



The Real Tool: The SVD

Images of the ...

Building Back the ...

The return of Cosines

The Singular Value ...

Cosine are the ...

What about these ...

Face example: Take 1

So what does the ...

[Home Page](#)

[Title Page](#)



Page 1 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)

PCA and the Singular Value Decomposition (SVD)

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— PCA and Beyond

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1. The Real Tool: The SVD

- SVD is for Singular Value Decomposition
- Generalizes the eigen-decomposition
- 1. The Geometry of the SVD (with the words example)
... and an illustration with images
- 2. The big questionWhat does the SVD optimizes?

The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

[Page 2 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



2. Images of the Components Building Back!

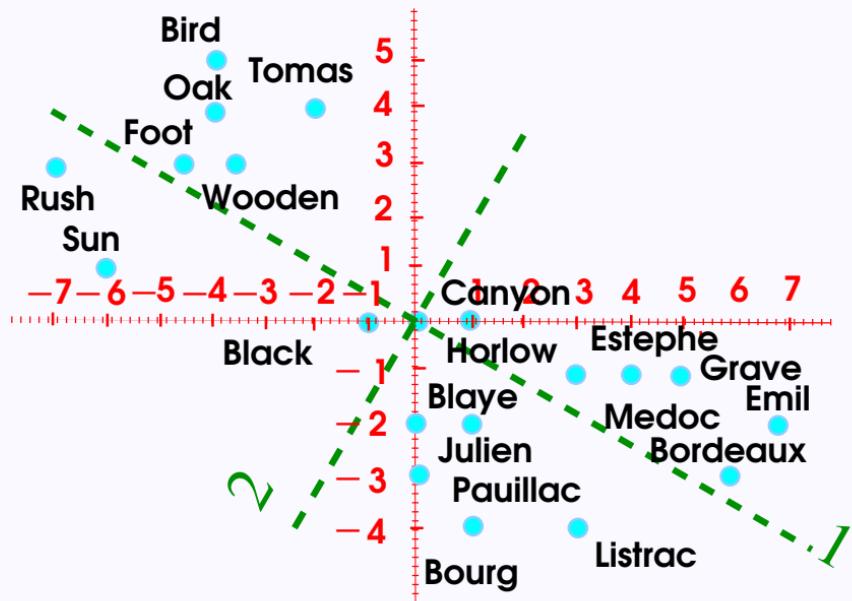


Figure 1: The Components in the space of the original variables.

The Real Tool: The SVD
Images of the...
Building Back the...
The return of Cosines
The Singular Value...
Cosine are the...
What about these...
Face example: Take 1
So what does the...

[Home Page](#)

[Title Page](#)

[«](#) [»](#)

[◀](#) [▶](#)

[Page 3 of 34](#)

[Go Back](#)

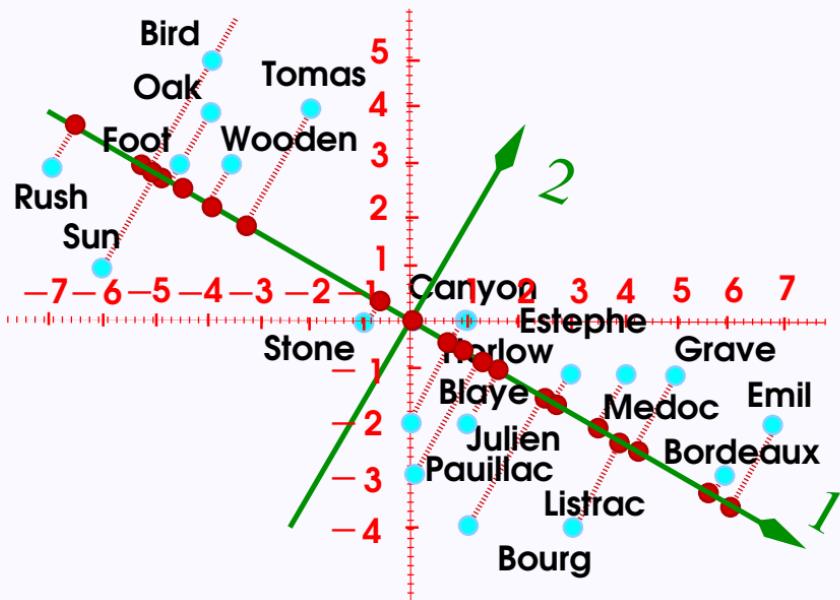
[Full Screen](#)

[Close](#)

[Quit](#)



The data according to the first component



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

«

»

◀

▶

Page 4 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

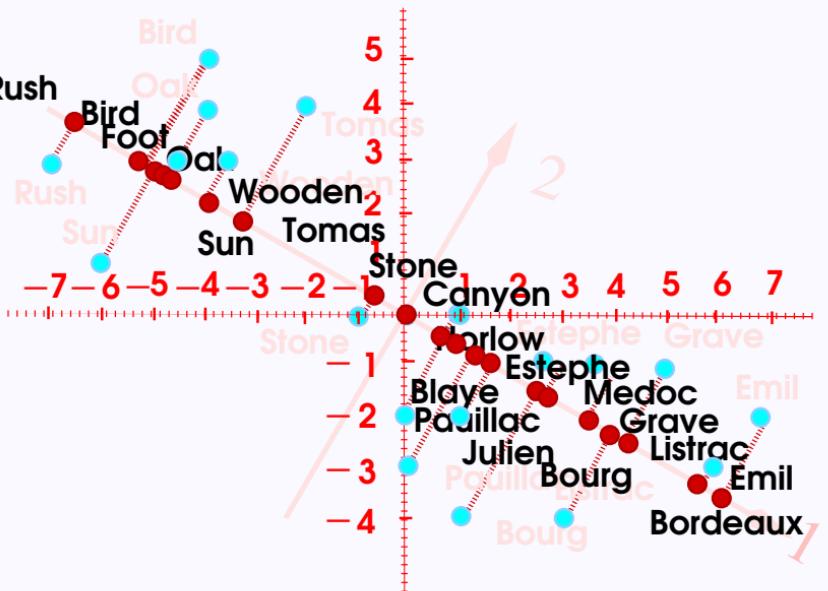
[Page 5 of 34](#)

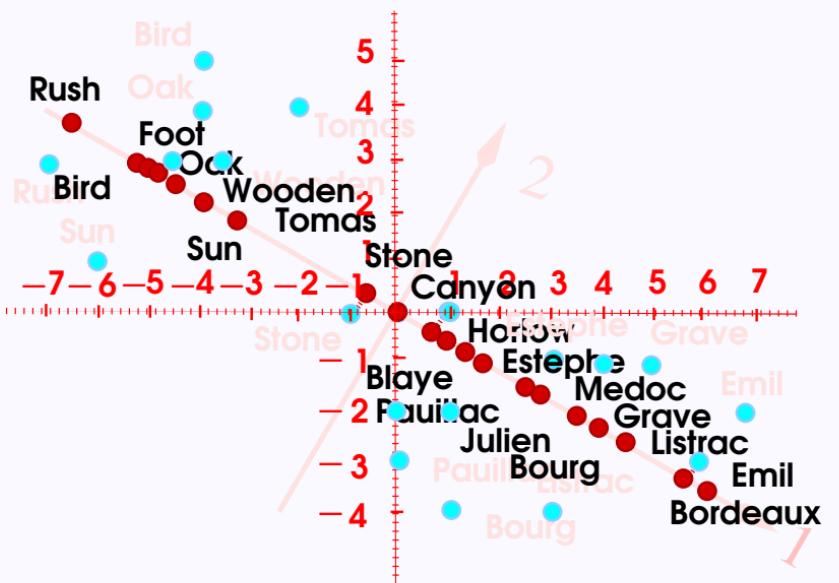
[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)





The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the ...

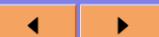
What about these...

Face example: Take 1

So what does the ...

[Home Page](#)

Title Page



Page 6 of 34

[Go Back](#)

Full Screen

Close

Quit



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

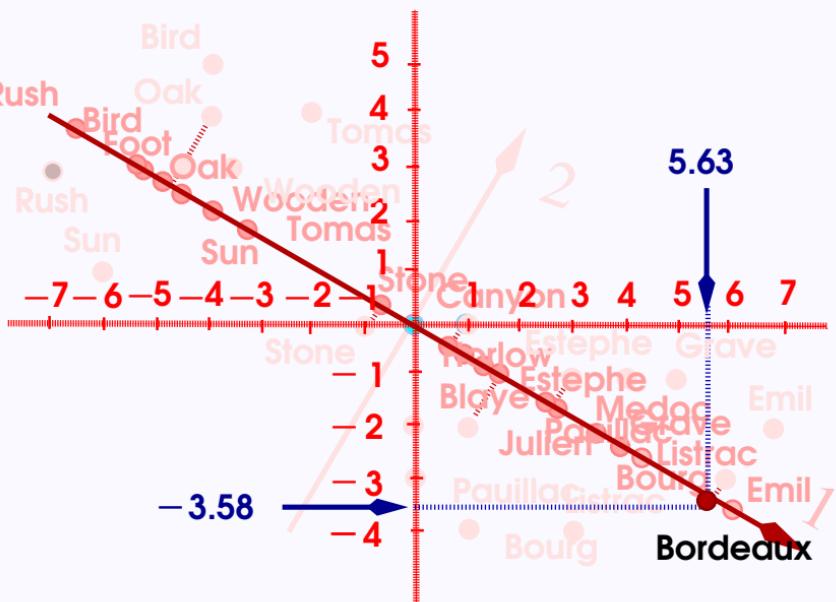
The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...



[Home Page](#)

[Title Page](#)

[«](#) [»](#)

[◀](#) [▶](#)

[Page 7 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



Table 1: Building back the data table one component at a time. Original variables, F_1 , data table according to F_1 F_2 , data table according to F_2 , \hat{w}_1 is w according to F_1 . The original data table is the sum of the “simple data tables.”

	w	y	F_1	\hat{w}_1	\hat{y}_1	F_2	\hat{w}_2	\hat{y}_2
Bordeaux	6	-3	6.67	5.63	-3.58	0.69	0.37	0.58
Black Stone	-1	0	-0.84	-0.71	0.45	-0.54	-0.29	-0.45
Listrac	3	-4	4.68	3.95	-2.51	-1.76	-0.95	-1.49
Canyon Creek	1	0	0.84	0.71	-0.45	0.54	0.29	0.45
Côte de Bourg	1	-4	2.99	2.52	-1.61	-2.84	-1.52	-2.39
Foot Hill	-4	3	-4.99	-4.21	2.68	0.38	0.21	0.32
Horlow	0	0	0.00	0.00	0.00	0.00	0.00	0.00
St Estephe	3	-1	3.07	2.59	-1.65	0.77	0.41	0.65
Wooden Hill	-3	3	-4.14	-3.49	2.22	0.92	0.49	0.78
Côte de Blaye	0	-2	1.07	0.91	-0.58	-1.69	-0.91	-1.42
Sun Set	-6	1	-5.60	-4.72	3.01	-2.38	-1.28	-2.01
Black Bird	-4	5	-6.06	-5.11	3.25	2.07	1.11	1.75
Médoc	4	-1	3.91	3.30	-2.10	1.30	0.70	1.10
St Julien	1	-2	1.92	1.62	-1.03	-1.15	-0.62	-0.97
Pauillac	0	-3	1.61	1.36	-0.86	-2.53	-1.36	-2.14
Gold Rush	-7	3	-7.52	-6.34	4.04	-1.23	-0.66	-1.04
Oak Vill	-4	4	-5.52	-4.66	2.96	1.23	0.66	1.04
Grave	5	-1	4.76	4.01	-2.55	1.84	0.99	1.55
St Emilion	7	-2	6.98	5.89	-3.75	2.07	1.11	1.75
Tomasello	-2	4	-3.83	-3.24	2.06	2.30	1.24	1.94

The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

Home Page

Title Page

◀ ▶

◀ ▶

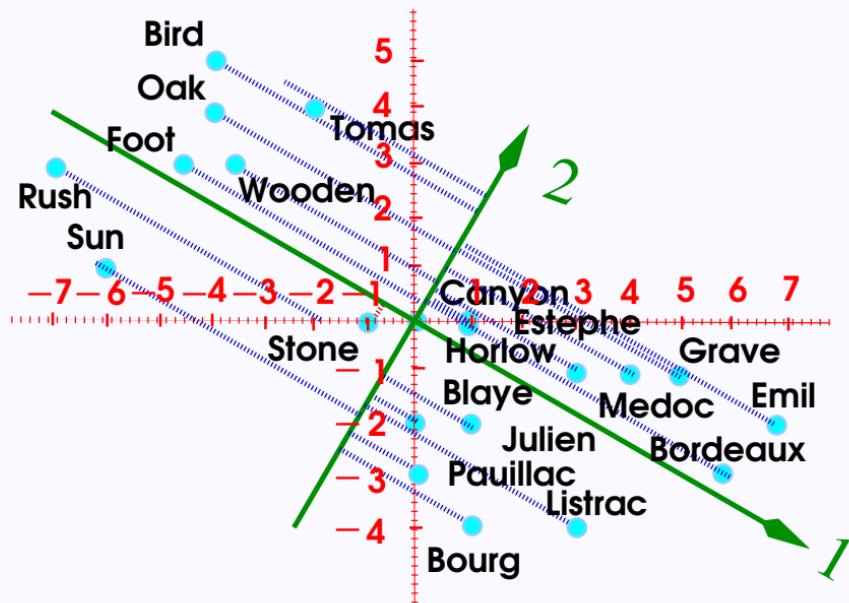
Page 8 of 34

Go Back

Full Screen

Close

Quit



The Real Tool: The SVD

Images of the ...

Building Back the ...

The return of Cosines

The Singular Value ...

Cosine are the ...

What about these ...

Face example: Take 1

So what does the ...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

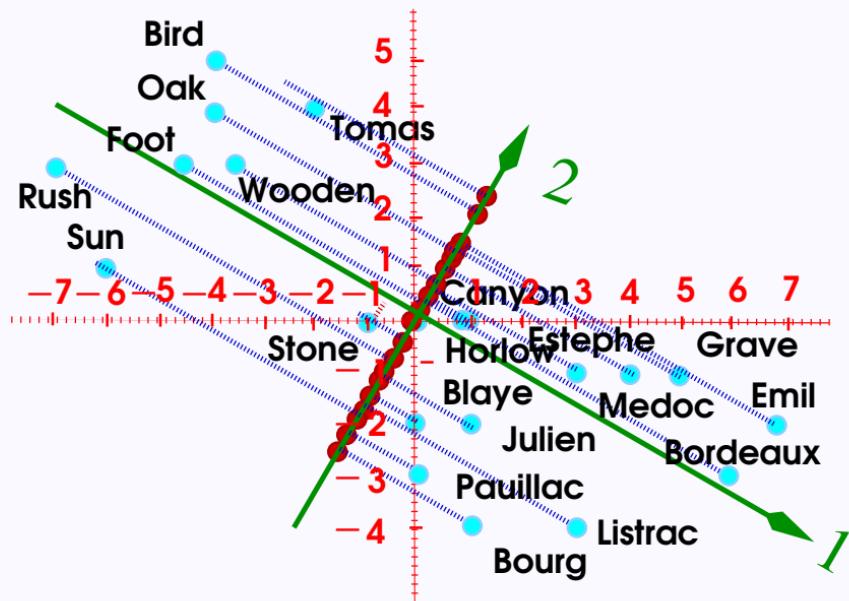
Page 9 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD
Images of the...
Building Back the...
The return of Cosines
The Singular Value...
Cosine are the...
What about these...
Face example: Take 1
So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

[Page 10 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

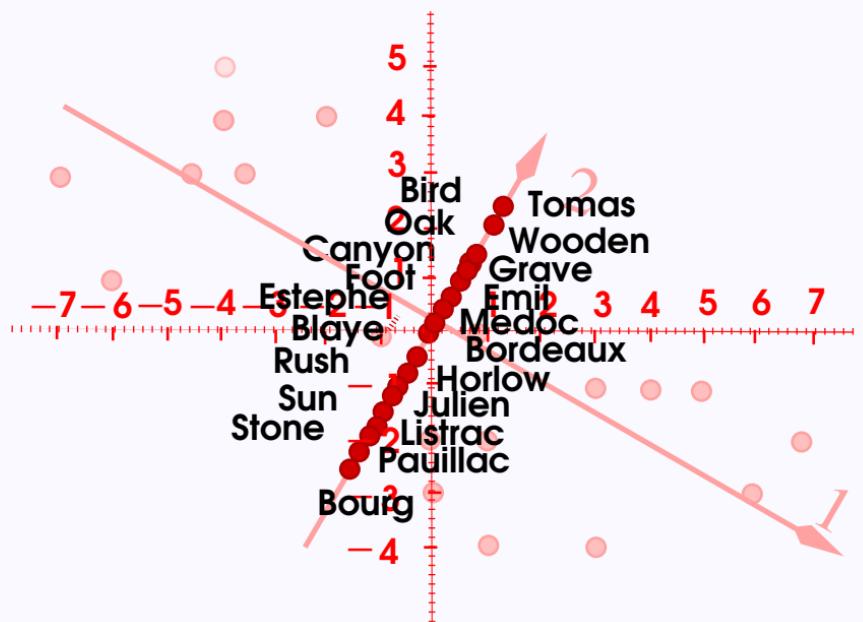
The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...



[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

Page 11 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

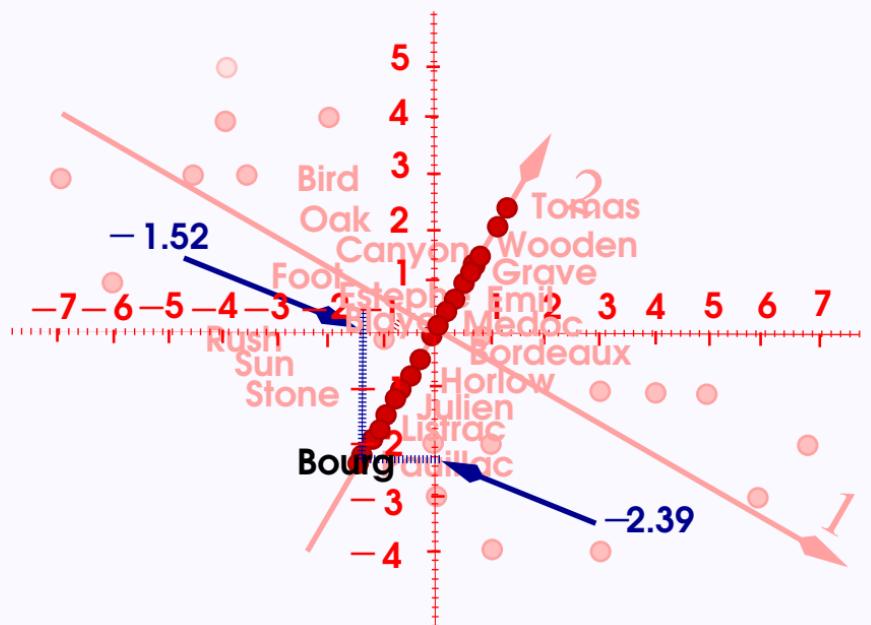
The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...



[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

[Page 12 of 34](#)

[Go Back](#)

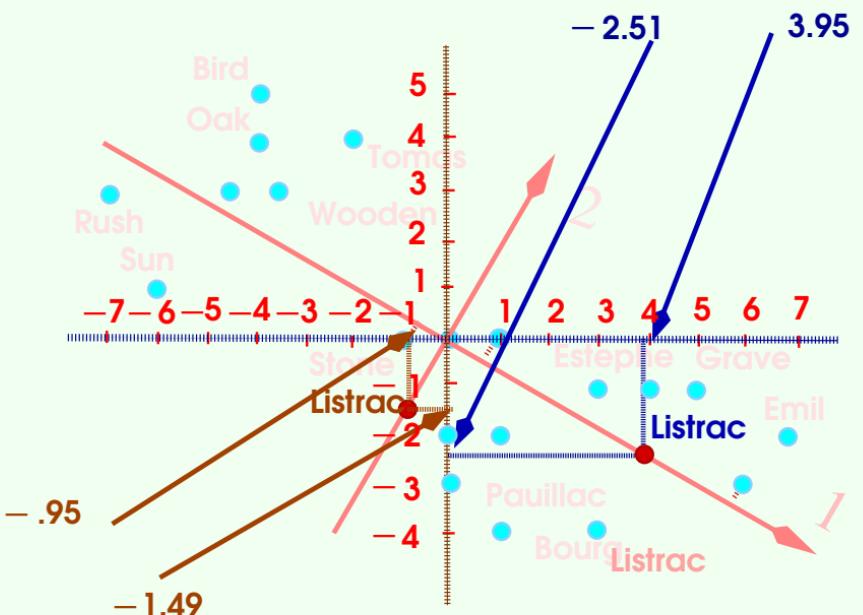
[Full Screen](#)

[Close](#)

[Quit](#)



3. Building Back the Data: Addition



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

◀

▶

◀

▶

Page 13 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

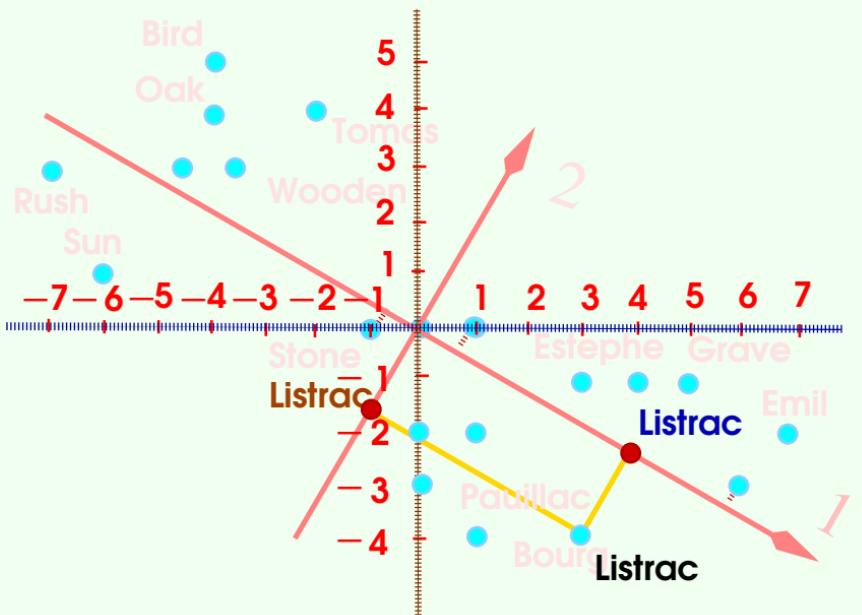
The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...



[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

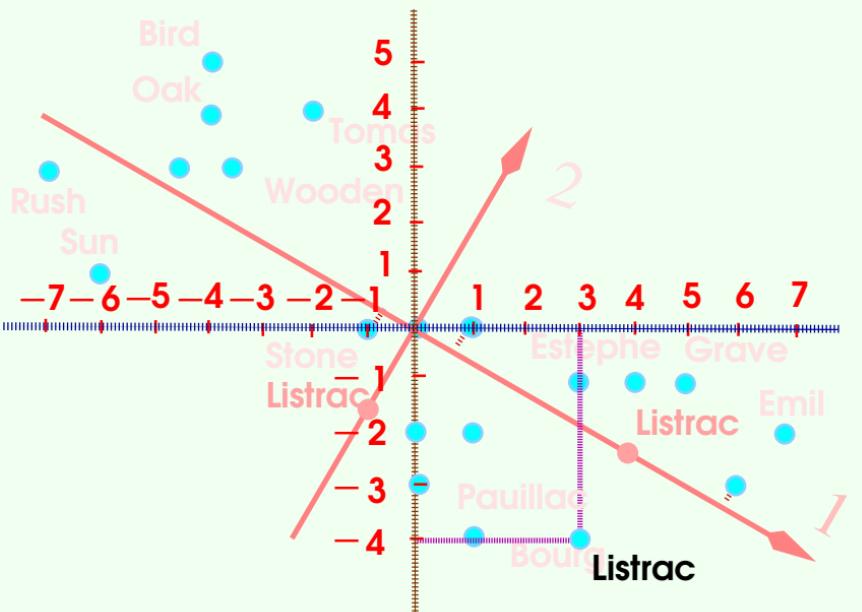
Page 14 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value.

Cosine are the ...

What about these ...

Face example: Take 1

So what does the ...

Home Page

Title Page



Page 15 of 34

[Go Back](#)

Full Screen

Close

[Quit](#)

4. The return of Cosines



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

Page 16 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

[Page 17 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)

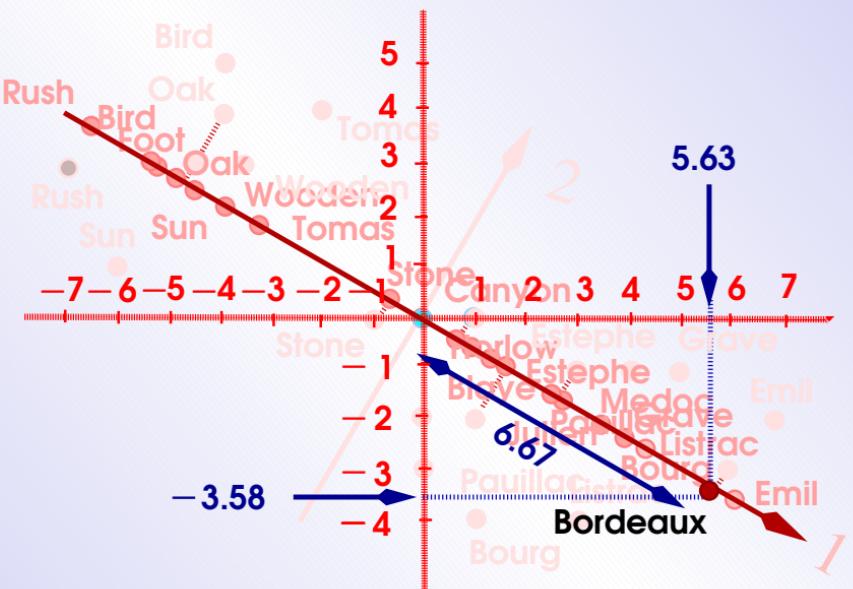


Figure 2: The coefficient of proportionality used to convert the value of F_1 into \hat{w}_1 or \hat{y}_1 is the cosine of the angle between the component and the original variables.



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

[Page 18 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)

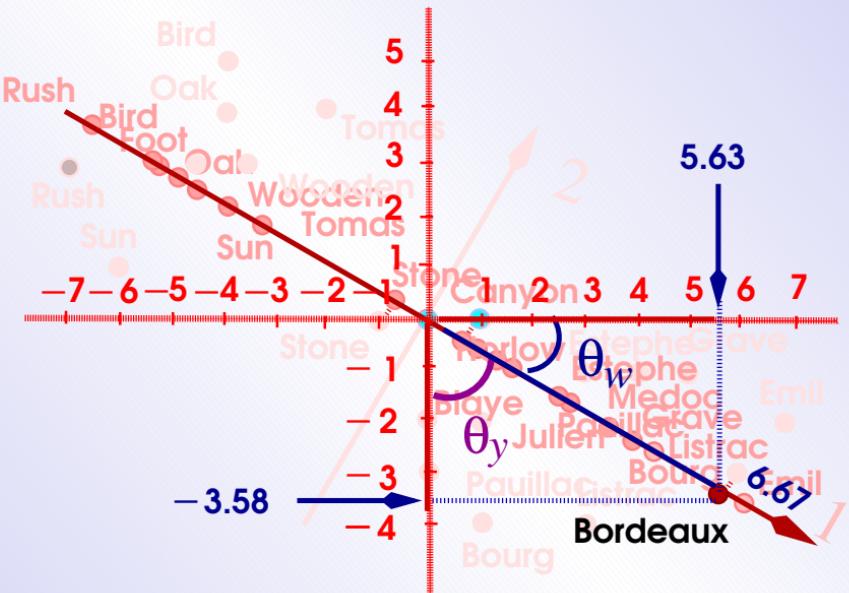


Figure 3: The coefficient of proportionality used to convert the value of F_1 into \hat{w}_1 or \hat{y}_1 is the cosine of the angle between the component and the original variables.



5. The Singular Value Decomposition: Take One!

$$\hat{w}_{\text{bordeaux},1} = .8437 \times F_{\text{bordeaux},1} = .8437 \times (6.6726) = 5.6294 .$$



$$\hat{y}_{\text{bordeaux},1} = -.5369 \times F_{\text{bordeaux},1} = -.5369 \times (6.6726) = -3.5824$$



these are also cosines:

$$\vartheta_{w,1} = 32^\circ \text{ (i.e., } \cos(32) = .8437)$$

$$\vartheta_{y,1} = 122^\circ \text{ (i.e., } \cos(122) = .5369)$$

The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

Page 19 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)



[Page 20 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



6. Cosine: the weights to build back everything

6.1. F from w and y

$w_{\text{bordeaux}} = 6$ and $y_{\text{bordeaux}} = -3$ as

$$F_{\text{bordeaux},1} = .8437 \times 6 + (-.5369) \times (-3) = 5.0620 + 1.6106 = 6.6726.$$



6.2. w and y from F

$F_{\text{bordeaux},1} = 6.6729$ and $F_{\text{bordeaux},2} = 0.6903$ as

$$w_{\text{bordeaux}} = .8437 \times 6.6726 + .5369 \times 0.6903 = 5.6294 + 0.3706 = 6.$$

The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

[Page 21 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)

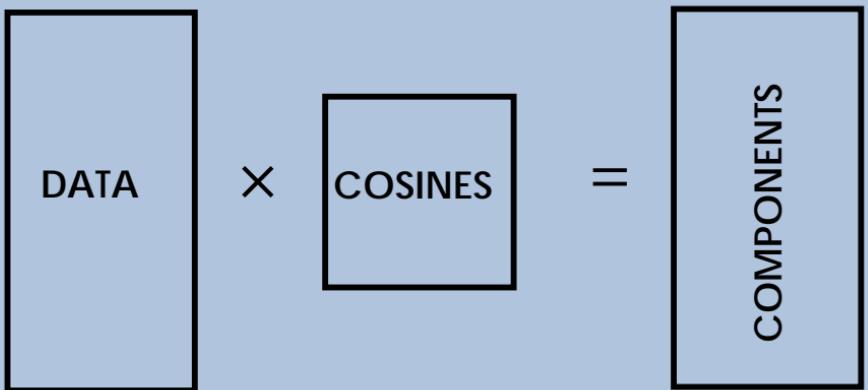


Figure 4: F from X and Q



[The Real Tool: The SVD](#)

[Images of the...](#)

[Building Back the...](#)

[The return of Cosines](#)

[The Singular Value...](#)

[Cosine are the...](#)

[What about these...](#)

[Face example: Take 1](#)

[So what does the...](#)

[Home Page](#)

[Title Page](#)



[Page 22 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)

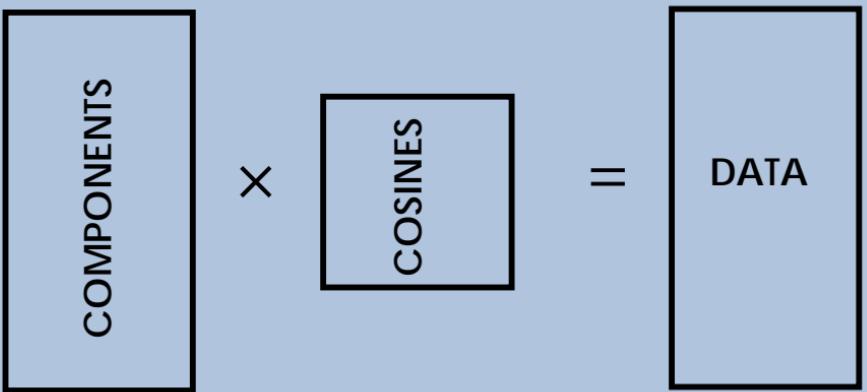


Figure 5: X from F and Q



[The Real Tool: The SVD](#)

[Images of the...](#)

[Building Back the...](#)

[The return of Cosines](#)

[The Singular Value...](#)

[Cosine are the...](#)

[What about these...](#)

[Face example: Take 1](#)

[So what does the...](#)

[Home Page](#)

[Title Page](#)



[Page 23 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

Home Page

Title Page



Page 24 of 34

Go Back

Full Screen

Close

Quit

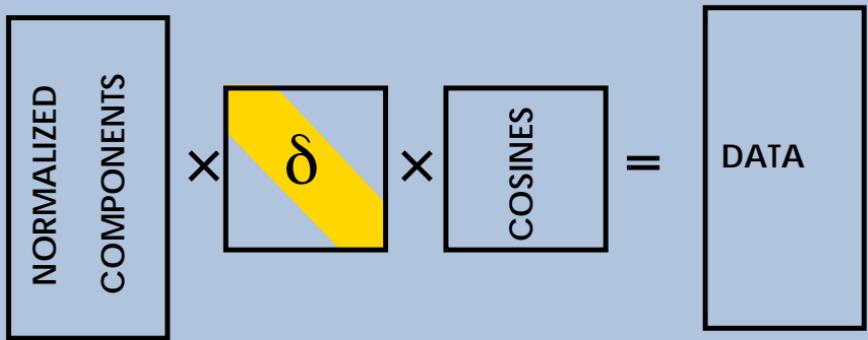


Figure 6: The SVD! $P\Delta Q^T = X$

7. What about these cosines and the loadings?

$$\text{Cosines} = \text{Loadings} \times \sqrt{\frac{SS_w}{\lambda}}$$



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

◀◀

▶▶

◀

▶

Page 25 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



8. Face example: Take 1

The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)



[Page 26 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the ...

Building Back the ...

The return of Cosines

The Singular Value ...

Cosine are the ...

What about these ...

Face example: Take 1

So what does the ...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

Page 27 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



Figure 7: The SVD! A 204 rows \times 290 columns = 59,610 pixels image.



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

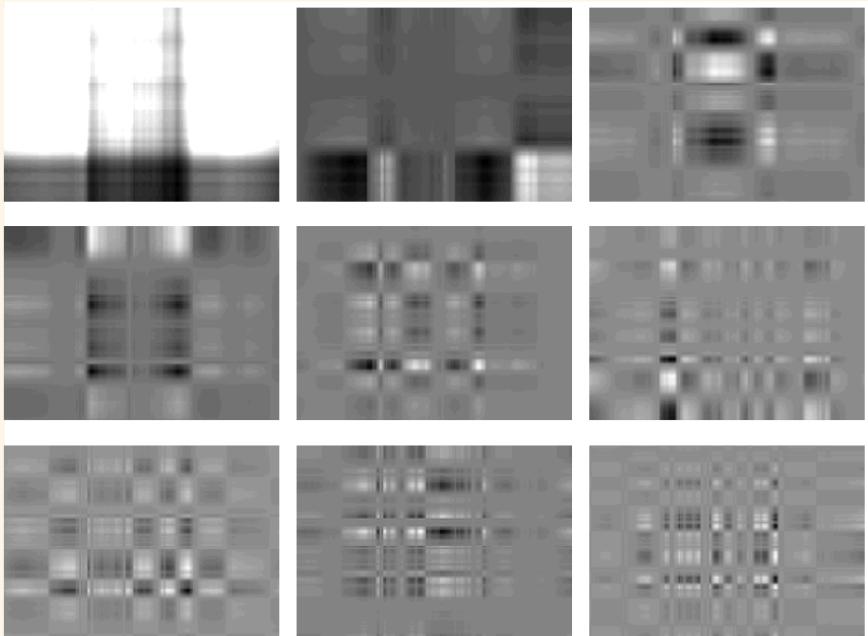


Figure 8: The SVD!

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

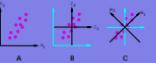
Page 28 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the ...

Building Back the ...

The return of Cosines

The Singular Value ...

Cosine are the ...

What about these ...

Face example: Take 1

So what does the ...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

[Page 29 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)

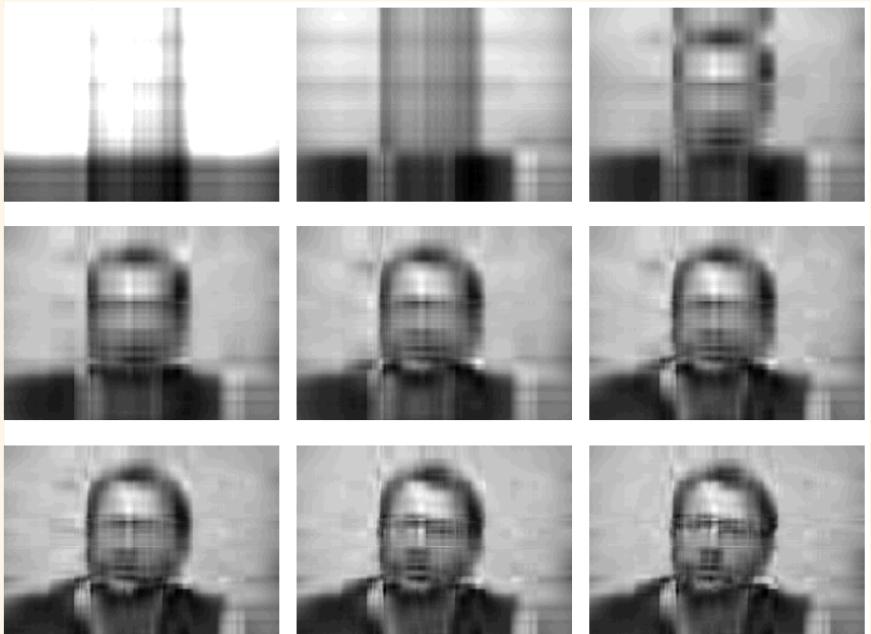


Figure 9: The SVD!

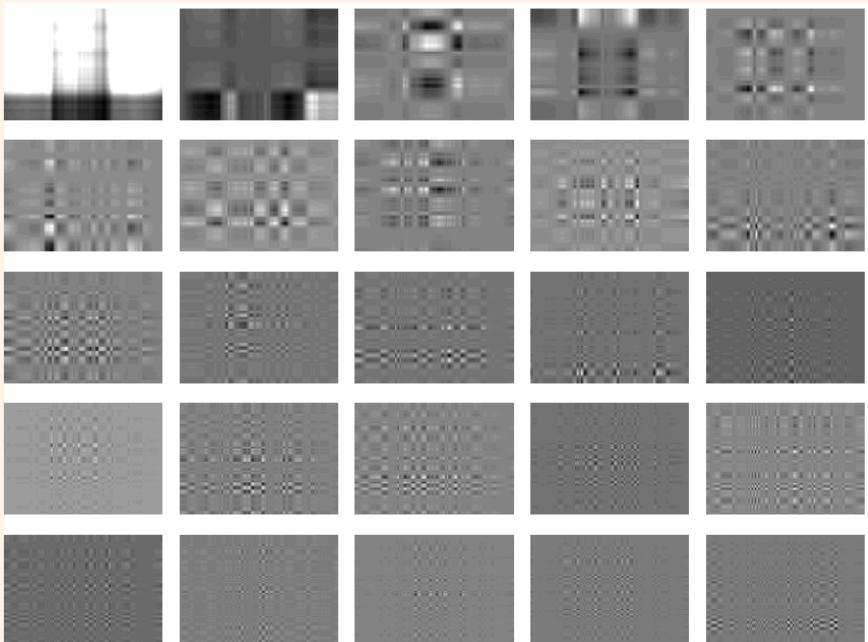


Figure 10: The SVD!

The Real Tool: The SVD
Images of the...
Building Back the...
The return of Cosines
The Singular Value...
Cosine are the...
What about these...
Face example: Take 1
So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

[Page 30 of 34](#)

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

Page 31 of 34

[Go Back](#)

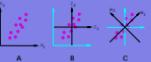
[Full Screen](#)

[Close](#)

[Quit](#)



Figure 11: The SVD!



The Real Tool: The SVD

Images of the...

Building Back the...

The return of Cosines

The Singular Value...

Cosine are the...

What about these...

Face example: Take 1

So what does the...

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

Page 32 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)



Figure 12: The SVD! Compression rate is around 80%.

9. So what does the SVD maximize?

Remember: $X = P\Delta Q^T$

So we want to find 2 vectors p and q such that

$\hat{X} = \delta pq^T = f q^T$ with $p^T p = q^T q = 1$

and $f = \delta p$

(i.e., \hat{X} is a rank one matrix) with

- $\arg \max_{p,q} = \delta = \text{trace} \left(X \times \hat{X}^T \right)$
- under the constraints that: $p^T p = q^T q = 1$

These are δ_1 , p_1 , and q_1 .



The Real Tool: The SVD

Images of the ...

Building Back the ...

The return of Cosines

The Singular Value ...

Cosine are the ...

What about these ...

Face example: Take 1

So what does the ...

- Now “deflate” $\hat{\mathbf{X}}$
- Get $\mathbf{X}^{[1]} = \mathbf{X} - \delta_1 \mathbf{p}_1 \mathbf{q}_1^T$
- Now get δ_2 , \mathbf{p}_2 , and \mathbf{q}_2 from $\mathbf{X}^{[1]}$. . .
- Keep on doing till there is nothing left of \mathbf{X}
- Et voilà!!

[Home Page](#)

[Title Page](#)

[◀◀](#) [▶▶](#)

[◀](#) [▶](#)

Page 34 of 34

[Go Back](#)

[Full Screen](#)

[Close](#)

[Quit](#)