《模式识别》

第三章 主成分分析

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课程目录（暂定）

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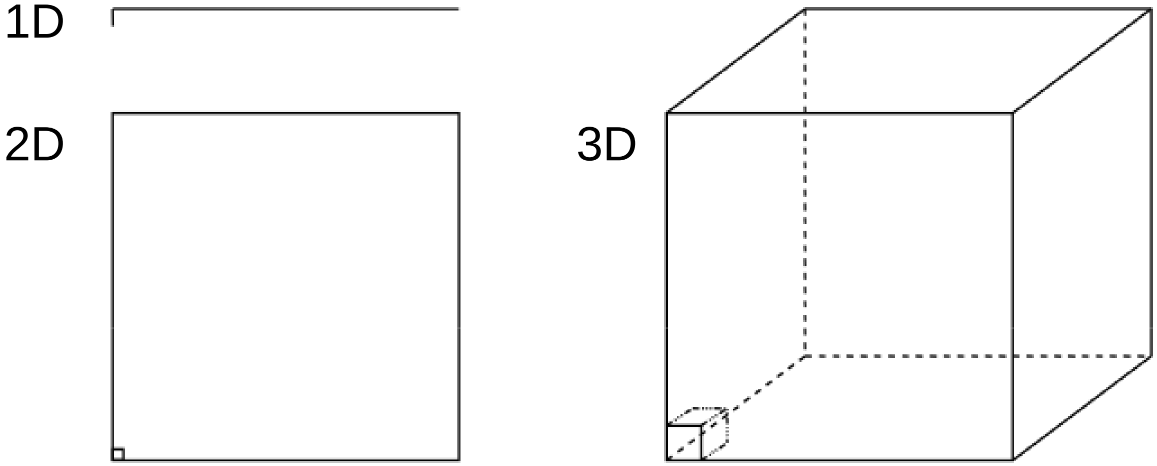
Recap: Curse of dimensionality

- Assume 5000 points uniformly distributed in the unit hypercube and we want to apply 5-NN. Suppose our query point is at the origin.
  - *In 1-dimension, we must go a distance of* $5/5000 = 0.001$ *on the average to capture 5 nearest neighbors.*
  - *In 2 dimensions, we must go* $\sqrt{0.001}$ *to get a square that contains 0.001 of the volume.*
  - *In d dimensions, we must go* $(0.001)^{1/d}$*.*



What we will learn today

- Singular value decomposition
- Principal Component Analysis (PCA)
- Image compression

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Singular Value Decomposition (SVD)

- There are several computer algorithms that can “factorize” a matrix, representing it as the product of some other matrices.
- The most useful of these is the Singular Value Decomposition.
- Represents any matrix A as a product of three matrices: $U\Sigma V^T$.
- Python command:
    - *[U,S,V]= numpy.linalg.svd(A)*

Singular Value Decomposition (SVD)

$$\boldsymbol{U\Sigma V^T = A}$$

- *Where $\boldsymbol{U}$ and $\boldsymbol{V}$ are rotation matrices, and $\boldsymbol{\Sigma}$ is a scaling matrix. For example:*

$$\begin{array}{ccccccc} U & & \Sigma & & V^T & & A \\ \begin{bmatrix}-.40 & .916\\ .916 & .40\end{bmatrix} & \times & \begin{bmatrix}5.39 & 0\\ 0 & 3.154\end{bmatrix} & \times & \begin{bmatrix}-.05 & .999\\ .999 & .05\end{bmatrix} & = & \begin{bmatrix}3 & -2\\ 1 & 5\end{bmatrix}\end{array}$$

https://en.wikipedia.org/wiki/Rotation_matrix

Singular Value Decomposition (SVD)

- Beyond 2 × 2 matrices:
  - *In general, if $\boldsymbol{A}$ is $m \times n$, then $\boldsymbol{U}$ will be $m \times m$, $\boldsymbol{\Sigma}$ will be $m \times n$, and $\boldsymbol{V^T}$ will be $n \times n$.*
  - *(Note the dimensions work out to produce $m \times n$ after multiplication)*

$$\overset{U}{\begin{bmatrix} -.39 & -.92 \\ -.92 & .39 \end{bmatrix}} \times \overset{\Sigma}{\begin{bmatrix} 9.51 & 0 & 0 \\ 0 & .77 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} = \overset{A}{\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}}$$

Singular Value Decomposition (SVD)

- $\boldsymbol{U}$ and $\boldsymbol{V}$ are always rotation matrices.
  - *Geometric rotation may not be an applicable concept, depending on the matrix. So we call them “unitary” matrices – each column is a unit vector.*
- $\boldsymbol{\Sigma}$ is a diagonal matrix
  - *The number of nonzero entries = rank of* **A**
  - *The algorithm always sorts the entries high to low*

$$\overset{U}{\begin{bmatrix} -.39 & -.92 \\ -.92 & .39 \end{bmatrix}} \times \overset{\Sigma}{\begin{bmatrix} 9.51 & 0 & 0 \\ 0 & .77 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} = \overset{A}{\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}}$$

SVD Applications

- We’ve discussed SVD in terms of geometric transformation matrices.
- But SVD of an image matrix can also be very useful.
- To understand this, we’ll look at a less geometric interpretation of what SVD is doing.

SVD Applications

$$\overset{U}{\begin{bmatrix} -.39 & -.92 \\ -.92 & .39 \end{bmatrix}} \times \overset{\Sigma}{\begin{bmatrix} 9.51 & 0 & 0 \\ 0 & .77 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} = \overset{A}{\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}}$$

- Look at how the multiplication works out, left to right:
- Column 1 of $\boldsymbol{U}$ gets scaled by the first value from $\boldsymbol{\Sigma}$.

$$\overset{U\Sigma}{\begin{bmatrix} -3.67 & -.71 & 0 \\ -8.8 & .30 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} \qquad \overset{A_{partial}}{\begin{bmatrix} 1.6 & 2.1 & 2.6 \\ 3.8 & 5.0 & 6.2 \end{bmatrix}}$$

- The resulting vector gets scaled by row 1 of $\boldsymbol{V^T}$ to produce a contribution to the columns of $\boldsymbol{A}$.

SVD Applications

$$\overset{U\Sigma}{\begin{bmatrix}-3.67 & -.71 & 0\\ -8.8 & .30 & 0\end{bmatrix}} \times \overset{V^T}{\begin{bmatrix}-.42 & -.57 & -.70\\ .81 & .11 & -.58\\ .41 & -.82 & .41\end{bmatrix}} \qquad \overset{A_{partial}}{\begin{bmatrix}1.6 & 2.1 & 2.6\\ 3.8 & 5.0 & 6.2\end{bmatrix}}$$

$$+ \quad \overset{U\Sigma}{\begin{bmatrix}-3.67 & -.71 & 0\\ -8.8 & .30 & 0\end{bmatrix}} \times \overset{V^T}{\begin{bmatrix}-.42 & -.57 & -.70\\ .81 & .11 & -.58\\ .41 & -.82 & .41\end{bmatrix}} \qquad \overset{A_{partial}}{\begin{bmatrix}-.6 & -.1 & .4\\ .2 & 0 & -.2\end{bmatrix}}$$

$$= \qquad \begin{bmatrix}1 & 2 & 3\\ 4 & 5 & 6\end{bmatrix}$$

- Each product of (*column i of* $\boldsymbol{U}$)·(*value i from* $\boldsymbol{\Sigma}$)·(*row i of* $\boldsymbol{V^T}$) produces a component of the final $\boldsymbol{A}$.

SVD Applications

$$\overset{U\Sigma}{\begin{bmatrix} -3.67 & -.71 & 0 \\ -8.8 & .30 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} \qquad \overset{A_{partial}}{\begin{bmatrix} 1.6 & 2.1 & 2.6 \\ 3.8 & 5.0 & 6.2 \end{bmatrix}}$$

$$\overset{A}{\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}}$$

$$\overset{U\Sigma}{\begin{bmatrix} -3.67 & -.71 & 0 \\ -8.8 & .30 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} \qquad \overset{A_{partial}}{\begin{bmatrix} -.6 & -.1 & .4 \\ .2 & 0 & -.2 \end{bmatrix}}$$

- We're building $\boldsymbol{A}$ as a linear combination of the columns of $\boldsymbol{U}$.
- Using all columns of $\boldsymbol{U}$, we'll rebuild the original matrix perfectly.
- But, in real-world data, often we can just use the first few columns of $\boldsymbol{U}$ and we'll get something close (e.g. the first $\boldsymbol{A_{partial}}$, above).

SVD Applications

$$\overset{U\Sigma}{\begin{bmatrix} -3.67 & -.71 & 0 \\ -8.8 & .30 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} \qquad \overset{A_{partial}}{\begin{bmatrix} 1.6 & 2.1 & 2.6 \\ 3.8 & 5.0 & 6.2 \end{bmatrix}}$$

$$\overset{A}{\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}}$$

$$\overset{U\Sigma}{\begin{bmatrix} -3.67 & -.71 & 0 \\ -8.8 & .30 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} \qquad \overset{A_{partial}}{\begin{bmatrix} -.6 & -.1 & .4 \\ .2 & 0 & -.2 \end{bmatrix}}$$

- We can call those first few columns of $\boldsymbol{U}$ the *Principal Components* of the data.
- They show the major patterns that can be added to produce the columns of the original matrix.
- The rows of $\boldsymbol{V^T}$ show how the *principal components* are mixed to produce the columns of the matrix.

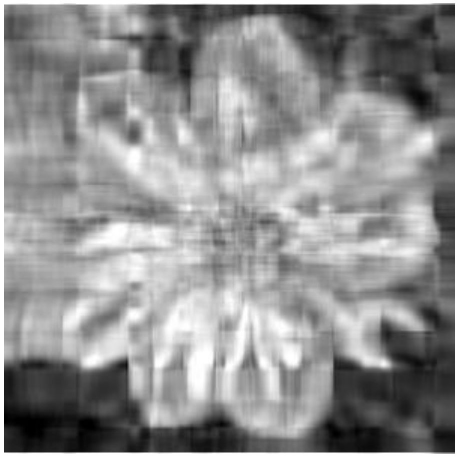
SVD Applications

$$\overset{U}{\begin{bmatrix} -.39 & -.92 \\ -.92 & .39 \end{bmatrix}} \times \overset{\Sigma}{\begin{bmatrix} 9.51 & 0 & 0 \\ 0 & .77 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} = \overset{A}{\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}}$$

We can look at $\boldsymbol{\Sigma}$ *to see that the first column has a large effect*

while the second column has a much smaller effect in this example

SVD Applications



- *For this image, using* **only the first 10** *of 300 principal components produces a recognizable reconstruction.*
- *So, SVD can be used for image compression.*

SVD for symmetric matrices

- If A is a symmetric matrix, it can be decomposed as the following:

$$A = \Phi\Sigma\Phi^T$$

- Compared to a traditional SVD decomposition, $U = V^T$ and is an orthogonal matrix.

Principal Component Analysis

$$\begin{array}{c} U\Sigma \\ \begin{bmatrix} -3.67 & -.71 & 0 \\ -8.8 & .30 & 0 \end{bmatrix} \end{array} \times \begin{array}{c} V^T \\ \begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix} \end{array} \qquad \begin{array}{c} A_{partial} \\ \begin{bmatrix} 1.6 & 2.1 & 2.6 \\ 3.8 & 5.0 & 6.2 \end{bmatrix} \end{array}$$

- Remember, columns of $\boldsymbol{U}$ are the *Principal Components* of the data: the major patterns that can be added to produce the columns of the original matrix.
- One use of this is to construct a matrix where each column is a separate data sample.
- Run SVD on that matrix, and look at the first few columns of $\boldsymbol{U}$ to see patterns that are common among the columns.
- This is called *Principal Component Analysis* (or PCA) of the data samples.

Principal Component Analysis

$$\overset{U\Sigma}{\begin{bmatrix} -3.67 & -.71 & 0 \\ -8.8 & .30 & 0 \end{bmatrix}} \times \overset{V^T}{\begin{bmatrix} -.42 & -.57 & -.70 \\ .81 & .11 & -.58 \\ .41 & -.82 & .41 \end{bmatrix}} \qquad \overset{A_{partial}}{\begin{bmatrix} 1.6 & 2.1 & 2.6 \\ 3.8 & 5.0 & 6.2 \end{bmatrix}}$$

- Often, raw data samples have a lot of redundancy and patterns.
- PCA can allow you to represent data samples as weights on the principal components, rather than using the original raw form of the data.
- By representing each sample as just those weights, you can represent just the “meat” of what’s different between samples.
- This minimal representation makes machine learning and other algorithms much more efficient.

How is SVD computed?

- For this class: tell PYTHON to do it. Use the result.
- But, if you're interested, one computer algorithm to do it makes use of Eigenvectors!

Eigenvector definition

- Suppose we have a square matrix A. We can solve for vector x and scalar λ such that $Ax = \lambda x$.
- In other words, find vectors where, if we transform them with A, the only effect is to scale them with no change in direction.
- These vectors are called eigenvectors, and the scaling factors λ are called eigenvalues.
- An $m \times m$ matrix will have $\leq m$ eigenvectors where λ is nonzero.

Finding eigenvectors

- Computers can find an x such that $Ax = \lambda x$ using this iterative algorithm:
  - X *= random unit vector*
  - *while(x hasn't converged)*
    - $X = Ax$
    - *normalize* x
- x will quickly converge to an eigenvector.
- Some simple modifications will let this algorithm find all eigenvectors.

Finding SVD

- Eigenvectors are for square matrices, but SVD is for all matrices
- To do svd(A), computers can do this:
  - *Take eigenvectors of AA^T (matrix is always square).*
    - *These eigenvectors are the columns of* **U***.*
    - *Square root of eigenvalues are the singular values (the entries of* **Σ***).*
  - *Take eigenvectors of A^TA (matrix is always square).*
    - *These eigenvectors are columns of* **V** *(or rows of* $\mathbf{V}^{\mathbf{T}}$*)*

Finding SVD

- Moral of the story: SVD is fast, even for large matrices
- It’s useful for a lot of stuff
- There are also other algorithms to compute SVD or part of the SVD
  - *Python’s np.linalg.svd() command has options to efficiently compute only what you need, if performance becomes an issue.*

A detailed geometric explanation of SVD is here: *http://www.ams.org/samplings/feature-column/fcarc-svd*

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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 – measure of the deviation from the mean for points in one dimension, e.g. heights.
- Covariance as a measure of how much each of the dimensions vary from the mean with respect to each other.
- 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.

Covariance

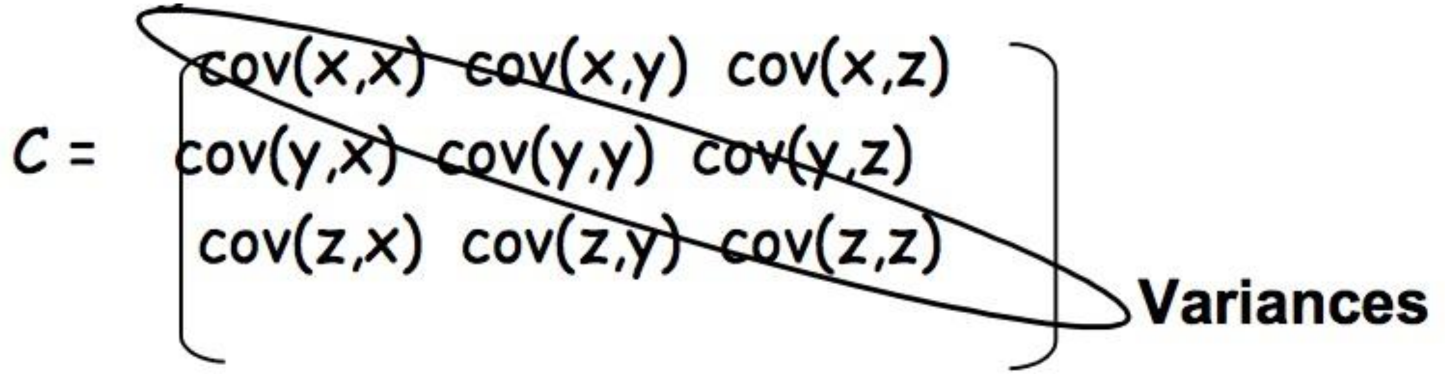
$$\text{covariance}\,(X,Y) = \frac{\sum_{i=1}^{n} (X_i - \bar{X})\,(Y_i - \bar{Y})}{(n-1)}$$

unbiased estimate

- So, if you had a 3-dimensional data set (x, y, z), then you could measure the covariance between the x and y dimensions, the y and z dimensions, and the x and z dimensions. Measuring the covariance between x and x , or y and y , or z and z would give you the variance of the x , y and z dimensions respectively.

Covariance matrix

- Representing Covariance between dimensions as a matrix, e.g. for 3 dimensions.



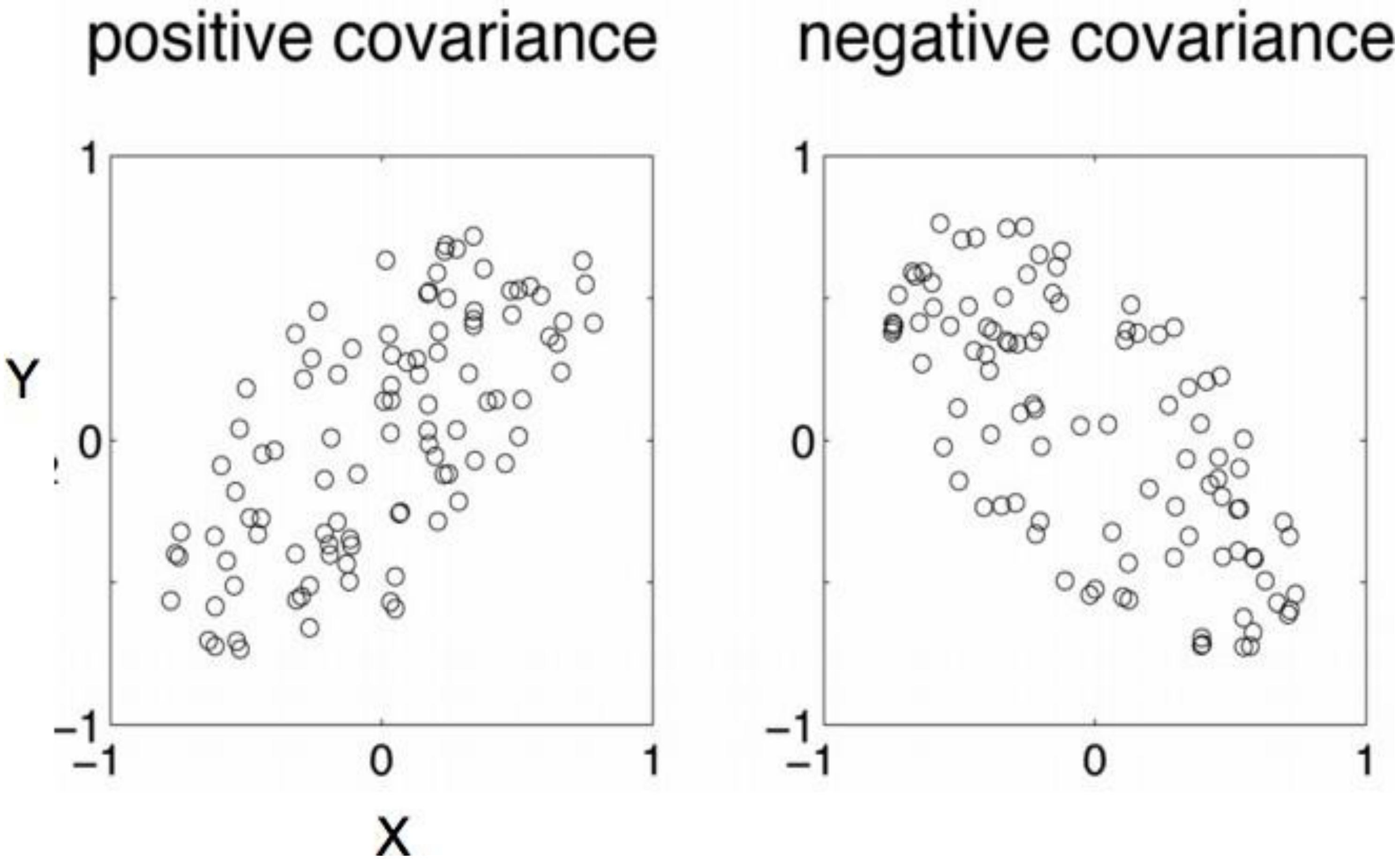
$$C = \begin{bmatrix} cov(x,x) & cov(x,y) & cov(x,z) \\ cov(y,x) & cov(y,y) & cov(y,z) \\ cov(z,x) & cov(z,y) & cov(z,z) \end{bmatrix}$$

- Diagonal is the variances of x, y and z.
- $cov(x, y) = cov(y, x)$ hence matrix is symmetrical about the diagonal.
- N-dimensional data will result in $N \times N$ covariance matrix.

Covariance

- What is the interpretation of covariance calculations?
    - *e.g.: 2 dimensional data set*
    - *x: number of hours studied for a subject*
    - *y: marks obtained in that subject*
    - *covariance value is say: 104.53*
    - *what does this value mean?*

Covariance interpretation



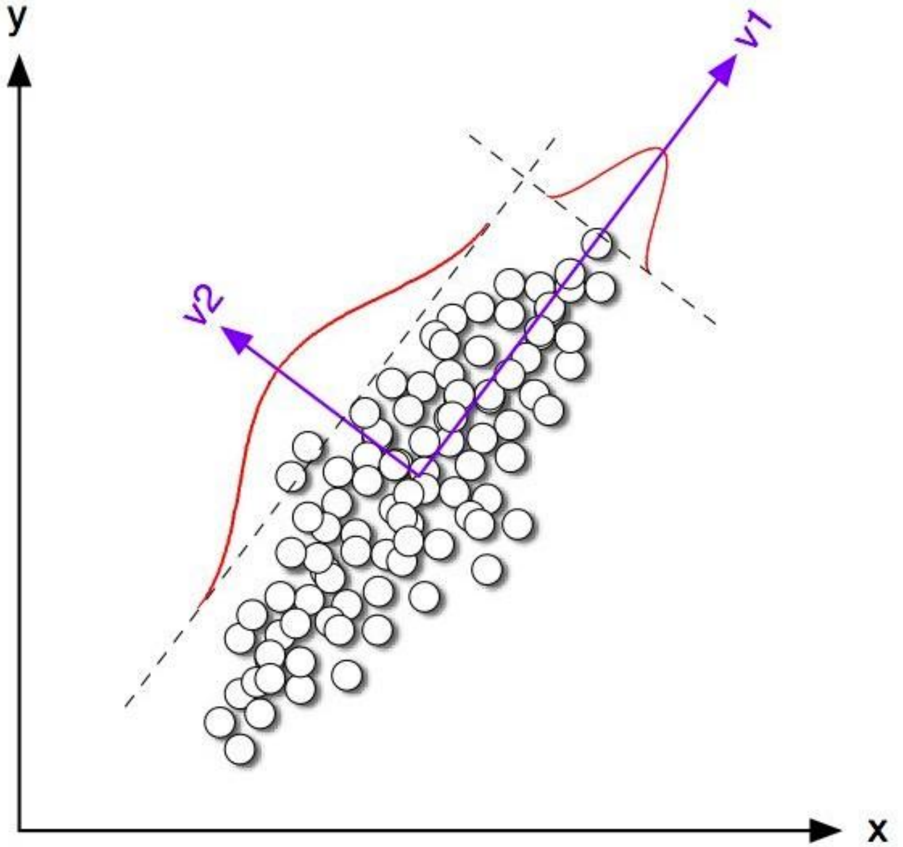
Covariance interpretation

- Exact value is not as important as it’s sign.
- 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. active social life vs performance in CS dept.
- If **covariance is zero**: the two dimensions are uncorrelated (not necessarily independent) of each other e.g. heights of students vs the marks obtained in a subject

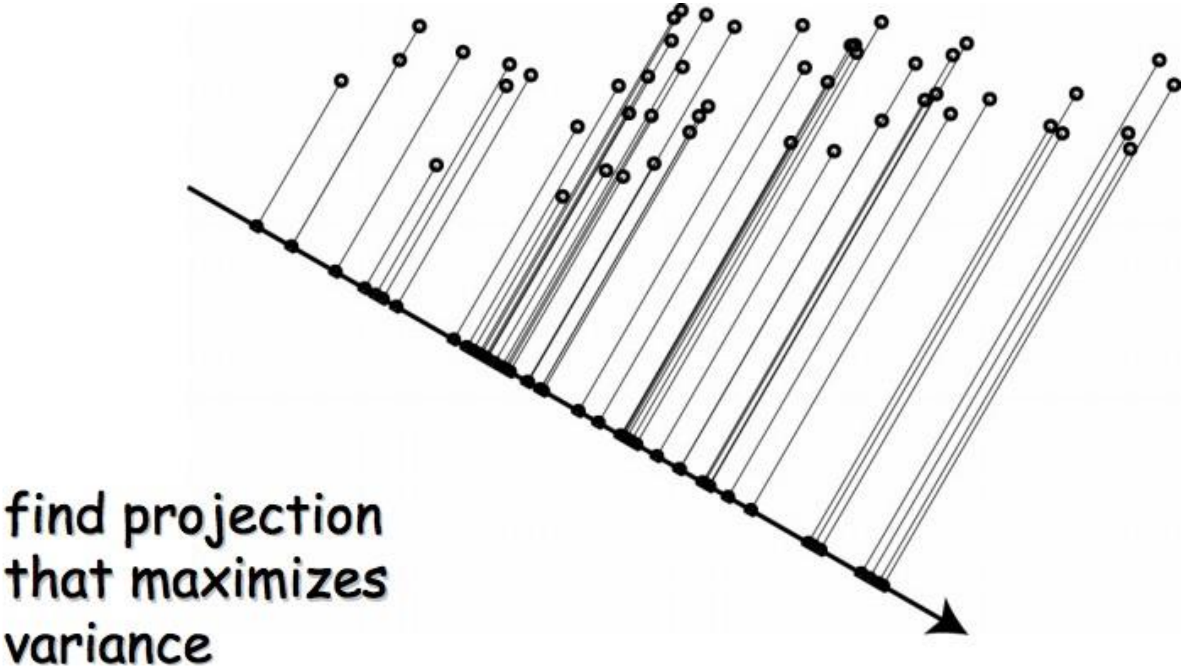
https://en.wikipedia.org/wiki/Covariance

Example data

Covariance between the two axis is high. Can we reduce the number of dimensions to just 1?

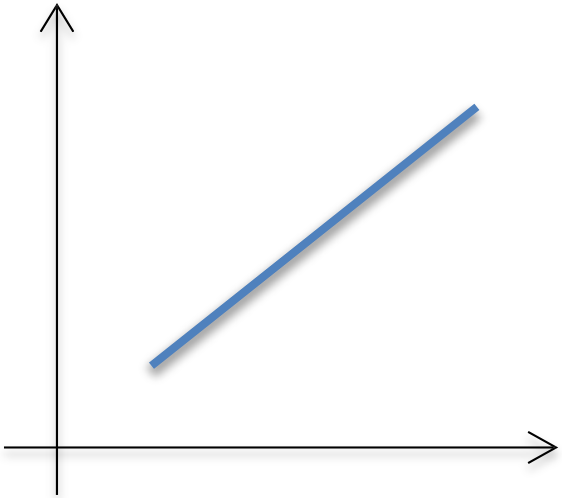


Geometric interpretation of PCA



Geometric interpretation of PCA

- Let's say we have a set of 2D data points x. But we see that all the points lie on a line in 2D.
- So, 2 dimensions are redundant to express the data. We can express all the points with just one dimension.



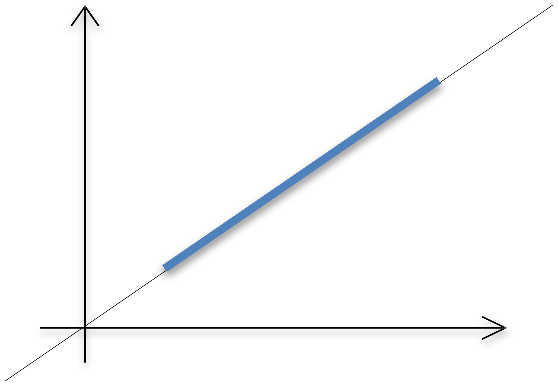
PCA: Principle Component Analysis

- 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 correlation between the points.*
  - *The tool for doing this is called PCA.*

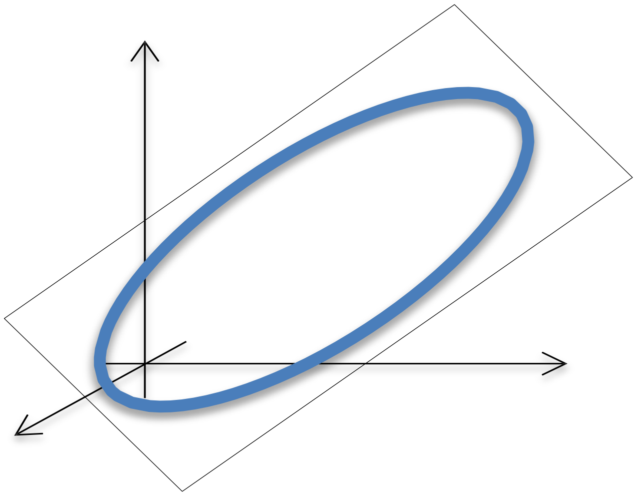
PCA Formulation

- Basic idea:
  - *If the data lives in a subspace, it is going to look very flat when viewed from the full space, e.g.*

1D subspace in 2D



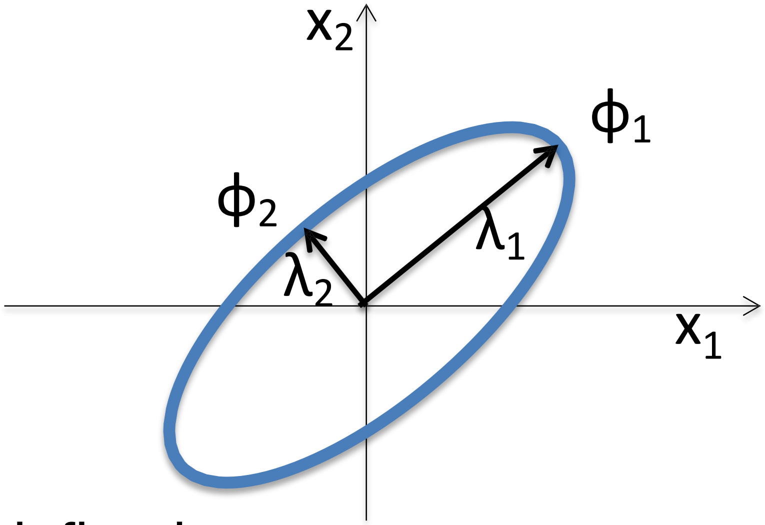
2D subspace in 3D



PCA Formulation

- Assume x is Gaussian with covariance Σ.
- Recall that a gaussian is defined with it's mean and variance:

$$\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$



- Recall that μ and Σ of a gaussian are defined as:

$$\boldsymbol{\mu} = \mathbf{E}[\mathbf{X}] = [\mathbf{E}[X_1], \mathbf{E}[X_2], \ldots, \mathbf{E}[X_k]]^{\mathrm{T}}$$

$$\boldsymbol{\Sigma} =: \mathbf{E}[(\mathbf{X} - \boldsymbol{\mu})(\mathbf{X} - \boldsymbol{\mu})^{\mathrm{T}}] = [\mathrm{Cov}[X_i, X_j]; 1 \leq i, j \leq k]$$

Formalization：最大化方差

- 方差是衡量新特征包含信息多少的度量
  - 有时也称为能量energy
- 优化目标函数 $J_2(\boldsymbol{w}) = \frac{1}{n}\sum_{i=1}^{n}\|\boldsymbol{w}^T(\boldsymbol{x}_i - \overline{\boldsymbol{x}})\|^2$
- 发现问题了吗?
  - $J_2(\boldsymbol{w})$可以是无穷大或者为0（平凡解）！
  - 最常用的解决办法：加上限制条件 $\|\boldsymbol{w}\|^2 = \boldsymbol{w}^T\boldsymbol{w} = 1$

$$\underset{\boldsymbol{w}}{\arg\max}\frac{1}{n}\sum_{i=1}^{n}\|(\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T\boldsymbol{w}\|^2$$

$$\text{s.t.} \qquad \boldsymbol{w}^T\boldsymbol{w} = 1$$

  - s.t. –subject to,表示约束条件constraint(s)

简化simplification、变换transformation

$$\|(\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T \boldsymbol{w}\|^2 = \left((\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T \boldsymbol{w}\right)^T \left((\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T \boldsymbol{w}\right)$$

$$= \boldsymbol{w}^T (\boldsymbol{x}_i - \overline{\boldsymbol{x}})(\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T \boldsymbol{w}$$

$$\frac{1}{n}\sum_{i=1}^{n} \|(\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T \boldsymbol{w}\|^2 = \boldsymbol{w}^T \sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \frac{1}{n} (\boldsymbol{x}_i - \overline{\boldsymbol{x}})(\boldsymbol{x}_i - \overline{\boldsymbol{x}})^T \boldsymbol{w}$$

$$= \boldsymbol{w}^T \Sigma \boldsymbol{w}$$

优化optimization

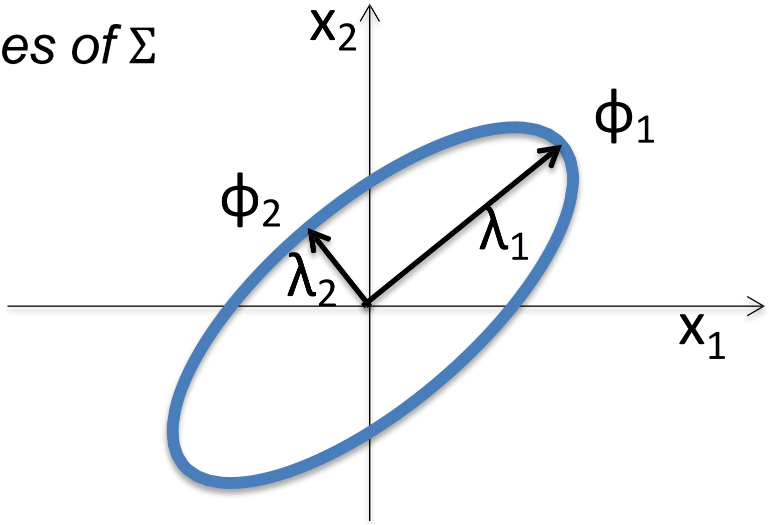
- 拉格朗日乘子法 Lagrange multipliers
  - 将有约束的优化问题转化为无约束的优化问题
- Lagrangian 拉格朗日函数

$$f(\mathbf{w},\lambda) = \mathbf{w}^T\Sigma\mathbf{w} - \lambda(\mathbf{w}^T\mathbf{w} - 1)$$

- λ：拉格朗日乘子Lagrange multiplier
- 最优的必要条件：$\frac{\partial f}{\partial \mathbf{w}} = \mathbf{0}$，$\frac{\partial f}{\partial \lambda} = 0$
- $\frac{\partial f}{\partial \mathbf{w}} = 2\Sigma\mathbf{w} - 2\lambda\mathbf{w} = \mathbf{0}$
  - 我们这里的前提条件是什么？
  - 应该想到用哪一个公式？
- $\Sigma\mathbf{w} = \lambda\mathbf{w}$,　　　　　$\mathbf{w}^T\mathbf{w} = 1$!

PCA Formulation

- If x is Gaussian with covariance Σ,
  - *Principal components* φ_i *are the eigenvectors of* Σ
  - *Principal lengths* λ_i *are the eigenvalues of* Σ



- by computing the eigenvalues we know the data is
  - *Not flat if* $\lambda_1 \approx \lambda_2$
  - *Flat if* $\lambda_1 >> \lambda_2$

J_1和J_2的等价关系

- 若干向量
  - $\boldsymbol{x}_i$：降维之前的向量
  - $\boldsymbol{w}^T(\boldsymbol{x}_i-\overline{\boldsymbol{x}})\boldsymbol{w}=a_i\boldsymbol{w}$：降维之后的向量
  - $\widehat{\boldsymbol{x}}$：在原空间中重建的向量
  - 目前的重建关系：$\boldsymbol{x}_i \approx \widehat{\boldsymbol{x}}_i=\overline{\boldsymbol{x}}+a_i\boldsymbol{w}$
- J_1的目的是使得$\widehat{\boldsymbol{x}}_i$和$\boldsymbol{x}_i$尽可能相差小($\overline{\boldsymbol{x}}$固定为均值)
  - $J_1(\boldsymbol{w},\boldsymbol{a})=\sum_{i=1}^{n}\frac{1}{n}\|\boldsymbol{x}_i-(\overline{\boldsymbol{x}}+a_i\boldsymbol{w})\|^2$
  - $\boldsymbol{w}$：投影方向， a_i：投影系数
- 最小化J_1得到的a_i和$\boldsymbol{w}$与J_2得到的结果完全一致！
  - 试着去证明!

PCA Algorithm (training)

- Given sample $\mathcal{D} = \{x_1, \dots, x_n\}, x_i \in \mathcal{R}^d$
  - Compute sample mean: $\hat{\mu} = \frac{1}{n}\sum_i x_i$.
  - Compute sample covariance: $\hat{\Sigma} = \frac{1}{n}\sum_i (x_i - \hat{\mu})(x_i - \hat{\mu})^T$.
  - Compute eigenvalues and eigenvectors of $\hat{\Sigma}$.

$$\hat{\Sigma} = \Phi\Lambda\Phi^T, \Lambda = diag(\sigma_1^2, \dots, \sigma_n^2), \Phi^T\Phi = I$$

  - Order eigenvalues $\sigma_1^2 > \cdots > \sigma_n^2$.
  - If, for a certain k, $\sigma_k \ll \sigma_1$, eliminate the eigenvalues and eigenvectors above k.

PCA Algorithm (testing)

- Given principal compoents $\Phi_i, i \in 1, \dots, k$ and a test sample $\mathcal{T} = \{t_1, \dots, t_n\}, t_i \in \mathcal{R}^d$
  - Subtract mean to each point $t_i' = t_i - \hat{\mu}$
  - Project onto eigenvector space $y_i = At_i'$, where

$$\mathbf{A} = \begin{bmatrix} \phi_1^T \\ \vdots \\ \phi_k^T \end{bmatrix}$$

  - Use $T' = \{y_1, \dots, y_n\}$ to estimate class conditional densities and do all further processing on y.

PCA by SVD

- An alternative manner to compute the principal components, based on singular value decomposition.
- Quick reminder: SVD
  - *Any real* $n \times m$ *matrix* ($n > m$) *can be decomposed as*

$$\boxed{A = \mathrm{M}\Pi\mathrm{N}^T}$$

  - *Where* M *is an* ($n \times m$) *column orthonormal matrix of left singular vectors (columns of* M*)*
  - Π *is an* ($m \times m$) *diagonal matrix of singular values*
  - N^T *is an* ($m \times m$) *row orthonormal matrix of right singular vectors (columns of* N*)*

$$\boxed{\mathrm{M}^T\mathrm{M} = I \qquad \mathrm{N}^T\mathrm{N} = I}$$

PCA by SVD

- To relate this to PCA, we consider the data matrix

$$\boxed{X = \begin{bmatrix} | & & | \\ x_1 & \dots & x_n \\ | & & | \end{bmatrix}}$$

- The sample mean is

$$\boxed{\mu = \frac{1}{n}\sum_i x_i = \frac{1}{n}\begin{bmatrix} | & & | \\ x_1 & \dots & x_n \\ | & & | \end{bmatrix}\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} = \frac{1}{n}X1}$$

PCA by SVD

- Center the data by subtracting the mean to each column of X
- The centered data matrix is

$$X_c = \begin{bmatrix} | & & | \\ x_1 & \cdots & x_n \\ | & & | \end{bmatrix} - \begin{bmatrix} | & & | \\ \mu & \cdots & \mu \\ | & & | \end{bmatrix}$$

$$= X - \mu 1^T = X - \frac{1}{n} X 1 1^T = X\left(I - \frac{1}{n} 1 1^T \right)$$

PCA by SVD

- The sample covariance matrix is

$$\Sigma = \frac{1}{n}\sum_i (x_i - \mu)(x_i - \mu)^T = \frac{1}{n}\sum_i x_i^c \left(x_i^c\right)^T$$

where x_i^c is the ith column of X_c

- This can be written as

$$\Sigma = \frac{1}{n}\begin{bmatrix} | & & | \\ x_1^c & \cdots & x_n^c \\ | & & | \end{bmatrix}\begin{bmatrix} - & x_1^c & - \\ & \vdots & \\ - & x_n^c & - \end{bmatrix} = \frac{1}{n} X_c X_c^T$$

PCA by SVD

- The matrix

$$X_c^T = \begin{bmatrix} - & x_1^c & - \\ & \vdots & \\ - & x_n^c & - \end{bmatrix}$$

is real ($n \times d$). Assuming $n > d$ it has SVD decomposition

$$X_c^T = \mathrm{M}\Pi\mathrm{N}^T \qquad \mathrm{M}^T\mathrm{M} = I \qquad \mathrm{N}^T\mathrm{N} = I$$

and

$$\Sigma = \frac{1}{n} X_c X_c^T = \frac{1}{n}\mathrm{N}\Pi\mathrm{M}^T\mathrm{M}\Pi\mathrm{N}^T = \frac{1}{n}\mathrm{N}\Pi^2\mathrm{N}^T$$

PCA by SVD

$$\boxed{\Sigma = \mathrm{N}\left(\frac{1}{n}\Pi^2\right)\mathrm{N}^T}$$

- Note that N is $(d \times d)$ and orthonormal, and Π^2 is diagonal. This is just the eigenvalue decomposition of Σ
- It follows that
    - *The eigenvectors of* Σ *are the columns of* N
    - *The eigenvalues of* Σ *are*

$$\boxed{\lambda_i = \frac{1}{n}\pi_i^2}$$

- This gives an alternative algorithm for PCA.

PCA by SVD

- In summary, computation of PCA by SVD
- Given X with one example per column
  - *Create the centered data matrix*

$$\boxed{X_c^T = \left(I - \frac{1}{n} 1 1^T \right) X^T}$$

  - *Compute its SVD*

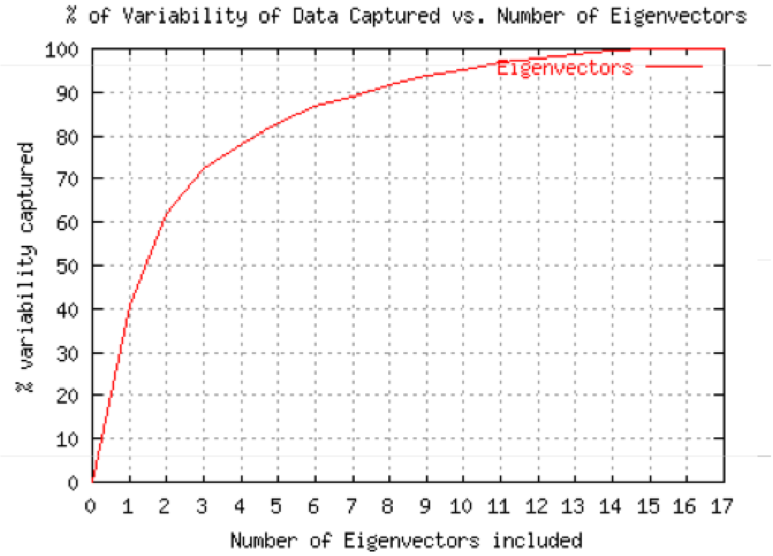
$$\boxed{X_c^T = \mathrm{M \Pi N}^T}$$

  - *Principal components are columns of N, eigenvalues are*

$$\boxed{\lambda_i = \frac{1}{n} \pi_i^2}$$

Rule of thumb for finding the number of PCA components

- A natural measure is to pick the eigenvectors that explain $p\%$ of the data variability.
  - *Can be done by plotting the ratio r_k as a function of k*



$$r_k = \sum_{i=1}^{k} \lambda_i^2 \Big/ \sum_{i=1}^{n} \lambda_i^2$$

  - *E.g. we need 3 eigenvectors to cover 70% of the variability of this dataset.*

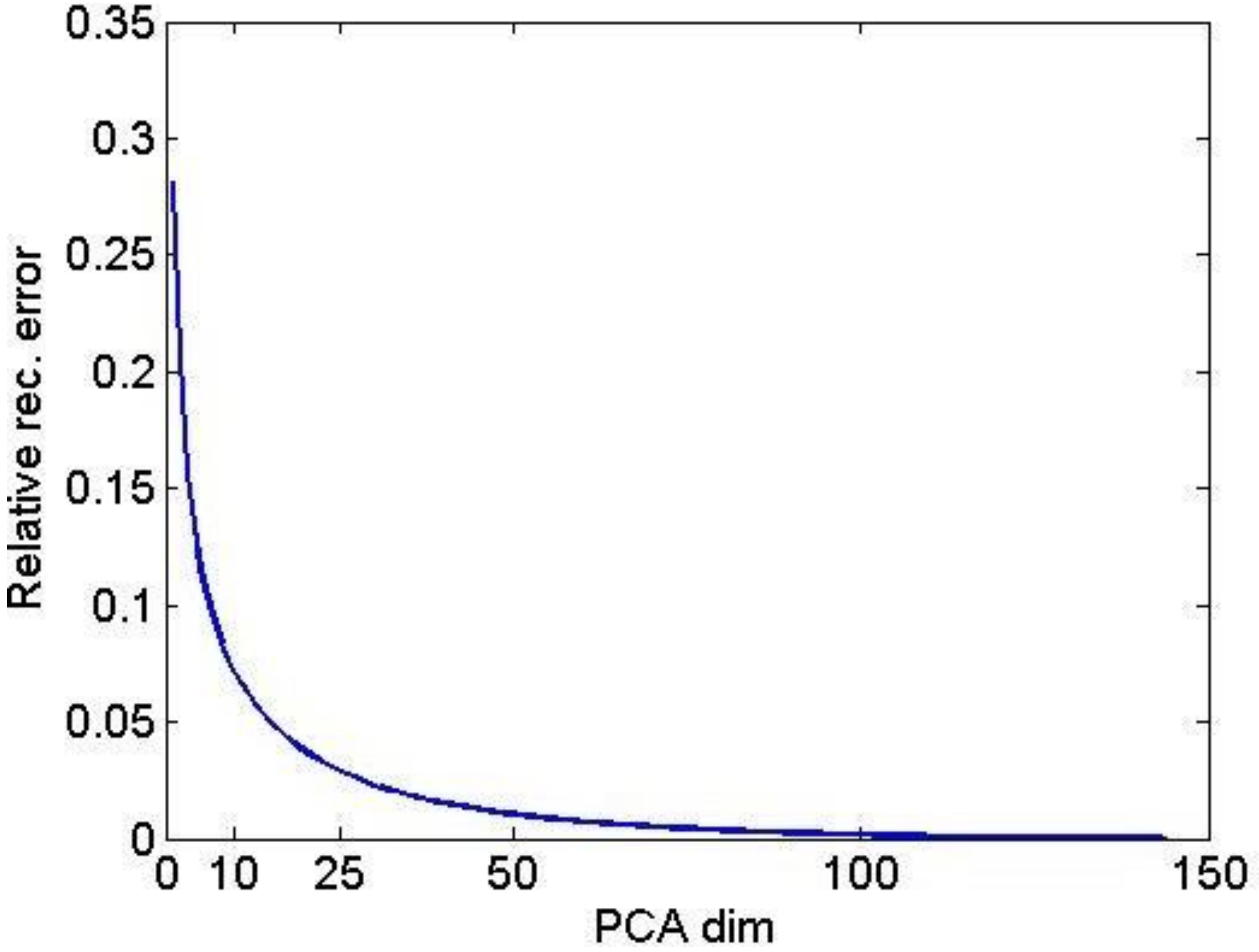
What we will learn today

- Singular value decomposition
- Principal Component Analysis (PCA)
- Image compression

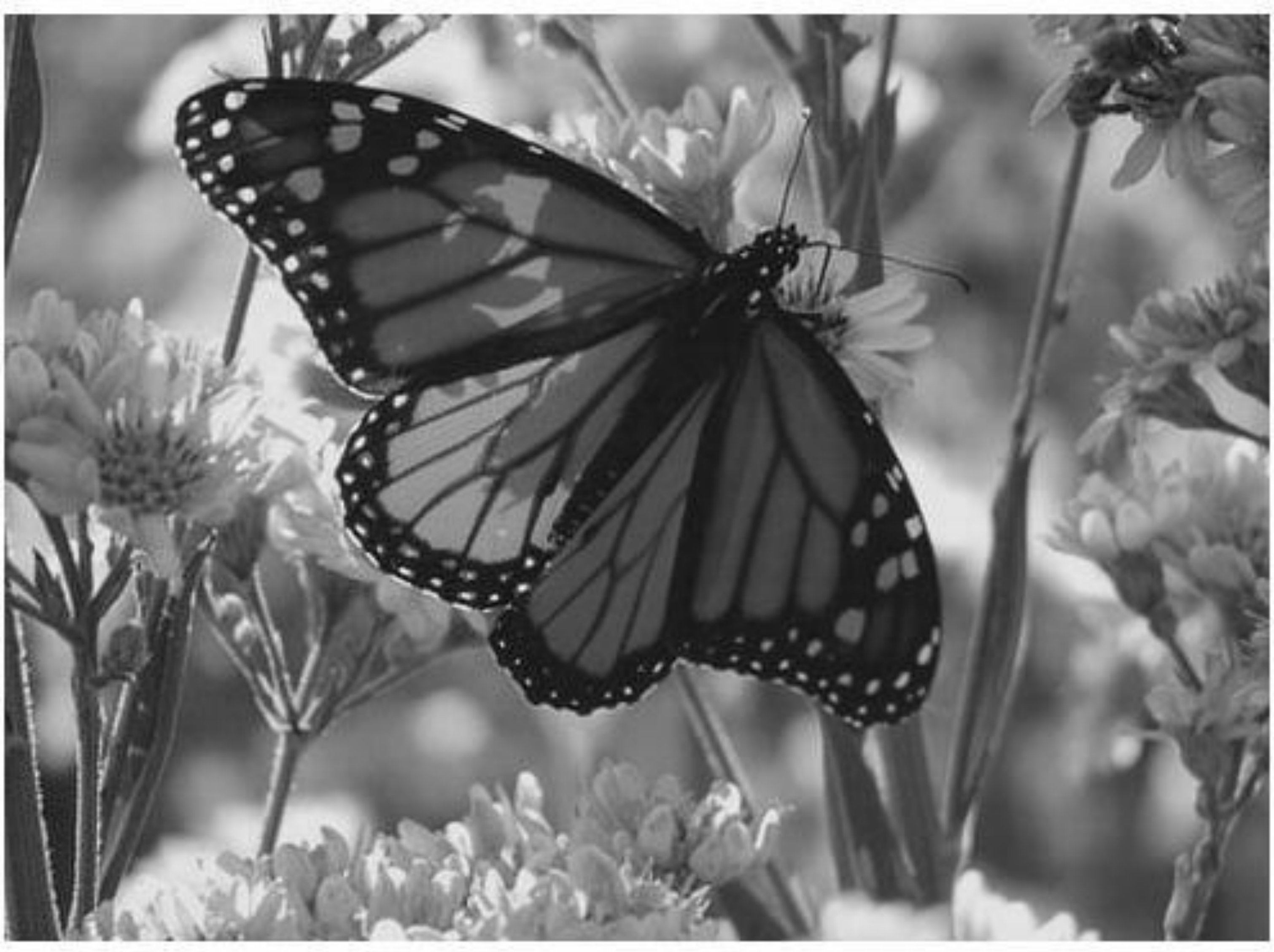
Original Image

- 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

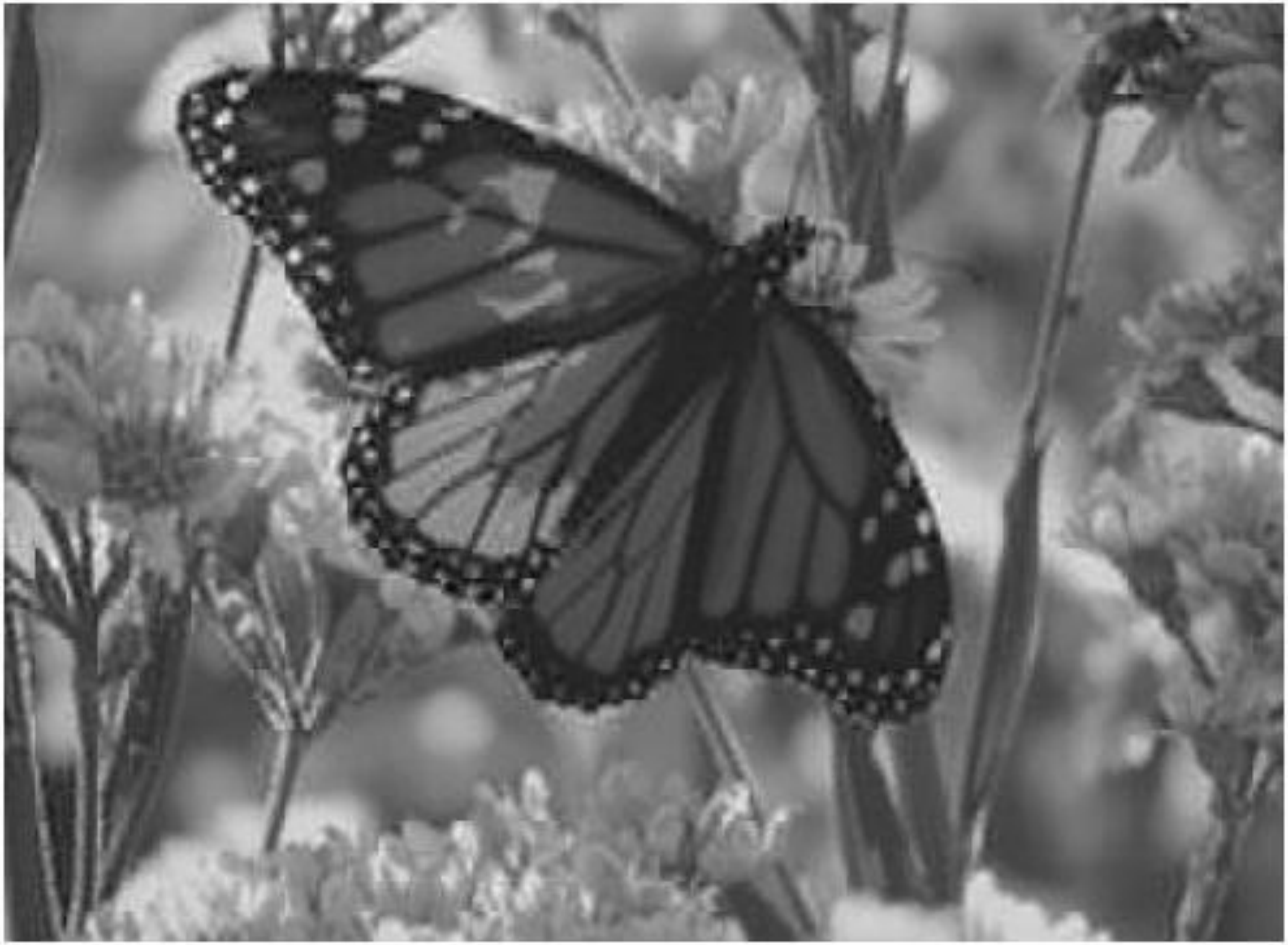
L_2 error and PCA dim



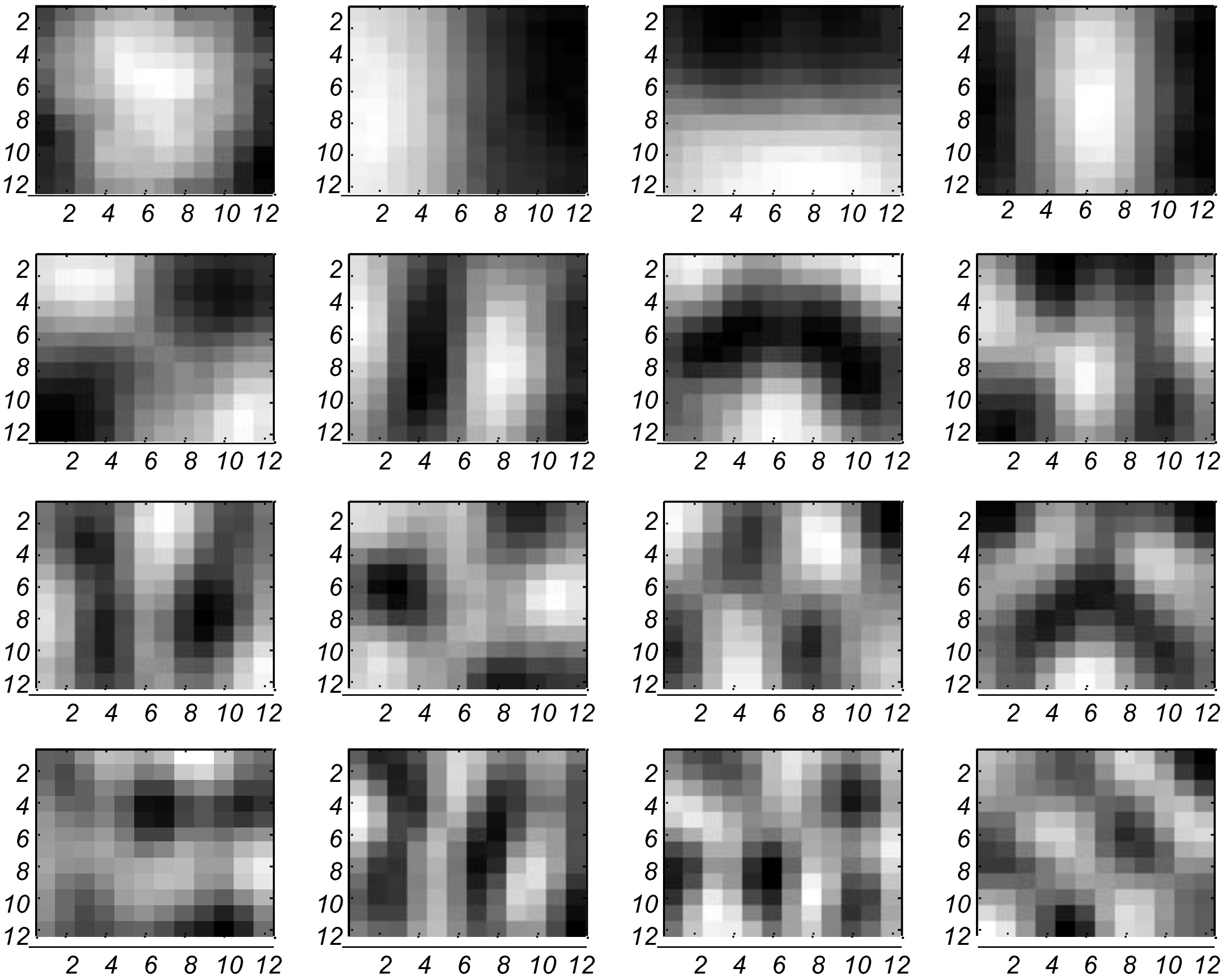
PCA compression: 144D → 60D



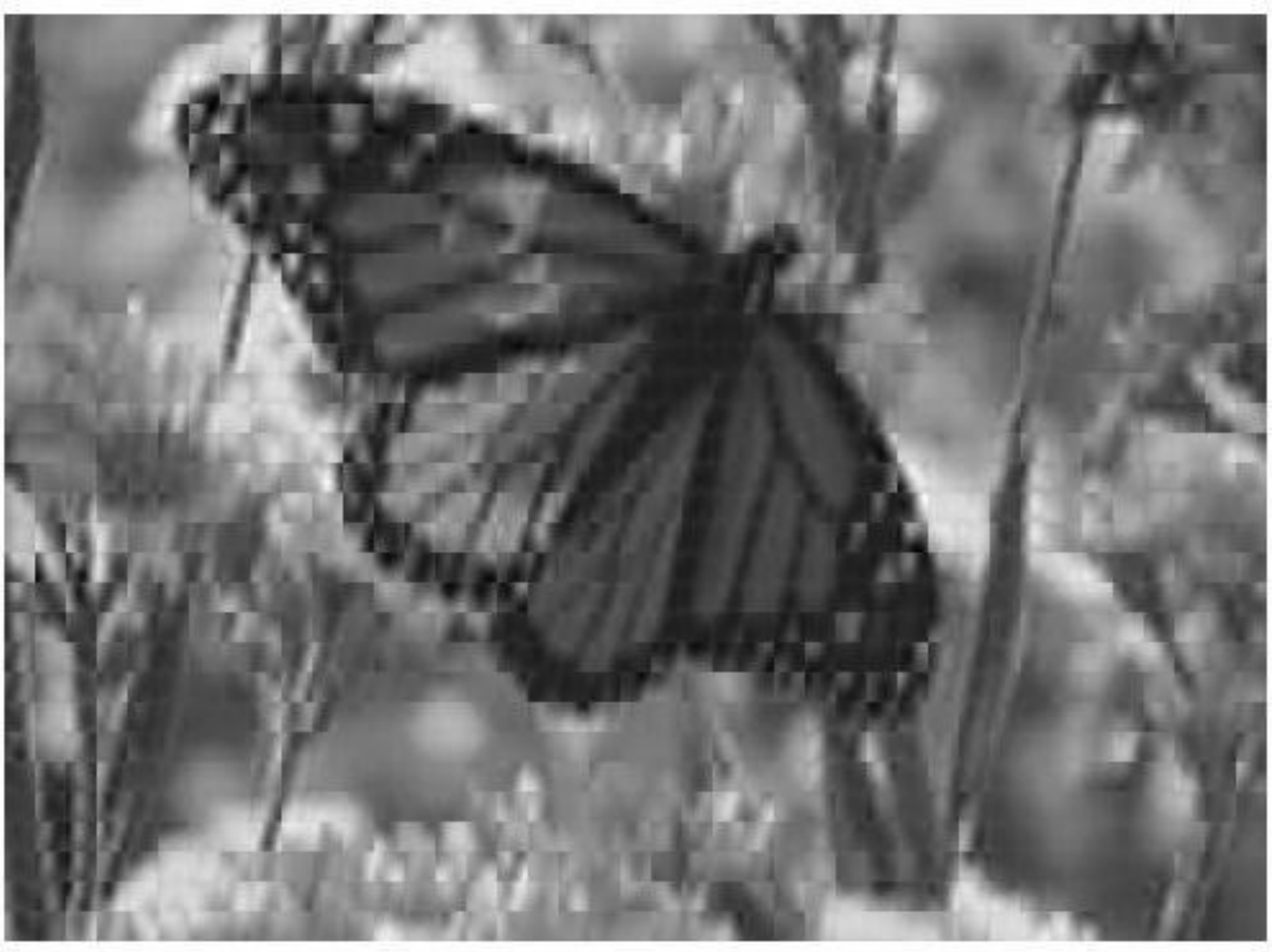
PCA compression: 144D → 16D



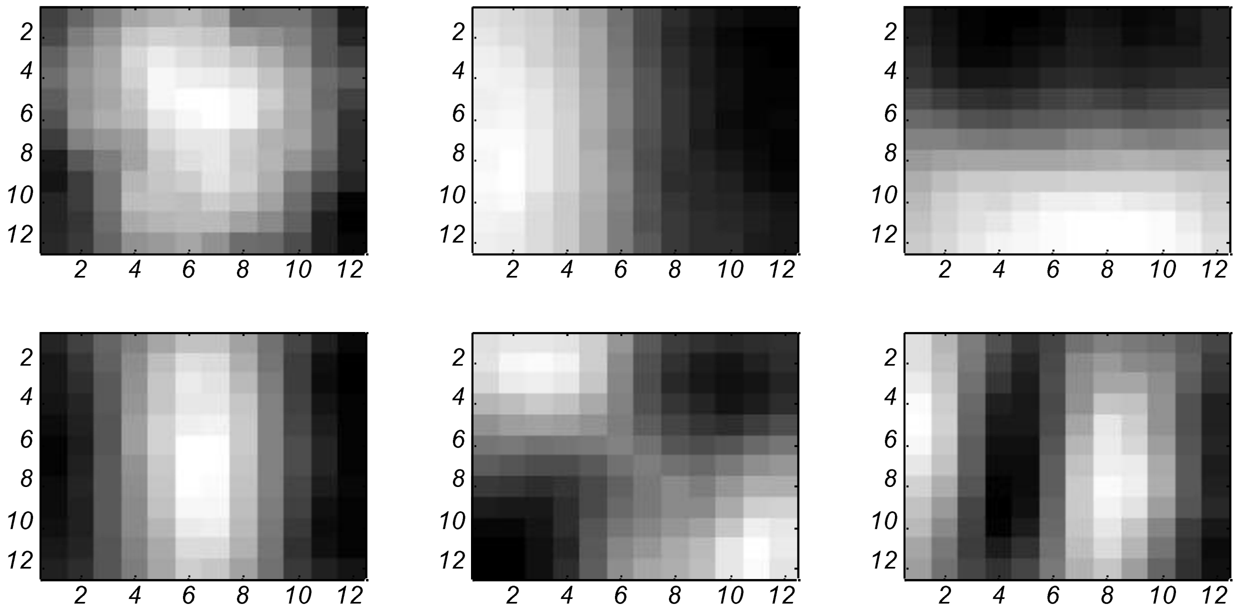
16 most important eigenvectors



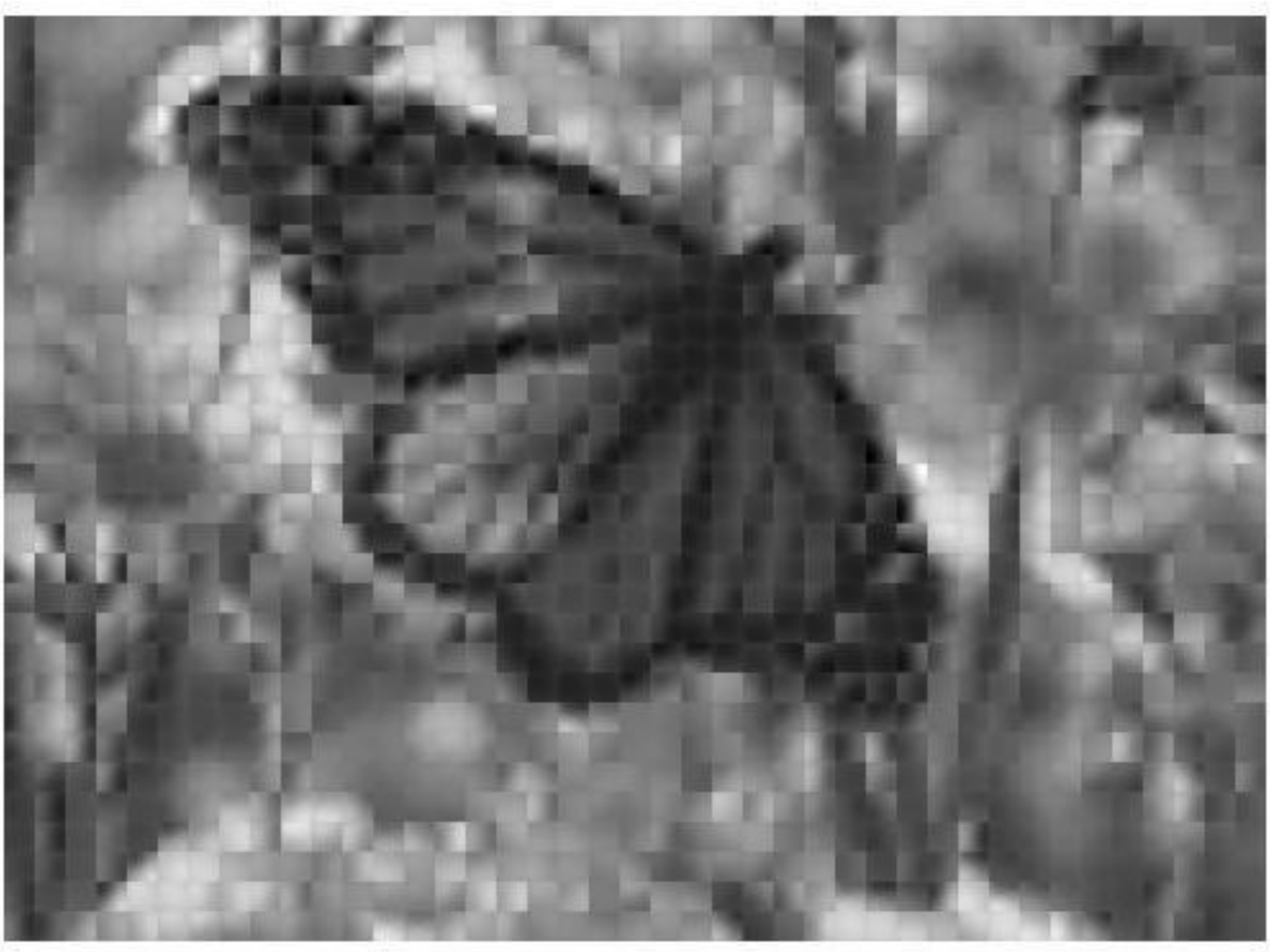
PCA compression: 144D → 6D



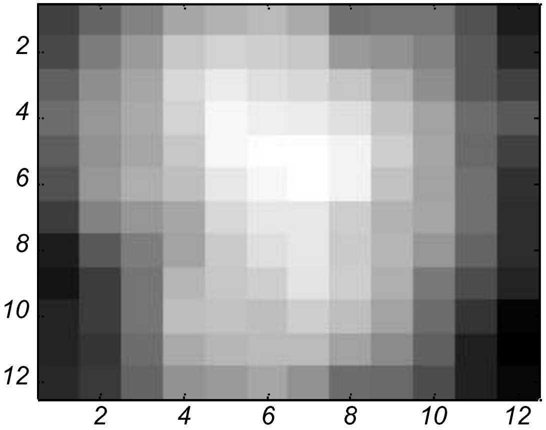
6 most important eigenvectors

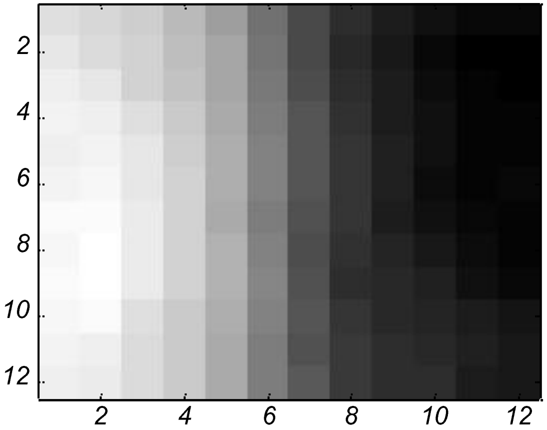


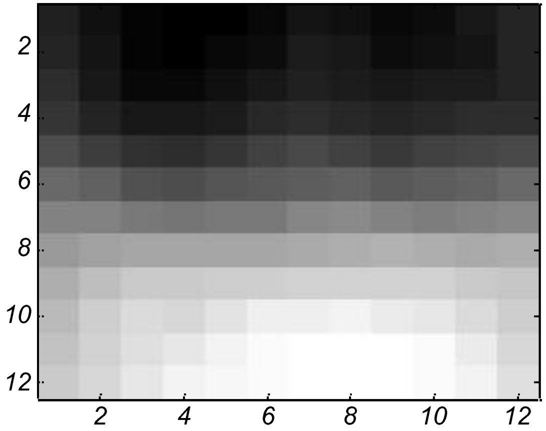
PCA compression: 144D → 3D



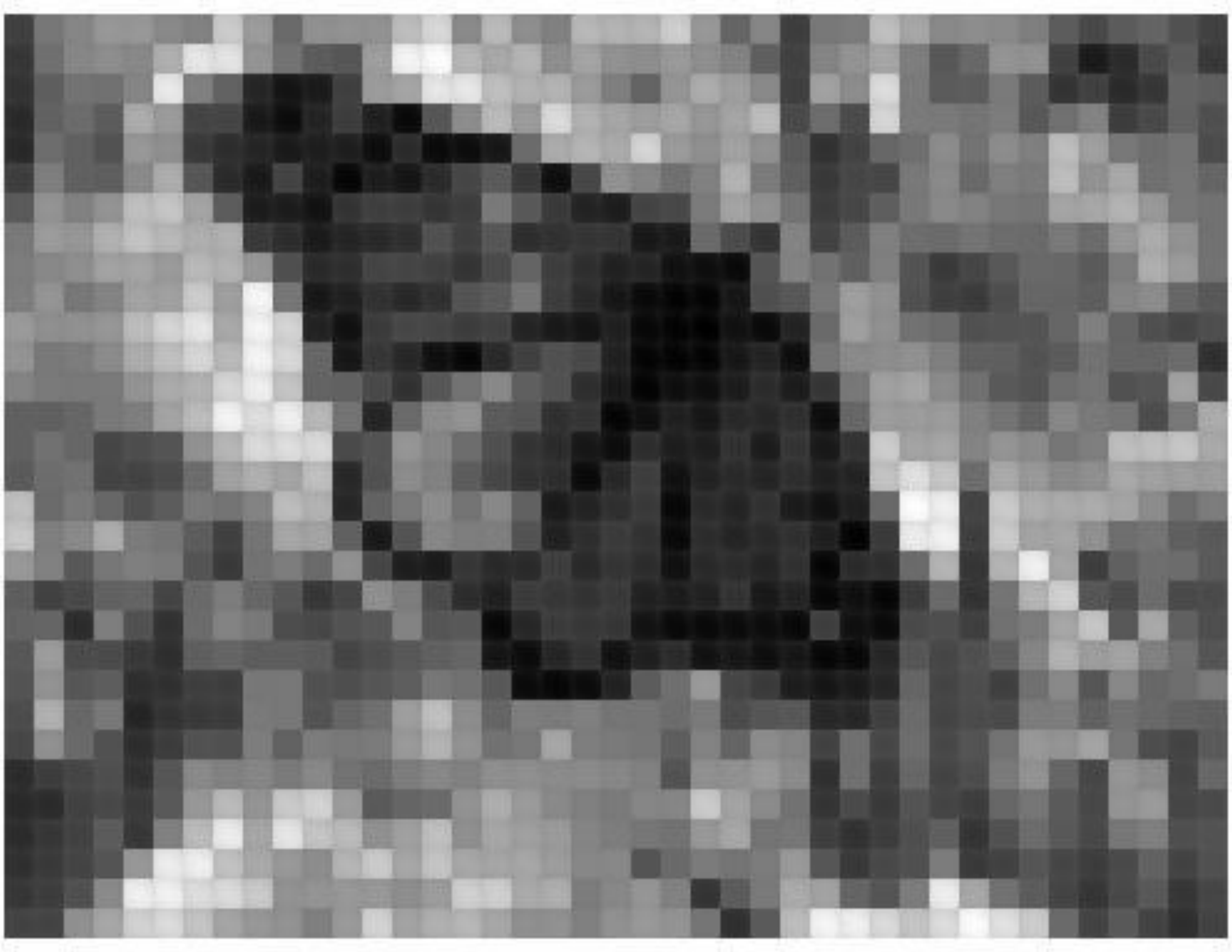
3 most important eigenvectors





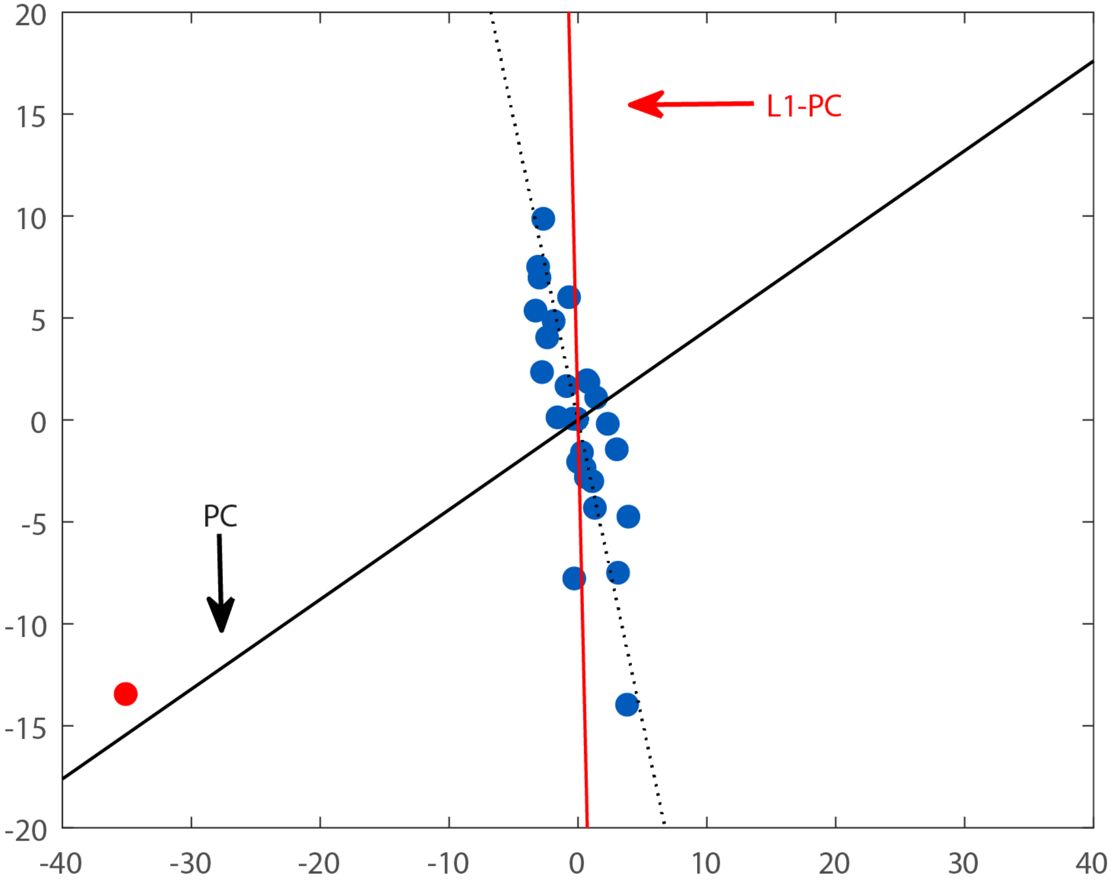


PCA compression: 144D → 1D



PCA vs L1 PCA

- Robustness



https://en.wikipedia.org/wiki/L1-norm_principal_component_analysis

What we have learned today

- Singular value decomposition
- Principal Component Analysis (PCA)
- Image compression