Tracking dominant symmetric matrices (including a new matrix factorization)

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Large Graphs and Networks
UCL Université catholique de Louvain

Eurasip lecture 2, Bari, August 2012

Goal

We want to approximate an $N \times N$ indefinite symmetric matrix H by a rank r factorization

$$H \approx UMU^T$$

where $U^T U = I_r$ and M is allowed to be indefinite as well

The optimal approximation is known

- $\Lambda(M)$ contains the r largest eigenvalues of H (in modulus)
- $\mathrm{Im}(U)$ is a basis for the corresponding eigenspace

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Goal :
Iterative procedure for large dense matrices in $\mathcal{O}(Nnr)$ complexity
($r \ll N$ is the rank of M and $n \leq N$ is the window size of the method)

"Sweeping" through H

We show only the columns and rows of U and H that are involved

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Rank $r = 3$ and we will use window size $n = 6$

step 1

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Start with leading $n \times n$ subproblem ($n = 6$ is the window size)

step 2

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Expand

step 2

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Expand also U (rank increases by 2)

step 3

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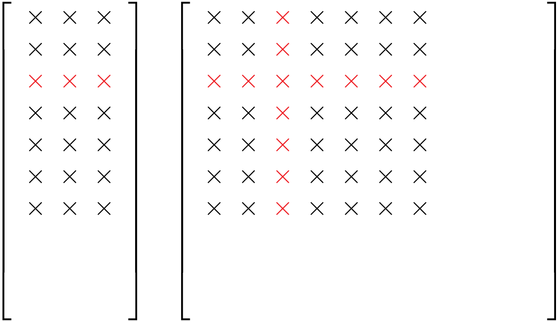
Downdate rank ...

step 4



... and also downsize window

step 4

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step 5

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Expand

step 6

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Downdate and downsize

step 7

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step 9

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Downdate and downsize

step 10

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step 11

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step 12

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Downdate and downsize

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Aim

Applications

- Tracking indefinite matrix problems
- Updating in sequential quadratic programming
- Updating saddle point problems

Aim

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Tools

- Updating increases $r \to r + 2$ and $n \to n + 1$
- Downdating restores the rank r (reduce by 2 again)
- Downsizing restores the window size n (optional)

The competitors

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but they suffer from the following disadvantages :

- updating bordered tridiagonal factorizations is expensive because of the updating of V
- deflating eigenvalues from a block diagonal is expensive because of the updating of D_{bl}

An anti-triangular decomposition

An anti-triangular decomposition

Theorem

Every $n \times n$ symmetric matrix H has a factorization $H = UMU^T$ where

$$M = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & Y^T \\ 0 & 0 & X & Z^T \\ 0 & Y & Z & W \end{bmatrix} \begin{matrix} \}n_0 \\ \}n_1 \\ \}n_2 \\ \}n_1 \end{matrix}, \quad X = eLL^T$$

where $U^T U = I_n$, $e = \pm 1$, $Y \in \mathbb{R}^{n_1 \times n_1}$, $L \in \mathbb{R}^{n_2 \times n_2}$ and $r = 2n_1 + n_2$

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$$\text{Ex}: \quad T = \left[\begin{array}{c|cc|ccc|cc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & \times \\ 0 & 0 & 0 & 0 & 0 & 0 & \times & \times \\ \hline 0 & 0 & 0 & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times & \times & \times \\ \hline 0 & 0 & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times & \times \end{array}\right]$$

Properties

$$M = \begin{array}{c} \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & Y^T \\ 0 & 0 & eLL^T & Z^T \\ 0 & Y & Z & W \end{array}\right] \end{array} \begin{array}{l} \}n_0 \\ \}n_1 \\ \}n_2 \\ \}n_1 \end{array} , \quad e = \pm 1$$

- $r = n_1 + n_2 + n_1$

Properties

$$M = \begin{array}{c} \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & Y^T \\ 0 & 0 & eLL^T & Z^T \\ 0 & Y & Z & W \end{array}\right] \begin{array}{l} \}n_0 \\ \}n_1 \\ \}n_2 \\ \}n_1 \end{array} \end{array}, \qquad e = \pm 1$$

- $r = n_1 + n_2 + n_1$
- L is full rank n_2 and can be chosen lower-triangular

Properties

$$M = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & Y^T \\ 0 & 0 & eLL^T & Z^T \\ 0 & Y & Z & W \end{bmatrix} \begin{matrix} \}n_0 \\ \}n_1 \\ \}n_2 \\ \}n_1 \end{matrix} , \qquad e = \pm 1$$

- $r = n_1 + n_2 + n_1$
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- Y is full rank n_1 and can be chosen anti-triangular

Properties

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- $r = n_1 + n_2 + n_1$
- L is full rank n_2 and can be chosen lower-triangular
- Y is full rank n_1 and can be chosen anti-triangular
- $InM_+ = (n_1 + n_2, n_1, n - r)$ and $InM_- = (n_1, n_1 + n_2, n - r)$

Properties

$$M = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & Y^T \\ 0 & 0 & eLL^T & Z^T \\ 0 & Y & Z & W \end{bmatrix} \begin{array}{l} \}n_0 \\ \}n_1 \\ \}n_2 \\ \}n_1 \end{array} , \quad e = \pm 1$$

- $r = n_1 + n_2 + n_1$
- L is full rank n_2 and can be chosen lower-triangular
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- $InM_+ = (n_1 + n_2, n_1, n - r)$ and $InM_- = (n_1, n_1 + n_2, n - r)$
- U is rectangular when removing zero rows/columns in M

Properties

$$M = \begin{array}{c} \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & Y^T \\ 0 & 0 & eLL^T & Z^T \\ 0 & Y & Z & W \end{array}\right] \begin{array}{l} \}n_0 \\ \}n_1 \\ \}n_2 \\ \}n_1 \end{array} \end{array}, \quad e = \pm 1$$

- $r = n_1 + n_2 + n_1$
- L is full rank n_2 and can be chosen lower-triangular
- Y is full rank n_1 and can be chosen anti-triangular
- $InM_+ = (n_1 + n_2, n_1, n - r)$ and $InM_- = (n_1, n_1 + n_2, n - r)$
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- The decomposition of a dense matrix requires $\mathcal{O}(n^3)$ flops

Properties

$$M = \begin{array}{c} \left[\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & Y^T \\ 0 & 0 & eLL^T & Z^T \\ 0 & Y & Z & W \end{array} \right] \end{array} \begin{array}{l} \}n_0 \\ \}n_1 \\ \}n_2 \\ \}n_1 \end{array}, \quad e = \pm 1$$

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For $\begin{bmatrix} 0 & B^T \\ B & A \end{bmatrix}$ one just requires a QR of B to get a (permuted) M

Proof (for e=1)

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the maximal non-negative subspace containing it, is unique

(see Gohberg-Lancaster-Rodman)

Some examples

Let $H = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$

then neutral vectors are e.g. given by $u_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ a \\ b \\ \sqrt{a^2 + 2b^2} \end{bmatrix}$

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When all positive eigenvalues are equal and all negative eigenvalues are equal, M is unique and essentially diagonal !

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One easily obtains the rank $r+2$ factorization $\tilde{H} = \tilde{U}\tilde{M}\tilde{U}^T$ where

$$\tilde{U} := \left[\begin{array}{cc|c} u_\perp & U & \\ \hline & & 1 \end{array} \right], \quad \tilde{M} := \left[\begin{array}{c|c|c} 0 & 0 & \rho \\ \hline 0 & M_r & r \\ \hline \rho & r^T & \alpha \end{array} \right], \quad b = Ur + \rho u_\perp$$

comes from a Gram Schmidt orthogonalization of $[U|b]$

Updating + downdating problem

Notice that up to a symmetric permutation, $\tilde{T}$ is anti-triangular :

$$\tilde{T} := \begin{bmatrix} 0 & 0 & 0 & 0 & \rho \\ 0 & 0 & 0 & S & r_s \\ 0 & 0 & eLL^T & W & r_w \\ 0 & S^T & W^T & G & r_g \\ \rho & r_s^T & r_w^T & r_g^T & \alpha \end{bmatrix}$$

where the matrix size n_1 increased by 1 (and the rank of $\tilde{T}$ by 2)

We need to "chop off" $\tilde{T}$'s 2 eigenvalues of smallest modulus : λ_1, λ_2
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All of these steps can be performed in $\mathcal{O}(Nr)$ flops

Downsizing problem

- Let H_v be an orthogonal (Householder) transformation such that

$$H_v \mathbf{v} = \upsilon \; e_1, \qquad \upsilon = \mp \|\mathbf{v}\|_2, \quad \tilde{U} = \left[\begin{array}{c} \mathbf{v}^T \\ V \end{array} \right]$$

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- The batman factorization of the scaled $\tilde{T}$ then has to be restored
- Any row of $\tilde{U}$ can be chosen to be removed this way
- Choose the row of least norm to get a better approximation

Example (positive semi-definite)

The following matrix has rank 3

$$F(i,j) = \sum_{k=1}^{3} \exp\left(-\frac{(i-\mu_k)^2 + (j-\mu_k)^2}{2\sigma_k}\right), \qquad i,j = 1,\ldots,100,$$

with

$$\mu = \left[\begin{array}{ccc} 4 & 18 & 76 \end{array}\right], \quad \sigma = \left[\begin{array}{ccc} 10 & 20 & 5 \end{array}\right].$$

Let $F = Q\Lambda Q^T$ be its spectral decomposition and let $\tilde{\Delta} \in \mathbb{R}^{100\times 100}$ be a matrix of random numbers generated by the `matlab` function `randn`, and define $\Delta = \tilde{\Delta}/\|\tilde{\Delta}\|_2$. Consider the matrix

$$H = F + \varepsilon \Delta\Delta^T, \qquad \varepsilon = 1.0e-5$$

Example

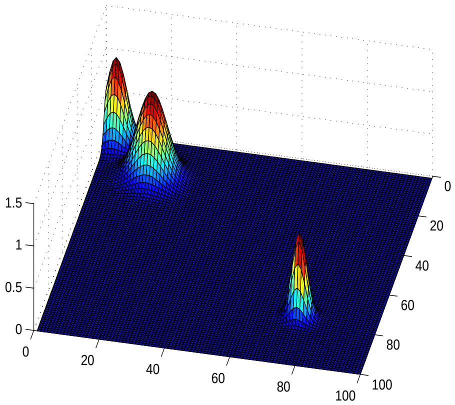

Figure: Graph of the size of the entries of the matrix H.

Example

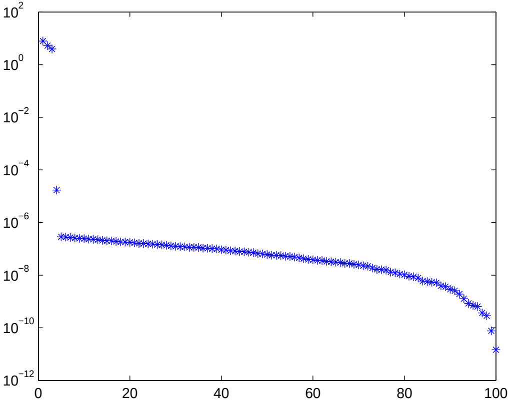

Figure: Distribution of the eigenvalues of the matrix H in logarithmic scale.

Example

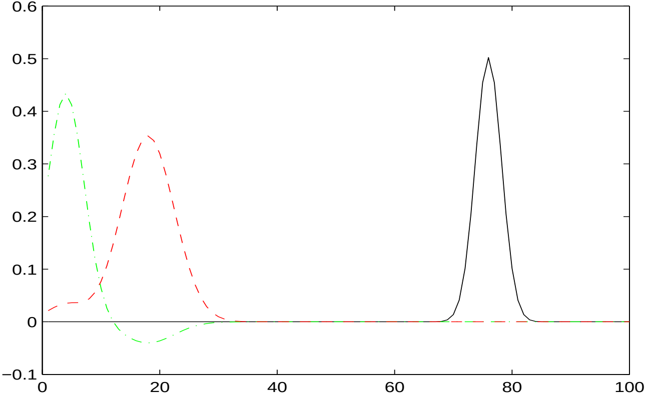

Figure: Plot of the three dominant eigenvectors of H

Example

Largest three eigenvalues of the matrix H (first column)

Largest three eigenvalues computed with our procedure (next cols) with rank $r = 3$ and window $n = 30, 40, 50$

λ_i	$\mu_i, n = 30$	$\mu_i, n = 40$	$\mu_i, n = 50$
7.949478e0	7.375113e0	7.820407e0	7.947127e0
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Reconstruction of dominant eigenvalues is quite good

The quality is improving with increasing window size n

Examples

We will consider a few examples of full decompositions
i.e. no downdating or downsizing

Ex1: $A = \mathrm{randn}(100); A = A + A'; \mathrm{Inertia}(A) = (50, 0, 50)$
Ex2: $A = \mathrm{rand}(100); A = A + A'; \mathrm{Inertia}(A) = (48, 0, 52)$
Ex3: A low rank
Ex4: A diagonal dominant

In each of the case we had good backward stability

$\frac{\|QMQ^T - A\|_2}{\|A\|_2}$	$\frac{\|LU - PA\|_2}{\|A\|_2}$	$\frac{\|QR - A\|_2}{\|A\|_2}$
2.49e-15	7.27e-16	1.12e-15

See movies

Random example

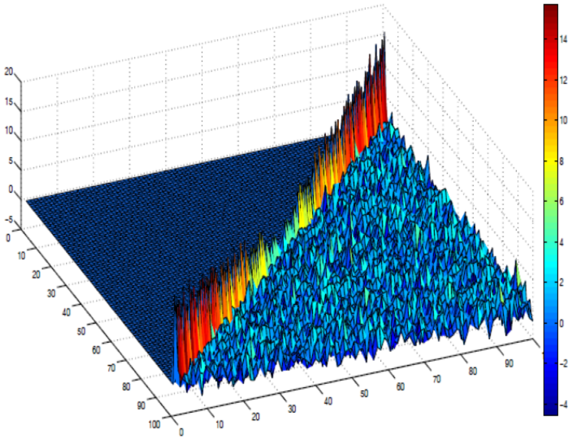


Figure: A random matrix $A = B + B^T$ with B generated by `randn(100,100)`

Random example

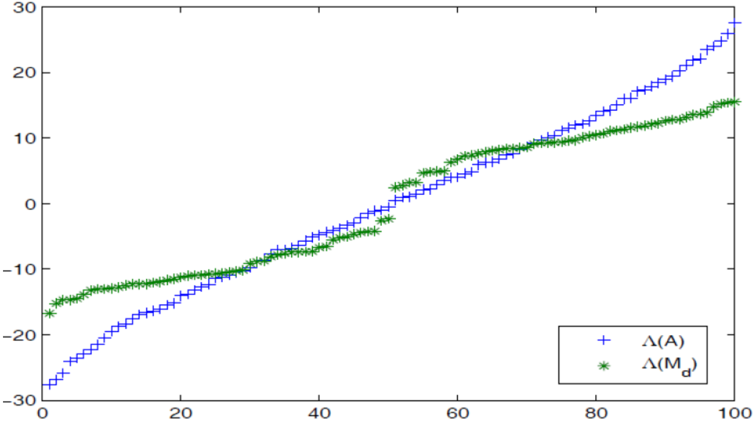


Figure: Eigenvalues and estimates based on the diagonal and anti-diagonal

Clustered example

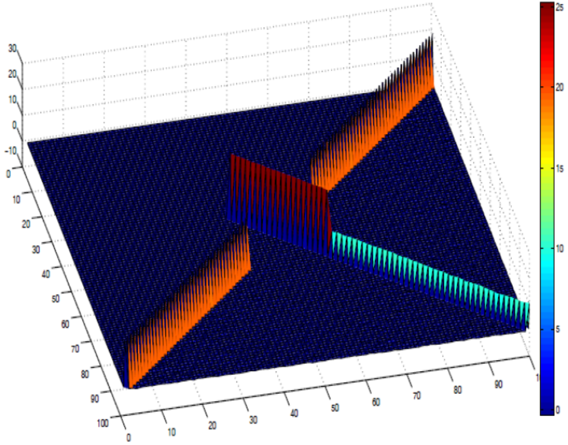
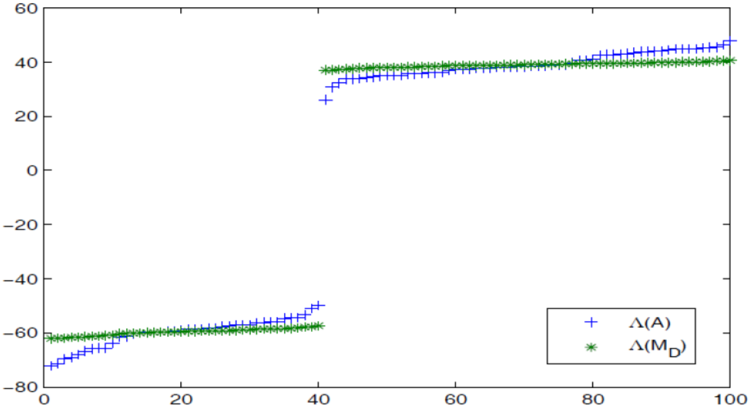


Figure: Matrix with a cluster of positive and a cluster of negative eigenvalues, generated by $A = U\mathit{diag}\left(-60I_{40}, 40I_{60}\right)U^{T} + E$ with $\|E\| \leq 1$

Clustered example



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- An efficient algorithm for computing incrementally the dominant eigenspace of a symmetric matrix
- The overall complexity of the incremental updating technique to compute an $N \times r$ basis matrix U for the dominant eigenspace of H, is reduced to $\mathcal{O}(N^2 r)$
- When using both incremental updating and downsizing to compute the dominant eigenspace of $\hat{H}_n$ (an $n \times n$ principal submatrix of H_N), the complexity is reduced to $\mathcal{O}(Nnr)$.

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