# Dominant feature extraction

Francqui Lecture 7-5-2010

Paul Van Dooren Université catholique de Louvain CESAME, Louvain-la-Neuve, Belgium Develop basic ideas for large scale dense matrices

Recursive procedures for

- Dominant singular subspace
- Multipass iteration
- Subset selection
- Dominant eigenspace of positive definite matrix
- Possible extensions

which are all based on solving cheap subproblems

Show accuracy and complexity results

Given  $A_{m \times n}$ , approximate it by a rank *k* factorization  $B_{m \times k}C_{k \times n}$  by solving

 $\min \|\boldsymbol{A} - \boldsymbol{B}\boldsymbol{C}\|_2, \quad k \ll m, n$ 



This has several applications in Image compression, Information retrieval and Model reduction (POD)

# Information retrieval



# Proper Orthogonal decomposition (POD)

Compute a state trajectory for one "typical" input

Collect the principal directions to project on



Quartz reactor



Snap shots of "typical" states Ten dominant "states"



We pass once over the data with a window of length *k* and perform along the way a set of windowed SVD's of dimension  $m \times (k + \ell)$ 



Step 1 : expand by appending  $\ell$  columns (Gram Schmidt) Step 2 : contract by deleting the  $\ell$  least important columns (SVD) Append column  $a_+$  to the current approximation  $URV^T$  to get

$$\begin{bmatrix} URV^{T} & a_{+} \end{bmatrix} = \begin{bmatrix} U & a_{+} \end{bmatrix} \begin{bmatrix} R & 0 \\ & 1 \end{bmatrix} \begin{bmatrix} V^{T} & \\ & 1 \end{bmatrix}$$

Update with Gram Schmidt to recover a new decomposition  $\hat{U}\hat{R}\hat{V}^{T}$ :



using 
$$\hat{r} = U^T a_+$$
,  $\hat{a} = a_+ - U\hat{r}$ ,  $\hat{a} = \hat{u}\hat{\rho}$  (since  $a_+ = U\hat{r} + \hat{u}\hat{\rho}$ )

Now remove the  $\ell$  smallest singular values of this new  $\hat{U}\hat{R}\hat{V}^{T}$  via

$$\hat{U}\hat{R}\hat{V}^{\mathsf{T}} = (\hat{U}G_u)(G_u^{\mathsf{T}}\hat{R}G_v)(G_v^{\mathsf{T}}\hat{V}^{\mathsf{T}}) =$$



and keeping  $U_+R_+V_+^{T}$  as best approximation of  $\hat{U}\hat{R}\hat{V}^{T}$  (just delete the  $\ell$  smallest singular values)

The Gram Schmidt update (expansion) requires 4mk flops per column (essentially for the products  $\hat{r} = U^T a_+$ ,  $\hat{a} = a_+ - U\hat{r}$ )

For  $G_u \hat{R} G_v = \begin{bmatrix} R_+ & 0 \\ \mu_i \end{bmatrix}$  one requires the left and right singular vectors of  $\hat{R}$  which can be obtained in  $O(k^2)$  flops per singular value (using inverse iteration)

Multiplying  $\hat{U}G_u$  and  $\hat{V}G_v$  requires 4mk flops per deflated column

The overall procedure requires 8mk flops per processed column and hence 8mnk flops for a rank *k* approximation to a  $m \times n$  matrix *A* 

One shows that 
$$A = U \begin{bmatrix} R & A_{12} \\ 0 & A_{22} \end{bmatrix} V^T$$
 where  $\| \begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix} \|_F^2$  is known

Let 
$$E := A - \hat{A} = U \Sigma V^T - \hat{U} \hat{\Sigma} \hat{V}^T$$
 and  $\mu := ||E||_2$ 

Let  $\hat{\mu} := \max \mu_i$  where  $\mu_i$  is the neglected singular value at step *i* 

One shows that the error norm

$$oldsymbol{\hat{\mu}} \leq \sigma_{oldsymbol{k}+1} \leq \mu \leq \sqrt{n-oldsymbol{k}} oldsymbol{\hat{\mu}} pprox oldsymbol{c} oldsymbol{\hat{\mu}}$$

$$\hat{\sigma}_i \leq \sigma_i \preceq \hat{\sigma}_i + \hat{\mu}^2 / 2\hat{\sigma}_i$$

 $\tan \theta_k \preceq \tan \hat{\theta}_k := \hat{\mu}^2 / (\hat{\sigma}_k^2 - \hat{\mu}^2), \quad \tan \phi_k \preceq \tan \hat{\phi}_k := \hat{\mu} \hat{\sigma}_1 / (\hat{\sigma}_k^2 - \hat{\mu}^2)$ 

where  $\theta_k$ ,  $\phi_k$  are the canonical angles of dimension k:

$$\cos \theta_k := \| \boldsymbol{U}^{\mathsf{T}}(:,k) \hat{\boldsymbol{U}} \|_2, \quad \cos \phi_k := \| \boldsymbol{V}^{\mathsf{T}}(:,k) \hat{\boldsymbol{V}} \|_2$$

#### **Examples**

#### The bounds get much better when the gap $\sigma_k - \sigma_{k+1}$ is large



#### How quickly do we track the subpaces ?



How  $\cos \theta_k^{(i)}$  evolves with the time step *i* 

### Example

#### Find the dominant behavior in an image sequence

Images can have up to 10<sup>6</sup> pixels

Each column of A is one image Original : m = 28341, n = 100



 ${\sf Approximation}: \ k=6$ 



Low Rank Incremental SVD can be applied in several passes, say to

$$\frac{1}{\sqrt{k}} \begin{bmatrix} A & A & \dots & A \end{bmatrix}$$

After the first block (or "pass") a good approximation of the dominant space  $\hat{U}$  has already been constructed

Going over to the next block (second "pass") will improve it, etc.

**Theorem** Convergence of the multipass method is linear, with approximate ratio of convergence  $\psi/(1 - \kappa^2) < 1$ , where

- $\psi$  measures orthogonality of the residual columns of A
- $\kappa$  is the ratio  $\sigma_k / \sigma_{k+1}$  of A

# **Convergence behavior**

#### for increasing gap between "signal" and "noise"



# **Convergence behavior**

#### for increasing orthogonality between "residual vectors"



# Ten dominant left singular vectors of ORL Database of faces (40 images, 10 subjects, $92 \times 112$ pixels = $10304 \times 400$ matrix)

#### Using MATLAB' SVD function



#### Using one pass of incremental SVD



Maximal angle : 16.3°, maximum relative error in sing. values : 4.8%

A useful and economical SVD approximation of  $A_{m,n}$ 

For matrices with columns that are very large or "arrive" with time

Complexity is proportional to mnk and the number of "passes"

Algorithms due to [1] Manjunath-Chandrasekaran-Wang (95) [2] Levy-Lindenbaum (00) [3] Chahlaoui-Gallivan-VanDooren (01) [4] Brand (03) [5] Baker-Gallivan-VanDooren (09)

Convergence analysis and accuracy in refs [3],[4],[5]

We want a "good approximation" of  $A_{mn}$  by a product  $B_{mk}P^T$  where  $P_{nk}$  is a "selection matrix" i.e. a submatrix of the identity  $I_n$ 

This seems connected to

$$\min \|\boldsymbol{A} - \boldsymbol{B} \boldsymbol{P}^{\mathsf{T}}\|_2$$

and maybe similar techniques can be used as for incremental SVD

Clearly, if B = AP, we just select a subset of the columns of A

Rather than minimizing  $||A - BP^T||_2$  we maximize vol(*B*) where

$$\operatorname{vol}(B) = \det(B^T B)^{\frac{1}{2}} = \prod_{i=1}^k \sigma_i(B), \qquad m \ge k$$

There are  $\binom{n}{k}$  possible choices and the problem is NP hard and there is no polynomial time approximation algorithm Gu-Eisenstat show that the Strong Rank Revealing QR factorization (SRRQR) solves the following simpler problem

*B* is sub-optimal if there is no swapping of a single column of *A* (yielding  $\hat{B}$ ) that has a larger volume (constrained minimum)

Here, we propose a simpler "recursive updating" algorithm that has complexity O(mnk) rather than  $O(mn^2)$  for Gu-Eisenstat

The idea is again based on a sliding window of size k + 1 (or  $k + \ell$ )

Sweep through columns of A while maintaining a "best" subset B

- Append a column of A to B, yielding  $B_+$
- Contract B<sub>+</sub> to B̂ by deleting the "weakest" column of B<sub>+</sub>

Let B = A(:, 1:k) to start with and let B = QR where R is  $k \times k$ 

Append the next column  $a_+$  of A to form  $B_+$  and update its decomposition using Gram Schmidt

$$B_{+} := \begin{bmatrix} QR & a_{+} \end{bmatrix} = \begin{bmatrix} Q & a_{+} \end{bmatrix} \begin{bmatrix} R & 0 \\ & 1 \end{bmatrix} = \begin{bmatrix} Q & \hat{q} \end{bmatrix} \begin{bmatrix} R & \hat{r} \\ & \hat{\rho} \end{bmatrix} = Q_{+}R_{+}$$

with  $\hat{r} = Q^T a_+$ ,  $\hat{a} = a_+ - Q\hat{r}$ ,  $\hat{a} = \hat{q}\hat{\rho}$  (since  $a_+ = Q\hat{r} + \hat{q}\hat{\rho}$ )

Contract  $B_+$  to  $\hat{B}$  by deleting the "weakest" column of  $R_+$ 

This can be done in  $O(mk^2)$  using Gu-Eisenstat's SRRQR method but an even simpler heuristic uses only O((m + k)k) flops Let  $R_+v = \sigma_{k+1}u$  be the singular vector pair corresponding to the smallest singular value  $\sigma_{k+1}$  of  $R_+$  and let  $v_i$  be the components of v

Let  $R_i$  be the submatrix obtained by deleting column *i* from  $R_+$  then

$$\frac{\sigma_{k+1}^2}{\sigma_1^2} + \left(1 - \frac{\sigma_{k+1}^2}{\sigma_1^2}\right) |v_i|^2 \le \frac{\operatorname{vol}^2(R_i)}{\prod_{j=1}^k \sigma_j^2} \le \frac{\sigma_{k+1}^2}{\sigma_k^2} + \left(1 - \frac{\sigma_{k+1}^2}{\sigma_k^2}\right) |v_i|^2$$

Maximizing  $|v_i|$  maximizes thus a lower bound on  $\text{vol}^2(R_i)$ In practice this is almost always optimal and guaranteed to be so if

$$\frac{\sigma_{k+1}^2}{\sigma_k^2} + \left(1 - \frac{\sigma_{k+1}^2}{\sigma_k^2}\right) |v_i|^2 \le \frac{\sigma_{k+1}^2}{\sigma_1^2} + \left(1 - \frac{\sigma_{k+1}^2}{\sigma_1^2}\right) |v_j|^2 \qquad \forall j \ne i$$

Start with B = A(:, 1:k) = QR where R is  $k \times k$ 

For j = k + 1 : n

- append column  $a_+ := A(:, j)$  to get  $B_+$
- update its QR decomposition to  $B_+ = Q_+ R_+$
- contract  $B_+$  to yield a new  $\hat{B}$  using the GKS heuristic
- update its QR decomposition to  $\hat{B} = \hat{Q}\hat{R}$

One can verify the optimality by performing a second pass

Notice that GKS is optimal when  $\sigma_{k+1} = 0$  since then

$$\operatorname{vol}(\boldsymbol{R}_i) = |\boldsymbol{v}_i| \prod_{j=1}^k \sigma_j$$

#### **Typical applications**

- Kernel Matrices (Machine Learning)
- Spectral Methods (Image Analysis)
- Correlation Matrices (Statistics and Signal Processing)
- Principal Component Analysis
- Karhunen-Loeve
- <mark>ا ا</mark>

We use  $K_N$  to denote the full  $N \times N$  positive definite matrix

# Sweeping through K

Suppose a rank *m* approximation of the dominant eigenspace of *K<sub>n</sub>* ∈ ℝ<sup>n×n</sup>, *n* ≫ *m*, is known,

$$K_n \approx A_n := U_n M_m U_n^T,$$

 $M_m \in \mathbb{R}^{m \times m}$  an spd matrix and  $U_n \in \mathbb{R}^{n \times m}$  with  $U_n^T U_n = I_m$ 

Suppose a rank *m* approximation of the dominant eigenspace of *K<sub>n</sub>* ∈ ℝ<sup>n×n</sup>, *n* ≫ *m*, is known,

$$K_n \approx A_n := U_n M_m U_n^T,$$

 $M_m \in \mathbb{R}^{m \times m}$  an spd matrix and  $U_n \in \mathbb{R}^{n \times m}$  with  $U_n^T U_n = I_m$ 

► Obtain the  $(n + 1) \times m$  eigenspace  $U_{n+1}$  of the  $(n + 1) \times (n + 1)$  kernel matrix  $K_{n+1}$ 

$$K_{n+1} = \begin{bmatrix} K_n & \mathbf{a} \\ \mathbf{a}^T & b \end{bmatrix} \approx \tilde{U}_{n+1,m+2} \tilde{M}_{m+2} \tilde{U}_{n+1,m+2}^T$$

Suppose a rank *m* approximation of the dominant eigenspace of *K<sub>n</sub>* ∈ ℝ<sup>n×n</sup>, *n* ≫ *m*, is known,

$$K_n \approx A_n := U_n M_m U_n^T,$$

 $M_m \in \mathbb{R}^{m \times m}$  an spd matrix and  $U_n \in \mathbb{R}^{n \times m}$  with  $U_n^T U_n = I_m$ 

► Obtain the  $(n + 1) \times m$  eigenspace  $U_{n+1}$  of the  $(n + 1) \times (n + 1)$  kernel matrix  $K_{n+1}$ 

$$K_{n+1} = \begin{bmatrix} K_n & \mathbf{a} \\ \mathbf{a}^T & b \end{bmatrix} \approx \tilde{U}_{n+1,m+2}\tilde{M}_{m+2}\tilde{U}_{n+1,m+2}^T$$

• Downdate  $\tilde{M}_{m+2}$  to get back to rank m

Suppose a rank *m* approximation of the dominant eigenspace of *K<sub>n</sub>* ∈ ℝ<sup>n×n</sup>, *n* ≫ *m*, is known,

$$K_n \approx A_n := U_n M_m U_n^T,$$

 $M_m \in \mathbb{R}^{m \times m}$  an spd matrix and  $U_n \in \mathbb{R}^{n \times m}$  with  $U_n^T U_n = I_m$ 

► Obtain the  $(n + 1) \times m$  eigenspace  $U_{n+1}$  of the  $(n + 1) \times (n + 1)$  kernel matrix  $K_{n+1}$ 

$$K_{n+1} = \begin{bmatrix} K_n & \mathbf{a} \\ \mathbf{a}^T & b \end{bmatrix} \approx \tilde{U}_{n+1,m+2} \tilde{M}_{m+2} \tilde{U}_{n+1,m+2}^T$$

- Downdate  $\tilde{M}_{m+2}$  to get back to rank m
- Downsize  $\tilde{U}_{n+1}$  to get back to size *n*

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

$[ \times \times \times \times ]$	Γ×	×	$\times$	$\times$	×	$\times$	$\times$	$\times$	$\times$	×
$\times \times \times \times$	×	$\times$	X							
$\times \times \times \times$	×	$\times$	×							
$\times \times \times \times$	×	$\times$	×							
$\times \times \times \times$	×	$\times$	×							
$\times \times \times \times$	×	$\times$	×							
$\times \times \times \times$	×	$\times$	×							
$\times \times \times \times$	×	$\times$	×							
$\times \times \times \times$	×	$\times$	×							
$\times \times \times \times$	×	$\times$	×							

Window size n = 5, rank k = 4



Start with leading  $n \times n$  subproblem



Expand



Downdate and downsize

$[ \times \times \times \times ]$	$[ \times \times$	$\times$ $\times$ $\times$
$\times$ $\times$ $\times$ $\times$	X X	$\times$ $\times$ $\times$
		~ ~ ~
		~ ~ ~
		$\times$ $\times$ $\times$
$\times \times \times \times$	$\times \times$	$\times$ $\times$ $\times$

$[ \times \times \times \times ]$	$] [ \times \times ]$	$\times$ $\times$ $\times$ $\times$
$\times \times \times \times$		$\times$ $\times$ $\times$ $\times$
$\times$ $\times$ $\times$ $\times$		× × × ×
$\times \times \times \times$		$\times$ $\times$ $\times$ $\times$
$\times \times \times \times$		$\times$ $\times$ $\times$ $\times$
	× ×	$\times$ $\times$ $\times$ $\times$
L	JL	

Expand

$\times$	$\times$	$\times$	×	Γ×	$\times$	$\times$	×	$\times$	×
×	×	×	×	×	×	×	×	Х	×
X	×	$\times$	×	×	×	×	×	×	×
×	×	×	×	×	×	×	×	$\times$	×
$\times$	$\times$	$\times$	$\times$	×	$\times$	×	$\times$	$\times$	×
X	×	×	×	×	×	×	X	Х	$\times$

Downdate and downsize

$\times \times \times \times$	$[ \times \times ]$	×	$\times$ $\times$	
× × × ×	× ×	×	× ×	
× × × × ×	× ×	×	× ×	
$\times$ $\times$ $\times$ $\times$	$\times \times$	×	$\times$ $\times$	
$\times$ $\times$ $\times$ $\times$	× ×	×	××	
$[ \times \times \times \times ]$	$[ \times \times ]$	×	$\times$ $\times$ $\times$	
-----------------------------------	---------------------	---	----------------------------	
$\times \times \times \times$	× ×	×	$\times$ $\times$ $\times$	
× × × ×	× ×	×	$\times$ $\times$ $\times$	
$\times \times \times \times$	× ×	×	$\times$ $\times$ $\times$	
$\times \times \times \times$	X X	×	$\times$ $\times$ $\times$	
	× ×	×	$\times$ $\times$ $\times$	

Expand

×	×	~							
	~	×	X	×	×	×	×	×	×
×	×	×	×	×	×	×	×	×	×
×	×	×	×	×	×	×	×	$\times$	×
×	×	$\times$	$\times$	×	×	$\times$	$\times$	$\times$	$\times$
×	$\times$	$\times$	×	×	×	$\times$	$\times$	$\times$	$\times$

Downdate and downsize

	-			
× × × ×	×	×	$\times$ $\times$ $\times$	
$\times$ $\times$ $\times$ $\times$	×	×	$\times$ $\times$ $\times$	
$\times \times \times \times$	×	×	$\times$ $\times$ $\times$	
$\times \times \times \times$	×	×	$\times$ $\times$ $\times$	
$\times \times \times \times$	×	×	$\times$ $\times$ $\times$	

				Γ						
×	×	×	×		×	×	×	×	×	×
×	×	×	×		×	×	×	×	×	×
×	×	×	Х		×	×	×	×	×	×
×	$\times$	$\times$	$\times$		×	×	$\times$	$\times$	$\times$	×
×	$\times$	$\times$	×		×	×	×	$\times$	$\times$	×
					×	×	×	×	×	×

Expand

1	Γ					
$\times$ $\times$ $\times$ $\times$	×	×	×	×	×	×
$\times$ $\times$ $\times$ $\times$	×	×	×	×	×	×
$\times$ $\times$ $\times$ $\times$	×	×	×	×	×	×
$\times$ $\times$ $\times$ $\times$	×	×	×	$\times$	$\times$	×
$\times \times \times \times$	×	×	×	$\times$	$\times$	×
$\times$ $\times$ $\times$ $\times$	×	×	×	Х	Х	×

Downdate and downsize

	-		-
× × × ×	×	×	$\times$ $\times$ $\times$
× × × ×	×	×	× × ×
× × × ×	×	×	$\times$ $\times$ $\times$
$\times \times \times \times$	×	×	$\times$ $\times$ $\times$
× × × ×	×	×	$\times$ $\times$ $\times$

[ ]	Γ			-
$\times \times \times \times$	×	×	X	× × ×
× × × ×	×	×	X	× × ×
$\times$ $\times$ $\times$ $\times$	×	×	×	× × ×
$\times$ $\times$ $\times$ $\times$	×	×	×	× × ×
$\times$ $\times$ $\times$ $\times$	×	×	×	$\times \times \times$
	×	×	×	× × ×

Expand

F 1 [	-			_
$\times \times \times \times$	×	×	× × :	××
× × × ×	×	×	× × :	××
$\times$ $\times$ $\times$ $\times$	×	×	× × :	× ×
$\times \times \times \times$	×	×	× × X	× ×
$\times \times \times \times$	×	×	× × X	× ×
$\times$ $\times$ $\times$ $\times$	×	×	××	× ×

Downdate and downsize

[ ]	Γ	]
$\times \times \times \times$		× × × ×
× × × ×	× ×	× × ×
× × × ×	××	× × ×
$\times \times \times \times$	X X	× × ×
	$L \times \times$	× × ×

Suppose a rank *m* approximation of the dominant eigenspace of *K<sub>n</sub>* ∈ ℝ<sup>n×n</sup>, *n* ≫ *m*, is known,

$$K_n \approx A_n := U_n M_m U_n^T,$$

 $M_m \in \mathbb{R}^{m \times m}$  an spd matrix and  $U_n \in \mathbb{R}^{n \times m}$  with  $U_n^T U_n = I_m$ 

► Obtain the  $(n + 1) \times m$  eigenspace  $U_{n+1}$  of the  $(n + 1) \times (n + 1)$  kernel matrix  $K_{n+1}$ 

$$K_{n+1} = \begin{bmatrix} K_n & \mathbf{a} \\ \mathbf{a}^T & b \end{bmatrix} \approx \tilde{U}_{n+1,m+2} \tilde{M}_{m+2} \tilde{U}_{n+1,m+2}^T$$

• Downdate  $M_{m+2}$  to delete the "smallest" two eigenvalues

## **Updating: Proposed algorithm**

## Since

$$\mathbf{a} = U_n U_n^T \mathbf{a} + (I_m - U_n U_n^T) \mathbf{a}$$
$$= U_n \mathbf{r} + \rho \mathbf{u}_{\perp},$$

with  $\mathbf{q} = (I_m - U_n U_n^T) \mathbf{a}$ ,  $\rho = \|\mathbf{q}\|_2$ ,  $\mathbf{u}_\perp = \mathbf{q}/\rho$ , we can write



# Updating: Proposed algorithm

### Let

$$M_m = Q_m \Lambda_m Q_m^T$$

### where

 $\Lambda_m = \operatorname{diag}(\mu_1, \mu_2, \ldots, \mu_m), \quad \mu_1 \geq \cdots \geq \mu_m > 0, \quad Q_m^T Q_m = I_m.$ 

### Let

$$M_m = Q_m \Lambda_m Q_m^T$$

#### where

 $\Lambda_m = \operatorname{diag}(\mu_1, \mu_2, \dots, \mu_m), \quad \mu_1 \geq \dots \geq \mu_m > 0, \quad Q_m^T Q_m = I_m.$ 

### Let

$$ilde{M}_{m+2} = ilde{Q}_{m+2} ilde{\Lambda}_{m+2} ilde{Q}_{m+2}^T$$

#### where

 $\tilde{\Lambda}_{m+2} = \operatorname{diag}(\tilde{\lambda}_1, \tilde{\lambda}_2, \dots, \tilde{\lambda}_{m+1}, \tilde{\lambda}_{m+2}), \quad \tilde{Q}_{m+2}^T \tilde{Q}_{m+2} = I_{m+2}$ 

### Let

$$M_m = Q_m \Lambda_m Q_m^T$$

#### where

 $\Lambda_m = \operatorname{diag}(\mu_1, \mu_2, \dots, \mu_m), \quad \mu_1 \geq \dots \geq \mu_m > 0, \quad Q_m^T Q_m = I_m.$ 

### Let

$$ilde{M}_{m+2} = ilde{Q}_{m+2} ilde{\Lambda}_{m+2} ilde{Q}_{m+2}^T$$

#### where

$$\tilde{\Lambda}_{m+2} = \operatorname{diag}(\tilde{\lambda}_1, \tilde{\lambda}_2, \dots, \tilde{\lambda}_{m+1}, \tilde{\lambda}_{m+2}), \quad \tilde{Q}_{m+2}^{\mathsf{T}} \tilde{Q}_{m+2} = I_{m+2}$$

By the interlacing property, we have

$$\tilde{\lambda}_1 \ge \mu_1 \ge \tilde{\lambda}_2 \ge \mu_2 \ge \cdots \ge \mu_m \ge \tilde{\lambda}_{m+1} \ge \mathbf{0} \ge \tilde{\lambda}_{m+2}$$

We want a simple orthogonal transformation H such that

$$H[\mathbf{v}_{m+1} \ \mathbf{v}_{m+2}] = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \hline \times & \mathbf{0} \\ \mathbf{0} & \times \end{bmatrix}, \qquad H\tilde{M}_{m+2}H^{\mathsf{T}} = \begin{bmatrix} \overline{M}_{m} \\ \hline \lambda_{m+1} \\ \lambda_{m+2} \end{bmatrix},$$

with  $\bar{M}_m \in \mathbb{R}^{m \times m}$ . Therefore

$$\boldsymbol{A}_{n+1} = \begin{bmatrix} \underline{U_n \mid \mathbf{u}_{\perp} \mid} \\ 1 \end{bmatrix} \boldsymbol{H}^T \begin{bmatrix} \underline{\bar{M}_m} \\ \lambda_{m+1} \\ \lambda_{m+2} \end{bmatrix} \boldsymbol{H} \begin{bmatrix} \underline{U_n^T} \\ \underline{\mathbf{u}_{\perp}^T} \\ 1 \end{bmatrix}$$

and the new updated decomposition is given by

$$\hat{A}_{n+1}=U_{n+1}\bar{M}_mU_{n+1}^T,$$

with  $U_{n+1}$  given by the first *m* columns of

$$\mathsf{f}\left[\frac{U_n \mid \mathsf{u}_\perp \mid}{1}\right] H^T$$

► It is not needed to compute the whole spectral decomposition of the matrix *M*<sub>m+2</sub>

- ► It is not needed to compute the whole spectral decomposition of the matrix  $\tilde{M}_{m+2}$
- To compute *H* only the eigenvectors v<sub>m+1</sub>, v<sub>m+2</sub> corresponding to λ<sub>m+1</sub>, λ<sub>m+2</sub> are needed

- ► It is not needed to compute the whole spectral decomposition of the matrix *M*<sub>m+2</sub>
- To compute *H* only the eigenvectors v<sub>m+1</sub>, v<sub>m+2</sub> corresponding to λ<sub>m+1</sub>, λ<sub>m+2</sub> are needed
- To compute these vectors cheaply, one needs to maintain (and update) the Cholesky factorization of

$$M_m = L_m L_m^T$$

- ► It is not needed to compute the whole spectral decomposition of the matrix *M*<sub>m+2</sub>
- To compute *H* only the eigenvectors v<sub>m+1</sub>, v<sub>m+2</sub> corresponding to λ<sub>m+1</sub>, λ<sub>m+2</sub> are needed
- To compute these vectors cheaply, one needs to maintain (and update) the Cholesky factorization of

$$M_m = L_m L_m^T$$

The eigenvectors are then obtained via inverse iteration and

- ► It is not needed to compute the whole spectral decomposition of the matrix *M*<sub>m+2</sub>
- To compute *H* only the eigenvectors v<sub>m+1</sub>, v<sub>m+2</sub> corresponding to λ<sub>m+1</sub>, λ<sub>m+2</sub> are needed
- To compute these vectors cheaply, one needs to maintain (and update) the Cholesky factorization of

$$M_m = L_m L_m^T$$

- The eigenvectors are then obtained via inverse iteration and
- H can then be computed as a product of Householder or Givens transformations

# **Updating Cholesky**

$$\begin{split} \tilde{M}_{m+2} &= \begin{bmatrix} \frac{M_m}{r} & \mathbf{r} \\ \frac{\mathbf{0}}{\mathbf{r}} & \rho \\ \mathbf{r}^T & \rho & \mathbf{b} \end{bmatrix} \\ &= \begin{bmatrix} \frac{L_m L_m^T}{r} & \mathbf{r} \\ \frac{\mathbf{0}}{\mathbf{r}} & \rho \\ \mathbf{r}^T & \rho & \mathbf{b} \end{bmatrix} \\ &= \begin{bmatrix} \frac{L_m}{\mathbf{0}} \\ \frac{\mathbf{0}}{\mathbf{r}} \\ \mathbf{t}^T \end{bmatrix} \begin{bmatrix} I_m \\ \mathbf{S}_c \end{bmatrix} \begin{bmatrix} \frac{L_m}{r} & \mathbf{0}_m | \mathbf{t} \\ \frac{\mathbf{0}}{r} \end{bmatrix} \\ &= \tilde{L}_{m+2} \tilde{D}_{m+2} \tilde{L}_{m+2}^T, \end{split}$$

.

where

$$\mathbf{t} = L_m^{-1} \mathbf{r}$$
 and  $S_c = \begin{bmatrix} \mathbf{0} & \rho \\ \rho & b - \mathbf{t}^T \mathbf{t} \end{bmatrix}$ .





$$\begin{bmatrix} \times \times \times \times \times \times \\ \vdots & \vdots & \vdots & \vdots \\ \times \times \times \times \times \times \end{bmatrix}$$





 $\begin{bmatrix} \times \times \times \times \times \times \\ \vdots & \vdots & \vdots & \vdots \\ \times \times \times \times \times \times \end{bmatrix}$ 





$$\begin{bmatrix} \times \times \times \times \times \times \\ \vdots & \vdots & \vdots & \vdots \\ \times \times \times \times \times \times \end{bmatrix}$$









$$\begin{bmatrix} \times \times \times \times \times \times \\ \vdots & \vdots & \vdots & \vdots \\ \times \times \times \times \times \times \end{bmatrix}$$





$$\begin{bmatrix} \times \times \times \times \times \times \\ \vdots & \vdots & \vdots & \vdots \\ \times \times \times \times \times \times \end{bmatrix}$$





$$\begin{bmatrix} \times \times \times \times \times \times \\ \vdots & \vdots & \vdots & \vdots \\ \times \times \times \times \times \times \end{bmatrix}$$










$$\begin{bmatrix} \times \times \times \times \times \times \\ \vdots & \vdots & \vdots & \vdots \\ \times \times \times \times \times \times \end{bmatrix}$$



$$\begin{bmatrix} \times \times \times \times & | & \times \times \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \times \times \times \times & | & \times \times \end{bmatrix}$$

• Let  $H_v$  be orthogonal such that

$$H_{\mathbf{v}}\mathbf{v} = \upsilon \; \mathbf{e}_{1,m}, \qquad \upsilon = \mp \|\mathbf{v}\|_{2}, \quad U_{n+1} = \begin{bmatrix} \mathbf{v}^{T} \\ V \end{bmatrix}.$$

• Let  $H_v$  be orthogonal such that

$$H_{\mathbf{v}}\mathbf{v} = v \mathbf{e}_{1,m}, \qquad v = \mp \|\mathbf{v}\|_2, \quad U_{n+1} = \begin{bmatrix} \mathbf{v}^T \\ V \end{bmatrix}.$$

► Then

$$U_{n+1}H_{\nu} = \begin{bmatrix} \upsilon & 0 & \cdots & 0 \\ \hline VH_{\nu} & \end{bmatrix}.$$

• Let  $H_v$  be orthogonal such that

$$H_{v}\mathbf{v} = \upsilon \ \mathbf{e}_{1,m}, \qquad \upsilon = \mp \|\mathbf{v}\|_{2}, \quad U_{n+1} = \begin{bmatrix} \mathbf{v}^{T} \\ V \end{bmatrix}.$$

Then

$$U_{n+1}H_{v} = \begin{bmatrix} v & 0 & \cdots & 0 \\ \hline VH_{v} & \end{bmatrix}.$$

► To retrieve the orthonormality of  $VH_v$ , it is sufficient to divide its first column of by  $\sqrt{1-v^2}$  and therefore multiply the first column and row of  $M_m$  by the same quantity

• Let  $H_v$  be orthogonal such that

$$H_{\mathbf{v}}\mathbf{v} = \upsilon \; \mathbf{e}_{1,m}, \qquad \upsilon = \mp \|\mathbf{v}\|_2, \quad U_{n+1} = \begin{bmatrix} \mathbf{v}^T \\ V \end{bmatrix}.$$

Then

$$U_{n+1}H_{v} = \begin{bmatrix} v & 0 & \cdots & 0 \\ \hline VH_{v} & \end{bmatrix}.$$

- ► To retrieve the orthonormality of  $VH_v$ , it is sufficient to divide its first column of by  $\sqrt{1-v^2}$  and therefore multiply the first column and row of  $M_m$  by the same quantity
- ► If the matrix  $M_m$  is factored as  $L_m L_m^T$  this reduces to multiplying the first entry of  $L_m$  by  $\sqrt{1 v^2}$

• Let  $H_v$  be orthogonal such that

$$H_{v}\mathbf{v} = \upsilon \ \mathbf{e}_{1,m}, \qquad \upsilon = \mp \|\mathbf{v}\|_{2}, \quad U_{n+1} = \begin{bmatrix} \mathbf{v}^{T} \\ V \end{bmatrix}.$$

Then

$$U_{n+1}H_{v} = \begin{bmatrix} v & 0 & \cdots & 0 \\ \hline VH_{v} & \end{bmatrix}.$$

- ► To retrieve the orthonormality of  $VH_v$ , it is sufficient to divide its first column of by  $\sqrt{1-v^2}$  and therefore multiply the first column and row of  $M_m$  by the same quantity
- ► If the matrix  $M_m$  is factored as  $L_m L_m^T$  this reduces to multiplying the first entry of  $L_m$  by  $\sqrt{1 v^2}$
- Any row of  $U_{n+1}$  can be chosen to be removed this way

#### When there is no downsizing

$$\|K_{n} - A_{n}\|_{F}^{2} \leq \eta_{n} := \sum_{i=m+1}^{\tilde{n}} \lambda_{i}^{(\tilde{n})^{2}} + \sum_{i=\tilde{n}+1}^{n} \delta_{i}^{(+)^{2}} + \sum_{i=\tilde{n}+1}^{n} \delta_{i}^{(-)^{2}},$$
$$\|K_{n} - A_{n}\|_{2} \leq \zeta_{n} := \lambda_{m+1}^{(\tilde{n})} + \sum_{i=\tilde{n}+1}^{n} \max\left\{\delta_{i}^{(+)}, \delta_{i}^{(-)}\right\},$$

where

$$\begin{aligned} A_{n} &:= U_{n} M_{m} U_{n}^{T}, \quad \delta_{i}^{(+)} = \lambda_{i}^{(m+1)}, \quad \delta_{i}^{(-)} = \lambda_{i}^{(m+2)}, \\ \|K_{\tilde{n}} - A_{\tilde{n}}\|_{F}^{2} &= \sum_{i=m+1}^{\tilde{n}} \lambda_{i}^{(\tilde{n})^{2}}, \quad \|K_{\tilde{n}} - A_{\tilde{n}}\|_{2} = \lambda_{m+1}^{(\tilde{n})}. \end{aligned}$$

# In relation to the original spectrum $K_N$ one obtains the approximate bounds

$$\sum_{i=m+1}^{N} \lambda_i^2 \leq \|K_N - A_N\|_F^2 \lesssim (N-m) \lambda_{m+1}^2.$$

and

$$\lambda_{m+1} \leq \|K_N - A_N\|_2 \lessapprox c\lambda_{m+1},$$

When donwsizing the matrix as well, there are no guaranteed bounds

The matrix considered in this example is a Kernel Matrix constructed from the Abalone benchmark data set http://archive.ics.uci.edu/ml/support/Abalone, with radial basis kernel function

$$k(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x} - \mathbf{y}\|_2^2}{100}\right),$$

The matrix considered in this example is a Kernel Matrix constructed from the Abalone benchmark data set http://archive.ics.uci.edu/ml/support/Abalone, with radial basis kernel function

$$k(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x} - \mathbf{y}\|_2^2}{100}\right),$$

This data set has 4177 training instances



**Figure:** Distribution of the largest 100 eigenvalues of the Abalone matrix in logarithmic scale.

**Table:** Largest 9 eigenvalues of the Abalone matrix  $K_N$  (second column), of  $A_N$  obtained with updating with  $\tilde{n} = 500$ , m = 9 (third column) and with  $\tilde{n} = 500$ , m = 20 (fourth column), respectively.

$\lambda_i$	$\mu_i, \tilde{n} = 500, m = 9$	$\mu_i, \tilde{n} = 500, m = 20$
4.14838108255808e+3	4.14838108255812e+3	4.1483810825580 <mark>5</mark> e+3
2.77142467123926e+1	2.771424671239 <mark>35</mark> e+1	2.771424671239 <mark>08</mark> e+1
3.96946486354603e-1	3.9694648 <mark>5174339</mark> e-1	3.96946486354 <mark>575</mark> e-1
2.82827838600384e-1	2.82827838240747e-1	2.82827838601794e-1
8.76354938729571e-2	8.76354893664714e-2	8.763549387 <mark>30078</mark> e-2
4.48191766538717e-2	4.48191002296202e-2	4.4819176653 <mark>7462</mark> e-2
3.95005821149249e-2	3.95005033082028e-2	3.9500582114 <mark>5827</mark> e-2
3.44916594206443e-2	3.44915746496473e-2	3.44916594206 <mark>963</mark> e-2
1.22751950123456e-2	1.22750932394003e-2	1.22751950116852e-2



**Figure:** Plot of the sequences of  $\delta_n^{(+)}$  (blue line),  $\delta_n^{(-)}$  (green line),  $\eta_n$  (red solid line),  $\lambda_{m+1}$  (cyan solid line) and  $||\mathcal{K}_N - \mathcal{A}_N||_F$  (magenta solid line).

**Table:** Angles between the eigenvectors corresponding to the largest 9 eigenvalues of  $K_N$ , computed by the function eigs of matlab and those computed by the proposed algorithm for  $\tilde{n} = 500$ , m = 9 (second column) and  $\tilde{n} = 500$ , m = 20 (third column).

i	$\angle(\mathbf{x}_i, \tilde{\mathbf{x}}_i)$	$\angle(\mathbf{x}_i, \hat{\mathbf{x}}_i)$
1	3.6500e-08	8.4294e-08
2	3.9425e-08	2.9802e-08
3	2.3774e-06	5.1619e-08
4	2.5086e-06	2.9802e-08
5	3.0084e-05	1.1151e-07
6	2.0446e-04	4.2147e-08
7	2.0213e-04	1.4901e-08
8	3.4670e-04	8.1617e-08
9	5.9886e-04	2.1073e-08

The following matrix has rank 3

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

with

$$\mu = \begin{bmatrix} 4 & 18 & 76 \end{bmatrix}, \quad \sigma = \begin{bmatrix} 10 & 20 & 5 \end{bmatrix}.$$

Let  $F = Q \wedge Q^T$  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  $\Delta = \tilde{\Delta}/\|\tilde{\Delta}\|_2$ . For this example, the considered SPD matrix is

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



**Figure:** Graph of the size of the entries of the matrix  $K_N$ .



**Figure:** Distribution of the eigenvalues of the matrix  $K_N$  in logarithmic scale.



Figure: Plot of the three dominant eigenvectors of  $K_N$ 



**Figure:** Plot of the sequences of  $\delta_n^{(+)}$  (blue dash dotted line),  $\delta_k^{(-)}$  (green dotted line),  $\eta_n$  (red solid line),  $\lambda_{m+1}$  (cyan solid line) and  $||K_N - A_N||_F$  (black solid line).

**Table:** Largest three eigenvalues of the matrix  $K_N$  (first column). Largest three eigenvalues computed with downdating procedure with minimal norm, with m = 3 and  $\tilde{n} = 30, 40, 50$  (second, third and fourth column), respectively. Largest three largest eigenvalues of  $K_N$  computed with the "former" downdating procedure (fifth column).

$\lambda_i$	$\mu_i, \tilde{n} = 30$	$\mu_i, \tilde{n} = 40$	$\mu_i, \tilde{n} = 50$	$\mu_i, \tilde{n} = 50$
7.949478e0	7.375113e0	7.820407e0	7.94 <mark>7127</mark> e0	3.963329e0
5.261405e0	5.2 <mark>55163</mark> e0	5.26 <mark>0243</mark> e0	5.261 <mark>384</mark> e0	5.417202e-6
3.963329e0	3.9 <mark>48244</mark> e0	3.963 <mark>213</mark> e0	3.963329e0	4.824060e-6

 A fast algorithm for to compute incrementally the dominant eigenspace of a positive definite matrix

- A fast algorithm for to compute incrementally the dominant eigenspace of a positive definite matrix
- Improvement on Hoegaerts, L., De Lathauwer, L., Goethals I., Suykens, J.A.K., Vandewalle, J., & De Moor, B. Efficiently updating and tracking the dominant kernel principal components. Neural Networks, 20, 220–229, 2007.

- A fast algorithm for to compute incrementally the dominant eigenspace of a positive definite matrix
- Improvement on Hoegaerts, L., De Lathauwer, L., Goethals I., Suykens, J.A.K., Vandewalle, J., & De Moor, B. Efficiently updating and tracking the dominant kernel principal components. Neural Networks, 20, 220–229, 2007.
- ► The overall complexity of the incremental updating technique to compute an  $N \times m$  basis matrix  $U_N$  for the dominant eigenspace of  $K_N$ , is reduced from  $(m + 4)N^2m + O(Nm^3)$  to  $6N^2m + O(Nm^2)$ .

- A fast algorithm for to compute incrementally the dominant eigenspace of a positive definite matrix
- Improvement on Hoegaerts, L., De Lathauwer, L., Goethals I., Suykens, J.A.K., Vandewalle, J., & De Moor, B. Efficiently updating and tracking the dominant kernel principal components. Neural Networks, 20, 220–229, 2007.
- ► The overall complexity of the incremental updating technique to compute an  $N \times m$  basis matrix  $U_N$  for the dominant eigenspace of  $K_N$ , is reduced from  $(m + 4)N^2m + O(Nm^3)$  to  $6N^2m + O(Nm^2)$ .

▶ When using both incremental updating and downsizing to compute the dominant eigenspace of  $\hat{K}_{\tilde{n}}$  (an  $\tilde{n} \times \tilde{n}$  principal submatrix of  $K_N$ ), the complexity is reduced  $(12m + 4)N\tilde{n}m + O(Nm^3)$  to  $16N\tilde{n}m + O(Nm^2)$ .

- A fast algorithm for to compute incrementally the dominant eigenspace of a positive definite matrix
- Improvement on Hoegaerts, L., De Lathauwer, L., Goethals I., Suykens, J.A.K., Vandewalle, J., & De Moor, B. Efficiently updating and tracking the dominant kernel principal components. Neural Networks, 20, 220–229, 2007.
- ► The overall complexity of the incremental updating technique to compute an  $N \times m$  basis matrix  $U_N$  for the dominant eigenspace of  $K_N$ , is reduced from  $(m + 4)N^2m + O(Nm^3)$  to  $6N^2m + O(Nm^2)$ .
- ▶ When using both incremental updating and downsizing to compute the dominant eigenspace of  $\hat{K}_{\tilde{n}}$  (an  $\tilde{n} \times \tilde{n}$  principal submatrix of  $K_N$ ), the complexity is reduced  $(12m + 4)N\tilde{n}m + O(Nm^3)$  to  $16N\tilde{n}m + O(Nm^2)$ .
- ▶ This is in both cases essentially a reduction by a factor *m*.

Gu, Eisenstat, An efficient algorithm for computing a strong rank revealing QR factorization, SIAM SCISC, 1996

Chahlaoui, Gallivan, Van Dooren, *An incremental method for computing dominant singular subspaces*, SIMAX, 2001

Hoegaerts, De Lathauwer, Goethals, Suykens, Vandewalle, De Moor, *Efficiently updating and tracking the dominant kernel principal components* Neural Networks, 2007.

Mastronardi, Tyrtishnikov, Van Dooren, *A fast algorithm for updating and downsizing the dominant kernel principal components*, SIMAX, 2010

Baker, Gallivan, Van Dooren, *Low-rank incrmenetal methods for computing dominant singular subspaces*, submitted, 2010

Ipsen, Van Dooren, *Polynomial Time Subset Selection Via Updating*, in preparation, 2010