

Principle Components Analysis

Dimensionality reduction

Why reduce the number of features in a data set?

- ① It reduces storage and computation time.
- ② High-dimensional data often has a lot of redundancy.
- ③ Remove noisy or irrelevant features.

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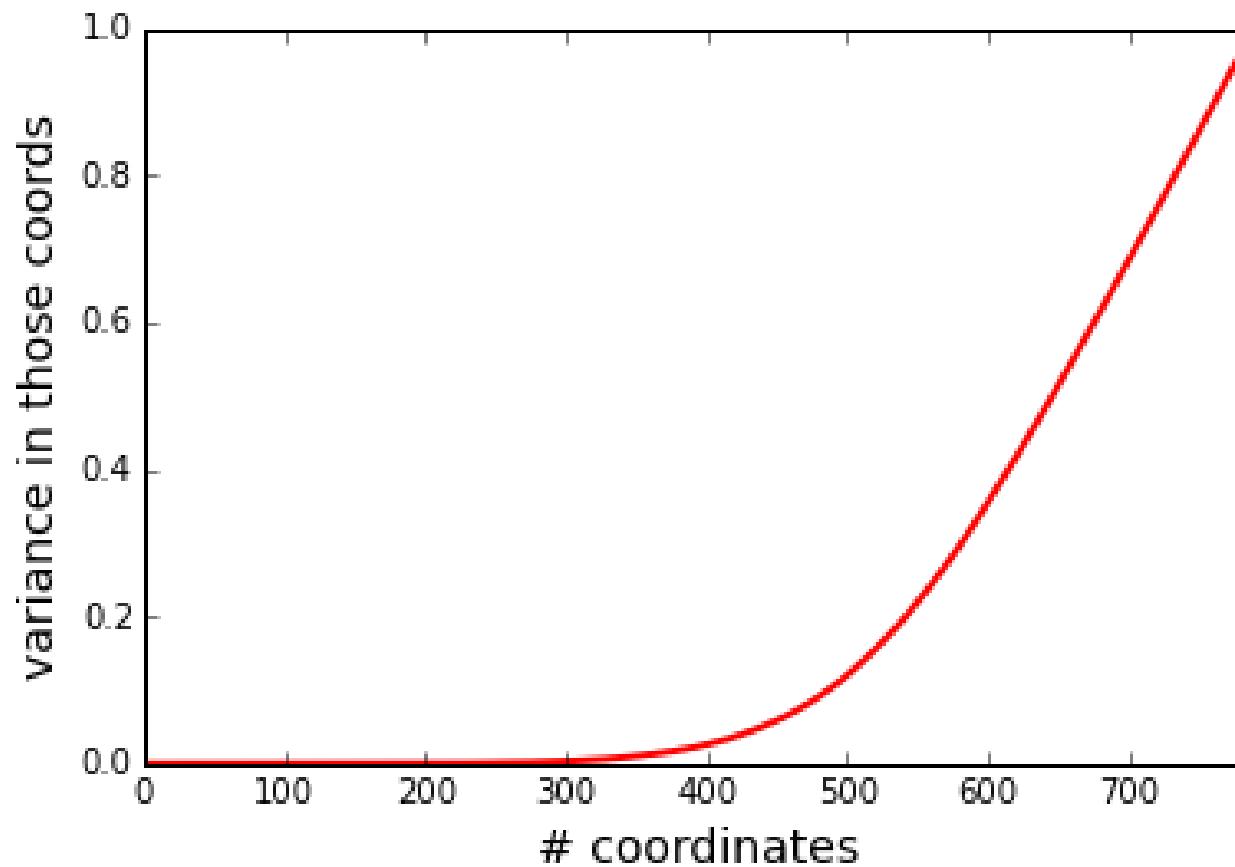
Those with lowest variance...

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?

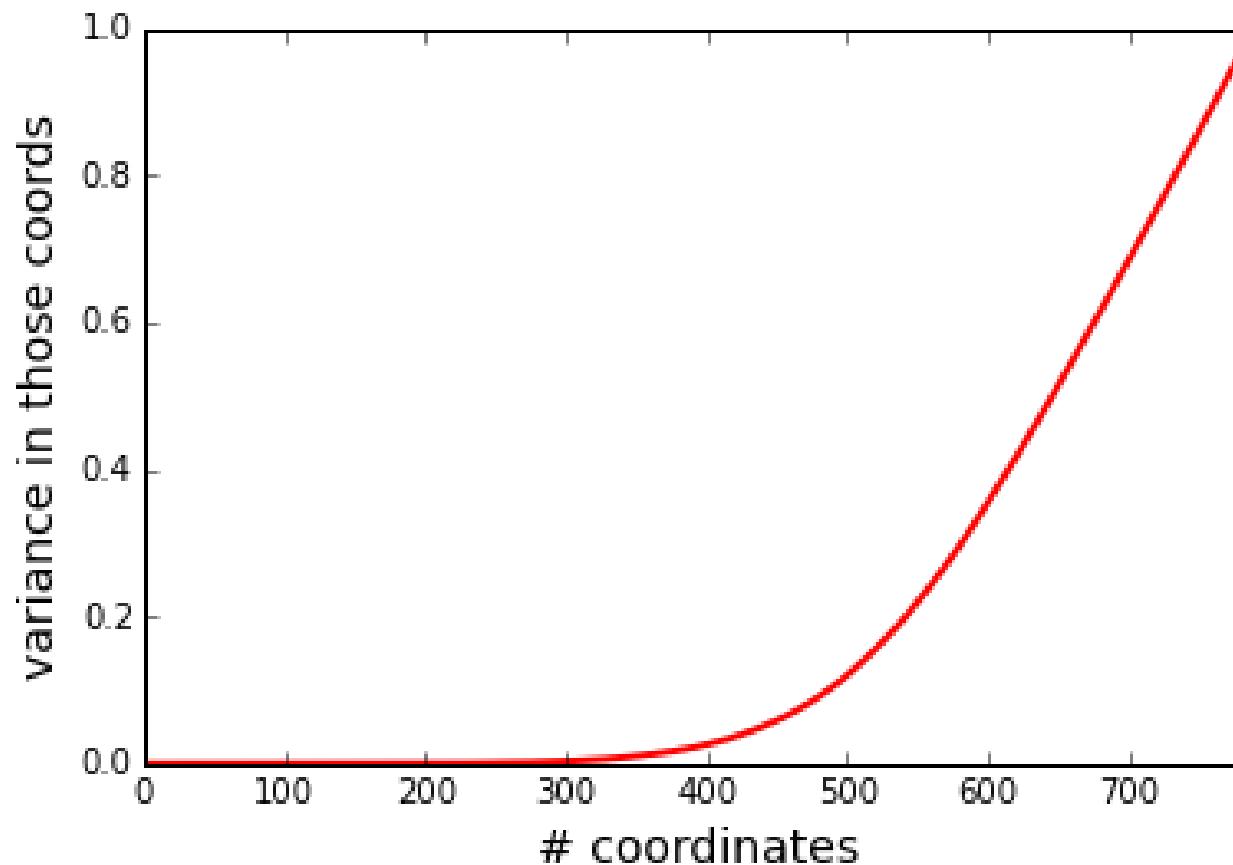
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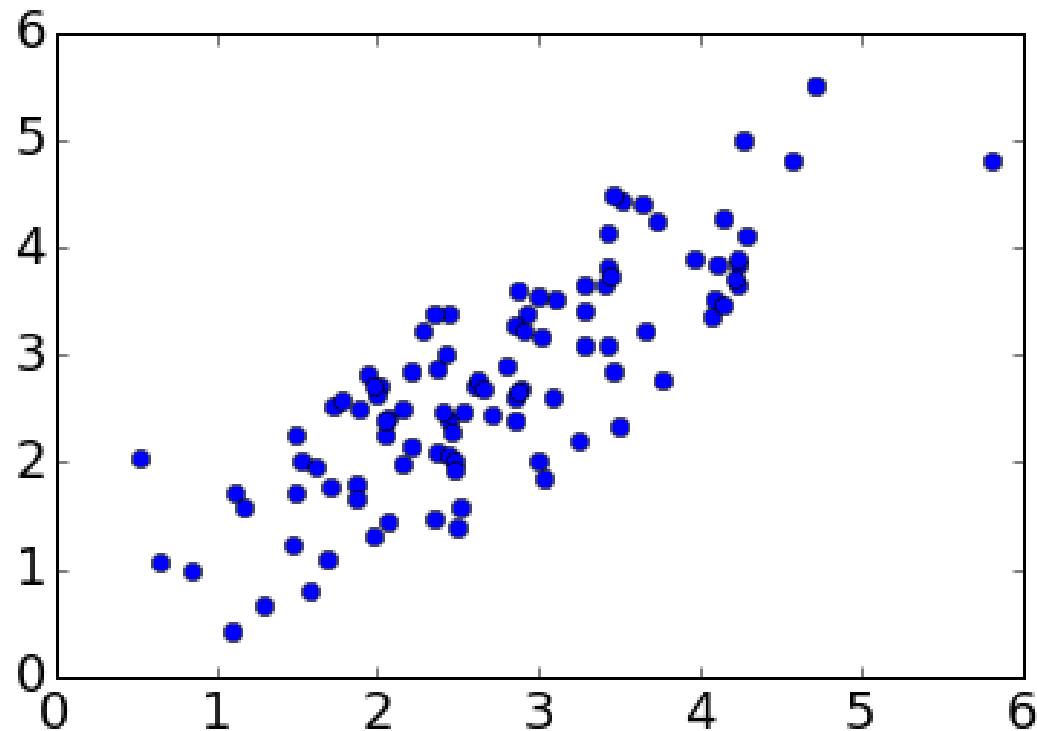
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Could easily drop 300-400 pixels...

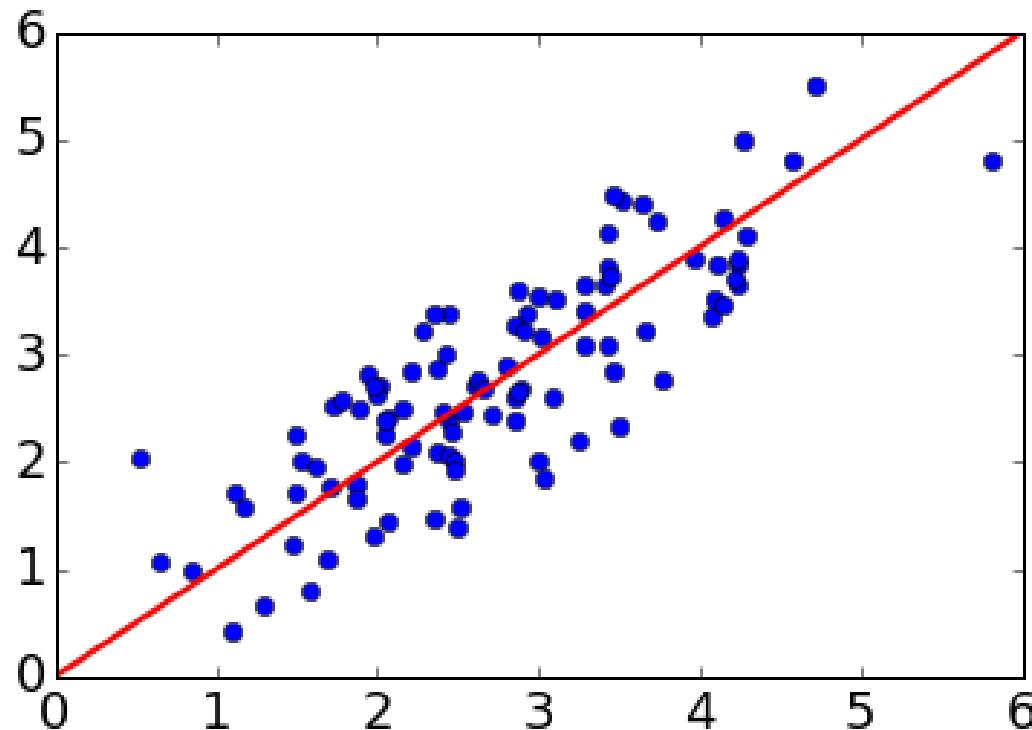
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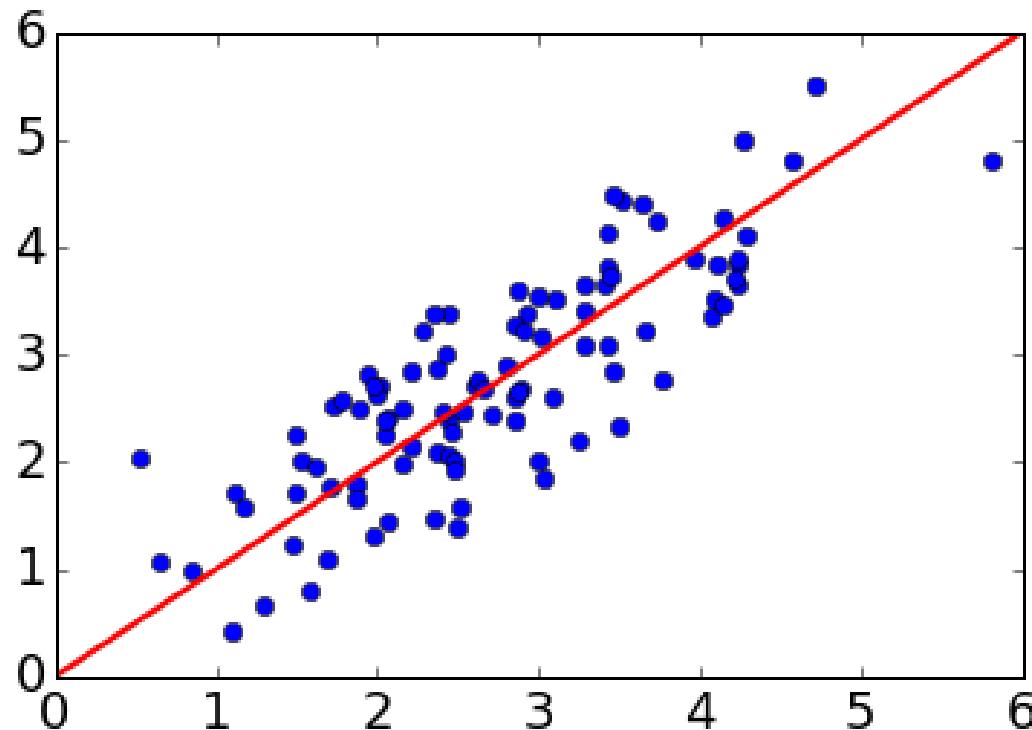
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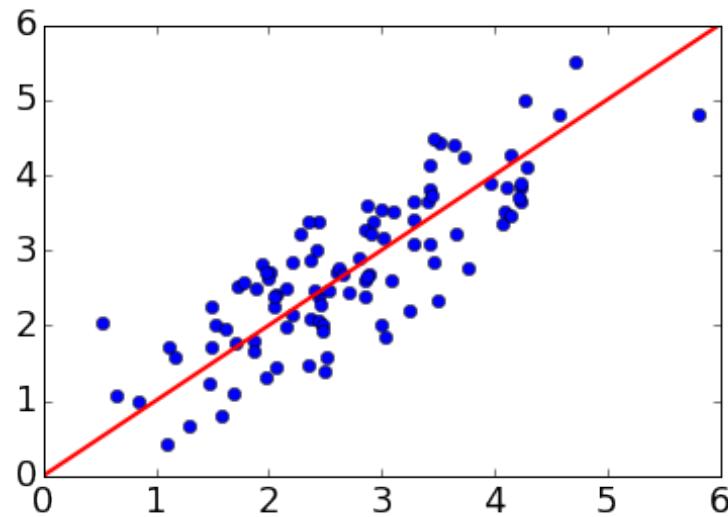
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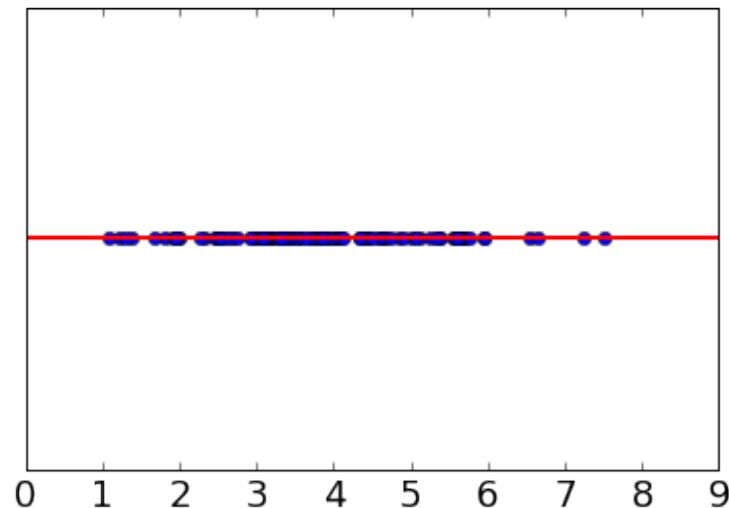


This is the **direction of maximum variance**.

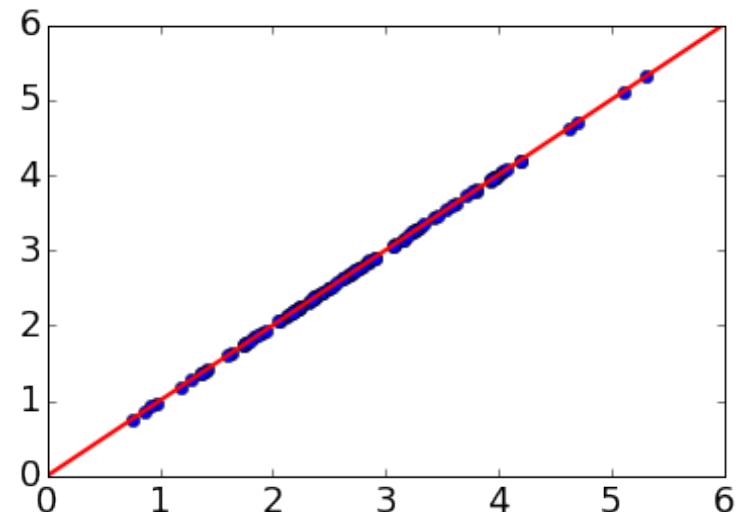
Two types of projection



Projection onto \mathbb{R} :

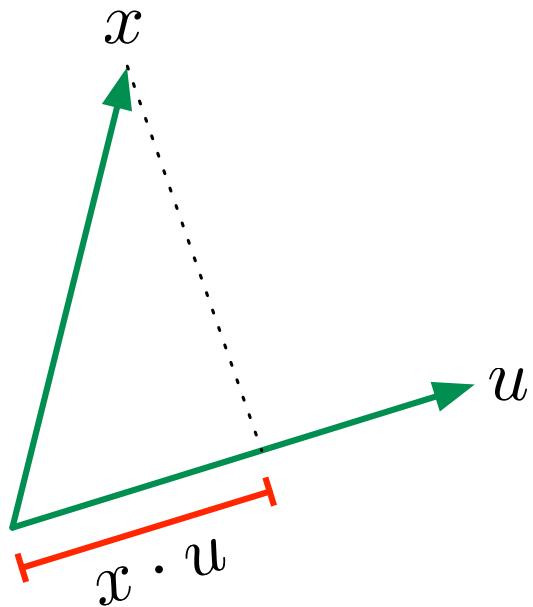


Projection onto a 1-d line in \mathbb{R}^2 :



Projection: formally

What is the projection of $x \in \mathbb{R}^p$ onto direction $u \in \mathbb{R}^p$ (where $\|u\| = 1$)?

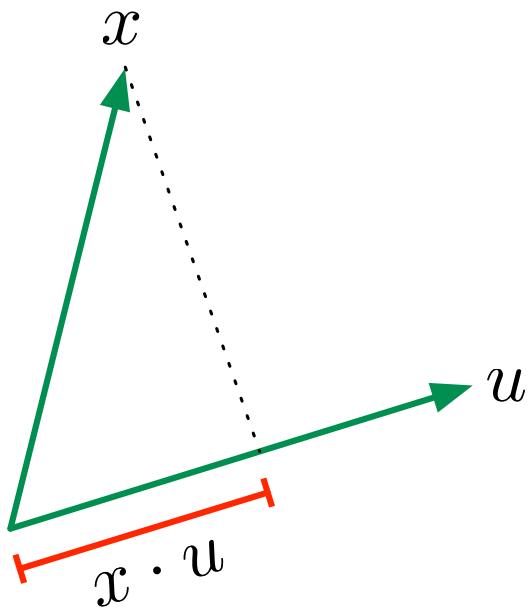


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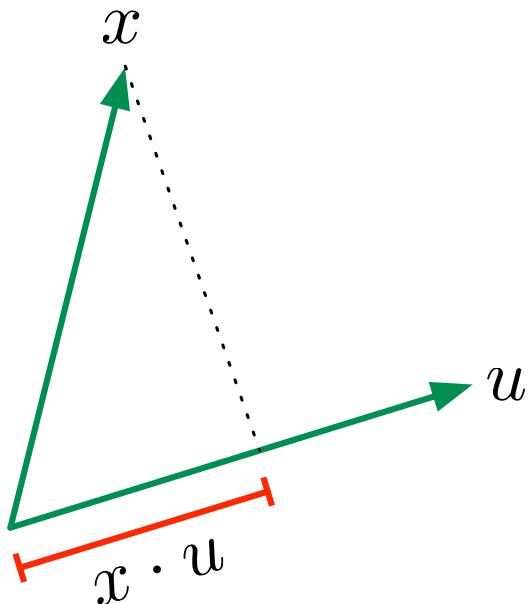
As a one-dimensional value:

$$x \cdot u = u \cdot x = u^T x = \sum_{i=1}^p u_i x_i.$$



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As a p -dimensional vector:

$$(x \cdot u)u = uu^T x$$

“Move $x \cdot u$ units in direction u ”

Matrix notation

The compact way for representing projections and rotations

Inner Products

Row vector $\mathbf{a} = (a_1, a_2 \dots, a_n)$

$$\text{Column vector } \mathbf{b}^T = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$
$$\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^n a_i b_i = \mathbf{a}\mathbf{b}^T = (a_1, a_2 \dots, a_n) \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Orthogonality and norm

$\mathbf{a} \cdot \mathbf{b} = 0$ a and b are **orthogonal** vectors

Norm $\|\mathbf{a}\|_2^2 \doteq \mathbf{a} \cdot \mathbf{a} = \sum_{i=1} \mathbf{a}_i^2$

Unit vector $\|\mathbf{a}\|_2 = 1$

matrix-vector product

$$A = \begin{pmatrix} a_{1,1}, a_{1,2}, \dots, a_{1,m} \\ a_{2,1}, a_{2,2}, \dots, a_{2,m} \\ \vdots \\ \vdots \\ a_{n,1}, a_{n,2}, \dots, a_{n,m} \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \vdots \\ \vdots \\ \mathbf{a}_n \end{pmatrix}$$

$$A\mathbf{b}^T = \begin{pmatrix} \mathbf{a}_1 \mathbf{b}^T \\ \mathbf{a}_2 \mathbf{b}^T \\ \vdots \\ \vdots \\ \mathbf{a}_n \mathbf{b}^T \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^m a_{1,i} b_i \\ \sum_{i=1}^m a_{2,i} b_i \\ \vdots \\ \vdots \\ \sum_{i=1}^m a_{n,i} b_i \end{pmatrix}$$

matrix-matrix product

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$$B = \begin{pmatrix} b_{1,1}, b_{1,2}, \dots, b_{1,l} \\ b_{2,1}, b_{2,2}, \dots, b_{2,l} \\ \vdots \\ \vdots \\ b_{m,1}, b_{m,2}, \dots, b_{m,l} \end{pmatrix} = (\mathbf{b}_1^T, \mathbf{b}_2^T, \dots, \mathbf{b}_l^T)$$

$$AB = \begin{pmatrix} (\mathbf{a}_1 \cdot \mathbf{b}_1), (\mathbf{a}_1 \cdot \mathbf{b}_2), \dots, (\mathbf{a}_1 \cdot \mathbf{b}_l) \\ (\mathbf{a}_2 \cdot \mathbf{b}_1), (\mathbf{a}_2 \cdot \mathbf{b}_2), \dots, (\mathbf{a}_2 \cdot \mathbf{b}_l) \\ \vdots \\ \vdots \\ (\mathbf{a}_n \cdot \mathbf{b}_1), (\mathbf{a}_n \cdot \mathbf{b}_2), \dots, (\mathbf{a}_n \cdot \mathbf{b}_l) \end{pmatrix}$$

diagonal matrices

$$D\mathbf{b}^T = \begin{pmatrix} \lambda_1, 0, 0, \dots, 0 \\ 0, \lambda_2, 0, \dots, 0 \\ 0, 0, \lambda_3, \dots, 0 \\ \vdots \\ \vdots \\ 0, 0, 0, \dots, \lambda_n \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix} = \begin{pmatrix} \lambda_1 b_1 \\ \lambda_2 b_2 \\ \cdot \\ \cdot \\ \cdot \\ \lambda_n b_n \end{pmatrix}$$

$$I\mathbf{b}^T = \begin{pmatrix} 1, 0, 0, \dots, 0 \\ 0, 1, 0, \dots, 0 \\ 0, 0, 1, \dots, 0 \\ \vdots \\ \vdots \\ 0, 0, 0, \dots, 1 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix}$$

Orthonormal Matrices

A is a square matrix ($n \times n$)

$$A = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \cdot \\ \cdot \\ \cdot \\ \mathbf{a}_n \end{pmatrix} \quad A^T = (\mathbf{a}_1^T, \mathbf{a}_2^T, \dots, \mathbf{a}_n^T)$$

$$AA^T = I$$

The rows of A define an orthonormal basis

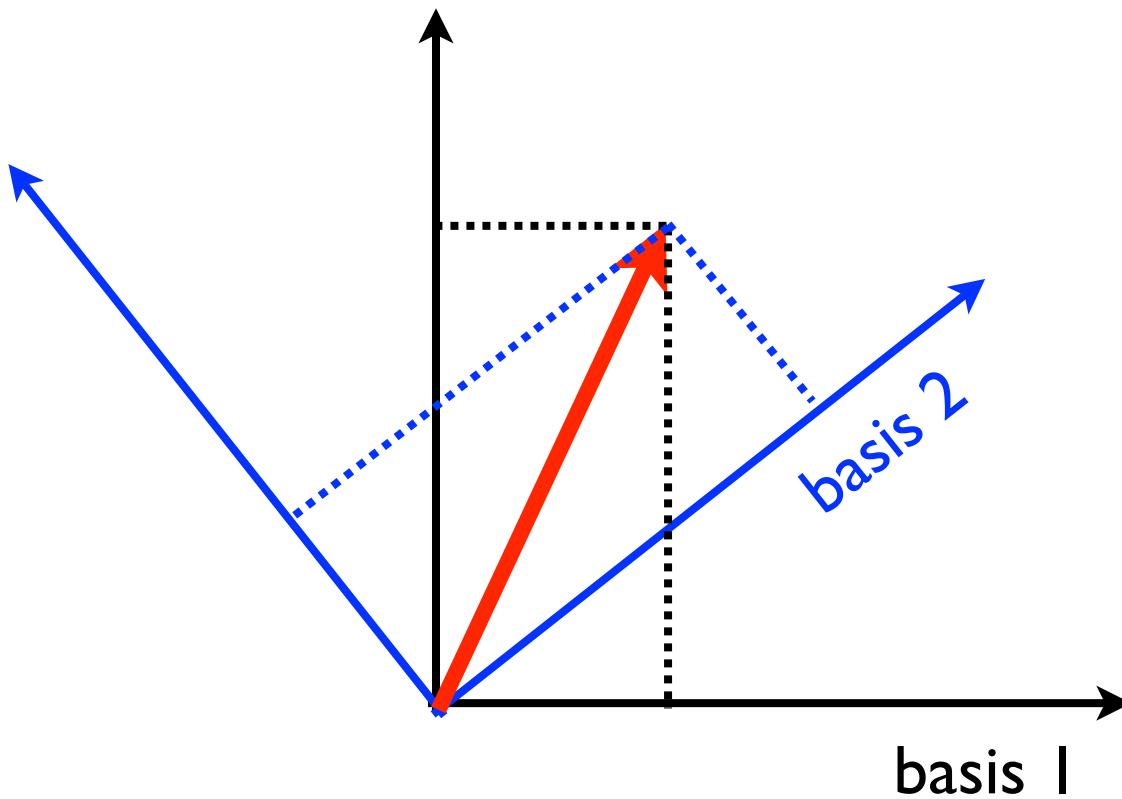
$$\forall i \neq j, \mathbf{a}_i \cdot \mathbf{a}_j = \|\mathbf{a}_i\|_2^2 = 1, \mathbf{a}_i \cdot \mathbf{a}_j = 0$$

Orthonormal matrices and vector bases

- A set of n orthogonal unit vectors in \mathbb{R}^n defines an orthonormal basis.
- Multiplying a vector by an orthonormal matrix corresponds to expressing it in terms of the orthonormal basis.

Changing basis in \mathbb{R}^2

basis = coordinate system



Eigenvectors and Eigenvalues

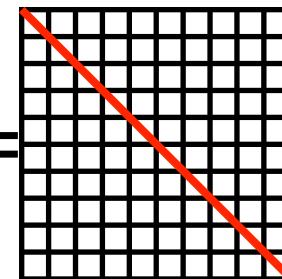
the vector \mathbf{a} is an **eigenvector** of the matrix \mathbf{M} with **eigenvalue** λ if

$$\mathbf{M}\mathbf{a} = \lambda\mathbf{a}$$

In words: the application of \mathbf{M} to \mathbf{a} amounts to changing the **length** of \mathbf{a} by a factor of λ without changing \mathbf{a} 's **direction**

Decomposing Symmetric Matrices

A symmetric matrix $\mathbf{M} =$



\mathbf{M} can be written in the form

$$M = A^T \begin{pmatrix} \lambda_1, 0, 0, \dots, 0 \\ 0, \lambda_2, 0, \dots, 0 \\ 0, 0, \lambda_3, \dots, 0 \\ \vdots \\ \vdots \\ 0, 0, 0, \dots, \lambda_n \end{pmatrix} A$$

\mathbf{A} is an orthonormal matrix consisting of the eigenvectors of \mathbf{M}

Interpretation of the decomposition

1. the operation $A^T D A a$ equals:
2. transform a into basis defined by A
3. multiply each coordinate i by λ_i
4. transform back to original basis

The covariance matrix

- A symmetric matrix that captures the pairwise relations between observations.

The observations matrix

Suppose our data consists of n p -dimensional vectors.
For example, for weather data, each observation can
be a 365 dimensional vector. $p=365$

$$\mathbf{X} = \begin{pmatrix} & & & \text{p variables} \\ x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix} \quad \text{n observations}$$

Subtracting the average observation vector

observation matrix:
$$\begin{pmatrix} x_{11} & \dots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \dots & x_{np} \end{pmatrix} = \begin{pmatrix} \vec{o}_1 \\ \vdots \\ \vec{o}_n \end{pmatrix}$$

The average observation vector: $\vec{\mu} = \begin{pmatrix} \mu_1 & \dots & \mu_p \end{pmatrix} = \frac{1}{n} \sum_{i=1}^n \vec{o}_i = \frac{1}{n} \sum_{i=1}^n \begin{pmatrix} x_{i1} & \dots & x_{ip} \end{pmatrix}$

Average corrected observation matrix:
$$\begin{pmatrix} x_{11} - \mu_1 & \dots & x_{1p} - \mu_p \\ \vdots & \ddots & \vdots \\ x_{n1} - \mu_1 & \dots & x_{np} - \mu_p \end{pmatrix} = \begin{pmatrix} \vec{o}_1 - \vec{\mu} \\ \vdots \\ \vec{o}_n - \vec{\mu} \end{pmatrix}$$

The mean vector for the average corrected observation matrix is the zero vector.

self outer product

Row vector $\mathbf{a} = (a_1, a_2 \dots, a_n)$

Self Inner Product

$$\mathbf{a} \cdot \mathbf{a} = \mathbf{a}\mathbf{a}^T = \sum_{i=1}^n a_i^2 \text{ is a scalar}$$

Self Outer product

$$\mathbf{a} \otimes \mathbf{a} = \mathbf{a}^T \mathbf{a} = \begin{pmatrix} a_1a_1 & \cdots & a_na_1 \\ \vdots & \ddots & \vdots \\ a_na_1 & \cdots & a_na_n \end{pmatrix} \text{ is an } n \times n \text{ matrix}$$

The covariance matrix

$$\text{Cov}(\mathbf{X}) \doteq \frac{1}{n} \sum_{i=1}^n (\vec{x}_i - \vec{\mu}) \otimes (\vec{x}_i - \vec{\mu})$$

As each outer product yields a symmetric matrix
the Covariance matrix is also symmetric.

We can apply the orthonormal decomposition.

i.e. $\text{Cov}(x) = A^T D A$

Interpretation of principle components

- distribution of random vector \mathbf{x} defines covariance matrix $\text{cov}(\mathbf{x})$
- decomposition $\text{cov}(\mathbf{x}) = \mathbf{A}^T \mathbf{D} \mathbf{A}$ changes the coordinate system of \mathbf{x}
- defines a new random vector $\mathbf{y} = \mathbf{A}\mathbf{x}$
- $\text{cov}(\mathbf{y}) = \mathbf{D}$
- $\text{var}(y_i) = \lambda_i, \forall i \neq j: \text{cov}(y_i, y_j) = 0$

The best k -dimensional projection

Let Σ be the $p \times p$ covariance matrix of X . Its **eigendecomposition** can be computed in $O(p^3)$ time and consists of:

- real **eigenvalues** $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p$
- corresponding **eigenvectors** $u_1, \dots, u_p \in \mathbb{R}^p$ that are orthonormal: that is, each u_i has unit length and $u_i \cdot u_j = 0$ whenever $i \neq j$.

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Theorem: Suppose we want to map data $X \in \mathbb{R}^p$ to just k dimensions, while capturing as much of the variance of X as possible. The best choice of projection is:

$$x \mapsto (u_1 \cdot x, u_2 \cdot x, \dots, u_k \cdot x),$$

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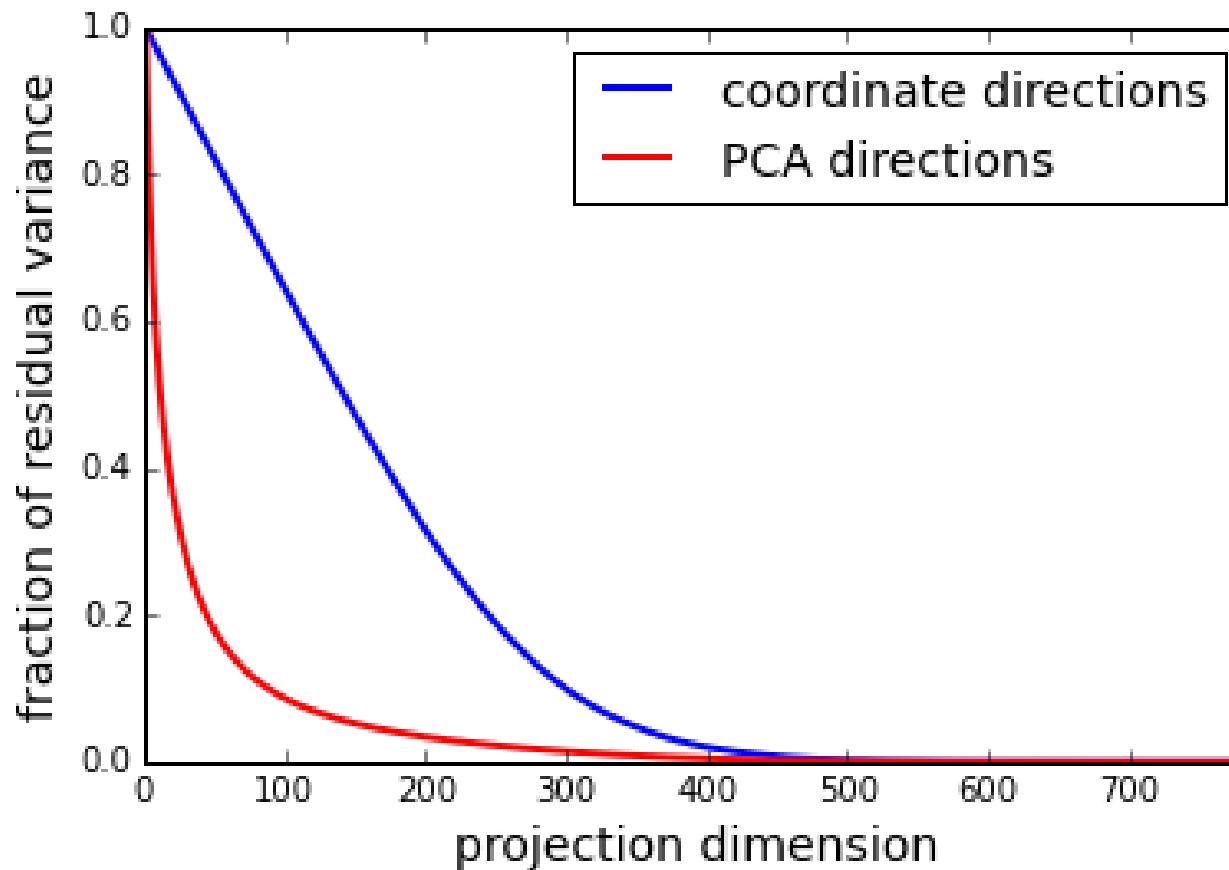
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Projecting the data in this way is **principal component analysis** (PCA).

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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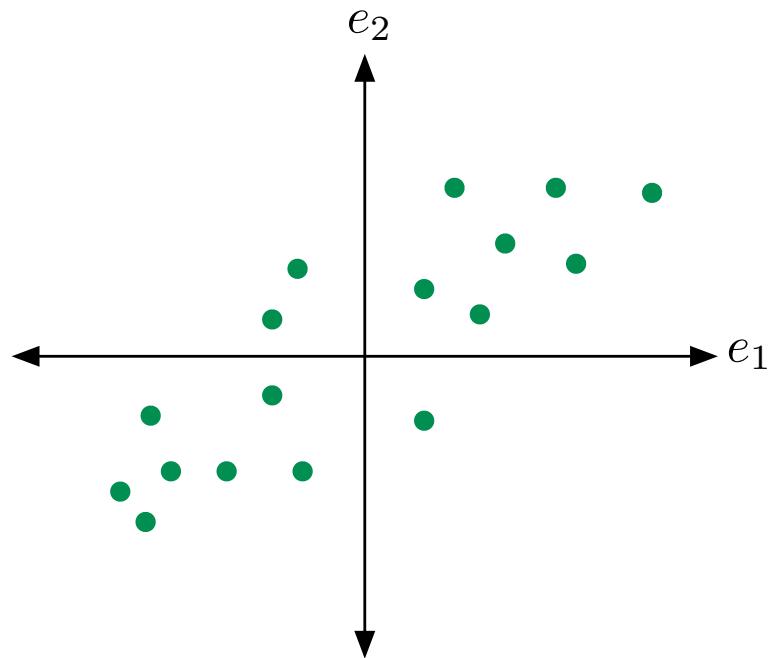


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A: Image x is reconstructed as $UU^T x$, where U is a $p \times k$ matrix whose columns are the top k eigenvectors of Σ .

Principal component analysis: recap

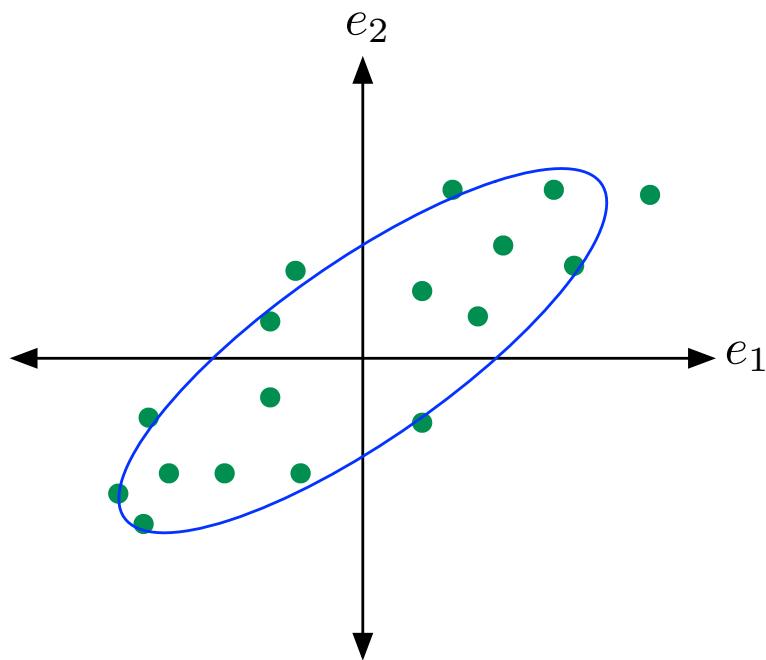
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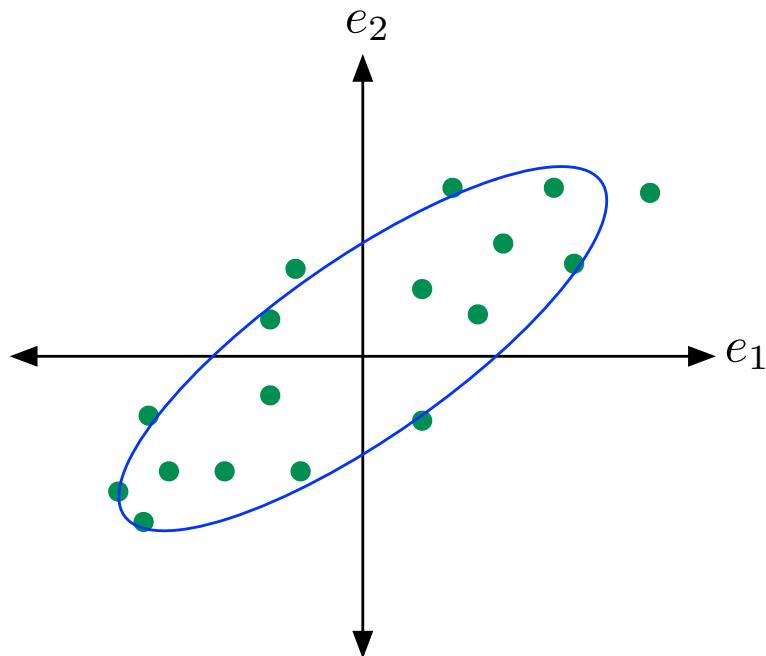
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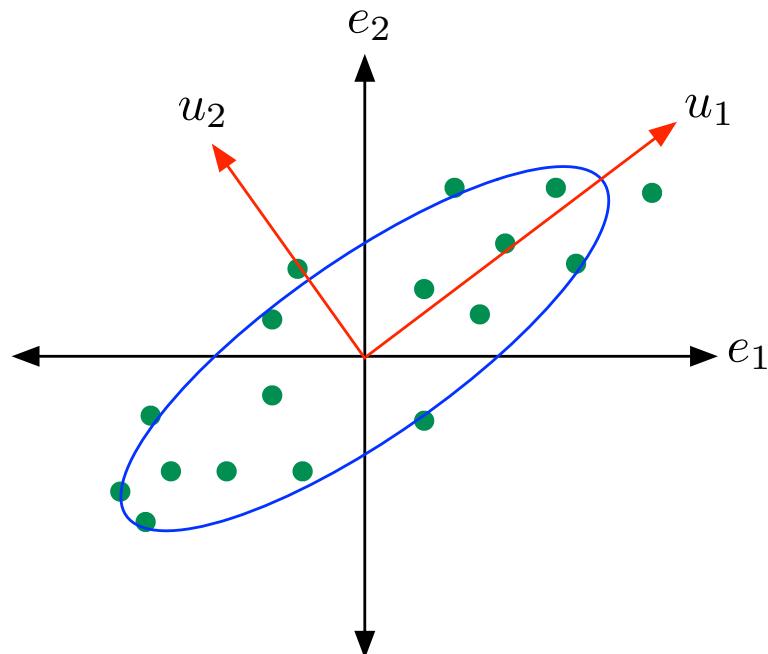
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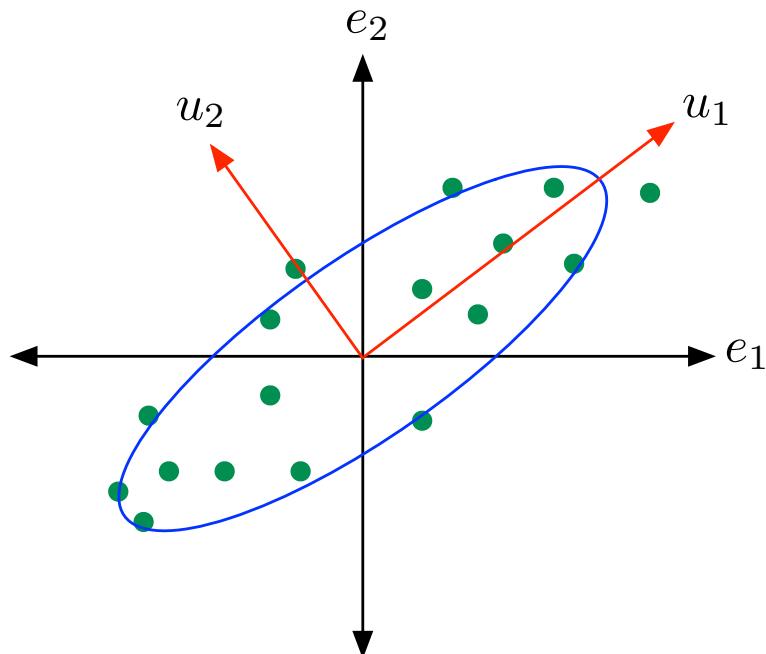
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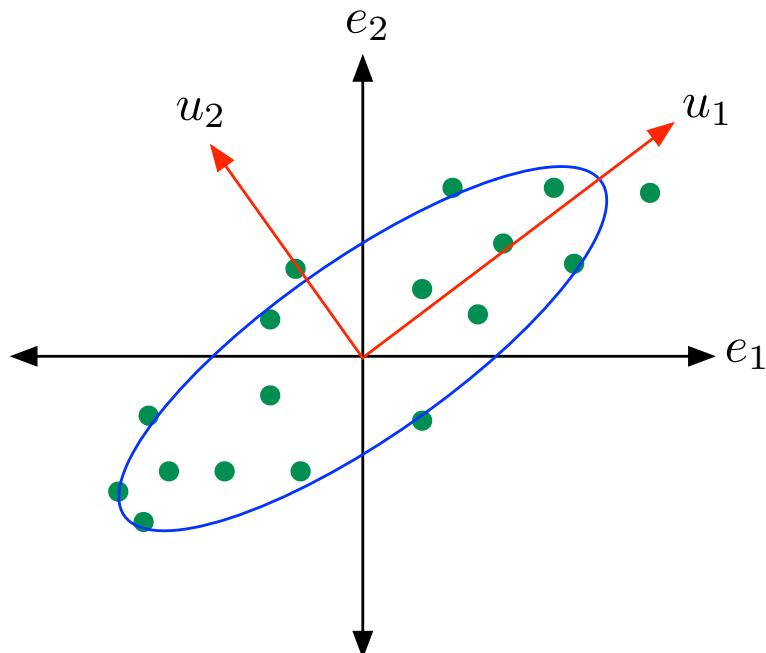
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What is the covariance of
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Example: personality assessment

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- Step: group these words into (approximate) synonyms. This is done by manual clustering. e.g. Norman (1967):

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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- Other ideas: factor analysis, independent component analysis, ...

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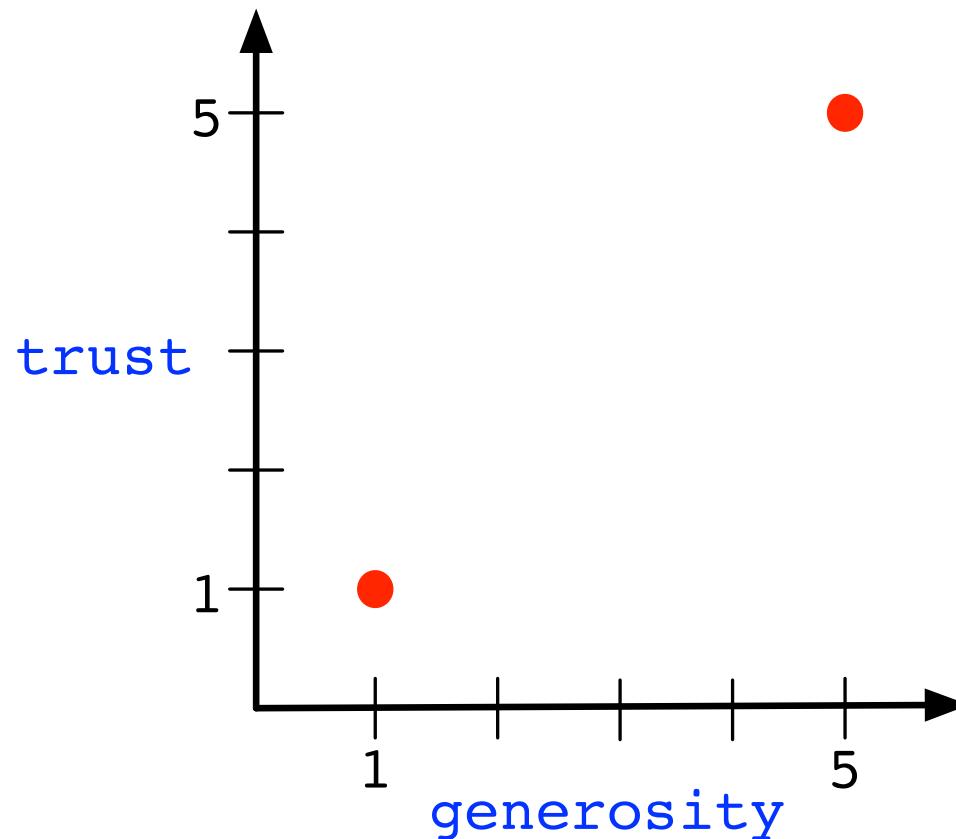
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Many of these yield similar results

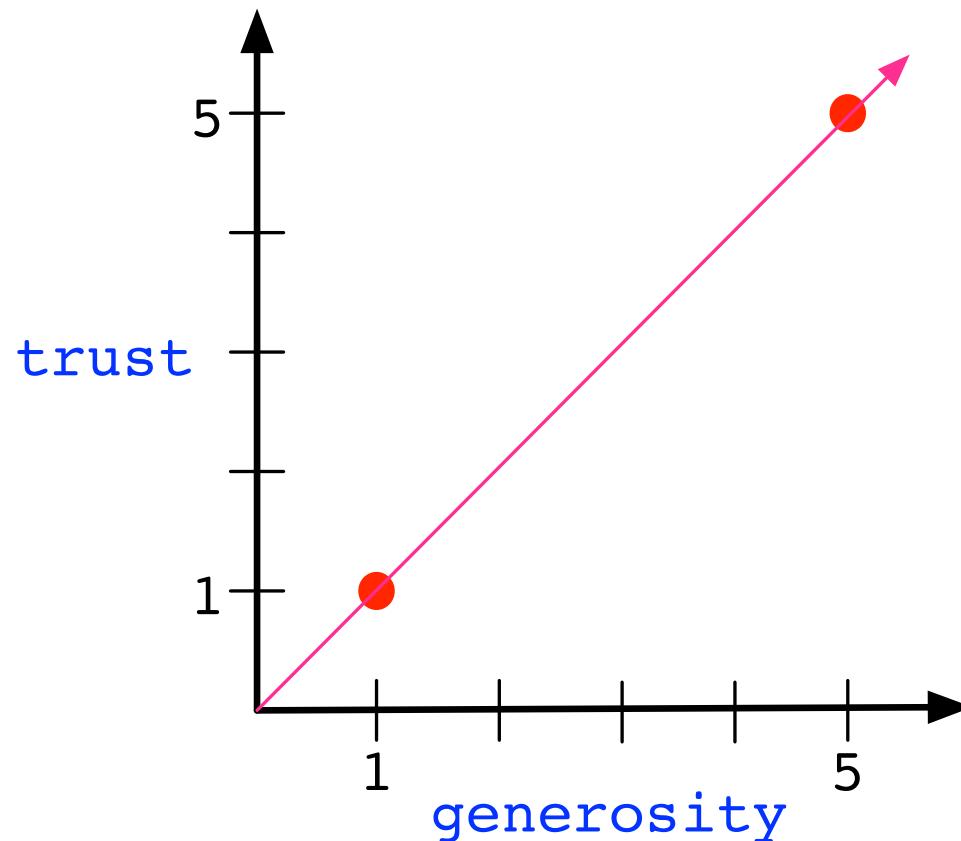
What does PCA accomplish?

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



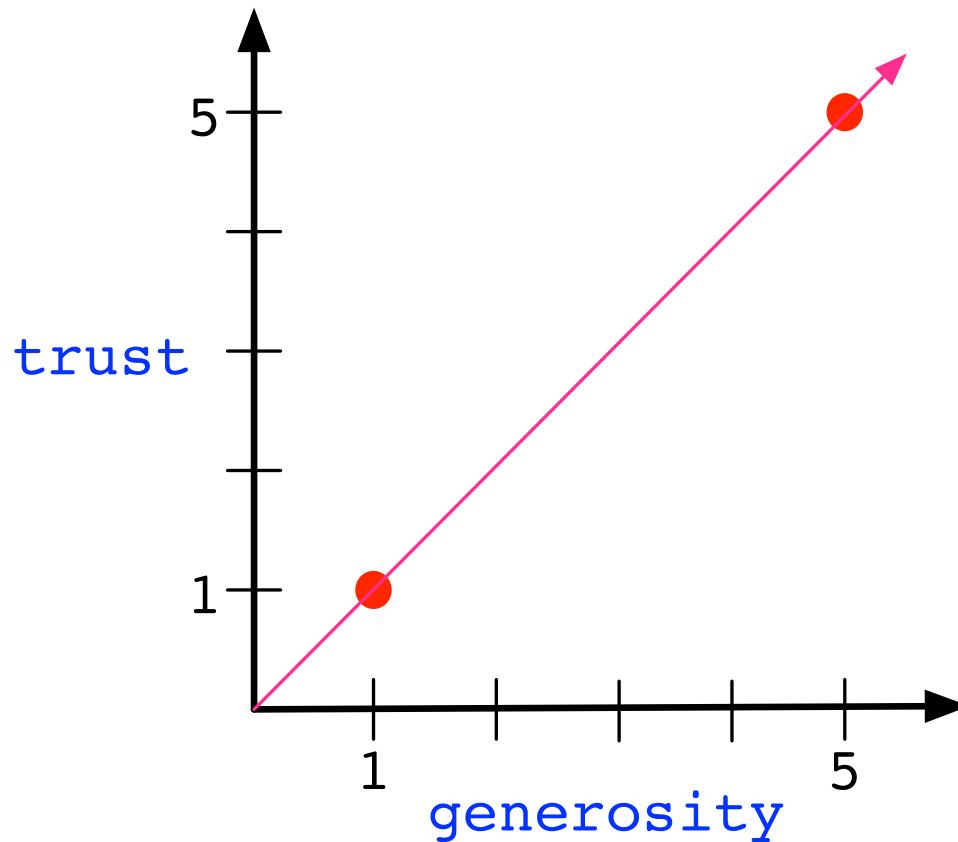
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Example: suppose two traits (generosity, trust) are highly correlated, to the point where each person either answers “1” to both or “5” to both.



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



This single PCA dimension entirely accounts for the two traits.

The “Big Five” taxonomy

Extraversion		Agreeableness		Conscientiousness		Neuroticism		Oppenness/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 Planful	-.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 Slipshot	.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.

Extraversion

Low

High

-.83 Quiet	.85 Talkative
-.80 Reserved	.83 Assertive
-.75 Shy	.82 Active
-.71 Silent	.82 Energetic
-.67 Withdrawn	.82 Outgoing
-.66 Retiring	.80 Outspoken
	.79 Dominant
	.73 Forceful
	.73 Enthusiastic
	.68 Show-off
	.68 Sociable
	.64 Spunky
	.64 Adventurous
	.62 Noisy
	.58 Bossy

Agreeableness

Low	High
-.52 Fault-finding	.87 Sympathetic
-.48 Cold	.85 Kind
-.45 Unfriendly	.85 Appreciative
-.45 Quarrelsome	.84 Affectionate
-.45 Hard-hearted	.84 Soft-hearted
-.38 Unkind	.82 Warm
-.33 Cruel	.81 Generous
-.31 Stern*	.78 Trusting
-.28 Thankless	.77 Helpful
-.24 Stingy*	.77 Forgiving
	.74 Pleasant
	.73 Good-natured
	.73 Friendly
	.72 Cooperative
	.67 Gentle
	.66 Unselfish
	.56 Praising
	.51 Sensitive

Conscientiousness

Low	High
-.58 Careless	.80 Organized
-.53 Disorderly	.80 Thorough
-.50 Frivolous	.78 Planful
-.49 Irresponsible	.78 Efficient
-.40 Slipshot	.73 Responsible
-.39 Undependable	.72 Reliable
-.37 Forgetful	.70 Dependable
	.68 Conscientious
	.66 Precise
	.66 Practical
	.65 Deliberate
	.46 Painstaking
	.26 Cautious*

Neuroticism

Low

High

-.39 Stable*	.73 Tense
-.35 Calm*	.72 Anxious
-.21 Contented*	.72 Nervous
.14 Unemotional*	.71 Moody
	.71 Worrying
	.68 Touchy
	.64 Fearful
	.63 High-strung
	.63 Self-pitying
	.60 Temperamental
	.59 Unstable
	.58 Self-punishing
	.54 Despondent
	.51 Emotional

Oppenness/Intellect

Low

High

- | | |
|-----------------------|--------------------|
| -.74 Commonplace | .76 Wide interests |
| -.73 Narrow interests | .76 Imaginative |
| -.67 Simple | .72 Intelligent |
| -.55 Shallow | .73 Original |
| -.47 Unintelligent | .68 Insightful |
| | .64 Curious |
| | .59 Sophisticated |
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| | .45 Witty* |
| | .45 Resourceful* |
| | .37 Wise |
| | .33 Logical* |
| | .29 Civilized* |
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