Principal Component Analysis

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Covariance

- Variance and Covariance are a measure of the “spread” of a set of points around their center of mass (mean)

- **Variance** is a measure of the deviation from the mean for points in one dimension e.g. variance in the measuring the length of the same object by different people.

- **Covariance** is a measure of how much each of the dimensions vary from the mean with respect to each other.

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Covariance

- Covariance is measured between 2 dimensions to see if there is a relationship between the 2 dimensions e.g. number of hours studied & marks obtained.

- The covariance between one dimension and itself is the variance

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Covariance

Cov dim (1, 2)

$$(X[1] - \bar{x}[1])(X[2] - \bar{x}[2])$$

$$\text{Covariance}(X, Y) = \frac{\sum_{i=1}^{n}(X - \bar{X})(Y - \bar{Y})}{n}$$

Cov dim 2, 3
1, 3

- For a 3-dimensional data set (x, y, z), one can measure the covariance between:
  - x and y dimensions,
  - y and z dimensions, and
  - x and z dimensions.

- Covariance is symmetrical: $\text{Cov}(X, Y) = \text{Cov}(Y, X)$

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Covariance Matrix

- Covariance between various dimensions is typically represented as a 2D **covariance matrix (C)**. For a 3-dimensional data (X, Y, Z):

$$C = \begin{bmatrix} \mathrm{Cov}(X,X) & \mathrm{Cov}(X,Y) & \mathrm{Cov}(X,Z) \\ \mathrm{Cov}(Y,X) & \mathrm{Cov}(Y,Y) & \mathrm{Cov}(Y,\mathrm{Z}) \\ \mathrm{Cov}(Z,X) & \mathrm{Cov}(Z,Y) & \mathrm{Cov}(Z,Z) \end{bmatrix}$$

- Diagonal elements are the variances of X, Y and Z.

- The covariance matrix C is is symmetrical about the diagonal

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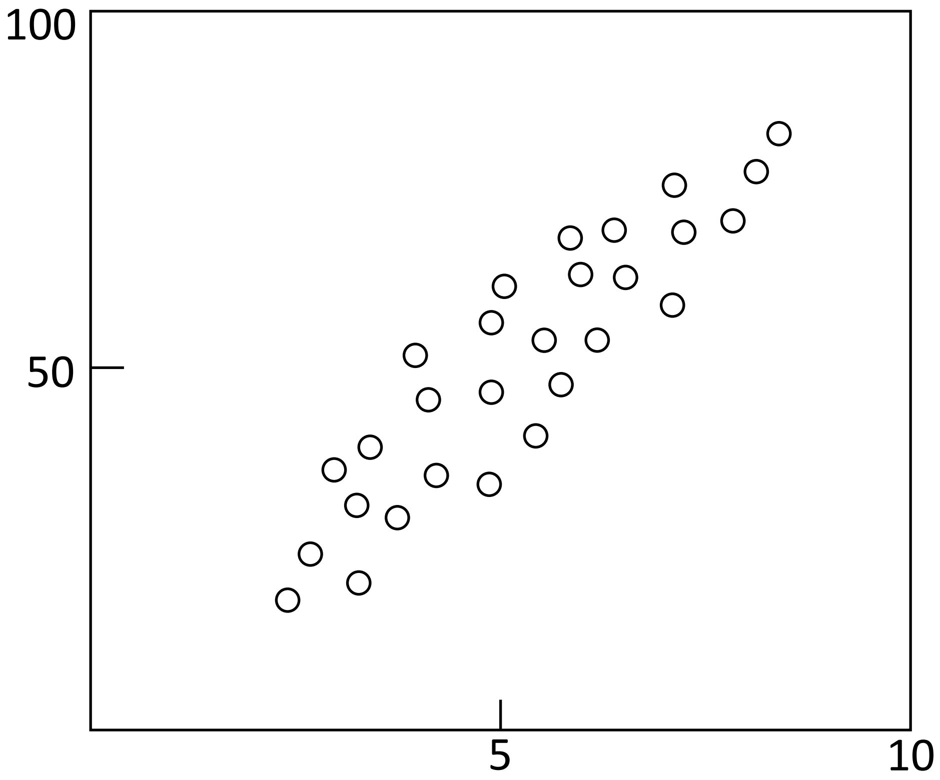
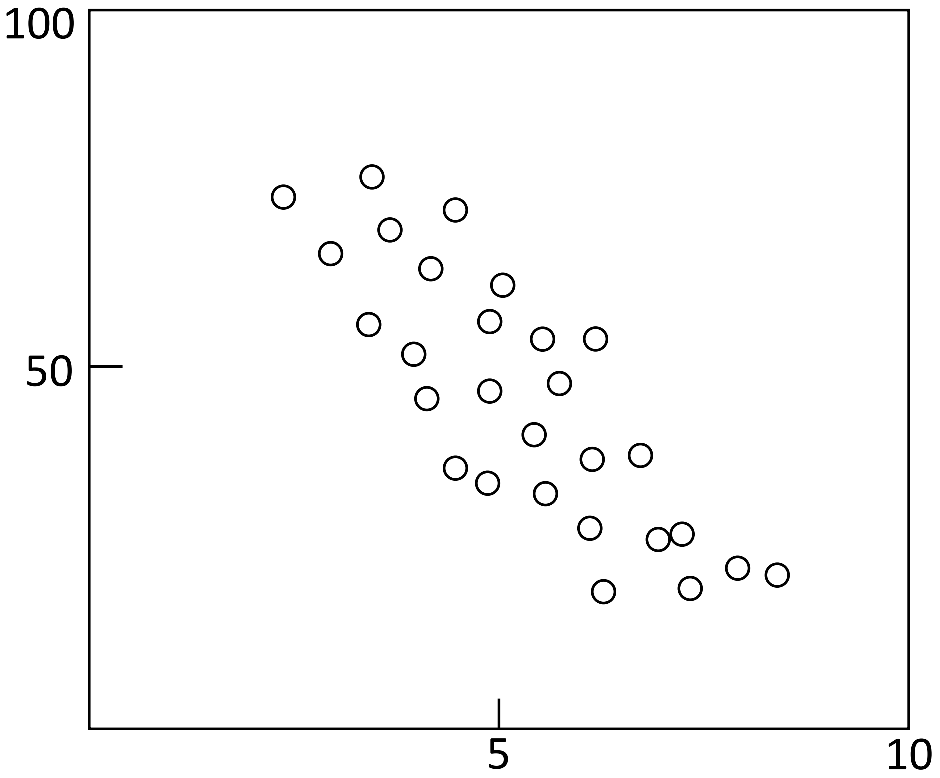
Interpreting Covariance

- **Example:** A 2-dimensional data set.
  - x: number of hours studied for a subject
  - y: marks obtained in that subject





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Interpreting Covariance

- A positive value of covariance indicates both dimensions increase or decrease together e.g. as the number of hours studied increases, the marks in that subject increase.

- A negative value indicates while one increases the other decreases, or vice-versa e.g. number of hours on facebook vs performance in CS dept.

- If covariance is zero: the two dimensions are independent of each other e.g. heights of students vs the marks obtained in a subject

Interpreting Covariance

Q. Why bother with calculating covariance when we could just plot the 2 values to see their relationship?

A. Covariance calculations are used to find relationships between dimensions in high dimensional data sets (usually greater than 3) where visualization is difficult.

each Image = vector
1 million pixels
1 million dimension

covariance between x & y

covariance between intensities at two locations in a image

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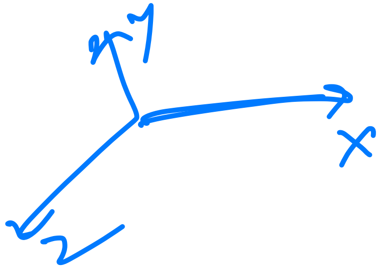
$A = (x, y, z)$



PCA

- Principal components analysis (PCA) is a technique that can be used to simplify a dataset

- It is a linear transformation that chooses a new coordinate system for the data set such that greatest variance by any projection of the data set comes to lie on the first axis (then called the first principal component), the second greatest variance on the second axis, and so on.

- PCA can be used for reducing dimensionality by eliminating the later principal components.

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PCA: Toy Example

- Consider following 3D points:

1	2	4	3	5	6
2	4	8	6	10	12
3	6	12	9	15	18

- Number of integers to be stored: 18

PCA: Toy Example

- How about the following representation?

$$\begin{bmatrix}1\\2\\3\end{bmatrix} = 1 * \begin{bmatrix}1\\2\\3\end{bmatrix} \qquad \begin{bmatrix}2\\4\\6\end{bmatrix} = 2 * \begin{bmatrix}1\\2\\3\end{bmatrix} \qquad \begin{bmatrix}4\\8\\12\end{bmatrix} = 4 * \begin{bmatrix}1\\2\\3\end{bmatrix}$$

$$\begin{bmatrix}3\\6\\9\end{bmatrix} = 3 * \begin{bmatrix}1\\2\\3\end{bmatrix} \qquad \begin{bmatrix}5\\10\\15\end{bmatrix} = 5 * \begin{bmatrix}1\\2\\3\end{bmatrix} \qquad \begin{bmatrix}6\\12\\18\end{bmatrix} = 6 * \begin{bmatrix}1\\2\\3\end{bmatrix}$$

- Number of integers to be stored: 9

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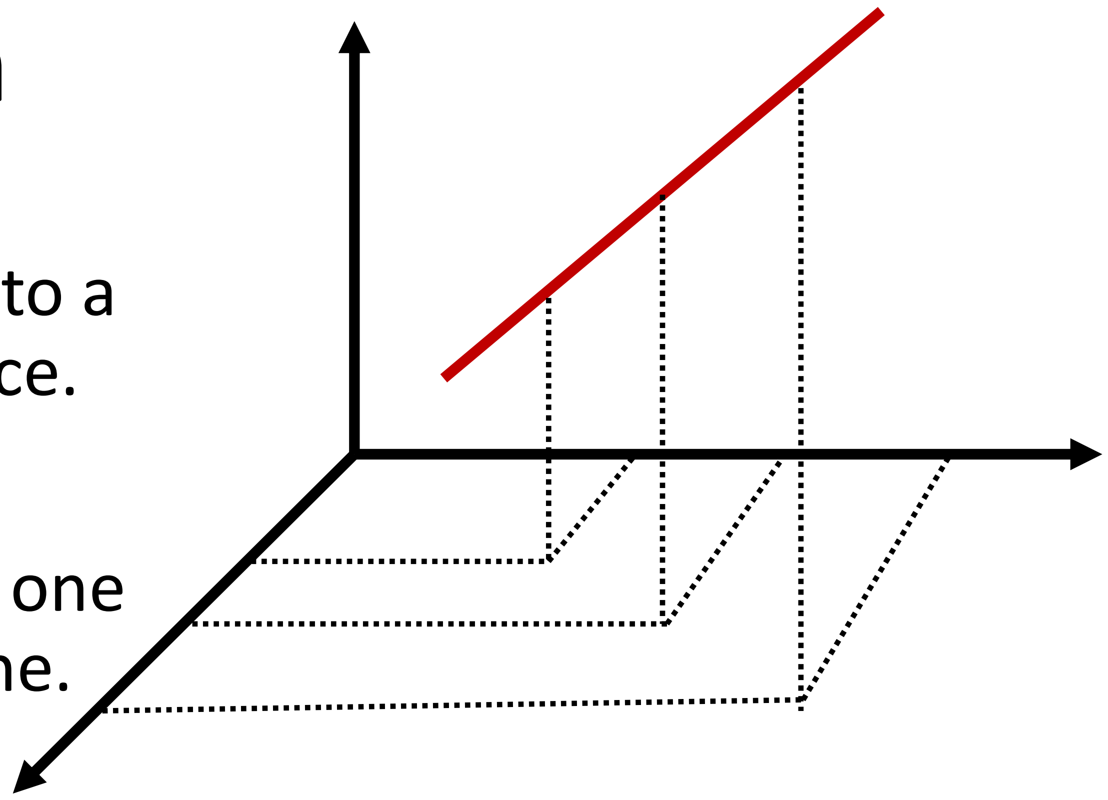
Geometrical Interpretation



- View each point in 3D space. But in this example, all the points happen to belong to a line: a 1D subspace of the original 3D space.
- Consider a new coordinate system where one of the axes is along the direction of the line.
- In this coordinate system, every point has only one non-zero coordinate.
- We only need to store the direction of the line (3 integers) and the non-zero coordinate for each of the 6 points (6 integers).

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Principal Component Analysis

- Given a set of points, how do we know if they can be compressed like in the previous example?

- The answer is to look into the covariance matrix

- The tool for doing this is called PCA

Principal Component Analysis

- By finding the eigenvalues and eigenvectors of the covariance matrix, we find that the eigenvectors with the largest eigenvalues correspond to the dimensions that have the largest variance in the dataset.
- This is the principal component.
- PCA is a useful statistical technique that has found applications in:
  - fields such as face recognition and image compression
  - finding patterns in data of high dimension.

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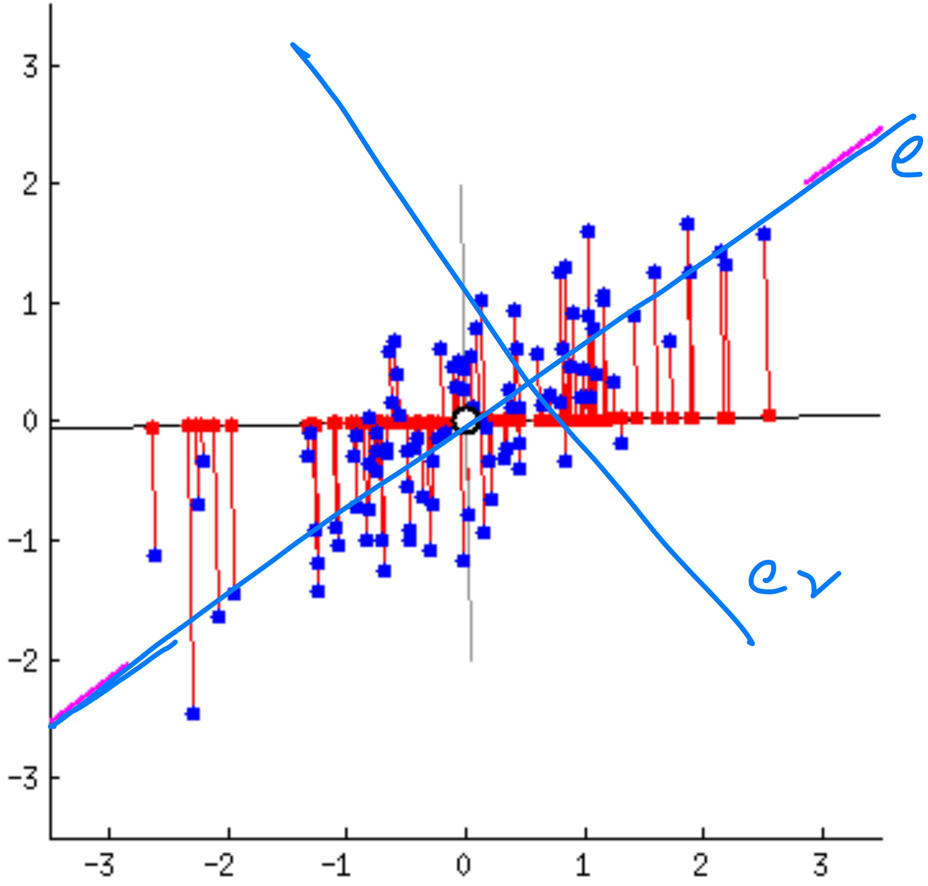
Principal Component Analysis



$x_i = a_1^i e_1 + a_2^i e_2$

small

million

10 vectors

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PCA Theorem

- Let $x_1, x_2, \ldots, x_n$ be a set of n, $d \times 1$ vectors and let $\bar{x}$ be their average:

x_i^T

$$x_i = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{id} \end{bmatrix} \qquad \bar{x} = \frac{1}{n}\sum_{i=1}^{i=n} \begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{id} \end{bmatrix}$$

d dimensional

$$\bar{x}_j = \bar{x}[j] = \frac{1}{n}\sum_{i=1}^{n} x_{ij}$$

- Let X be the $d \times n$ matrix with columns: $[x_1 - \bar{x} \quad x_2 - \bar{x} \quad \ldots \quad x_n - \bar{x}]$

d

$d \times n$

Covariance Matrix

- Let $Q = XX^T$ be the $d \times d$ covariance matrix:

$$Q = [x_1 - \bar{x} \quad x_2 - \bar{x} \quad \ldots \quad x_n - \bar{x}] \begin{bmatrix} (x_1 - \bar{x})^T \\ (x_2 - \bar{x})^T \\ \vdots \\ (x_n - \bar{x})^T \end{bmatrix}$$

- Also called **Scatter Matrix** in the context of PCA.

- Q is square as well as symmetric

- Q can be very large (in vision, d is often the number of pixels in an image!)

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PCA Theorem

Theorem:

Each x_j can be written as: $x_j = \bar{x} + \sum_{i=1}^{i=d} g_{ji} e_i$, where e_i are the d eigenvectors of Q with non-zero eigenvalues.

x_i $\hat{x}$

- The eigenvectors $e_1, e_2, \dots, e_d$ span an **eigenspace**.

- $e_1, e_2, \dots, e_d$ are $d \times 1$ orthonormal vectors.

- The scalars g_{ji} are the coordinates of x_j in the eigenspace:

$$g_{ji} = (x_j - \bar{x}).e_i$$

dot product

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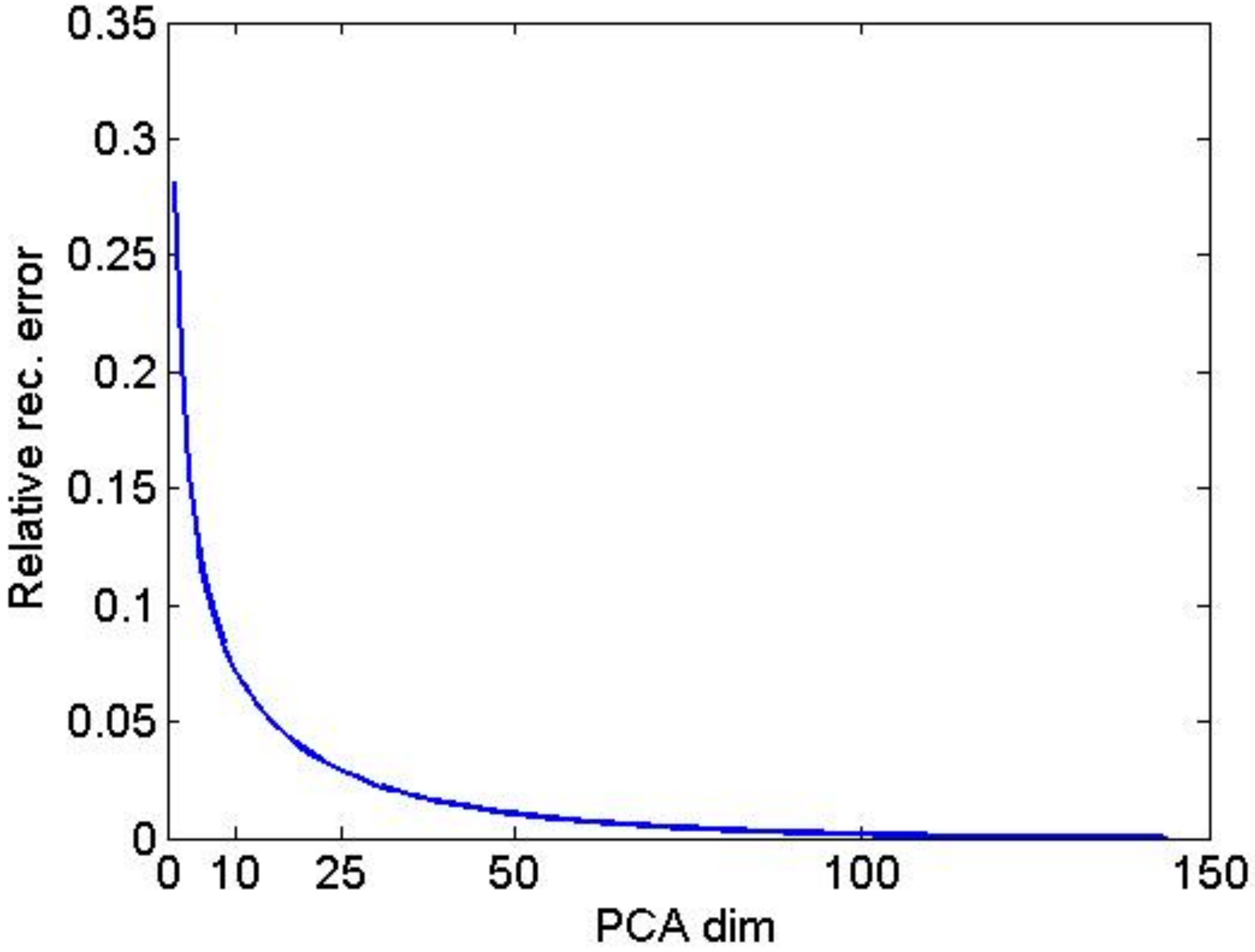
Using PCA to Compress Data

- Expressing x in terms of $e_1, \ldots e_d$ has not changed the size of the data
- If the points are highly correlated many of the coordinates of x will be zero or close to zero (if they indeed lie in a lower-dimensional linear subspace)
- Sort the eigenvectors e_i according to the their eigenvalue: $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_\mathrm{d}$
- Assuming $\lambda \approx 0, \text{if } i > k$: $x_j \approx \bar{x} + \sum_{i=1}^{i=k} g_{ji} e_i$

L_2 error and PCA dim



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PCA compression: 144D → 60D

Divide the image into a grid of 12X12 cells (144 dimensions) and represent each cell using PCA

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PCA compression: 144D → 16D

16

14400 x 16 + 16 x 144

eigenvector 16 x 144

14400

120 x 120

1440 x 1440

144 → 16

x_i

$a_1^i e_1 + a_2^i e_2 \cdots$

$a_{16}^i e_{16}$

$+ a_{144}^i e_{144}$

x_m

x_1

d

144

$\hat{x}_1$

x_i

x_i

$\frac{144}{16}$

e_i = 144 d

e_1 e_{16}

x_j = 144

$x_j = \sum c_i^j e_i$

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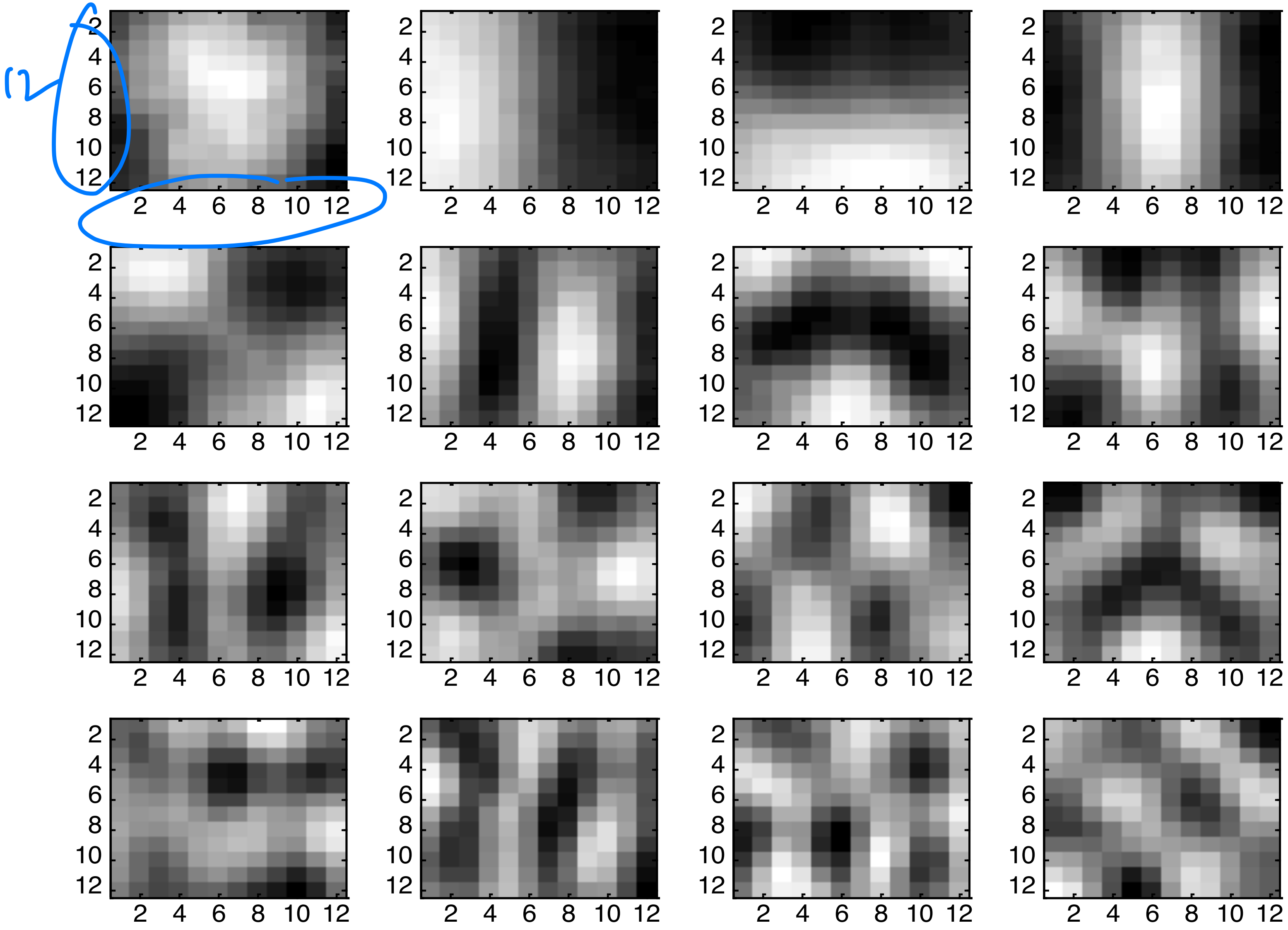
16 most important eigenvectors

x_i $[e_1 \quad e_{16}]$ $[c^i]$



16 eigenvectors

PCA compression: 144D → 6D

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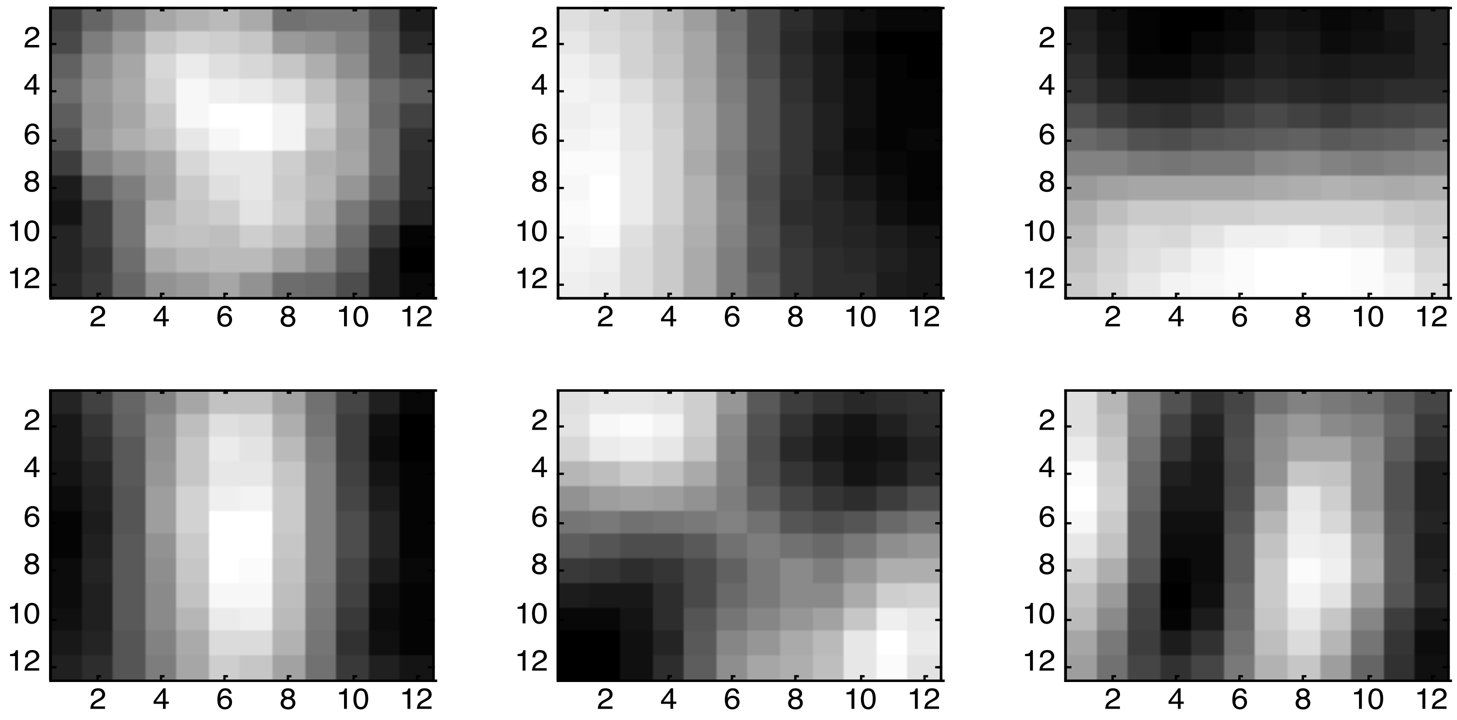
6 most important eigenvectors



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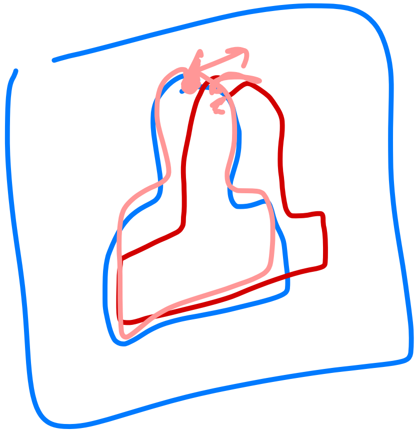
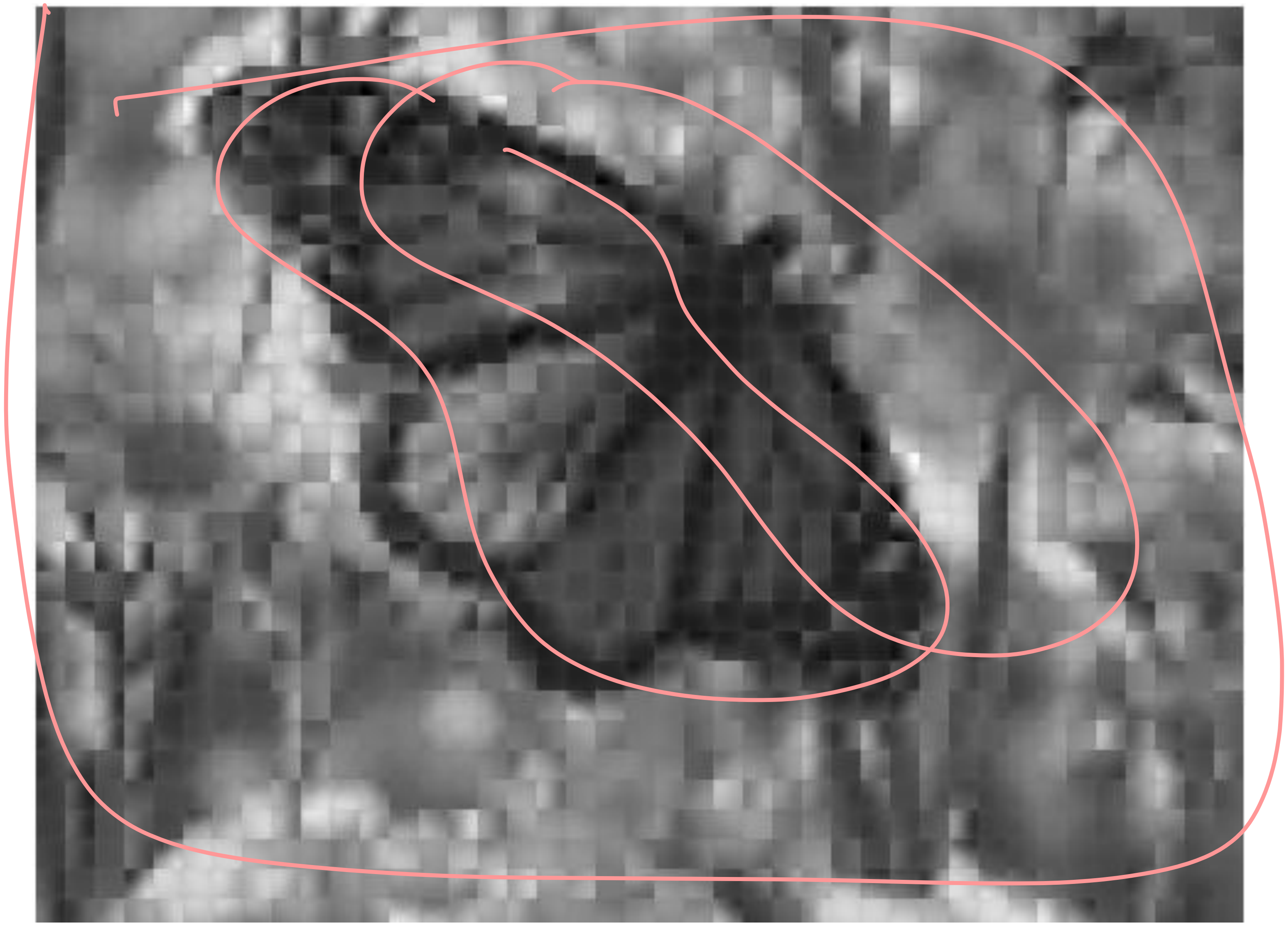
PCA compression: 144D → 3D





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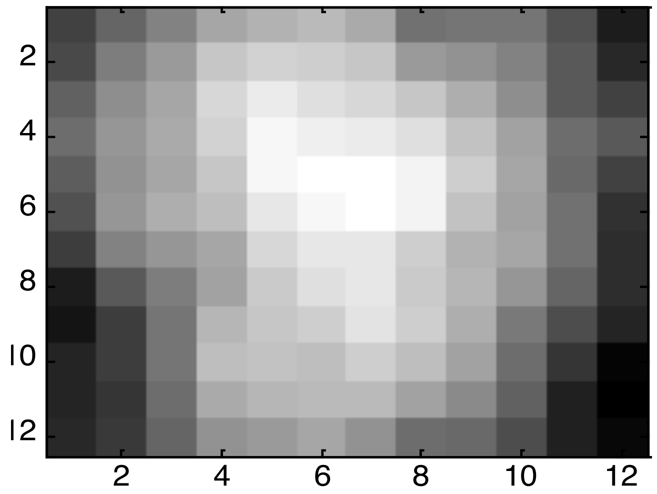
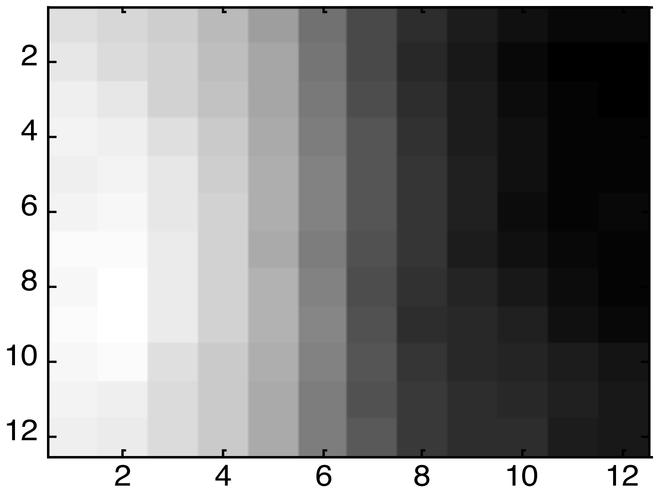
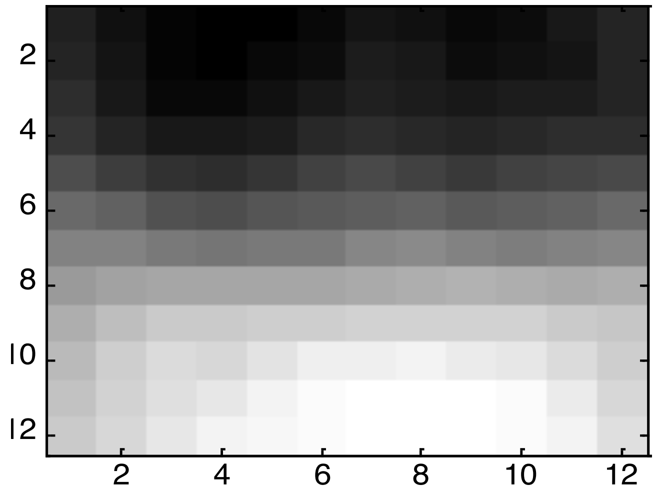
3 most important eigenvectors







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PCA compression: 144D → 1D