$\frac{1}{2} \| Ax - B \|_2^2$

Nonnegative least squares

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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

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
Questions?
Some references I


D. Gillis and J. H. Bowles. Parallel implementation of the ORASIS algorithm for remote sensing data analysis.

Some references II

P. Gemperline.  
*Practical guide to chemometrics.*  

L. L. Gunderson.  
*Intraoperative irradiation: techniques and results.*  

B. Jian, B. C. Vemuri, and E. Özarslan.  
A mixture of Wisharts (mow) model for multifiber reconstruction.  

The short $t_2$ component in normal-appearing white matter in multiple sclerosis.  
Some references III

R. L. Parker.  
*Geophysical inverse theory.*  

O. Pisaturo, R. Moedckli, and F. O. Bochud.  
Monte Carlo based independent monitor unit calculation in IMRT.  

A. Ramirez-Manzanares, M. Rivera, and J. C. Gee.  
Denoising intra-voxel Axon fiber orientations by means of ECQMMF method.  

M. S. B. Sehgal, I. Gondal, and L. Dooley.  
Collateral missing value estimation: robust missing value estimation for consequent microarray data processing.  
Some references IV

M. J. Schulz and D. J. Inman.
Techniques in active dynamic structural control to optimize structural controllers and structural parameters.

E. J. Simmonds and D. N. MacLennan.
*Fisheries acoustics: theory and practice.*

S. Timotheou.
Nonnegative least squares learning for the random neural network.

N. Vo, B. Moran, and S. Challa.
Nonnegative least-squares classifier for face recognition.
Some references V

H. Wozniak and D. Pfenniger.
Distribution of Kolmogorov-Sinaï entropy in self-consistent models of barred galaxies.