analysis.
In A. J. Plaza and C.-I. Cheng, editors, *High performance computing in remote sensing.* CRC Press, 2008.

Some references II



P. Gemperline.

Practical guide to chemometrics.

CRC Press, 2008.



L. L. Gunderson.

Intraoperative irradiation: techniques and results.

Humana Press, 1999.



B. Jian, B. C. Vemuri, and E. Özarlan.

A mixture of Wisharts (mow) model for multifiber reconstruction.

In D. Laidlaw and J. Weickert, editors, *Visualization and Processing of Tensor Fields: Advances and Perspectives*, 2009.



A. MacKay, C. Laule, I. Vavasour, B. Mädler, A. Trabouise, D. Paty, W. Moore, and D. Li.

The short t_2 component in normal-appearing white matter in multiple sclerosis.

In M. Filippi, G. Comi, and M. Rovaris, editors, *Normal-appearing white and grey matter damage in multiple sclerosis*. Springer, 2004.

Some references III



R. L. Parker.

Geophysical inverse theory.

Princeton University Press, 1994.



O. Pisaturo, R. Moedckli, and F. O. Bochud.

Monte Carlo based independent monitor unit calculation in IMRT.

In World Congress on Medical Physics and Biomedical Engineering (IFMBE), volume 25, pages 441–444, 2009.



A. Ramirez-Manzanares, M. Rivera, and J. C. Gee.

Denosing intra-voxel Axon fiber orientations by means of ECQMMF method.

In MICAI 2009, LNAI 5845, pages 303–312, 2009.



M. S. B. Sehgal, I. Gondal, and L. Dooley.

Collateral missing value estimation: robust missing value estimation for consequent microarray data processing.

In Advances in Artificial Intelligence (AI), LNAI 3809, pages 274–283, 2005.

Some references IV



M. J. Schulz and D. J. Inman.

Techniques in active dynamic structural control to optimize structural controllers and structural parameters.

In C. T. Leondes, editor, *Structural dynamic systems computational techniques and optimization: Dynamic analysis and control techniques*. CRC Press, 1999.



E. J. Simmonds and D. N. MacLennan.

Fisheries acoustics: theory and practice.

Wiley-Blackwell, 2005.



S. Timotheou.

Nonnegative least squares learning for the random neural network.

In *ICANN 2008*, LNCS 5163, pages 195–204, 2008.



N. Vo, B. Moran, and S. Challa.

Nonnegative leastu-square classifier for face recognition.

In *Advances in Neural Networks: ISNN*, LNCS 5553, pages 449–456, 2009.

Some references V



H. Wozniak and D. Pfenniger.

Distribution of Kolmogorov-Sinai entropy in self-consistent models of barred galaxies.

In *Celestial Mechanics and Dynamical Astronomy*, pages 149–158, 1999.