Implementations of Fisher's Linear Discriminant Analysis from the Numerical Point of View

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Outline

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Motivation Example

- protein folding classification into 42 groups
- frequencies of 20 amino acids as predictors
  - 20 singles, 400 pairs, 8000 triples, . . .
- expensive data-collection
  - just hundreds of examples - 268
- classical $p \gg n$ issue in microarray, document classification etc.

Problems

- matrix storage
- computational cost
  - matrix multiplications, inversions
  - computing inner products
  - optimalization, QP, . . .
- . . . no straightforward using of $p < n$ methods

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Fisher's Criterion I

- variance . . . $\text{Var}(\boldsymbol{X}) = \boldsymbol{\Sigma} = \text{E}_{\boldsymbol{X}}\left[(\boldsymbol{X}-\boldsymbol{\mu})(\boldsymbol{X}-\boldsymbol{\mu})^T\right]$
- decomposition (between- and within-variance)
  $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_B + \boldsymbol{\Sigma}_W$

$$\boldsymbol{\Sigma}_B = \sum_{k=1}^{K} \pi_k (\boldsymbol{\mu}_k - \boldsymbol{\mu})(\boldsymbol{\mu}_k - \boldsymbol{\mu})^T$$

$$\boldsymbol{\Sigma}_W = \sum_{k=1}^{K} \pi_k \text{E}_{\boldsymbol{X}|G}\left[(\boldsymbol{X}-\boldsymbol{\mu}_k)(\boldsymbol{X}-\boldsymbol{\mu}_k)^T\right]$$

- total variance after projection . . .
  $\text{Var}(\mathbf{c}^T\boldsymbol{X}) = \mathbf{c}^T\boldsymbol{\Sigma}_B\mathbf{c} + \mathbf{c}^T\boldsymbol{\Sigma}_W\mathbf{c}$
- Fisher's criterion

$$\max_{\mathbf{c}\in\mathbb{R}^p} \frac{\mathbf{c}^T\boldsymbol{\Sigma}_B\mathbf{c}}{\mathbf{c}^T\boldsymbol{\Sigma}_W\mathbf{c}} \quad \text{s. t.} \quad \mathbf{c} \neq \mathbf{0}$$

Fisher's Criterion II

- generalized eigenproblem with matrix pencil $(\mathbf{\Sigma}_B, \mathbf{\Sigma}_W)$
- (ordered) ν-eigenvectors give projected matrix $\mathbf{C} = \mathbf{C}_\nu$

1. estimate
   - $\mu, \mu_k, \mathbf{\Sigma}_B, \mathbf{\Sigma}_W$

$$\boldsymbol{B} \equiv \frac{(\boldsymbol{GM} - \mathbf{1}\bar{\mathbf{x}})^T(\boldsymbol{GM} - \mathbf{1}\bar{\mathbf{x}})}{g-1}, \quad \boldsymbol{W} \equiv \frac{(\mathrm{X} - \boldsymbol{GM})^T(\mathrm{X} - \boldsymbol{GM})}{n-g}$$

   - $\boldsymbol{B}, \boldsymbol{W} \in \mathbb{R}^{p \times p}$, $\boldsymbol{B}, \boldsymbol{W} \geq 0$
   - $\mathrm{rank}(\boldsymbol{B}) \leq K - 1$, $r = \mathrm{rank}(\boldsymbol{W}) \leq \min\{n, p\}$
2. solve $\boldsymbol{B}\mathbf{c} - \lambda\boldsymbol{W}\mathbf{c} = 0$ to obtain $\mathbf{C}$
   - find $K - 1$ largest eigenpairs
3. compute
   - all distances $||\widetilde{\mathbf{x}} - \widetilde{\mu}_k||^2 = ||\mathbf{x} - \mu_k||^2_{\mathbf{CC}^T}$
   - find group label through minimum

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The $p \gg n$ case

- if $\boldsymbol{W}$ nonsingular $\Rightarrow$ transformation to a standard eigenproblem, e. g.

$$(\boldsymbol{W}^{-1}\boldsymbol{B} - \lambda\mathbf{I})\mathbf{c} = 0$$

- in the $p \gg n$ case $\boldsymbol{W}$ is singular $\Rightarrow$
  - transformation not possible
  - very challenging eigenproblem
    - may even happen that

$$\det(\boldsymbol{B} - \lambda\boldsymbol{W}) = 0 \qquad \forall\,\lambda \in \mathbb{C}\,!$$

pair $\{\boldsymbol{B}, \boldsymbol{W}\}$ is called singular matrix pencil

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Underlying Linear Algebra

- Generalized Schur Decomposition [Moler, Stewart - 1973]:

$$\boldsymbol{Q}^T(\boldsymbol{B}-\boldsymbol{W})\boldsymbol{Z} = \boldsymbol{T} - \boldsymbol{S}$$

  - $\boldsymbol{Q}$, $\boldsymbol{Z}$ orthogonal, $\boldsymbol{T}$, $\boldsymbol{S}$ upper triangular
  - singularity $\Rightarrow$ possible zeros on main diagonals of $\boldsymbol{T}$ and $\boldsymbol{S}$

1. $t_{ii} \neq 0 \neq s_{ii} \Rightarrow \det(\boldsymbol{T} - \frac{t_{ii}}{s_{ii}}\boldsymbol{S}) = 0$, $\frac{t_{ii}}{s_{ii}}$ …finite eigenvalue
2. $t_{ii} = 0$, $s_{ii} \neq 0 \Rightarrow \det(\boldsymbol{T} - 0 \cdot \boldsymbol{S}) = 0$, 0 …finite —"—
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- how to determine the $K-1$ largest eigenvalues???

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$$Q^T(B - W)Z = T - S$$

- Q, Z orthogonal, T, S upper triangular
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Relation with FLDA

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   $(\boldsymbol{B} - \frac{t_{ii}}{s_{ii}}\boldsymbol{W})\mathbf{c} = 0 \quad \Rightarrow \quad \mathbf{c}^T\boldsymbol{B}\mathbf{c} = \frac{t_{ii}}{s_{ii}}\mathbf{c}^T\boldsymbol{W}\mathbf{c}$
   - $\lambda = \frac{t_{ii}}{s_{ii}}$ ... ratio of between- to within-variance
   - complement of null-spaces of $\boldsymbol{B}$, $\boldsymbol{W}$
2. finite zero
   $(\boldsymbol{B} - 0 \cdot \boldsymbol{W})\mathbf{c} = 0 \quad \Rightarrow \quad \mathbf{c}^T\boldsymbol{B}\mathbf{c} = 0$
   - opposite of FLDA aim
   - null-space of $\boldsymbol{B}$
3. infinite
   $\mathbf{c}^T\boldsymbol{B}\mathbf{c} = \lambda\mathbf{c}^T\boldsymbol{W}\mathbf{c}$ for $\lambda = \infty$ "$\Rightarrow$" $\mathbf{c}^T\boldsymbol{W}\mathbf{c} = 0$
   - wanted for FLDA, quality depends on $\mathbf{c}^T\boldsymbol{B}\mathbf{c}$
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   - complement of null-spaces of $\boldsymbol{B}$, $\boldsymbol{W}$
2. finite zero
   $(\boldsymbol{B} - 0 \cdot \boldsymbol{W})\mathbf{c} = 0 \quad \Rightarrow \quad \mathbf{c}^T\boldsymbol{B}\mathbf{c} = 0$
   - opposite of FLDA aim
   - null-space of $\boldsymbol{B}$
3. infinite
   $\mathbf{c}^T\boldsymbol{B}\mathbf{c} = \lambda\mathbf{c}^T\boldsymbol{W}\mathbf{c}$ for $\lambda = \infty$ " $\Rightarrow$ " $\mathbf{c}^T\boldsymbol{W}\mathbf{c} = 0$
   - wanted for FLDA, quality depends on $\mathbf{c}^T\boldsymbol{B}\mathbf{c}$
   - null-space of $\boldsymbol{W}$
4. any value is eigenvalue
   $\mathbf{c}^T\boldsymbol{B}\mathbf{c} = \lambda\mathbf{c}^T\boldsymbol{W}\mathbf{c} \quad \forall\lambda \in \mathbb{C}$ " $\Rightarrow$ " $\mathbf{c}^T\boldsymbol{W}\mathbf{c} = 0 = \mathbf{c}^T\boldsymbol{B}\mathbf{c}$
   - uninteresting for FLDA
   - common null-space of $\boldsymbol{B}$, $\boldsymbol{W}$

Relation with FLDA

1. finite nonzero
   $(\boldsymbol{B} - \frac{t_{ii}}{s_{ii}} \boldsymbol{W})\mathbf{c} = 0 \quad \Rightarrow \quad \mathbf{c}^T \boldsymbol{B} \mathbf{c} = \frac{t_{ii}}{s_{ii}} \mathbf{c}^T \boldsymbol{W} \mathbf{c}$
   - $\lambda = \frac{t_{ii}}{s_{ii}}$ ... ratio of between- to within-variance
   - complement of null-spaces of $\boldsymbol{B}$, $\boldsymbol{W}$
2. finite zero
   $(\boldsymbol{B} - 0 \cdot \boldsymbol{W})\mathbf{c} = 0 \quad \Rightarrow \quad \mathbf{c}^T \boldsymbol{B} \mathbf{c} = 0$
   - opposite of FLDA aim
   - null-space of $\boldsymbol{B}$
3. infinite
   $\mathbf{c}^T \boldsymbol{B} \mathbf{c} = \lambda \mathbf{c}^T \boldsymbol{W} \mathbf{c} \quad \text{for} \quad \lambda = \infty \quad " \Rightarrow " \quad \mathbf{c}^T \boldsymbol{W} \mathbf{c} = 0$
   - wanted for FLDA, quality depends on $\mathbf{c}^T \boldsymbol{B} \mathbf{c}$
   - null-space of $\boldsymbol{W}$
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   $\mathbf{c}^T \boldsymbol{B} \mathbf{c} = \lambda \mathbf{c}^T \boldsymbol{W} \mathbf{c} \quad \forall \lambda \in \mathbb{C} \quad " \Rightarrow " \quad \mathbf{c}^T \boldsymbol{W} \mathbf{c} = 0 = \mathbf{c}^T \boldsymbol{B} \mathbf{c}$
   - uninteresting for FLDA
   - common null-space of $\boldsymbol{B}$, $\boldsymbol{W}$

Introduction

- here only methods from R, Matlab
  - linked with LAPACK-libraries
  - all methods are backward stable
- common approaches . . . "eliminate" singularity
- slight modification of $\boldsymbol{W}$ while preserving crucial information . . . regularization
- most methods based on spectral decomposition

$$\boldsymbol{W} = \boldsymbol{Q}\,\mathrm{diag}(\lambda_1, \ldots, \lambda_r, 0, \ldots, 0)\boldsymbol{Q}^T, \quad \boldsymbol{Q}^T\boldsymbol{Q} = \mathbf{I},$$

where $r = \mathrm{rank}(\boldsymbol{W})$

Outline

Pseudoinverse

- let $\boldsymbol{\Lambda}_r = \mathrm{diag}(\lambda_1, \ldots, \lambda_r)$
- partition $\boldsymbol{Q} = (\boldsymbol{Q}_r, \boldsymbol{Q}_N)$, where $\boldsymbol{Q}_N$ spans null-space of $\boldsymbol{W}$
- transformation to standard eigenproblem with

$$\boldsymbol{W}^+ = \boldsymbol{Q}_r \boldsymbol{\Lambda}_r^{-1} \boldsymbol{Q}_r^T$$

Pseudoinverse - properties

+ smaller eigenproblem (dimension r)
+ no need to search for an optimal regularization parameter
– only finite eigenpairs (discards null-space of $\boldsymbol{W}$)

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Implementation I - Non-symmetric transformation

- solve standard eigenproblem

$$(\boldsymbol{Q}_r \boldsymbol{\Lambda}_r^{-1} \boldsymbol{Q}_r^T \boldsymbol{B} - \lambda \mathbf{I})\mathbf{c} = 0$$

- cost of nonsymmetric QR-method: $\pm 25p^3$ flops
- eigenvalues and -vectors can be ill-conditioned
- store several $p \times p$ matrices
- see e. g. [Cheng et al. - 1992]

Implementation II - Symmetric transformation

- solve standard eigenproblem

$$(\boldsymbol{\Lambda}_r^{-1/2}\boldsymbol{Q}_r^T\boldsymbol{B}\boldsymbol{Q}_r\boldsymbol{\Lambda}_r^{-1/2} - \lambda\mathbf{I})\mathbf{c}^* = 0,$$

$$\mathbf{c} = \frac{\boldsymbol{Q}_r\boldsymbol{\Lambda}_r^{1/2}\mathbf{c}^*}{\|\boldsymbol{Q}_r\boldsymbol{\Lambda}_r^{1/2}\mathbf{c}^*\|}$$

- cost of symmetric QR-method: $\pm 9p^3$ flops
- only eigenvectors can be ill-conditioned
- store $\boldsymbol{W}$, $\boldsymbol{Q} \in \mathbb{R}^{p \times p}$, but transformed eigenproblem is $r \times r$
- see e.g. [Krzanowski et al. - 1995]

Implementation III - SVD-implementation I

- exploits the given structure of $\boldsymbol{B}$ and $\boldsymbol{W}$, e. g.

$$\boldsymbol{W} = \left(\frac{X - \boldsymbol{GM}}{\sqrt{n-g}}\right)^T \frac{X - \boldsymbol{GM}}{\sqrt{n-g}} = \boldsymbol{Q\Lambda Q}^T$$

- use SVD instead of eigen decomposition
- cost: $\pm 4p^2n$ flops or $\pm 14pn^2$ flops for "economy size SVD"

Implementation III - SVD-implementation II

- only eigenvectors can be ill-conditioned
- storage: 1 $n \times p$ matrix, 1 $n \times r$ matrix
- here everywhere economy size SVD
- `lda()` function in R-environment with default parameters
  - pseudoinverse method
  - SVD implementation

Outline

Epsilon-perturbation I

- consider $\boldsymbol{Q}\boldsymbol{\Lambda}_\varepsilon\boldsymbol{Q}^T$ instead of $\boldsymbol{Q}_r\boldsymbol{\Lambda}_r\boldsymbol{Q}_r^T$,

  $$\text{where } \boldsymbol{\Lambda}_\varepsilon = \operatorname{diag}(\lambda_1, \ldots, \lambda_r, \varepsilon, \ldots, \varepsilon)$$

  see e. g. [Cheng et al. - 1992]
- transformation of modified generalized eigenproblem

  $$(\boldsymbol{B} - \lambda\boldsymbol{Q}\boldsymbol{\Lambda}_\varepsilon\boldsymbol{Q}^T)\mathbf{c} = 0$$

Epsilon-perturbation - properties

+ no exclusion of any null-spaces
– large eigenproblem (dimension p)
– need for regularization parameter ε
– too small $\varepsilon \Rightarrow$ ill-conditioned eigenproblem

Epsilon-perturbation I

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– large eigenproblem (dimension p)
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Epsilon-perturbation II

- nonsymmetric & symmetric implementations: as before, only forming transformed eigenproblem is little more expensive
- SVD implementation: as before, BUT
  - store $p \times p$ matrix $\boldsymbol{Q}$
  - cannot exploit economy SVD: $\pm 4p^2n$

Outline

Null-space I

- vectors $\mathbf{c}$ in the null-space of $\boldsymbol{W}$ satisfy $\mathbf{c}^T \boldsymbol{W} \mathbf{c} = 0$
- if $\mathbf{c}^T \boldsymbol{B} \mathbf{c}$ is large $\Rightarrow$ can be used for projection
- find largest eigenvalues of $\boldsymbol{B}$ in null-space of $\boldsymbol{W}$ by solving

$$(\boldsymbol{Q}_N^T \boldsymbol{B} \boldsymbol{Q}_N - \mathbf{I})\mathbf{c} = 0$$

see e. g. [Guo et al. - 2003]

The Null-space method - properties

+ does not need a regularization parameter
– solves an eigenproblem of dimension $p - r$
– discards finite eigenvalues of original problem

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Null-space II

- symmetric implementation: as for Epsilon perturbation, but storage and cost a little cheaper
- SVD
  - storage: 1 $p \times (p - r)$ matrix
  - cost of 1 full SVD: $4p^2n$

Outline

Common Null-space Elimination I

- ...numerical analysists recommend [Parlett - 1998]
- common null-space of $\boldsymbol{B}$, $\boldsymbol{W}$ $\Rightarrow$ ill-posed eigenproblem
- project onto complement of common null-space
- $\boldsymbol{B}x = 0 \quad \wedge \quad \boldsymbol{W}x = 0 \quad \Leftrightarrow \quad (\boldsymbol{B} + \boldsymbol{W})x = 0$, because $\boldsymbol{B}, \boldsymbol{W} \geq 0$
- compute spectral decomposition $\boldsymbol{B} + \boldsymbol{W}$
- let $\boldsymbol{P}$ contain eigenvectors for non-zero eigenvalues
- solve the projected problem

$$(\boldsymbol{P}^T\boldsymbol{B}\boldsymbol{P} - \lambda\boldsymbol{P}^T\boldsymbol{W}\boldsymbol{P})\mathbf{c}^* = 0, \quad \mathbf{c} = \boldsymbol{P}\mathbf{c}^*$$

- vector selection by considering $\mathbf{c}^T\boldsymbol{B}\mathbf{c}$, $\mathbf{c}^T\boldsymbol{W}\mathbf{c}$

Common Null-space Elimination II

Common Null-space Elimination - properties

+ problem smaller than n ($\ll p$)
+ no exclusion of null-space of $\boldsymbol{W}$

Implementation with QZ:

- storage: only $p \times n$ matrices
- cost: order $pn^2 + n^3$
- both eigenvalues and -vectors can be ill-conditioned

Common Null-space Elimination II

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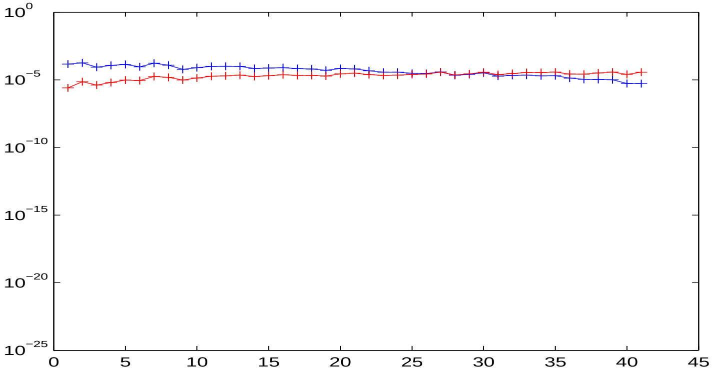
Numerical Experiment

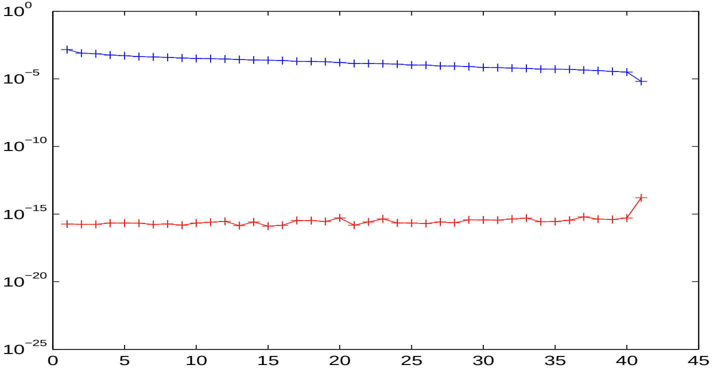
- protein fold classification problem
- sample size $n = 268$
    - 143 in training set
    - 125 in test set
- $p = 400$ predictors
- $K = 42$ classes

Pseudoinverse



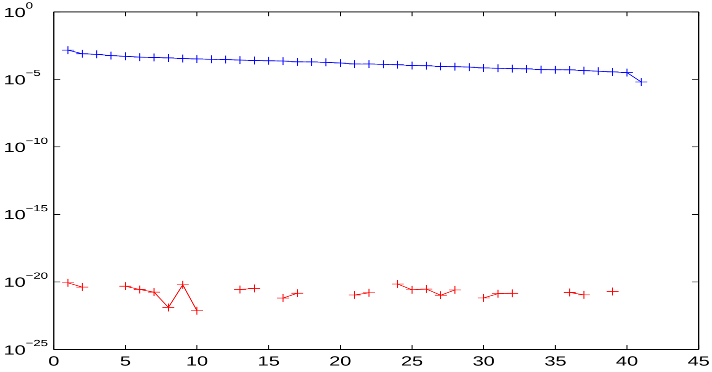
blue curve: $\mathbf{c}^T \boldsymbol{B} \mathbf{c}$, red curve: $\mathbf{c}^T \boldsymbol{W} \mathbf{c}$

Epsilon-perturbation



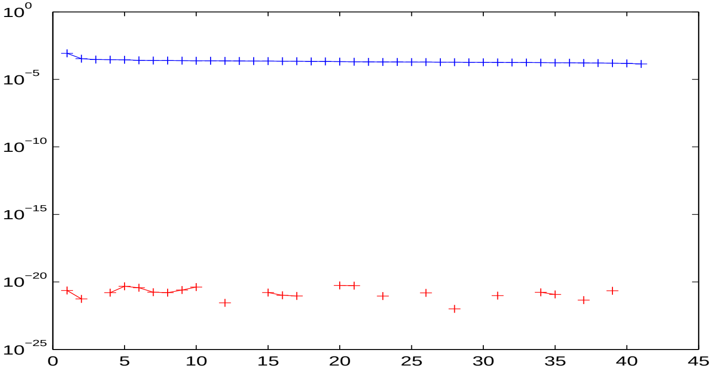
blue curve: $\mathbf{c}^T \boldsymbol{B} \mathbf{c}$, red curve: $\mathbf{c}^T \boldsymbol{W} \mathbf{c}$

Null-Space



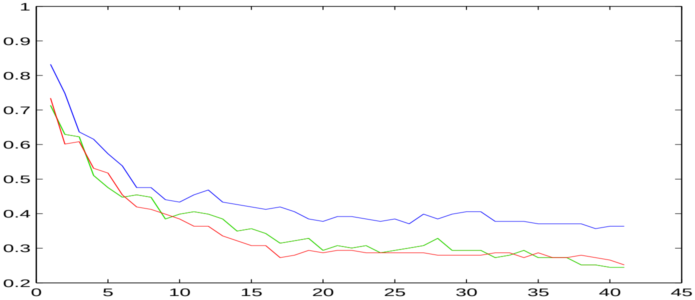
blue curve: $\mathbf{c}^T \boldsymbol{B} \mathbf{c}$, red curve: $\mathbf{c}^T \boldsymbol{W} \mathbf{c}$

Common Null-Space Elimination



blue curve: $\mathbf{c}^T \boldsymbol{B} \mathbf{c}$, red curve: $\mathbf{c}^T \boldsymbol{W} \mathbf{c}$

Error Rates of Classifi ers



blue curve: Pseudoinverse, green curve: both Epsilon and Null-space, red curve: Common Null-space elimination

- two middle methods: error rate of 24%
- can compete with Support Vector Machine strategy 23.2% (other over 28.8%, see e. g. [Markowetz et al. - 2003])

Conclusions

- Generalized Schur decomposition as a theoretical tool for better understanding of FLDA
  - covers all proposed methods
- Common-null space elimination
  - seems most appropriate, not only theoretically, but also experimentally and numerically
- in addition we found...
  - pseudoinverse method (R) for $p \gg n$ needs not be the best at all!
  - exploitation of structure with SVD

Open Questions & Future work

- choice and influence of regularization parameter in perturbation technique
- main challenge for nearby future is extension to very large problems
    - sparsity!!!
    - exploitation of special structure
- generalization to nonlinear cases
    - kernels method for Fisher [Baudat, Anouar - 2000]

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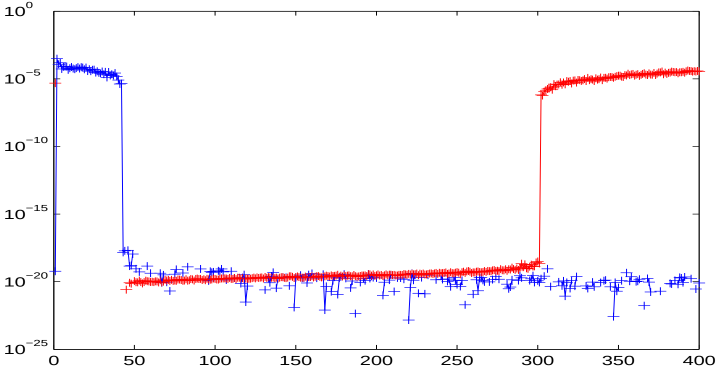
Generalized Schur Decomposition (by QZ)



blue curve: diagonal of $\boldsymbol{T}(\boldsymbol{B})$, red curve: diagonal of $\boldsymbol{S}(\boldsymbol{W})$