

制約条件付きの非線形の近さの数値実験
—国際学会講演報告—

橋本 明浩
新潟県立看護大学（基盤科学）

A Numerical Simulation on closeness under constraints

Akihiro Hashimoto
Information Science, Niigata College of Nursing

キーワード：近さ（Closeness），制約（Constraints）

抄録

非線形制約条件化の下での近さの概念について研究を行い，国際学会で報告したので，その内容を紹介し若干の考察を加える．

研究目的

自然科学においては，モデルを想定し，モデルのパラメタ推定をある規準の下で行う．具体例としては，回帰分析法，AIC（Akaike's Information Criterion）による比較，（Hashimoto [1974]），主成分分析法等である．このような手法を統計学的手法と呼んでいるが，情報数理的な考え方をすれば，いずれも「非線形最適化問題」に定式化される．すなわち，最適化する目的関数が残差平方和，尤度，相関係数であると考えることができる．ところで，パラメタに関しては実験的，社会的な制約により，何らかの制約条件が課せられていることが多く，この場合は「制約条件付きの非線形最適化問題」を解く必要がある．線形制約条件の下での研究については，C. R. Rao [1986] 等，多く報告されているが，非線形制約条件の下での非線形最適化問題については未報告部分が多く，数学的な困難さもあって，実際的な非線形制約条件の下での非線形最適化問題の研究がなされていない．そこで，現実的な制約等を考慮した制約条件付き最適化問題の研究を考え，本年度は香港の国際統計学会で講演を行ったので，これを紹介し若干の考察を加える．

研究方法および結果等

理論的研究については平成 14 年度学長特別研究費研究報告書，参考文献で示す考察を加え厳密を得ることができた．そこで実際の入学試験データをもとに数値実験をおこない付録図表に示す結果を得た．この結果をふまえ以下のベルヌイ学会で報告した．

場所 香港科学学術大学

日時 平成 15 年 12 月 18－23 日

報告内容は付録に与える.

むすび

非線形問題について多くの質問がなされたが, 問題の複雑さ特殊事例等の共通理解を深められ有意義であった. 今後は数値実験の結果をふまえて理論的な解析, 分布論までも研究の対象として考えていきたい.

謝辞

本研究は千葉大学田栗正章教授, 宮埜壽夫教授との共同研究でなされたものであり, 両先生に感謝する. また研究の場を与えていただいた学長, 委員会の皆様に深く感謝する.

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Maximization of Correlation under Quadratic and Linear Constraints

A. Hashimoto, H. Miyano
and
M. Taguri
Japan

December 18-20, 2003

EAPR Conference 2003, Hong Kong Univ. of Sci. & Tech.

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Description of our problem

The motivation of this study is to devise a new method for improving predictive validity of tests, such as entrance examination

Measure of predictive validity

y_i : Score of subject i on external criteria Y

z_i : Score vector of subject i on p test items

$Z = (z_1, z_2, \dots, z_n)'$ $y = (y_1, y_2, \dots, y_n)'$

Measure = Correlation of Zw and y

w : p dimensional weight vector

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Problem on sample space

Find the weight vector w which maximizes the correlation R_0 of Zw and y under the constraints

$$Aw = d \quad \text{and} \quad (w - w_0)' B^{-1} (w - w_0) \leq 1$$

$$R_0 = \frac{y'(I_n - Q_n)Zw}{\sqrt{y'(I_n - Q_n)y} \sqrt{w'Z'(I_n - Q_n)Zw}}$$

$$Q_n = 11'/n, \quad 1 = (1, 1, \dots, 1)'$$

w_0 : Fixed weight vector (e.g., current weight)

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Using singular value decomposition

$$(I_n - Q_n)Z = U\Lambda V'$$

where Λ is a diagonal matrix of non-zero singular values and defining

$$x = \Lambda V'w, \quad x_0 = \Lambda V'w_0, \quad \text{and} \quad b = U'y,$$

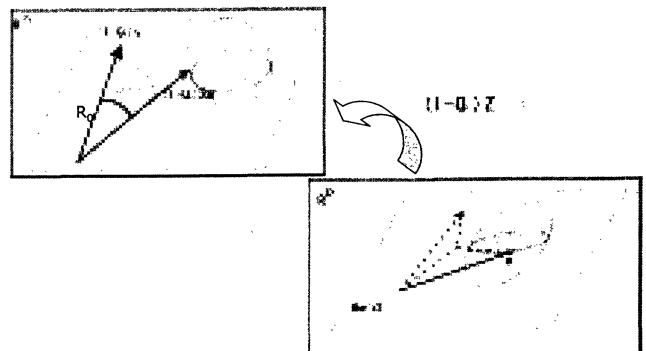
we have a translated form of our problem on parameter space; that is,

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Schematic illustration of translation



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Equivalent problem on parameter space (1)

Find the vector \mathbf{x} which maximizes

$$|R_1| = \frac{|\mathbf{b}'\mathbf{x}|}{\|\mathbf{b}\| \|\mathbf{x}\|}$$

under linear and quadratic constraints

$$F\mathbf{x} = \mathbf{d}, (\mathbf{x} - \mathbf{x}_0)'G^{-1}(\mathbf{x} - \mathbf{x}_0) \leq 1$$

where

$$F = AV\Lambda^{-1}, G^{-1} = \Lambda^{-1}V'B^{-1}V\Lambda^{-1}$$

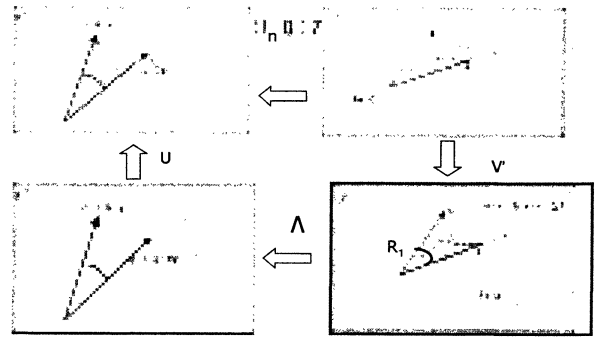
By using singular value decomposition of F , we have the following equivalent problem.

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Schematic illustration of translation



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Equivalent problem on parameter space (2)

Find the vector \mathbf{u} which maximizes

$$|R_2| = \frac{|\mathbf{h}'\mathbf{u}|}{\|\mathbf{h}\| \|\mathbf{u}\|}$$

under the quadratic constraint

$$(\mathbf{u} - \mathbf{u}_0)'H^{-1}(\mathbf{u} - \mathbf{u}_0) \leq 1$$

where \mathbf{u}_0 , \mathbf{h} and H are vectors or matrix defined by F , G^{-1} and \mathbf{x}_0

Our problem equals the maximization problem under quadratic constraint!

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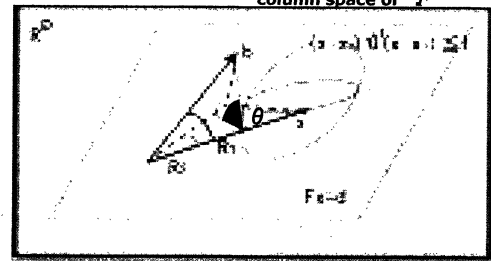
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Relationship between two correlation coefficients

$$R_2 = R_1 \cos \theta$$

θ : Angle between \mathbf{b} and the column space of F



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Optimal solution

Let \mathbf{u}^* be an optimal \mathbf{u} then optimal weight vector \mathbf{w}^* is given by

$$\mathbf{w}^* = V\Lambda^{-1}V_f' \begin{pmatrix} \Lambda_f^{-1}U_f'\mathbf{d} \\ \mathbf{u}^* \end{pmatrix}$$

where U_f , V_f and Λ_f are the matrices specified by the singular value decomposition of F ;

$$F = U_f(\Lambda_f, O)V_f'$$

Λ_f : Diagonal matrix of nonzero singular values

O : Zero matrix

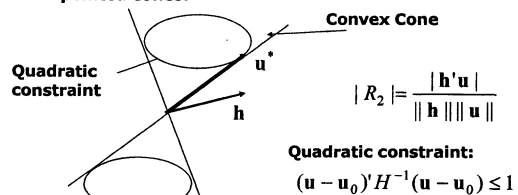
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Computing \mathbf{u}^*

As shown in our previous paper (Hashimoto et al., 2000), the non-trivial optimal can be obtained by solving the correlation maximization problem under the constraint specified by the union of two convex pointed cones.



$$|R_2| = \frac{|\mathbf{h}'\mathbf{u}|}{\|\mathbf{h}\| \|\mathbf{u}\|}$$

Quadratic constraint:

$$(\mathbf{u} - \mathbf{u}_0)'H^{-1}(\mathbf{u} - \mathbf{u}_0) \leq 1$$

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Algorithm for computing optimal weight

Compute S.V.D. of data matrix

$$(I_n - Q_n)Z = U\Lambda V'$$

Compute S.V.D. of $F = AV\Lambda^{-1}$

$$F = U_f(\Lambda_f, O)Y_f'$$

Rewrite the problem as a problem under one quadratic constraint

Using Hashimoto's algorithm, compute its solution to have optimal weight vector

$$w^* = V\Lambda^{-1}V_f' \begin{pmatrix} \Lambda_f^{-1}U_f'd \\ u^* \end{pmatrix}$$

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Numerical example

Entrance examination data:

$n : 198$ candidates ; $p : 5$ subjects

$$w_0 = (0.2, 0.2, 0.2, 0.2, 0.2)'$$

$$B = \sigma I, \quad \sigma = (0.050, 0.063, \dots, 0.250)$$

$$(w - w_0)'B^{-1}(w - w_0) \leq 1$$

$$A = (1, 1, 1, 1, 1) ; Aw = 1$$

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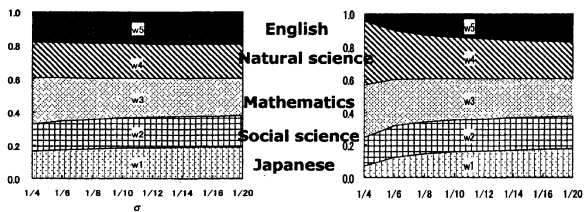
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Optimal weights compared with least squares solution

Least squares solution

Correlation maximized solution



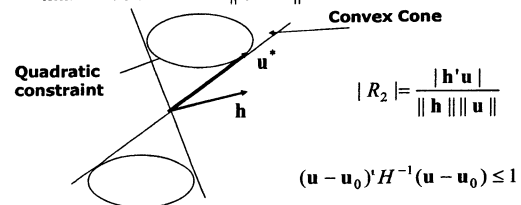
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Correlation maximization and least squares problems

If we translate the original problem defined on sample space to the equivalent problem on parameter space, that is the maximization of R_2 , then the maximization of angle between u and h is apparently equivalent to the minimization of $\|u - h\|^2$



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Concluding remarks

However, this least squares problem is hard to solve by traditional method, e.g., Lagrangean method.

So our main contributions are:

(1) Problem translation by Singular Value Decomposition

Problem in sample space with parameter constraints



(2) Development of Convex Cone Method for Optimization
Convex cone specified by the constraints

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