

PCA and SVD

Sanjoy Dasgupta

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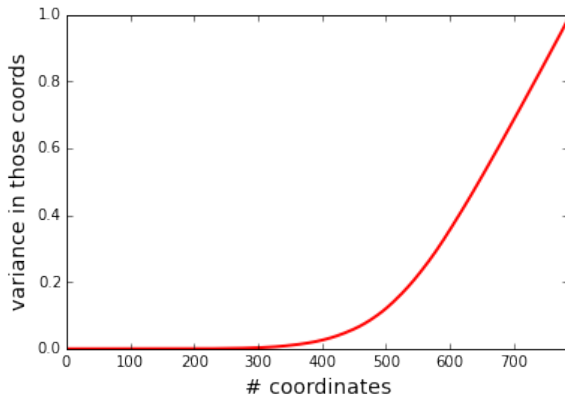
Those with lowest variance...

Eliminating low variance coordinates

Example: MNIST. What fraction of the total variance is contained in the 100 (or 200, or 300) coordinates with lowest variance?

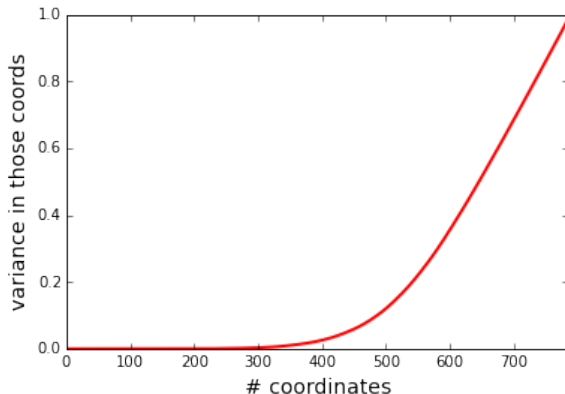
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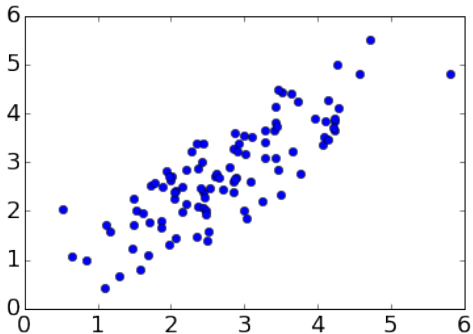
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Could easily drop 300-400 pixels...

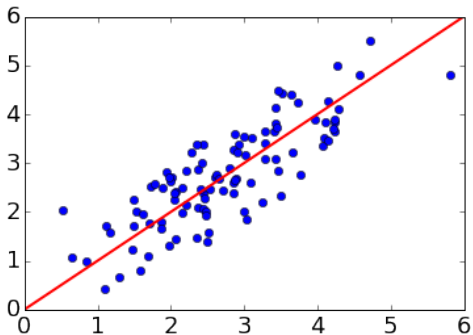
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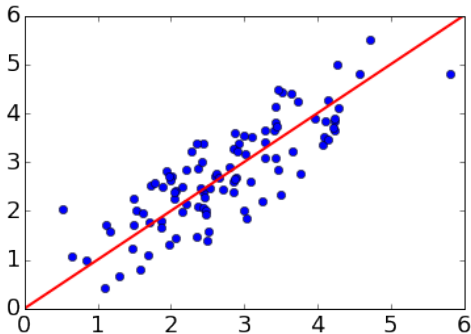
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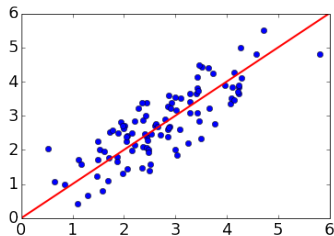
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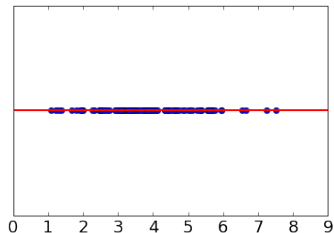


This is the **direction of maximum variance**.

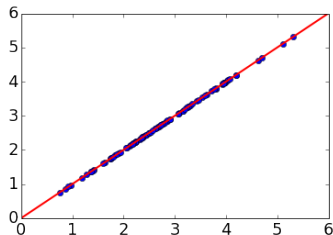
Two types of projection



Projection onto \mathbb{R} :

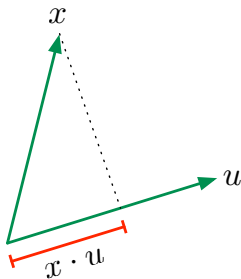


Projection onto a 1-d line in \mathbb{R}^2 :



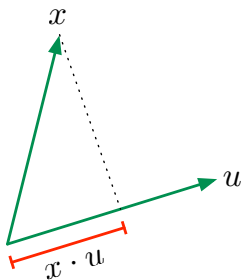
Projection: formally

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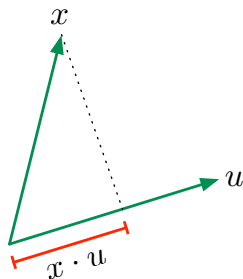


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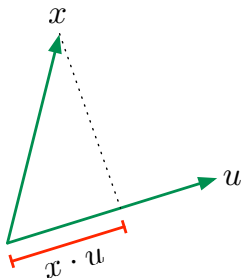
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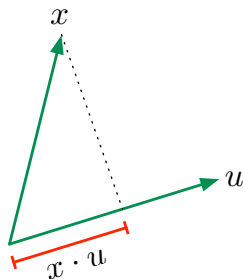
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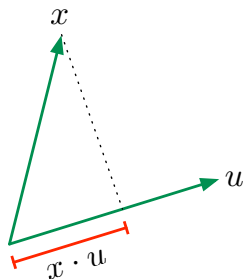
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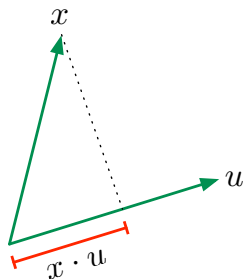
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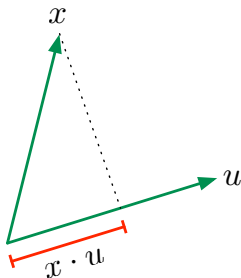
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$$(x \cdot u_1)u_1 + (x \cdot u_2)u_2 + \dots + (x \cdot u_k)u_k = UU^T x.$$

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But we'll generally project along non-coordinate directions.

The best single direction

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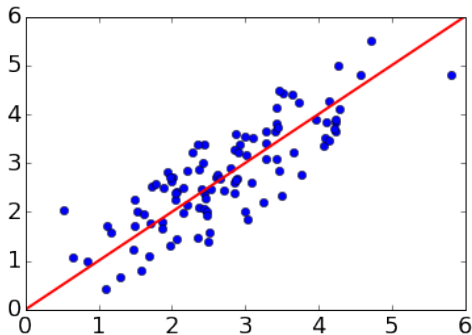
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Another theorem: $u^T \Sigma u$ is maximized by setting u to the first **eigenvector** of Σ . The maximum value is the corresponding **eigenvalue**.

Best single direction: example



This direction is the **first eigenvector** of the 2×2 covariance matrix of the data.

The best k -dimensional projection

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- real **eigenvalues** $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p$
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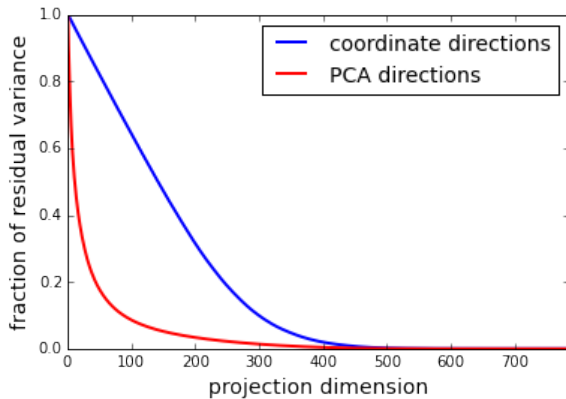
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Projecting the data in this way is **principal component analysis (PCA)**.

Example: MNIST

Contrast coordinate projections with PCA:



MNIST: image reconstruction



Reconstruct this original image from its PCA projection to k dimensions.

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A: Image x is reconstructed as $UU^T x$, where U is a $p \times k$ matrix whose columns are the top k eigenvectors of Σ .

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$$\underbrace{\begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 10 \end{pmatrix}}_M \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}}_x = \underbrace{\begin{pmatrix} 2x_1 \\ -x_2 \\ 10x_3 \end{pmatrix}}_{Mx}$$

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- 5 What about more general matrices that are symmetric but not necessarily diagonal? They also just scale coordinates separately, but in a **different coordinate system**.

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$$Mu = \lambda u$$

for some scaling constant λ . This λ is the **eigenvalue** associated with u .

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Notice that these eigenvectors form an orthonormal basis.

Eigenvectors of a real symmetric matrix

Theorem. Let M be any real symmetric $p \times p$ matrix. Then M has

- p eigenvalues $\lambda_1, \dots, \lambda_p$
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Example: consider the matrix

$$M = \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}$$

It has eigenvectors

$$u_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad u_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

and corresponding eigenvalues $\lambda_1 = 4$ and $\lambda_2 = 2$. (Check)

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Thus $Mx = U\Lambda U^T x$, which can be interpreted as follows:

- U^T rewrites x in the $\{u_i\}$ coordinate system
- Λ is a simple coordinate scaling in that basis
- U then sends the scaled vector back into the usual coordinate basis

Spectral decomposition: example

Apply spectral decomposition to the matrix M we saw earlier:

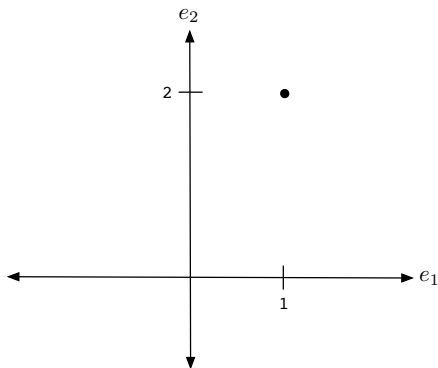
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$$M \begin{pmatrix} 1 \\ 2 \end{pmatrix} = ???$$

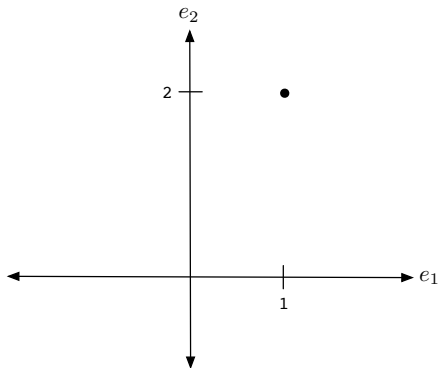


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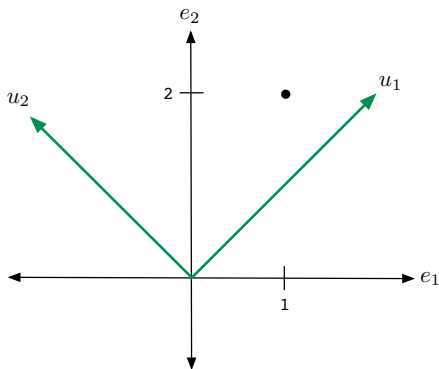


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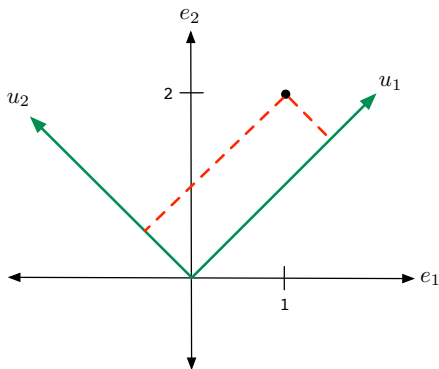


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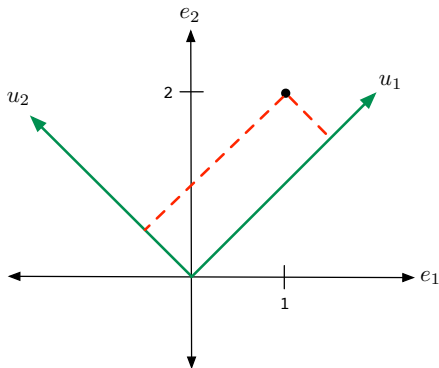


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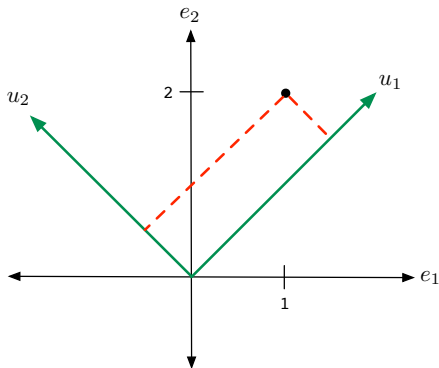


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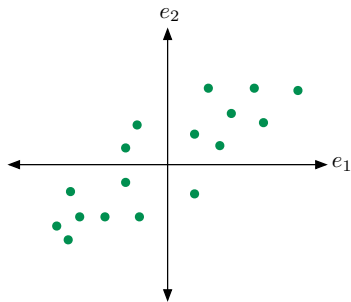
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Principal component analysis: recap

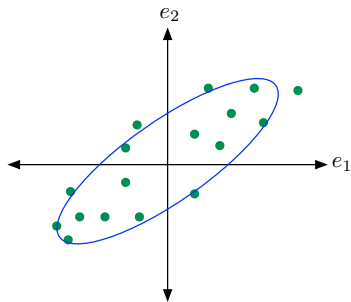
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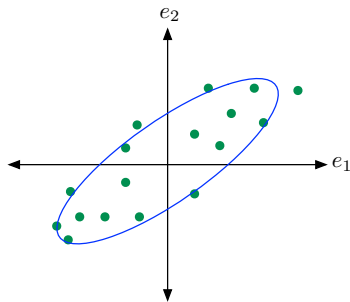
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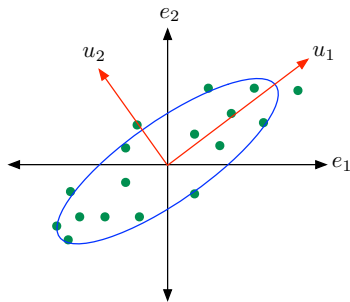
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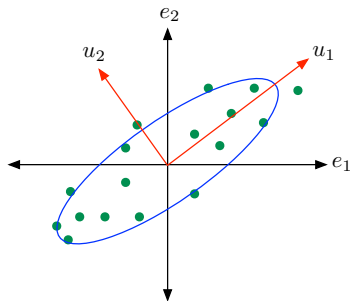
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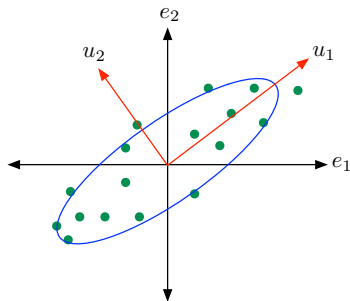
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What is the covariance of the projected data?

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Spirit	Jolly, merry, witty, lively, peppy
Talkativeness	Talkative, articulate, verbose, gossipy
Sociability	Companionable, social, outgoing
Spontaneity	Impulsive, carefree, playful, zany
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- Data collection: Ask a variety of subjects to what extent each of these words describes them.

Personality assessment: the data

Matrix of data (1 = strongly disagree, 5 = strongly agree)

	shy	merry	tense	boastful	forgiving	quiet
Person 1	4	1	1	2	5	5
Person 2	1	4	4	5	2	1
Person 3	2	4	5	4	2	2
		:				

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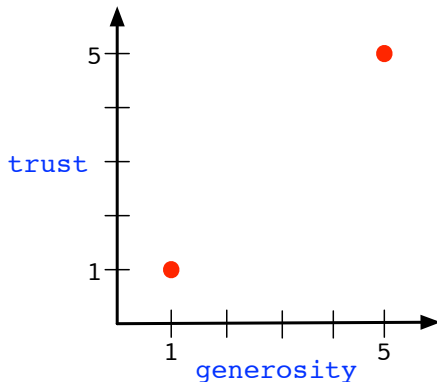
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Many of these yield similar results

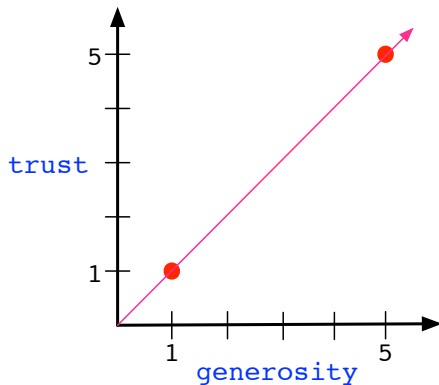
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Example: suppose two traits (generosity, trust) are highly correlated, to the point where each person either answers “1” to both or “5” to both.



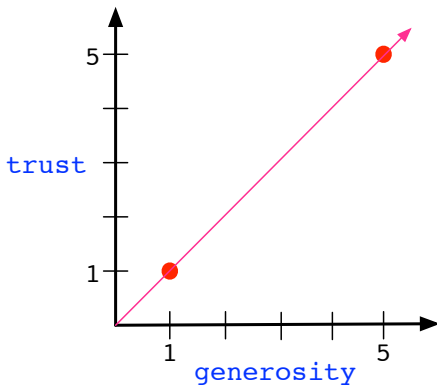
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This single PCA dimension entirely accounts for the two traits.

The “Big Five” taxonomy

[illegible]

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Extraversion		Agreeableness		Conscientiousness		Neuroticism		Openness/Intellect	
Low	High	Low	High	Low	High	Low	High	Low	High
-.83 Quiet	.85 Talkative	-.52 Fault-finding	.87 Sympathetic	-.58 Careless	.80 Organized	-.39 Stable*	.73 Tense	-.74 Commonplace	.76 Wide interests
-.80 Reserved	.83 Assertive	-.48 Cold	.85 Kind	-.53 Disorderly	.80 Thorough	-.35 Calm*	.72 Anxious	-.73 Narrow interests	.76 Imaginative
-.75 Shy	.82 Active	-.45 Unfriendly	.85 Appreciative	-.50 Frivolous	.78 Placid	-.21 Contented*	.72 Nervous	-.67 Simple	.72 Intelligent
-.71 Silent	.82 Energetic	-.45 Quarrelsome	.84 Affectionate	-.49 Irresponsible	.78 Efficient	.14 Unemotional*	.71 Moody	-.55 Shallow	.73 Original
-.67 Withdrawn	.82 Outgoing	-.45 Hard-hearted	.84 Soft-hearted	-.40 Slipshod	.73 Responsible		.71 Worrying	-.47 Unintelligent	.68 Insightful
-.66 Retiring	.80 Outspoken	-.38 Unkind	.82 Warm	-.39 Undependable	.72 Reliable		.68 Touchy		.64 Curious
	.79 Dominant	-.33 Cruel	.81 Generous	-.37 Forgetful	.70 Dependable		.64 Fearful		.59 Sophisticated
	.73 Forceful	-.31 Stern*	.78 Trusting		.68 Conscientious		.63 High-strung		.59 Artistic
	.73 Enthusiastic	-.28 Thankless	.77 Helpful		.66 Precise		.63 Self-pitying		.59 Clever
	.68 Show-off	-.24 Stingy*	.77 Forgiving		.66 Practical		.60 Temperamental		.58 Inventive
	.68 Sociable		.74 Pleasant		.65 Deliberate		.59 Unstable		.56 Sharp-witted
	.64 Spunky		.73 Good-natured		.46 Painstaking		.58 Self-punishing		.55 Ingenious
	.64 Adventurous		.73 Friendly		.26 Cautious*		.54 Despondent		.45 Witty*
	.62 Noisy		.72 Cooperative				.51 Emotional		.45 Resourceful*
	.58 Bossy		.67 Gentle						.37 Wise
			.66 Unselfish						.33 Logical*
			.56 Praising						.29 Civilized*
			.51 Sensitive						.22 Foresighted*
									.21 Polished*
									.20 Dignified*

Many applications, such as online match-making.

Singular value decomposition (SVD)

For **symmetric** matrices, such as covariance matrices, we have seen:

- Results about existence of eigenvalues and eigenvectors
- The fact that the eigenvectors form an alternative basis
- The resulting spectral decomposition, which is used in PCA

But what about arbitrary matrices $M \in \mathbb{R}^{p \times q}$?

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But what about arbitrary matrices $M \in \mathbb{R}^{p \times q}$?

Any $p \times q$ matrix (say $p \leq q$) has a **singular value decomposition**:

$$M = \underbrace{\begin{pmatrix} \uparrow & & \uparrow \\ u_1 & \cdots & u_p \\ \downarrow & & \downarrow \end{pmatrix}}_{p \times p \text{ matrix } U} \underbrace{\begin{pmatrix} \sigma_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_p \end{pmatrix}}_{p \times p \text{ matrix } \Lambda} \underbrace{\begin{pmatrix} \longleftarrow v_1 \longrightarrow \\ \vdots \\ \longleftarrow v_p \longrightarrow \end{pmatrix}}_{p \times q \text{ matrix } V^T}$$

- u_1, \dots, u_p are orthonormal vectors in \mathbb{R}^p
- v_1, \dots, v_p are orthonormal vectors in \mathbb{R}^q
- $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p$ are **singular values**

Matrix approximation

We can **factor** any $p \times q$ matrix as $M = UW^T$:

$$\begin{aligned} M &= \begin{pmatrix} \uparrow & & \uparrow \\ u_1 & \cdots & u_p \\ \downarrow & & \downarrow \end{pmatrix} \begin{pmatrix} \sigma_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_p \end{pmatrix} \begin{pmatrix} \longleftarrow v_1 \longrightarrow \\ \vdots \\ \longleftarrow v_p \longrightarrow \end{pmatrix} \\ &= \underbrace{\begin{pmatrix} \uparrow & & \uparrow \\ u_1 & \cdots & u_p \\ \downarrow & & \downarrow \end{pmatrix}}_{p \times p \text{ matrix } U} \underbrace{\begin{pmatrix} \longleftarrow \sigma_1 v_1 \longrightarrow \\ \vdots \\ \longleftarrow \sigma_p v_p \longrightarrow \end{pmatrix}}_{p \times q \text{ matrix } W^T} \end{aligned}$$

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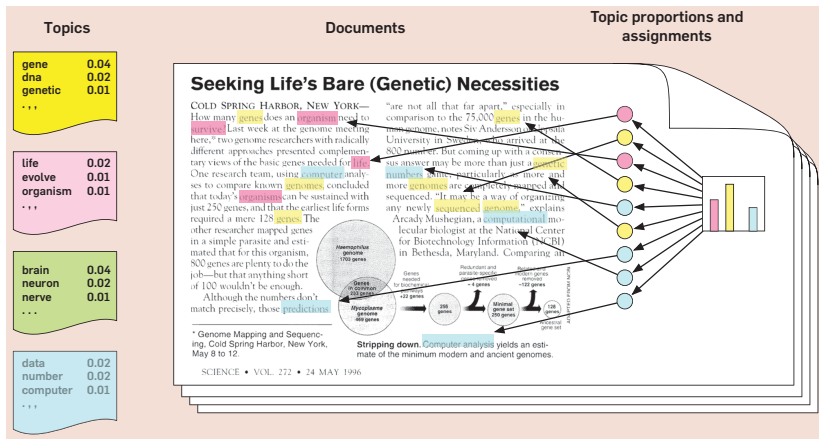
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A concise approximation to M : just take the first k columns of U and the first k rows of W^T , for $k < p$:

$$\hat{M} = \underbrace{\begin{pmatrix} \uparrow & & \uparrow \\ u_1 & \cdots & u_k \\ \downarrow & & \downarrow \end{pmatrix}}_{p \times k} \underbrace{\begin{pmatrix} \longleftarrow \sigma_1 v_1 \longrightarrow \\ \vdots \\ \longleftarrow \sigma_k v_k \longrightarrow \end{pmatrix}}_{k \times q}$$

Example: topic modeling

Blei (2012):



Latent semantic indexing (LSI)

Given a large corpus of n documents:

- Fix a vocabulary, say of V words.
- Bag-of-words representation for documents: each document becomes a vector of length V , with one coordinate per word.
- The corpus is an $n \times V$ matrix, one row per document.

	cat	dog	house	boat	garden	...
Doc 1	4	1	1	0	2	
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Let's find a concise approximation to this matrix M .

Latent semantic indexing, cont'd

Use SVD to get an approximation to M : for small k ,

$$\underbrace{\begin{pmatrix} \leftarrow \text{doc 1} \rightarrow \\ \leftarrow \text{doc 2} \rightarrow \\ \leftarrow \text{doc 3} \rightarrow \\ \vdots \\ \leftarrow \text{doc } n \rightarrow \end{pmatrix}}_{n \times V \text{ matrix } M} \approx \underbrace{\begin{pmatrix} \leftarrow \theta_1 \rightarrow \\ \leftarrow \theta_2 \rightarrow \\ \leftarrow \theta_3 \rightarrow \\ \vdots \\ \leftarrow \theta_n \rightarrow \end{pmatrix}}_{n \times k \text{ matrix } \Theta} \underbrace{\begin{pmatrix} \leftarrow \psi_1 \rightarrow \\ \vdots \\ \leftarrow \psi_k \rightarrow \end{pmatrix}}_{k \times V \text{ matrix } \Psi}$$

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Think of this as a *topic model* with k topics.

- ψ_j is a vector of length V describing topic j : coefficient ψ_{jw} is large if word w appears often in that topic.
- Each document is a combination of topics: θ_{ij} is the weight of topic j in document i .

Latent semantic indexing, cont'd

Use SVD to get an approximation to M : for small k ,

$$\underbrace{\begin{pmatrix} \leftarrow \text{doc 1} \rightarrow \\ \leftarrow \text{doc 2} \rightarrow \\ \leftarrow \text{doc 3} \rightarrow \\ \vdots \\ \leftarrow \text{doc } n \rightarrow \end{pmatrix}}_{n \times V \text{ matrix } M} \approx \underbrace{\begin{pmatrix} \leftarrow \theta_1 \rightarrow \\ \leftarrow \theta_2 \rightarrow \\ \leftarrow \theta_3 \rightarrow \\ \vdots \\ \leftarrow \theta_n \rightarrow \end{pmatrix}}_{n \times k \text{ matrix } \Theta} \underbrace{\begin{pmatrix} \leftarrow \psi_1 \rightarrow \\ \vdots \\ \leftarrow \psi_k \rightarrow \end{pmatrix}}_{k \times V \text{ matrix } \Psi}$$

Think of this as a *topic model* with k topics.

- ψ_j is a vector of length V describing topic j : coefficient ψ_{jw} is large if word w appears often in that topic.
- Each document is a combination of topics: θ_{ij} is the weight of topic j in document i .

Document i originally represented by i th row of M , a vector in \mathbb{R}^V .
Can instead use $\theta_i \in \mathbb{R}^k$, a more concise “semantic” representation.

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- Treat each row of \hat{M} as a data point in \mathbb{R}^q .
- We can think of the data as “simple” if it actually lies in a low-dimensional subspace.
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We can get \hat{M} directly from the singular value decomposition of M .

Low-rank approximation

Recall: Singular value decomposition of $p \times q$ matrix M (with $p \leq q$):

$$M = \begin{pmatrix} \uparrow & & \uparrow \\ u_1 & \cdots & u_p \\ \downarrow & & \downarrow \end{pmatrix} \begin{pmatrix} \sigma_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_p \end{pmatrix} \begin{pmatrix} \longleftarrow v_1 \longrightarrow \\ \vdots \\ \longleftarrow v_p \longrightarrow \end{pmatrix}$$

- u_1, \dots, u_p is an orthonormal basis of \mathbb{R}^p
- v_1, \dots, v_q is an orthonormal basis of \mathbb{R}^q
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The **best rank- k approximation** to M , for any $k \leq p$, is then

$$\hat{M} = \underbrace{\begin{pmatrix} \uparrow & & \uparrow \\ u_1 & \cdots & u_k \\ \downarrow & & \downarrow \end{pmatrix}}_{p \times k} \underbrace{\begin{pmatrix} \sigma_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_k \end{pmatrix}}_{k \times k} \underbrace{\begin{pmatrix} \leftarrow v_1 \rightarrow \\ \vdots \\ \leftarrow v_k \rightarrow \end{pmatrix}}_{k \times q}$$

Example: Collaborative filtering

Details and images from Koren, Bell, Volinsky (2009).

Recommender systems: matching customers with products.

- Given: data on prior purchases/interests of users
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Prototypical example: Netflix.

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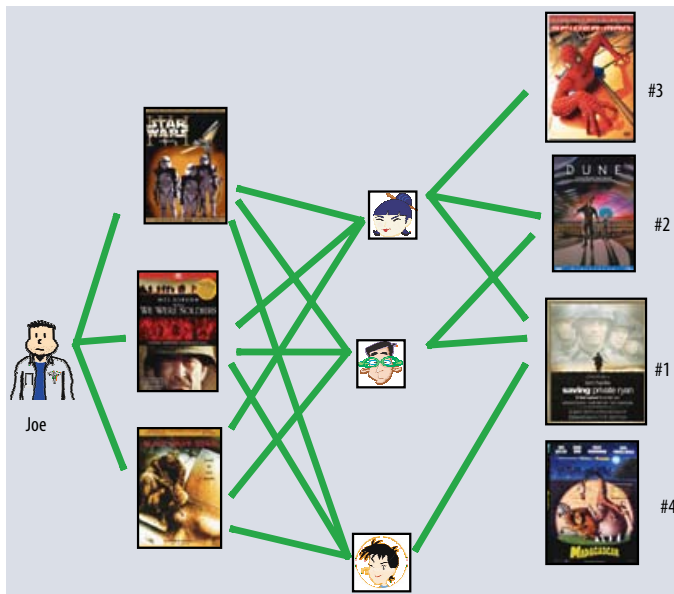
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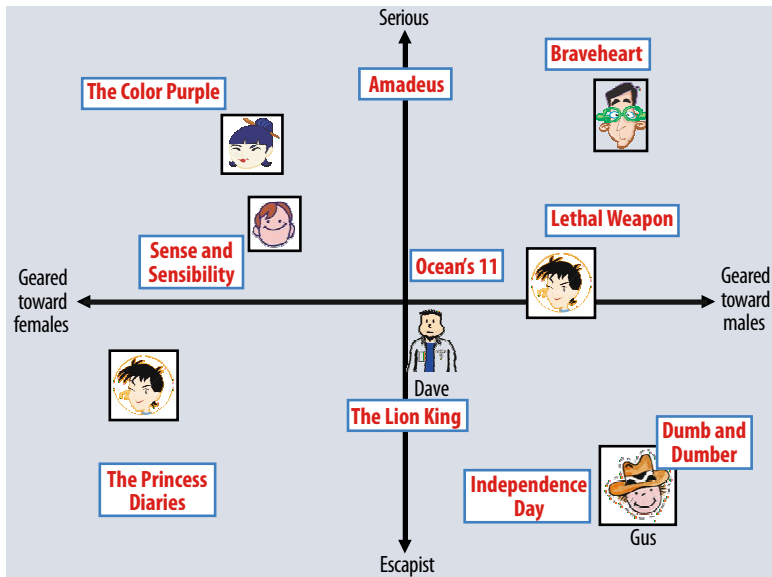
Two strategies for collaborative filtering:

- Neighborhood methods
- Latent factor methods

Neighborhood methods



Latent factor methods



The matrix factorization approach

User ratings are assembled in a large matrix M :

	<i>Star Wars</i>	<i>Matrix</i>	<i>Casablanca</i>	<i>Camelot</i>	<i>Godfather</i>	...
User 1	5	5	2	0	0	
User 2	0	0	3	4	5	
User 3	0	0	5	0	0	
		⋮				

- Not rated = 0, otherwise scores 1-5.
- For n users and p movies, this has size $n \times p$.
- Most of the entries are unavailable, and we'd like to predict these.

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Idea: Find the best low-rank approximation of M , and use it to fill in the missing entries.

User and movie factors

Best rank- k approximation is of the form $M \approx UW^T$:

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This “latent” representation embeds users and movies within the same k -dimensional space:

- Represent i th user by $u_i \in \mathbb{R}^k$
- Represent j th movie by $w_j \in \mathbb{R}^k$

Top two Netflix factors

