PCA

Chris Tralie

Duke University

July 11, 2017

Point Cloud Centroid

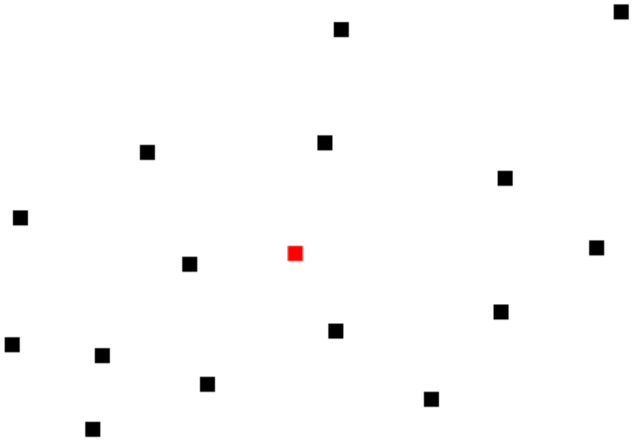
Given a collection of points $X = \{\vec{x}_i\}|_{i=1}^{N}$
Centroid $\vec{c}$ is the "mean point"

That is

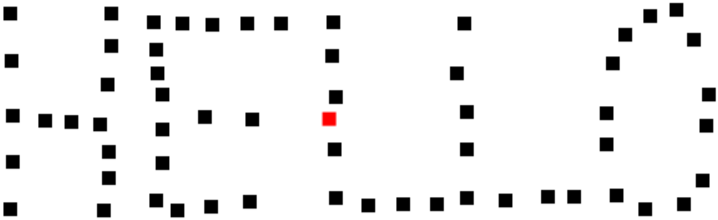
$$\vec{c}[k] = \frac{1}{N} \sum_{i=1}^{N} x_i[k]$$

Average each coordinate independently

Point Cloud Centroid



Point Cloud Centroid



Directions of Variance

Subtract off centroid, organize point cloud into $N \times d$ matrix, each point along a row

$$X = \begin{bmatrix} - & \vec{x_1} & - \\ - & \vec{x_2} & - \\ - & \vec{x_3} & - \\ \dots & \vdots & \dots \\ - & \vec{x_N} & - \end{bmatrix}$$

Directions of Variance

Subtract off centroid, organize point cloud into $N \times d$ matrix, each point along a row

$$X = \begin{bmatrix} - & \vec{x_1} & - \\ - & \vec{x_2} & - \\ - & \vec{x_3} & - \\ \dots & \vdots & \dots \\ - & \vec{x_N} & - \end{bmatrix}$$

Choose a unit column vector direction $u \in \mathbb{R}^{d \times 1}$
Then

$$d = Xu$$

gives projections onto u

Directions of Variance

$$d = Xu$$

gives projections onto u

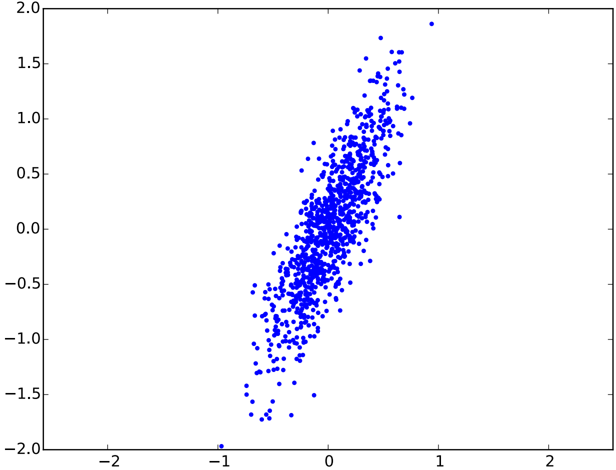
Directions of Variance

$$d = Xu$$

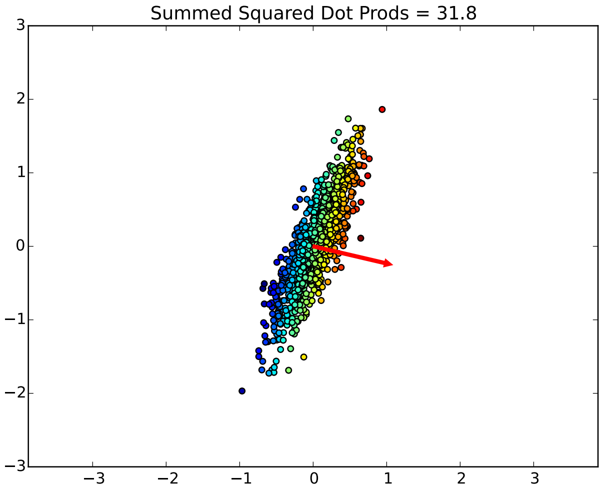
gives projections onto u
What is the sum of the squared norms of each projected point, in matrix form?

Directions of Variance: Example

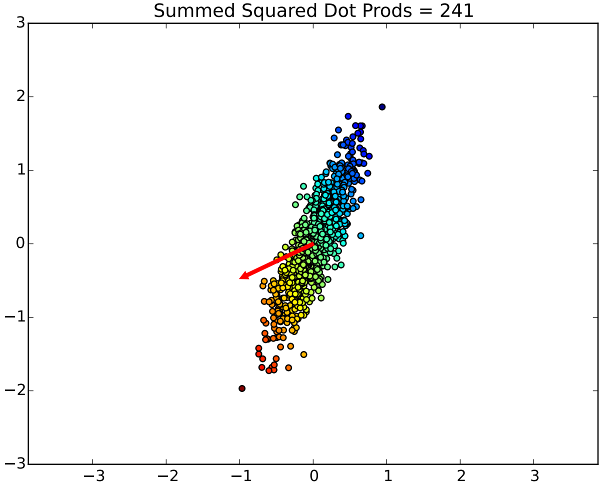
1000 point example in 2D, centroid is origin



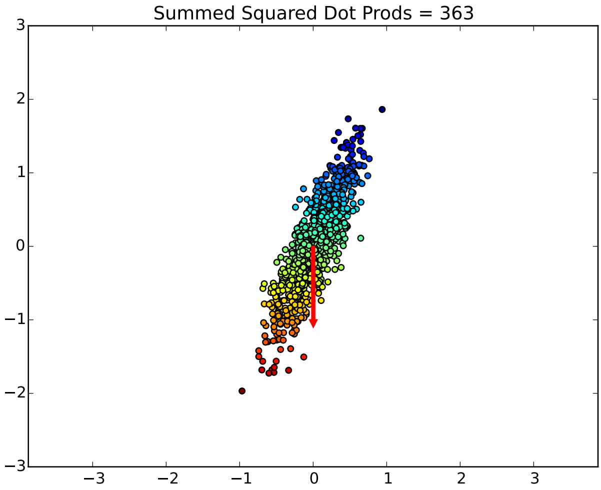
Directions of Variance: Example



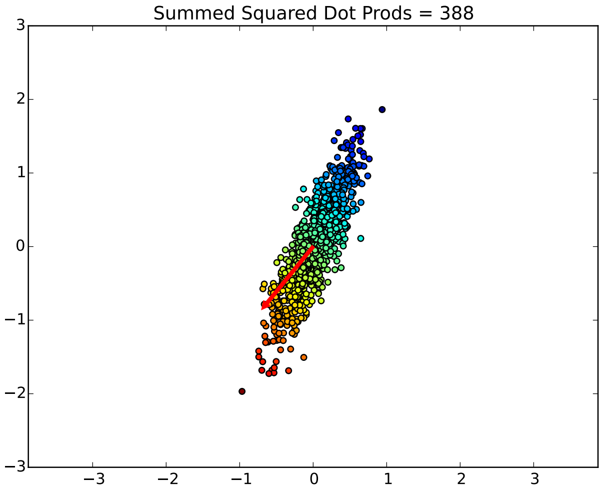
Directions of Variance: Example



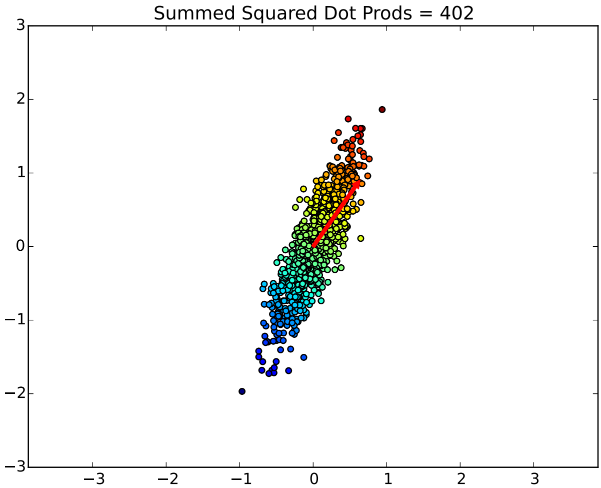
Directions of Variance: Example



Directions of Variance: Example

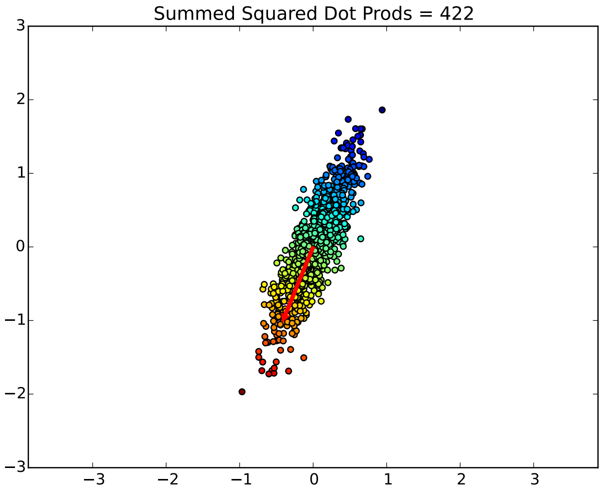


Directions of Variance: Example

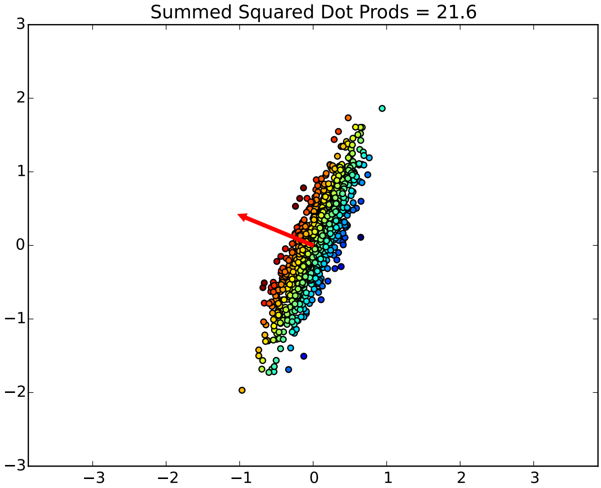


PCA Example

Largest direction of variance, $\lambda_1 = 422$



Smallest direction of variance, $\lambda_2 = 21.6$



PCA: Interactive Examples 2D/3D

http://www.ctralie.com/Teaching/COMPSCI290/Lectures/10_PCA/PCA2D.html

http://www.ctralie.com/Teaching/COMPSCI290/Materials/JSPCViewer/

PCA Pitfalls

Outliers!
(Show Demo Again)

PCA Pitfalls

Close Eigenvectors
"Multiplicity issues" for "near-isotropic" point clouds

Directions of Variance: Some More Math

$$d^T d = (Xu)^T (Xu) = u^T (X^T X) u = u^T A u$$

Directions of Variance: Some More Math

$$d^T d = (Xu)^T (Xu) = u^T (X^T X) u = u^T A u$$

- Note that $A = X^T X$ is symmetric.

Directions of Variance: Some More Math

$$d^T d = (Xu)^T (Xu) = u^T (X^T X) u = u^T A u$$

- Note that $A = X^T X$ is symmetric.
- It is also *positive semi-definite*. All eigenvalues are real and positive

Directions of Variance: Some More Math

$$d^T d = (Xu)^T (Xu) = u^T (X^T X) u = u^T A u$$

- Note that $A = X^T X$ is symmetric.
- It is also *positive semi-definite*. All eigenvalues are real and positive
- Let (v_1, λ_1), (v_2, λ_2), ..., (v_d, λ_d) be the d eigenvalue/eigenvector pairs. Then a direction u can be written as

$$u = a_1 v_1 + a_2 v_2 + \ldots + a_d v_d$$

Directions of Variance: Some More Math

$$u^T(X^TX)u = u^TAu$$

Let $u = a_1v_1 + a_2v_2 + \ldots + a_dv_d$
and all vs are unit-norm eigenvectors

Directions of Variance: Some More Math

$$u^T(X^TX)u = u^TAu$$

Let $u = a_1 v_1 + a_2 v_2 + \ldots + a_d v_d$
and all vs are unit-norm eigenvectors
Then

$$u^TAu = (a_1 v_1 + a_2 v_2 + \ldots + a_d v_d)^T A (a_1 v_1 + a_2 v_2 + \ldots + a_d v_d)$$

Directions of Variance: Some More Math

$$u^T(X^TX)u = u^TAu$$

Let $u = a_1v_1 + a_2v_2 + \ldots + a_dv_d$
and all vs are unit-norm eigenvectors
Then

$$u^TAu = (a_1v_1 + a_2v_2 + \ldots + a_dv_d)^TA(a_1v_1 + a_2v_2 + \ldots + a_dv_d)$$

$$u^TAu = (a_1v_1 + a_2v_2 + \ldots + a_dv_d)^T(a_1\lambda_1v_1 + a_2\lambda_2v_2 + \ldots + a_d\lambda_dv_d)$$

Directions of Variance: Some More Math

$$u^T(X^TX)u = u^TAu$$

Let $u = a_1v_1 + a_2v_2 + \ldots + a_dv_d$
and all vs are unit-norm eigenvectors
Then

$$u^TAu = (a_1v_1 + a_2v_2 + \ldots + a_dv_d)^T A(a_1v_1 + a_2v_2 + \ldots + a_dv_d)$$

$$u^TAu = (a_1v_1 + a_2v_2 + \ldots + a_dv_d)^T (a_1\lambda_1v_1 + a_2\lambda_2v_2 + \ldots + a_d\lambda_dv_d)$$

Remembering that all vs are orthogonal

Directions of Variance: Some More Math

$$u^T(X^TX)u = u^TAu$$

Let $u = a_1v_1 + a_2v_2 + \ldots + a_dv_d$
and all vs are unit-norm eigenvectors
Then

$$u^TAu = (a_1v_1 + a_2v_2 + \ldots + a_dv_d)^T A(a_1v_1 + a_2v_2 + \ldots + a_dv_d)$$

$$u^TAu = (a_1v_1 + a_2v_2 + \ldots + a_dv_d)^T (a_1\lambda_1v_1 + a_2\lambda_2v_2 + \ldots + a_d\lambda_dv_d)$$

Remembering that all vs are orthogonal

$$u^TAu = a_1^2\lambda_1 + a_2^2\lambda_2 + \ldots + a_d^2\lambda_d$$

Directions of Variance: Some More Math

$$u^T Au = a_1^2\lambda_1 + a_2^2\lambda_2 + \ldots + a_d^2\lambda_d$$

Assuming that $||u|| = 1 \implies (a_1^2 + a_2^2 + \ldots a_d^2) = 1$

Also assume that $\lambda_1 > \lambda_2 > \ldots > \lambda_d$

Raffle Point Question: What should the *a*s be to maximize the sum of squared dot products: $u^T Au$?

Principal Component Analysis Algorithm

1. Stack points in rows.

2. Compute the "covariance matrix" $A = X^T X$

3. Compute eigenvalues/eigenvectors of A, sorted in decreasing order

Orthogonal directions of variance are in the eigenvectors

Sum of squared dot products with directions are associated eigenvalues