Dimensionality Reduction

Motivation

- Clustering
  - One way to summarize a complex real-valued data point with a single categorical variable
- Dimensionality reduction
  - Another way to simplify complex high-dimensional data
  - Summarize data with a lower dimensional real valued vector

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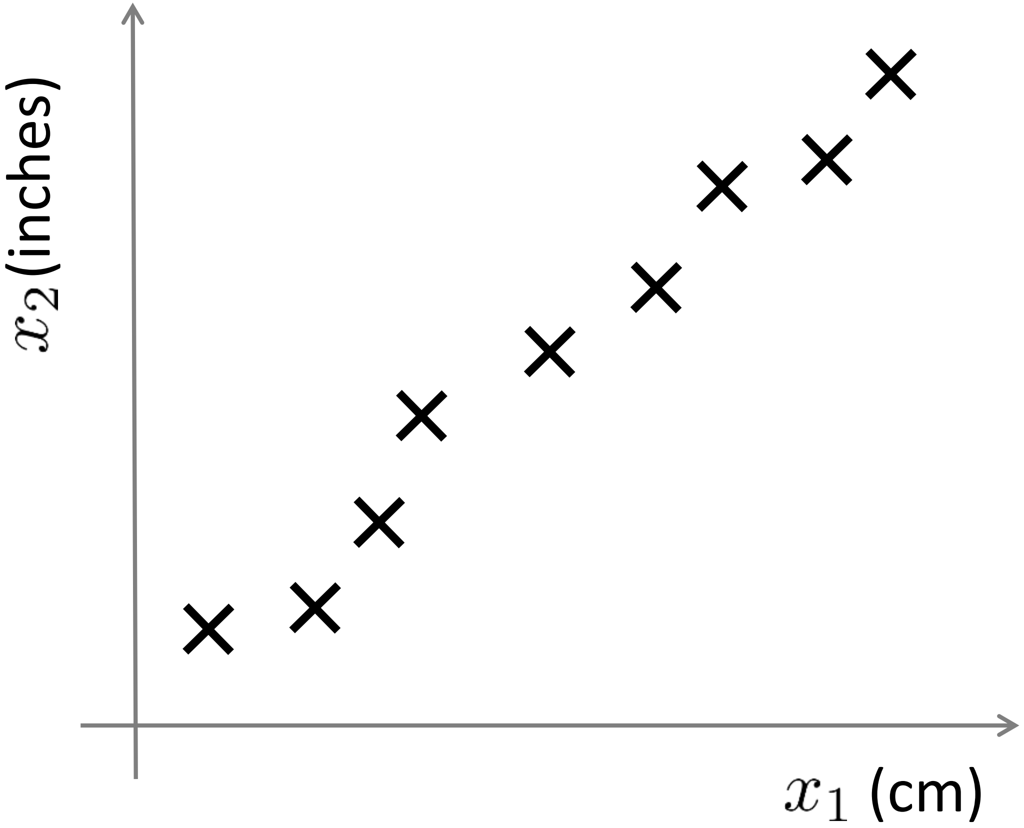
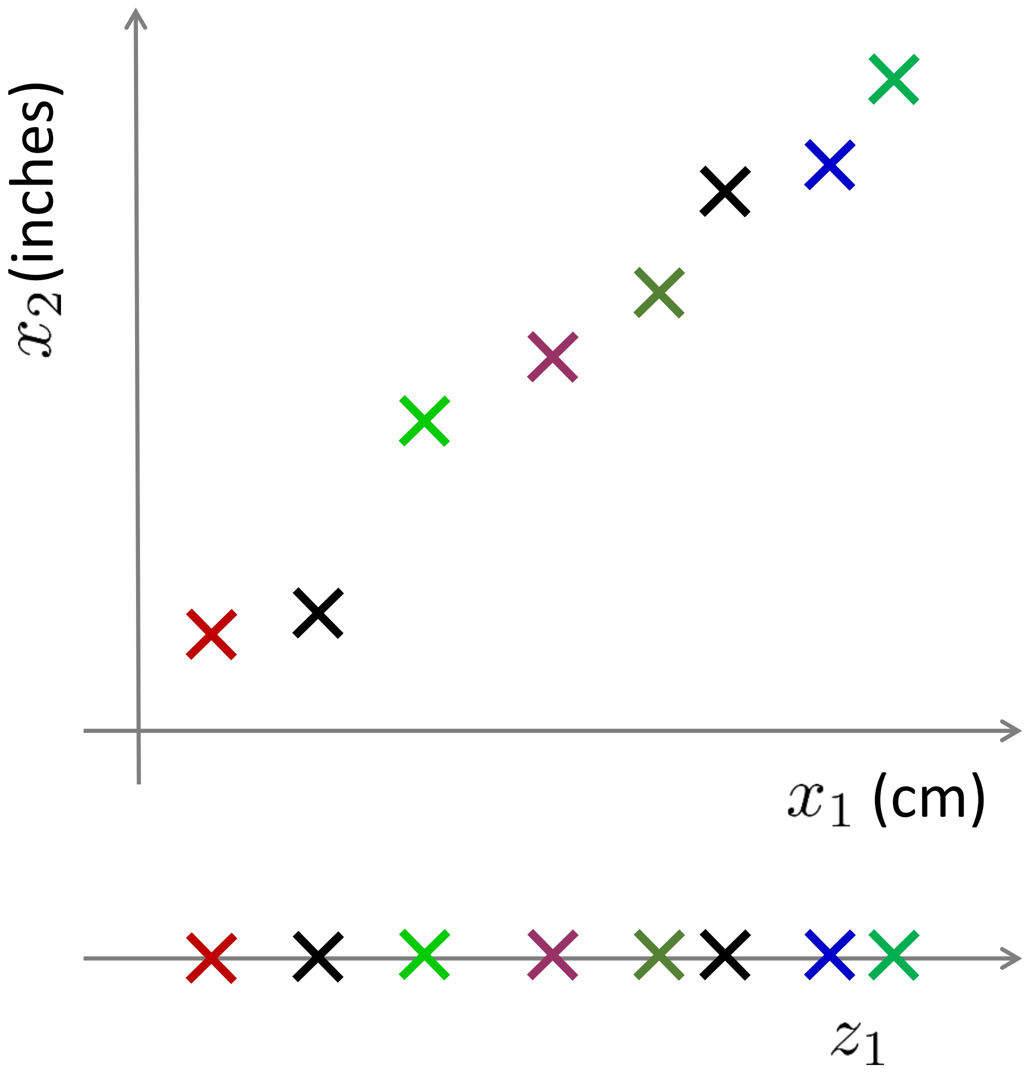
- Given data points in *d* dimensions
- Convert them to data points in *r*<*d* dimensions
- With minimal loss of information

Data Compression



Reduce data from
2D to 1D

Data Compression



Reduce data from 2D to 1D

$$x^{(1)} \rightarrow z^{(1)}$$
$$x^{(2)} \rightarrow z^{(2)}$$
$$\vdots$$
$$x^{(m)} \rightarrow z^{(m)}$$

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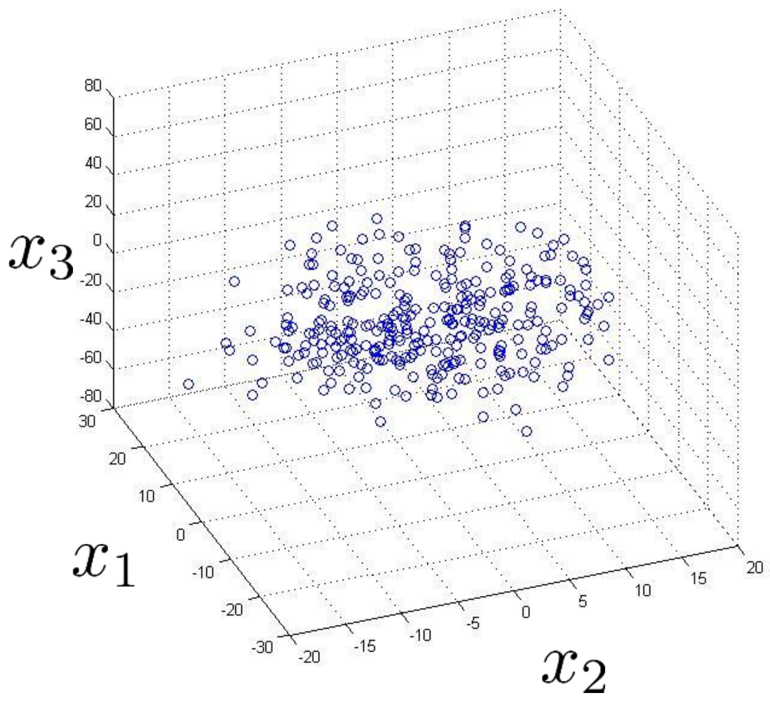
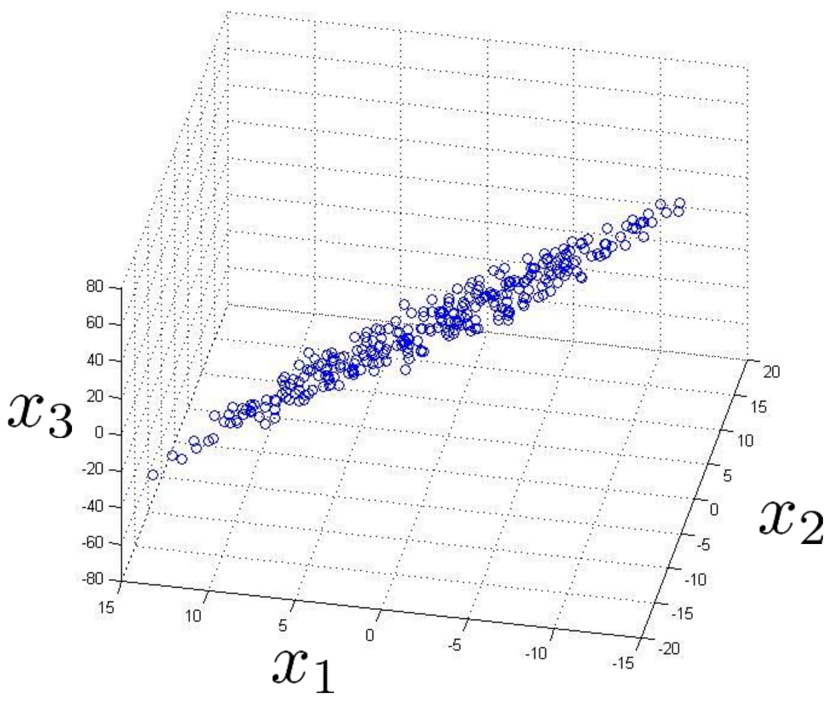
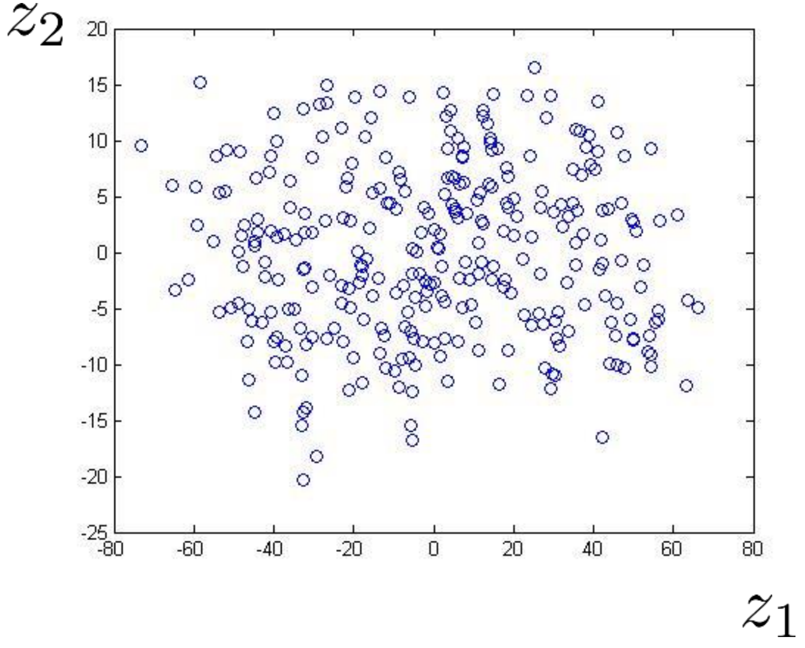
Data Compression

Reduce data from 3D to 2D







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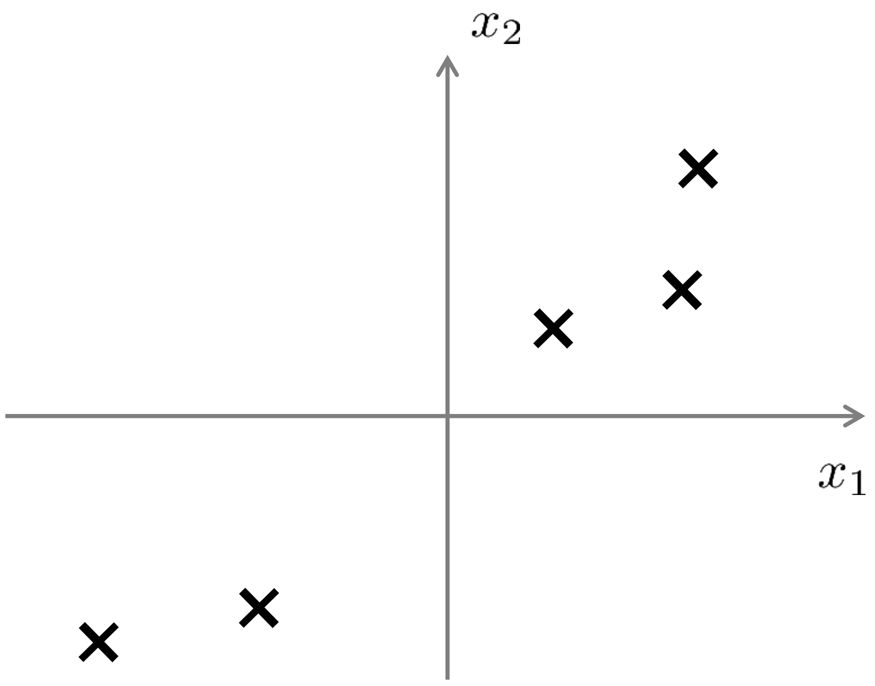
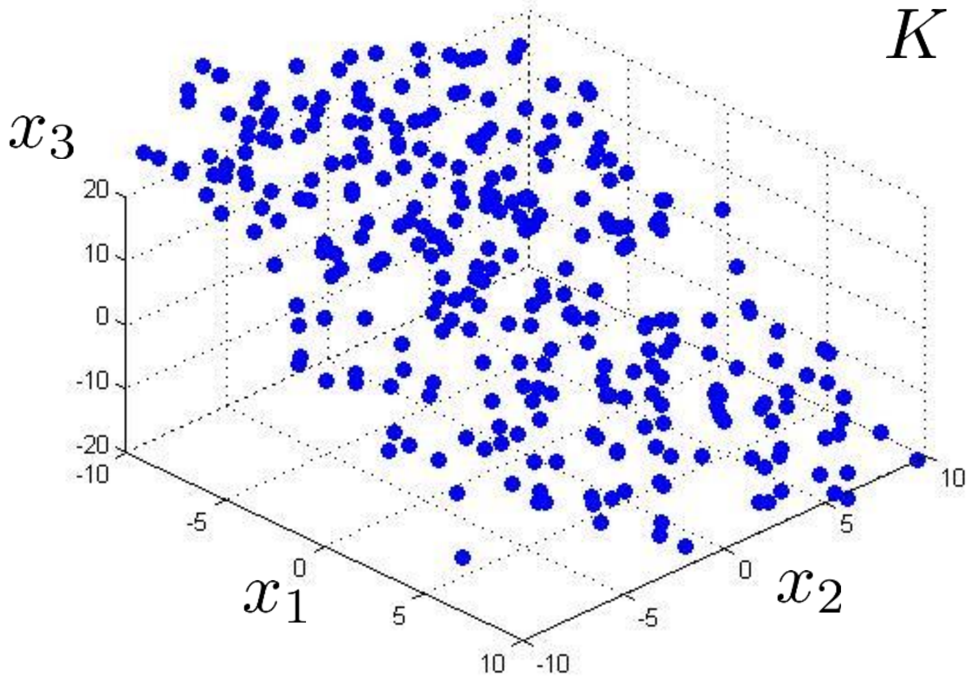
Principal Component Analysis (PCA) problem formulation

$$3D \to 2D$$
$$K = 2$$





Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.

Reduce from n-dimension to k-dimension: Find k vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error.

Principal Component Analysis

Goal: Find r-dim projection that best preserves variance

1. Compute mean vector μ and covariance matrix Σ of original points
2. Compute eigenvectors and eigenvalues of Σ
3. Select top r eigenvectors
4. Project points onto subspace spanned by them:

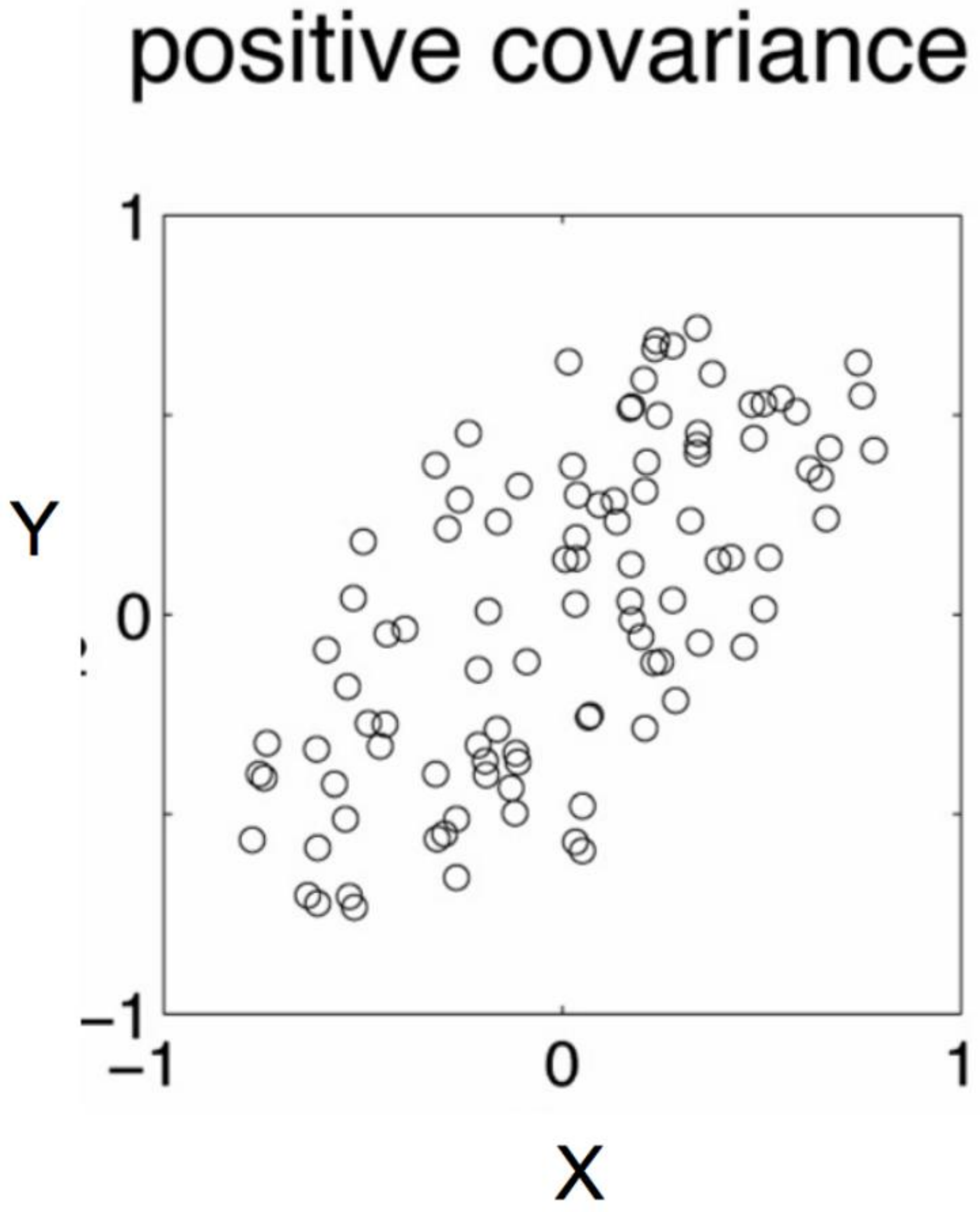
   $$y = A(x - \mu)$$

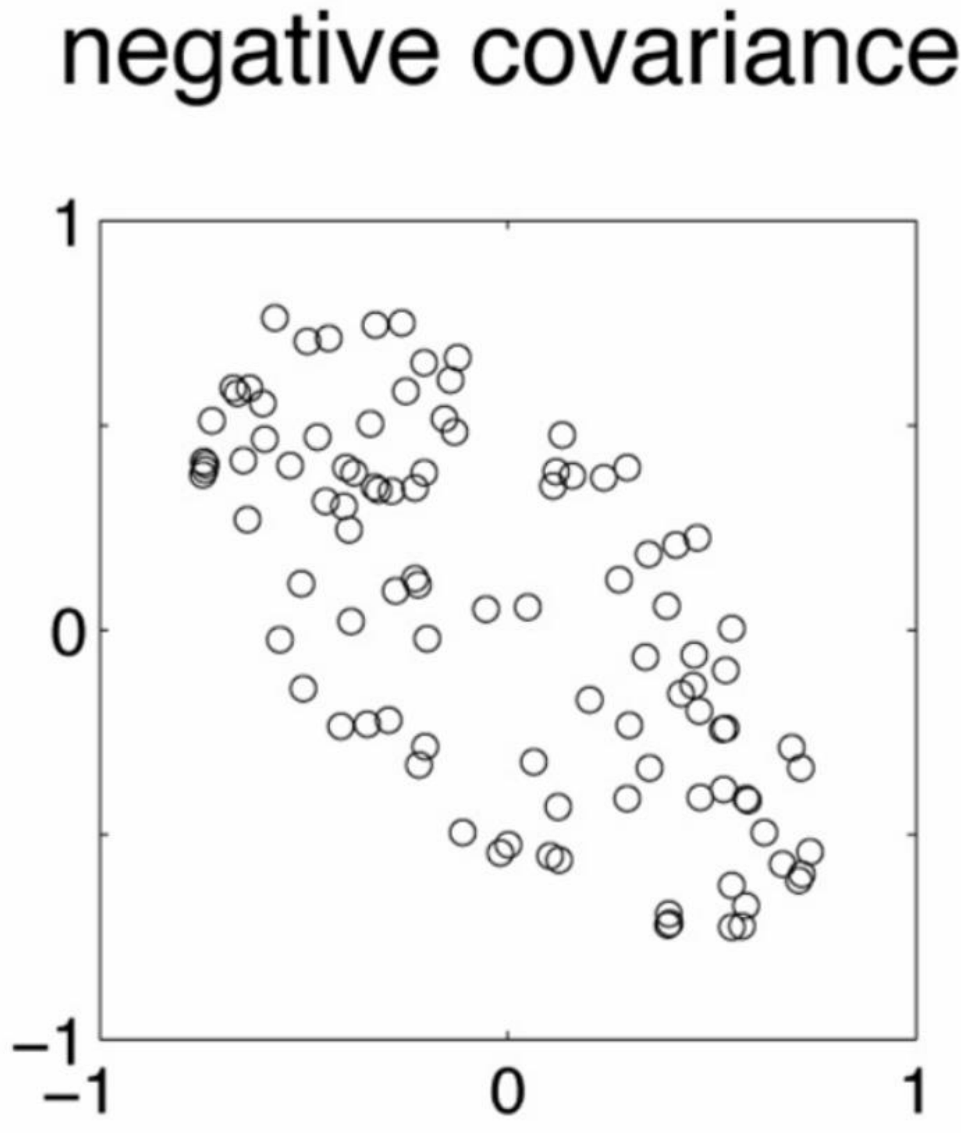
   where y is the new point, x is the old one, and the rows of A are the eigenvectors

Covariance

- Variance and Covariance:
  - Measure of the “spread” of a set of points around their center of mass(mean)
- Variance:
  - Measure of the deviation from the mean for points in one dimension
- Covariance:
  - Measure of how much each of the dimensions vary from the mean with **respect to each other**

- **Covariance is measured between two dimensions**
- **Covariance sees if there is a relation between two dimensions**
- **Covariance between one dimension is the variance**





Positive: Both dimensions increase or decrease together

Negative: While one increase the other decrease

Covariance

- Used to find relationships between dimensions in high dimensional data sets

$$q_{jk} = \frac{1}{N} \sum_{i=1}^{N} (X_{ij} - \underbrace{E(X_j)}_{\text{The Sample mean}})(X_{ik} - E(X_k))$$

Eigenvector and Eigenvalue

$Ax = \lambda x$

A: Square Matirx

λ: Eigenvector or characteristic vector

X: Eigenvalue or characteristic value

- ***The zero vector can not be an eigenvector***
- ***The value zero can be eigenvalue***

Eigenvector and Eigenvalue

Ax = λx

A: Square Matirx

λ: Eigenvector or characteristic vector

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Example

$$Show\ \ x = \begin{bmatrix} 2 \\ 1 \end{bmatrix} is\,an\,eigenvector\ for\ \ A = \begin{bmatrix} 2 & -4 \\ 3 & -6 \end{bmatrix}$$

$$Solution : Ax = \begin{bmatrix} 2 & -4 \\ 3 & -6 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$But\ \ for\ \ \lambda = 0,\ \ \lambda x = 0 \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$Thus, x\,is\,an\,eigenvector\,of\ A, and\,\lambda = 0\ is\,an\,eigenvalue.$$

Eigenvector and Eigenvalue

$Ax = \lambda x$ → $Ax - \lambda x = 0$

$(A - \lambda I)x = 0$

If we define a new matrix B: → $B = A - \lambda I$

$Bx = 0$

If B has an inverse: → $x = B^{-1}0 = 0$ ✗ **BUT! an eigenvector cannot be zero!!**

x will be an eigenvector of A if and only if B does not have an inverse, or equivalently det(B)=0 :

$$\boxed{\det(A - \lambda I) = 0}$$

Eigenvector and Eigenvalue

Example 1: Find the eigenvalues of

$$A = \begin{bmatrix} 2 & -12 \\ 1 & -5 \end{bmatrix}$$

$$|\lambda I - A| = \begin{vmatrix} \lambda - 2 & 12 \\ -1 & \lambda + 5 \end{vmatrix} = (\lambda - 2)(\lambda + 5) + 12$$

$$= \lambda^2 + 3\lambda + 2 = (\lambda + 1)(\lambda + 2)$$

two eigenvalues: –1, – 2

Note: The roots of the characteristic equation can be repeated. That is, $\lambda_1 = \lambda_2 = \ldots = \lambda_k$. If that happens, the eigenvalue is said to be of multiplicity k.

Example 2: Find the eigenvalues of

$$A = \begin{bmatrix} 2 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

$$|\lambda I - A| = \begin{vmatrix} \lambda - 2 & -1 & 0 \\ 0 & \lambda - 2 & 0 \\ 0 & 0 & \lambda - 2 \end{vmatrix} = (\lambda - 2)^3 = 0$$

λ = 2 is an eigenvector of multiplicity 3.

Principal Component Analysis

Input: $\mathbf{x} \in \mathbb{R}^D \colon\ \mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$

Set of basis vectors: $\mathbf{u}_1, \ldots, \mathbf{u}_K$

Summarize a *D* dimensional vector *X* with *K* dimensional feature vector *h(x)*

$$h(\mathbf{x}) = \begin{bmatrix} \mathbf{u}_1 \cdot \mathbf{x} \\ \mathbf{u}_2 \cdot \mathbf{x} \\ \cdots \\ \mathbf{u}_K \cdot \mathbf{x} \end{bmatrix}$$

Principal Component Analysis

$$\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_K]$$

Basis vectors are orthonormal

$$\mathbf{u}_i^T \mathbf{u}_j = 0$$
$$||\mathbf{u}_j|| = 1$$

New data representation *h(x)*

$$z_j = \mathbf{u}_j \cdot \mathbf{x}$$
$$h(\mathbf{x}) = [z_1, \ldots, z_K]^T$$

Principal Component Analysis

$$\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_K]$$

New data representation *h(x)*

$$h(\mathbf{x}) = \mathbf{U}^T \mathbf{x}$$

$$h(\mathbf{x}) = \mathbf{U}^T (\mathbf{x} - \mu_0)$$

Empirical mean of the data

$$\mu_0 = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_i$$

The space of all face images

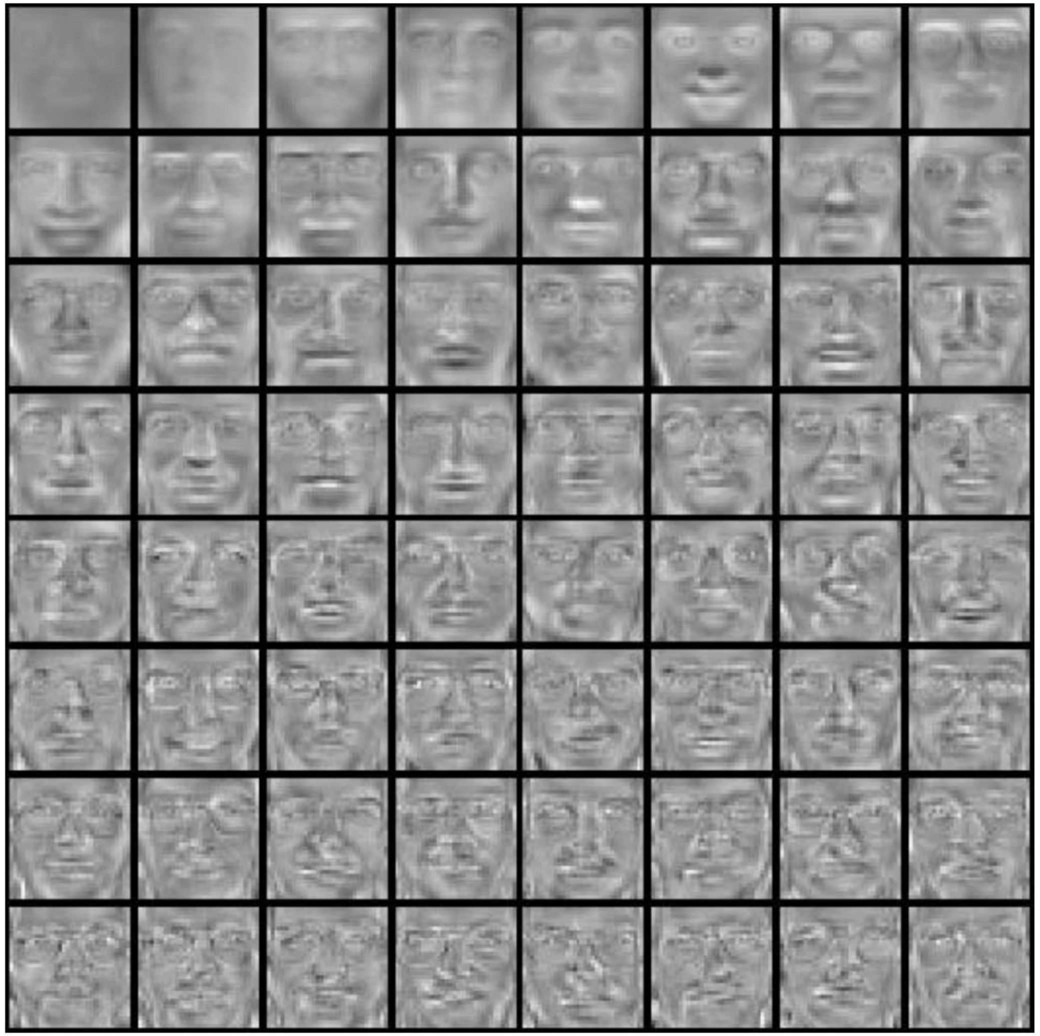
- When viewed as vectors of pixel values, face images are extremely high-dimensional
  - 100x100 image = 10,000 dimensions
  - Slow and lots of storage
- But very few 10,000-dimensional vectors are valid face images
- We want to effectively model the subspace of face images

slide by Derek Hoiem

Eigenfaces example

Top eigenvectors: $u_1, \ldots u_k$

Mean: μ



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Representation and reconstruction

- Face **x** in "face space" coordinates:

$$\mathbf{x} \rightarrow [\mathbf{u}_1^{\mathrm{T}}(\mathbf{x} - \mu), \ldots, \mathbf{u}_k^{\mathrm{T}}(\mathbf{x} - \mu)]$$
$$= \quad w_1, \ldots, w_k$$

- Reconstruction:

$$\hat{x} \quad = \quad \mu \quad + \quad w_1u_1+w_2u_2+w_3u_3+w_4u_4+ \ldots$$

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Reconstruction

P = 4

P = 200

P = 400

After computing eigenfaces using 400 face images from ORL face database

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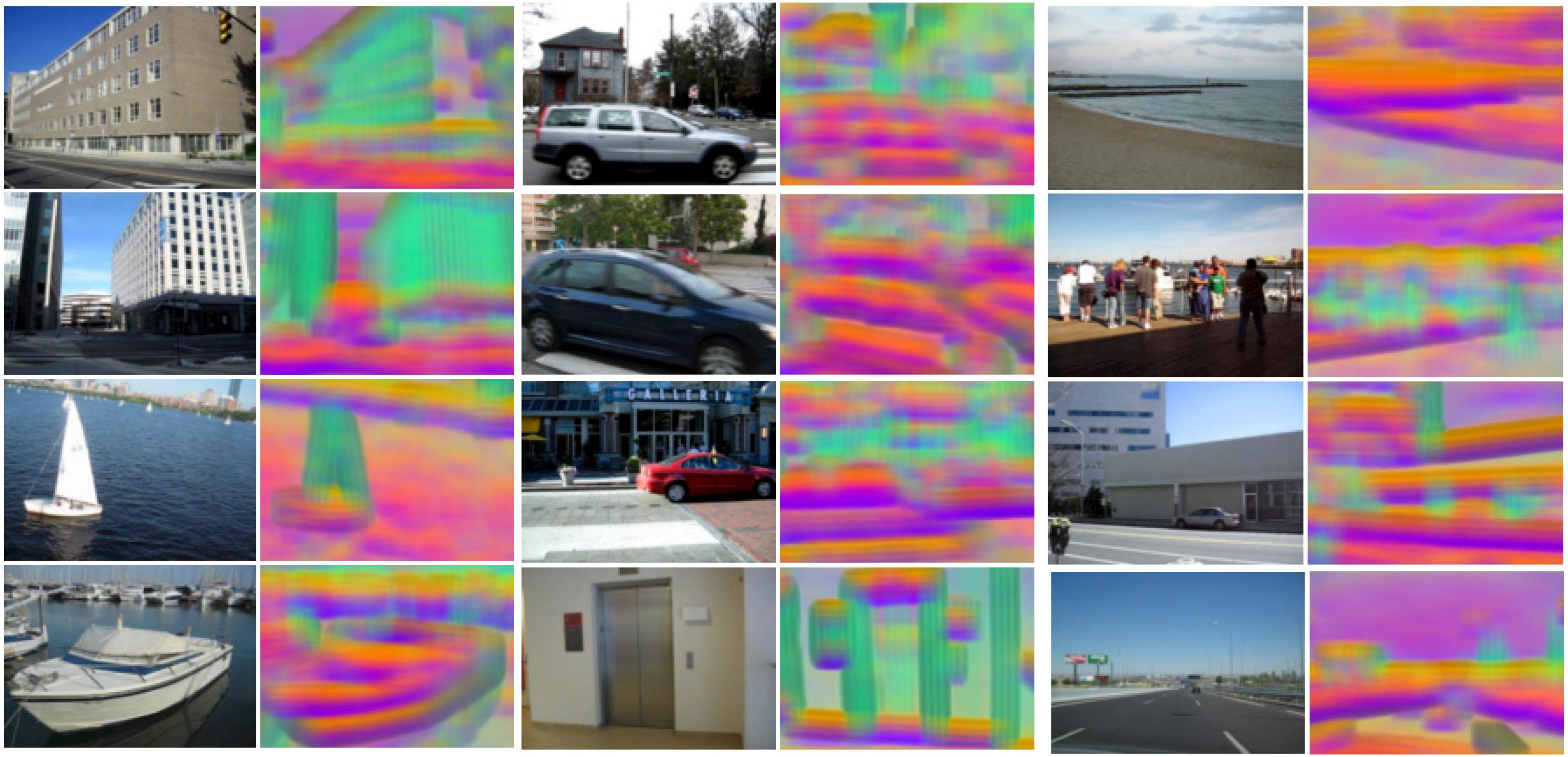
SIFT feature visualization



- The top three principal components of SIFT descriptors from a set of images are computed
- Map these principal components to the principal components of the RGB space
- pixels with similar colors share similar structures

Application: Image compression

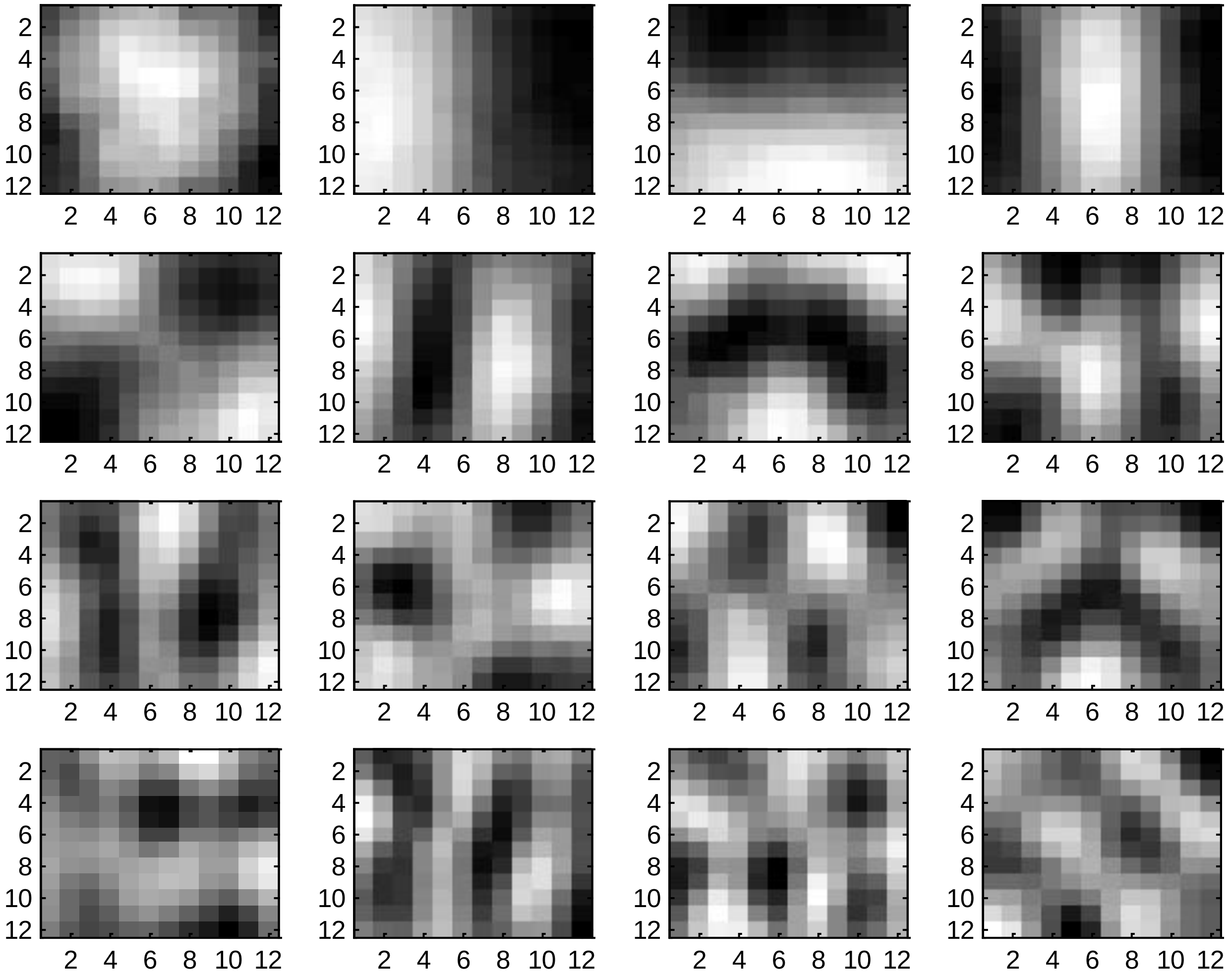
Original Image

- Divide the original 372x492 image into patches:
  - Each patch is an instance that contains 12x12 pixels on a grid
- View each as a 144-D vector

PCA compression: 144D → 60D

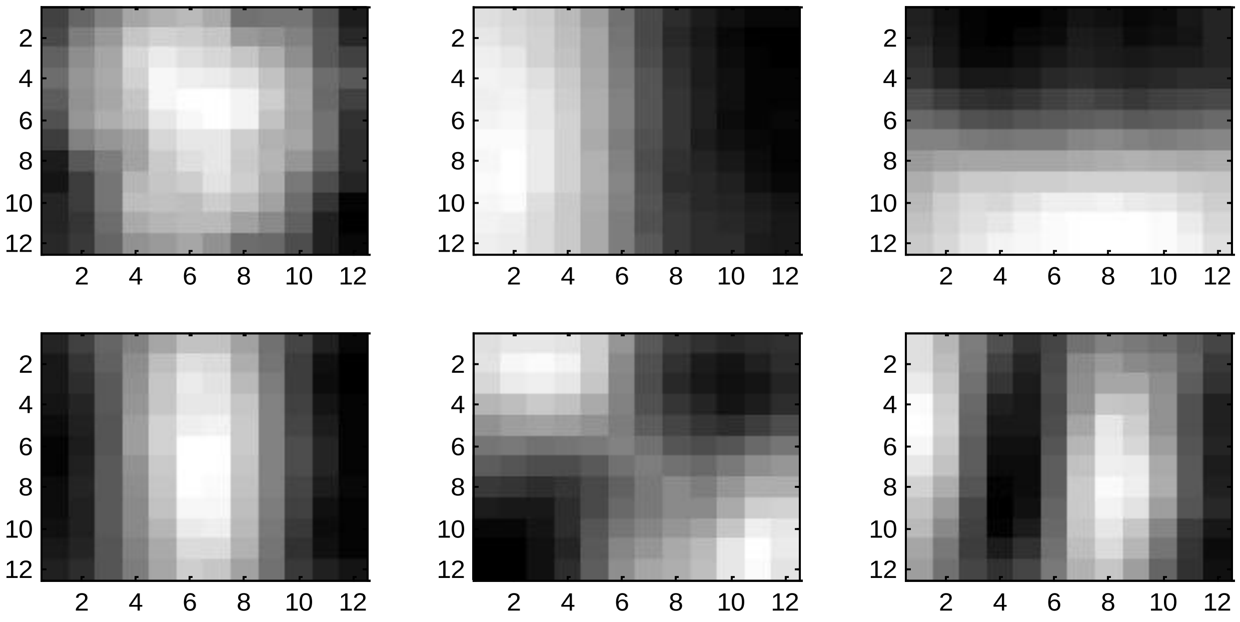
PCA compression: 144D → 16D

16 most important eigenvectors



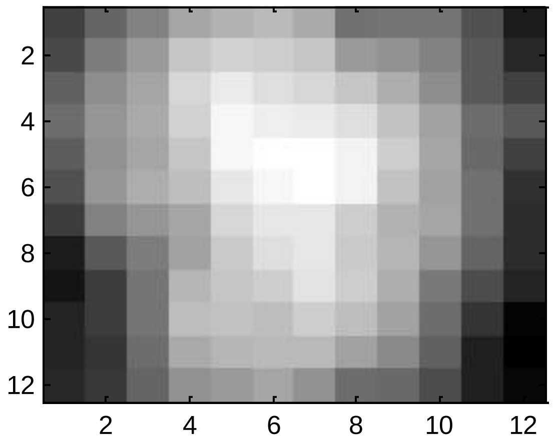
PCA compression: 144D) 6D

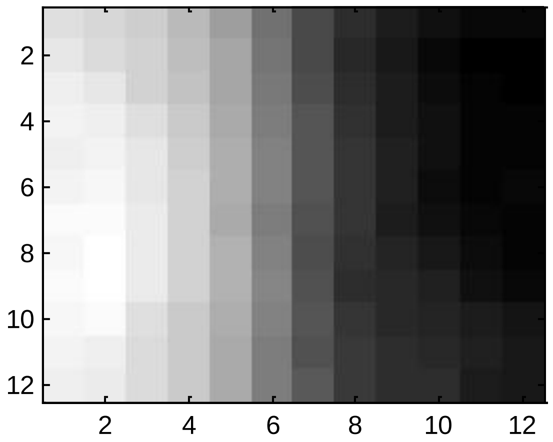
6 most important eigenvectors

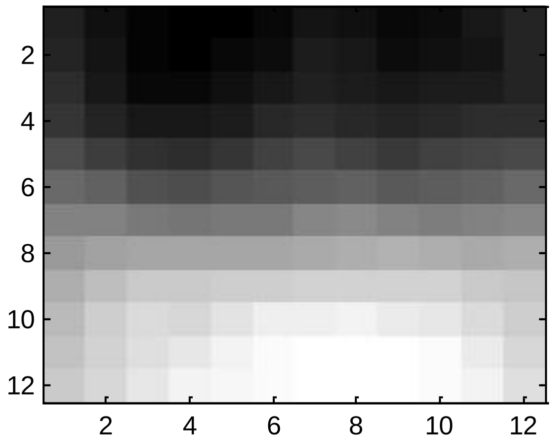


PCA compression: 144D → 3D

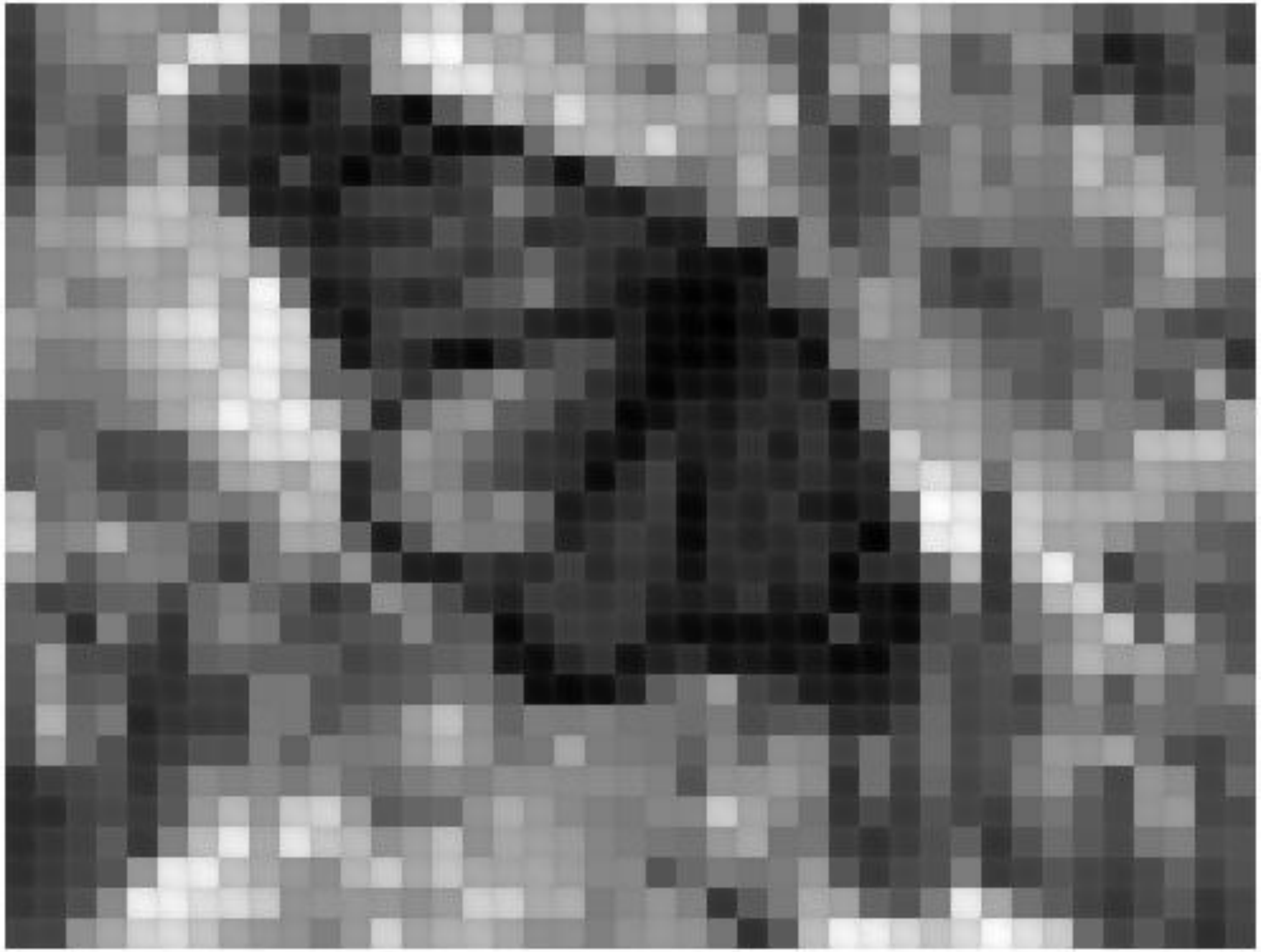
3 most important eigenvectors



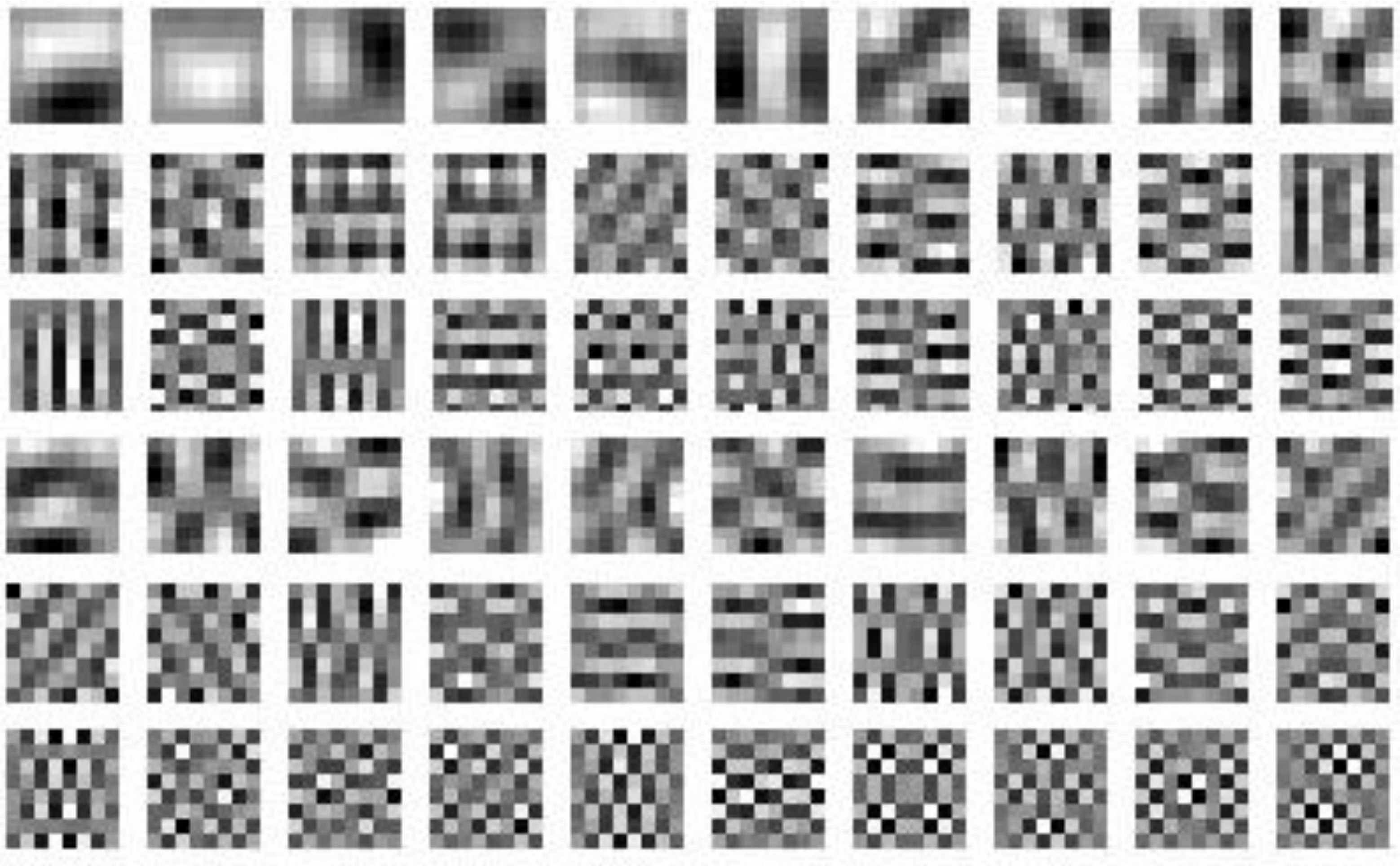




PCA compression: 144D → 1D

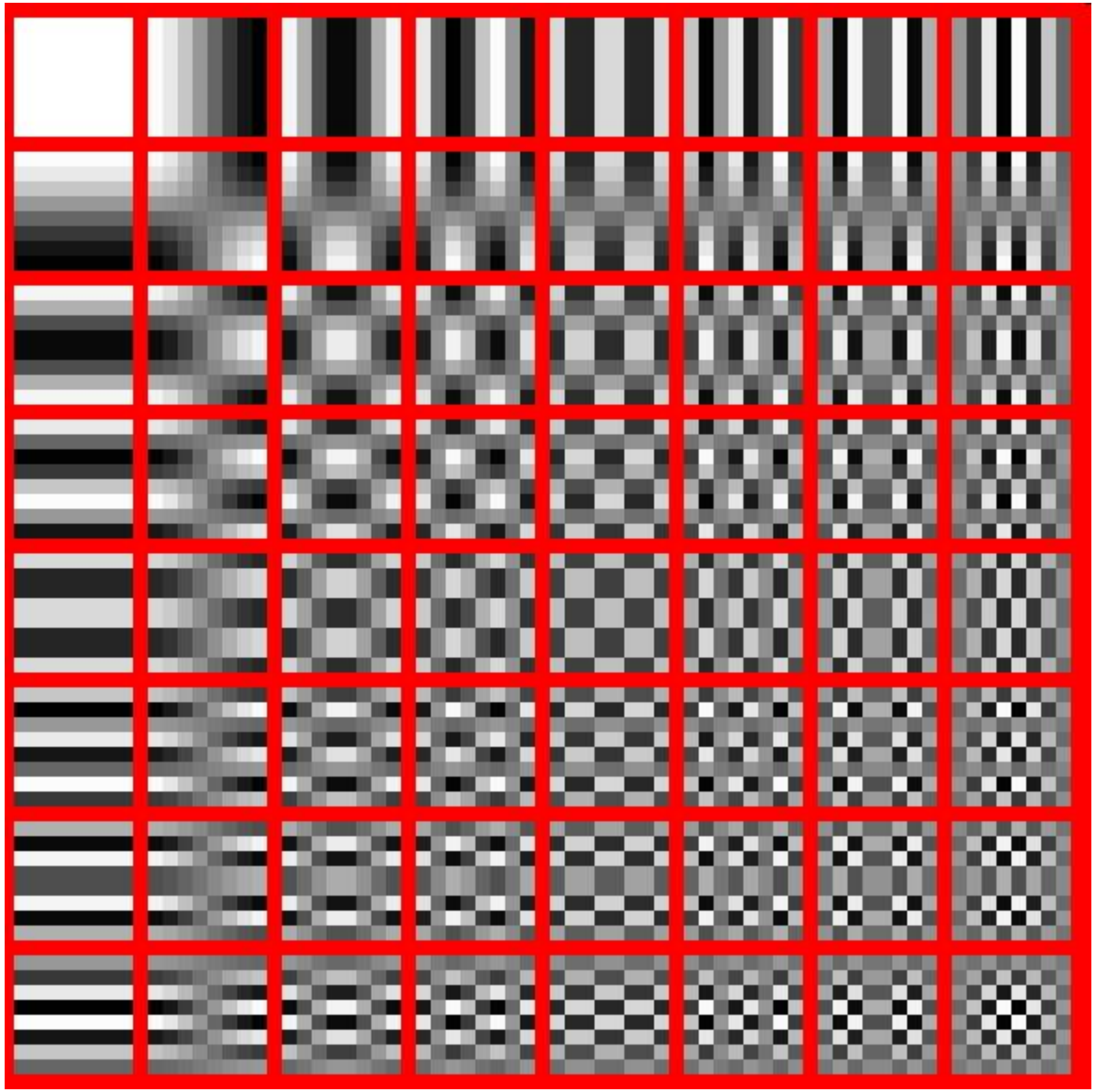


60 most important eigenvectors



Looks like the discrete cosine bases of JPG!...

2D Discrete Cosine Basis



http://en.wikipedia.org/wiki/Discrete_cosine_transform

Dimensionality reduction

- PCA (Principal Component Analysis):
  - Find projection that maximize the variance
- ICA (Independent Component Analysis):
  - Very similar to PCA except that it assumes non-Guassian features
- Multidimensional Scaling:
  - Find projection that best preserves inter-point distances
- LDA(Linear Discriminant Analysis):
  - Maximizing the component axes for class-separation
- …
- …