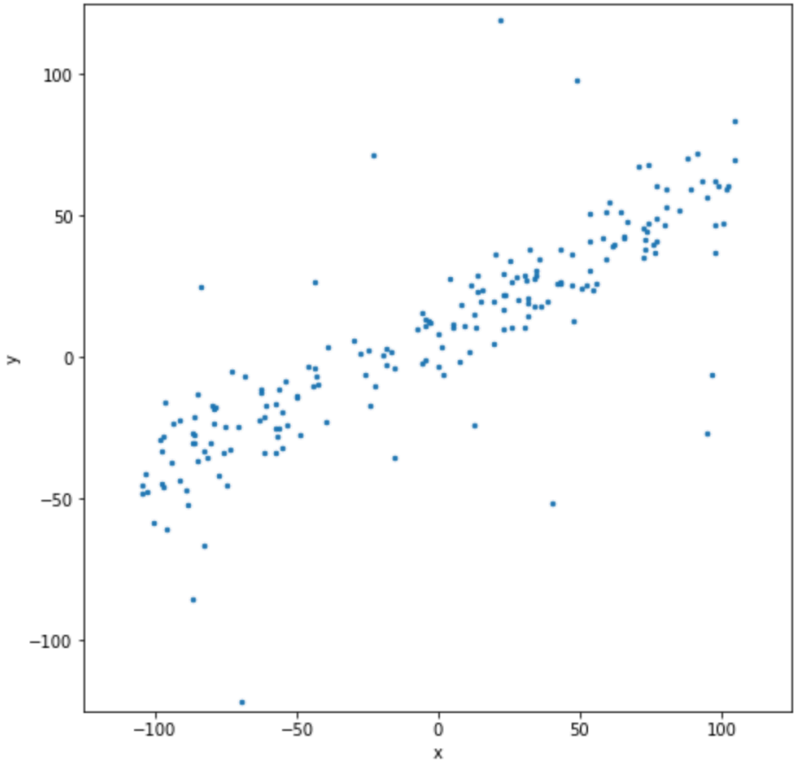
PRINCIPAL COMPONENTS ANALYSIS (PCA)

PRINCIPAL COMPONENTS ANALYSIS

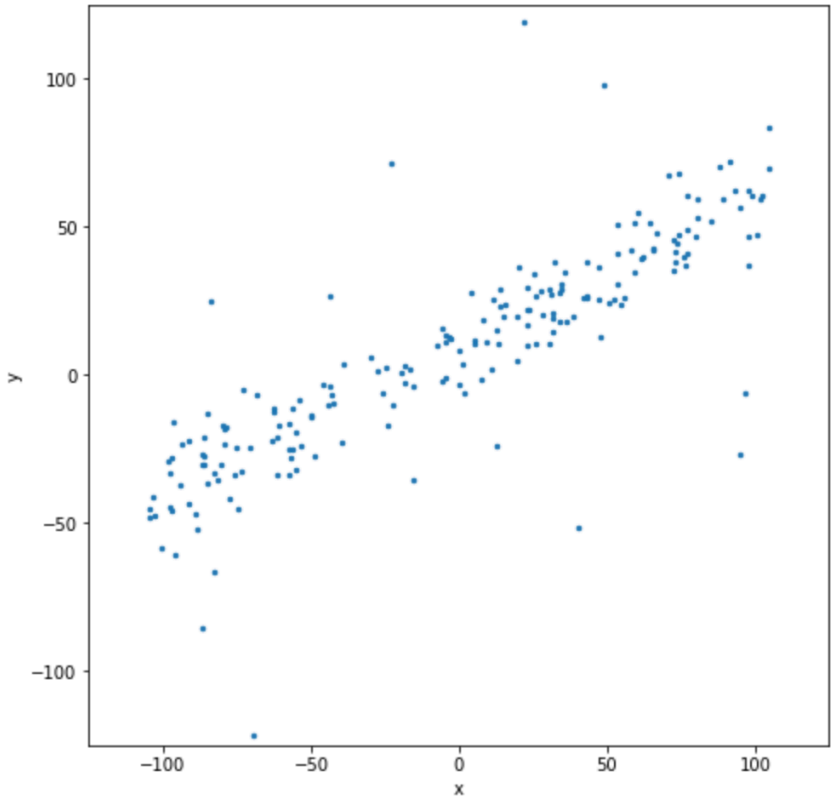
- Principal components analysis is a technique to compress data (reduce dimensionality) and is useful in classification.
- Goal is to find fewer basis vectors (called principal components) to represent the data.
- Most of the data variance (correlation between the original variables) is retained in the new dimensions.
- The principal components (new variables) are uncorrelated.

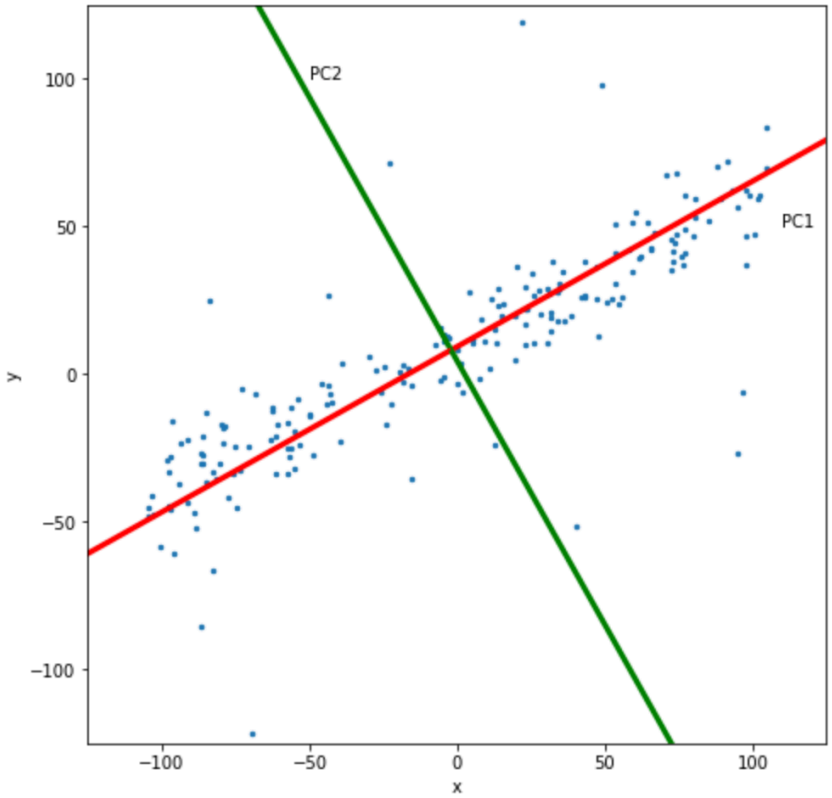
PCA - GEOMETRIC VIEW



n **observations in 2D space,**

PRINCIPAL COMPONENTS ANALYSIS - GEOMETRIC VIEW

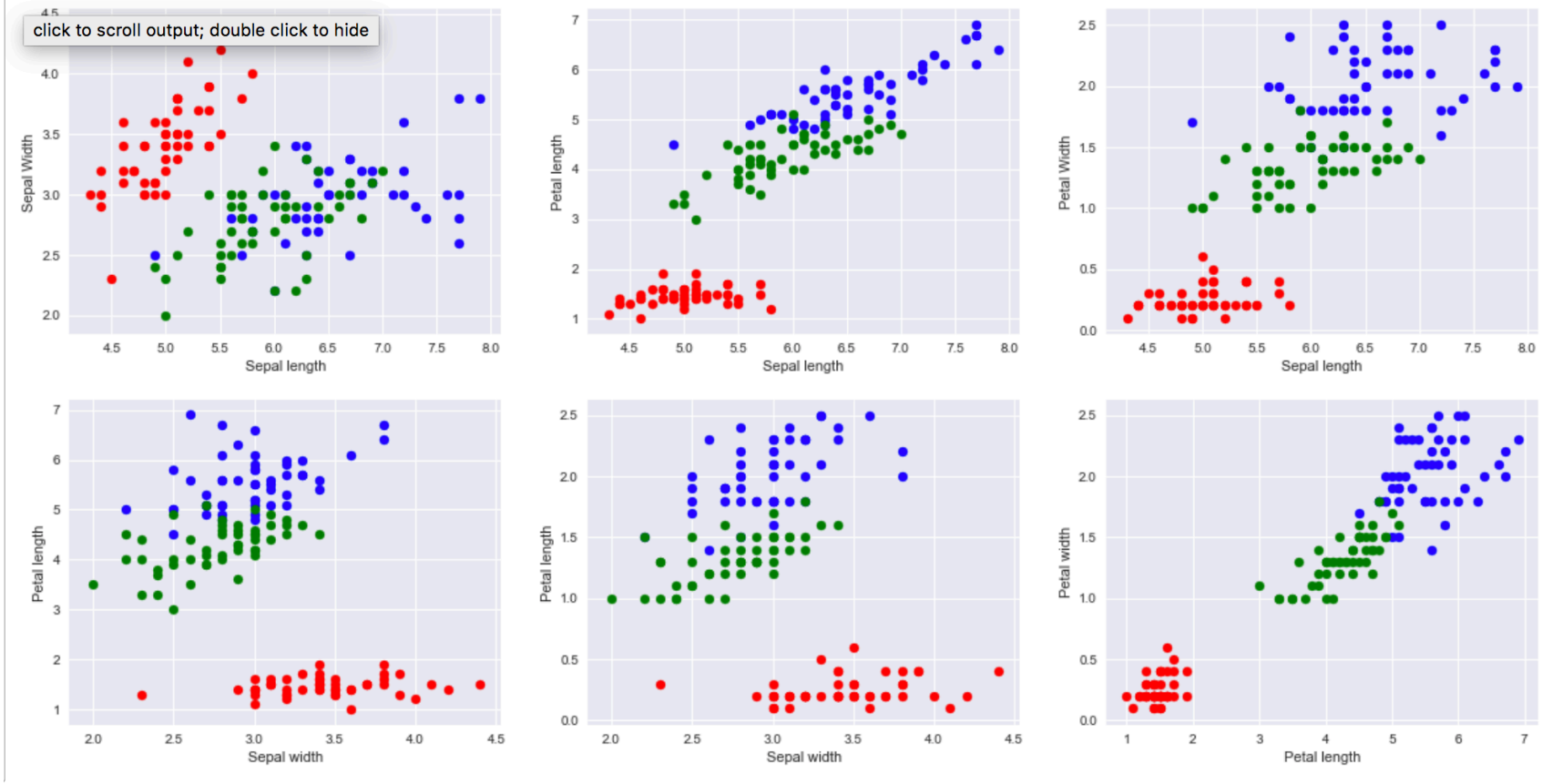




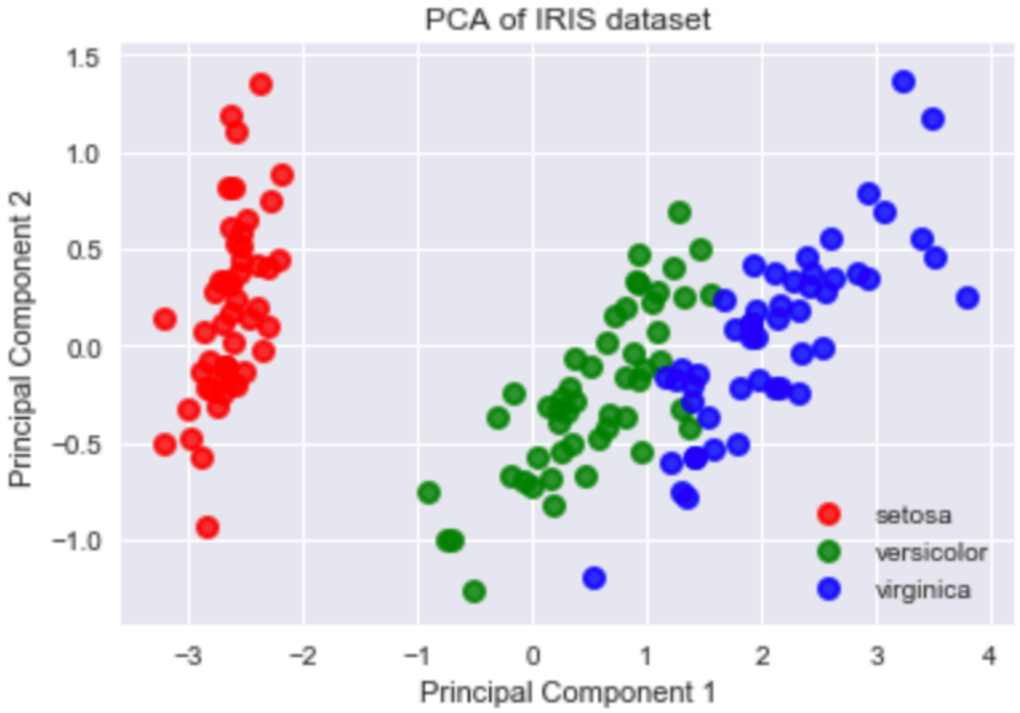
PCA - INTRODUCTION

	sepal_length	sepal_width	petal_length	petal_width	species
8	4.4	2.9	1.4	0.2	setosa
52	6.9	3.1	4.9	1.5	versicolor
35	5.0	3.2	1.2	0.2	setosa
127	6.1	3.0	4.9	1.8	virginica
96	5.7	2.9	4.2	1.3	versicolor

PCA - INTRODUCTION



PCA - INTRODUCTION



PRINCIPAL COMPONENT ANALYSIS

- A technique to find the directions along which the points (set of tuples) in high-dimensional data line up best.
- Treat a set of tuples as a matrix M and find the eigenvectors for M^TM (covariance matrix).
- The matrix of these eigenvectors can be thought of as a rigid rotation in a high-dimensional space.
- When this transformation is applied to the original data - the axis corresponding to the principal eigenvector is the one along which the points are most “spread out”.

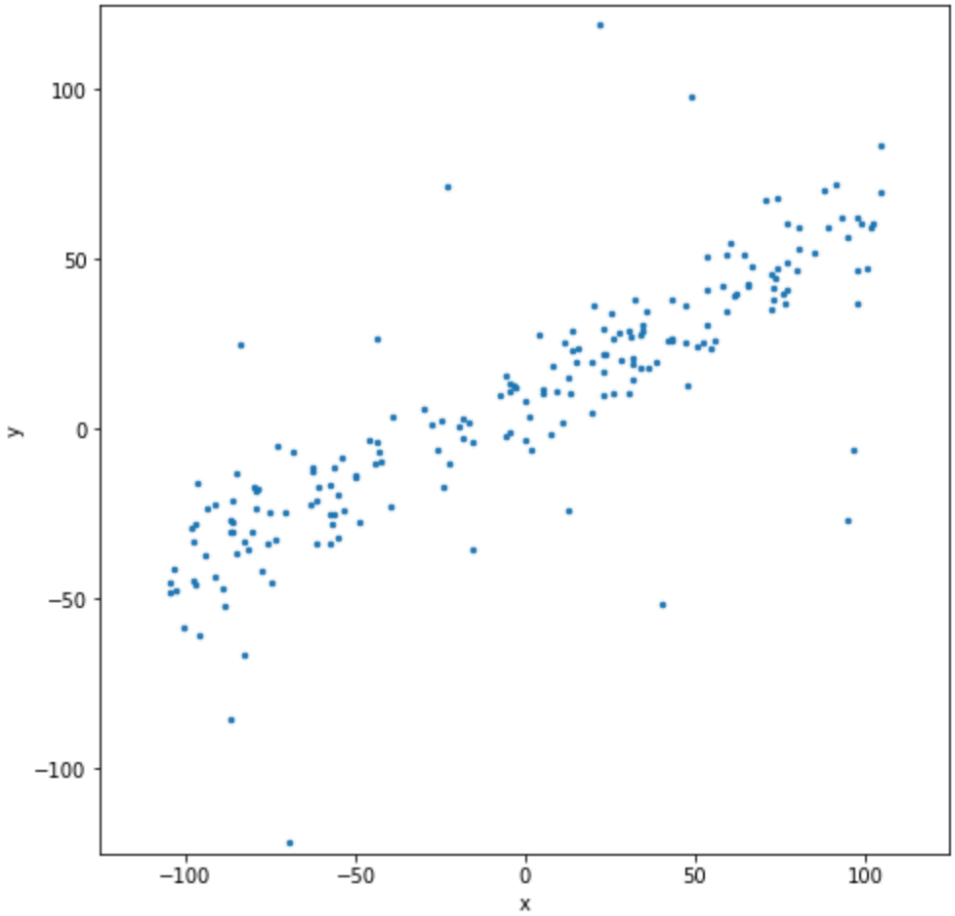
PRINCIPAL COMPONENT ANALYSIS

- When this transformation is applied to the original data - the axis corresponding to the principal eigenvector is the one along which the points are most “spread out”.
- This axis is the one along which variance of the data is maximized.
- Points can best be viewed as lying along this axis with small deviations from this axis.
- Likewise, the axis corresponding the second eigenvector is the axis along which the variance of distances from the first axis is greatest, and so on.

PRINCIPAL COMPONENT ANALYSIS

- Principal Component Analysis (PCA) is a dimensionality reduction method.
- The goal is to embed data in high dimensional space, onto a small number of dimensions.
- It most frequent use is in exploratory data analysis and visualization.
- It can also be helpful in regression (linear or logistic) where we can transform input variables into a smaller number of predictors for modeling.

PCA STEPS -
STEP 1 MEAN SUBTRACTION



PCA STEPS -
STEP 2 COVARIANCE MATRIX

```
array([[-84.07963403, -29.20401342],
       [-94.40799878, -24.21822549],
       [-20.0794366 , -18.24247399],
       [ 62.63769935,  46.8234735 ]])
```

top 5 rows of mean centered data

```
array([[3881.30854873, 1897.16347756],
       [1897.16347756, 1557.15527689]])
```

Eigen decomposition of covariance matrix, $X^T X$

PCA STEPS -
STEP 3 EIGEN VALUES & EIGEN VECTORS OF COVARIANCE MATRIX

```
eig_vals, eig_vecs = np.linalg.eig(cov)
```

```
eig_vals
```

```
array([4944.01310842,  494.4507172 ])
```

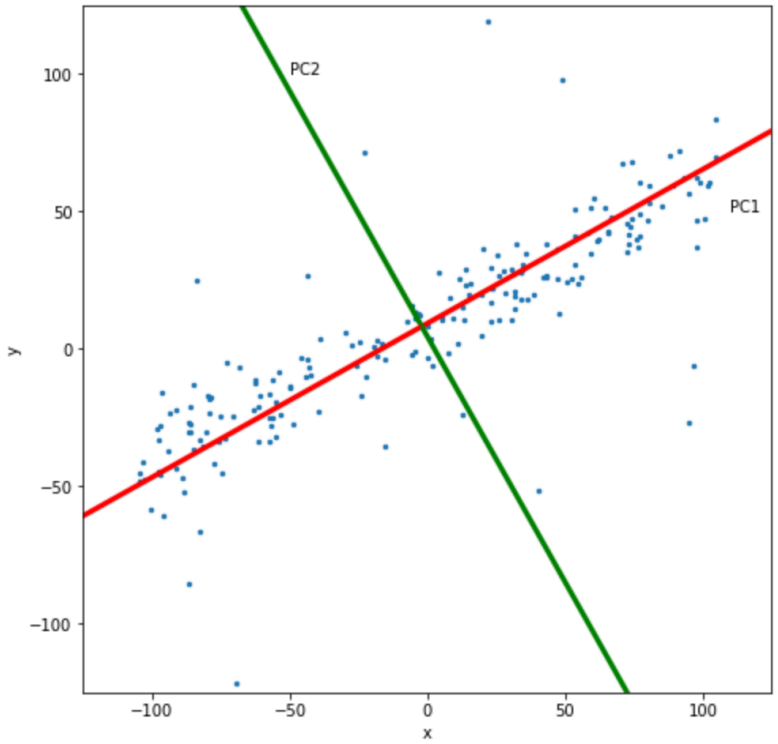
```
eig_vecs
```

```
array([[ 0.87244857, -0.48870594],
       [ 0.48870594,  0.87244857]])
```

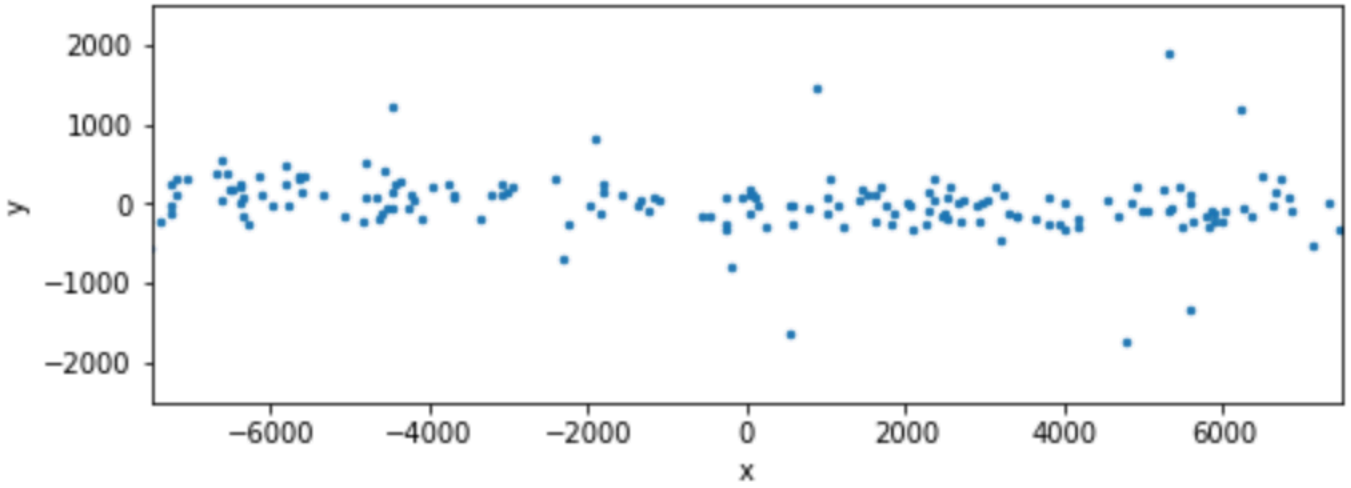
PCA STEPS -
STEP 4 - PRINCIPAL COMPONENTS

Multiply each eigen vector by its corresponding eigen value (usually square root)

Plot them on top of the data



PCA STEPS -
STEP 5 - PROJECT DATA ALONG DOMINANT PC



In general, transformed data, $T = WX^T$

Where X is our original data and W is the Principal components matrix
Each column of W is a principal component

PRINCIPAL COMPONENT ANALYSIS

- **Mathematically,**

  Given: Data set $\{x_1, x_2, \ldots, x_n\}$

  where, x_i **is the vector of p variable values for the i-th observation.**

  Return:

  Matrix $[\phi_1, \phi_2, \ldots, \phi_p]$

  of linear transformations that retain maximal variance.

  $\phi_1 = (\phi_{11}, \phi_{21}, \ldots, \phi_{p1})$

- **You can think of the first vector** ϕ_1 **as a linear transformation that embeds observations into 1 dimension**

$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \ldots + \phi_{p1}X_p$$

PRINCIPAL COMPONENT ANALYSIS

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$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \ldots + \phi_{p1}X_p$$

where ϕ_1 is selected so that the resulting dataset $\{z_i, \ldots, z_n\}$ has maximum variance.

- **In order for this to make sense, mathematically, data has to be centered**
  - **Each X_i has zero mean**
  - **Transformation vector ϕ_1 has to be normalized, i.e., $\sum_{j=1}^{p} \phi_{j1}^2 = 1$**

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- We can find ϕ_1 by solving an optimization problem:

$$\max_{\phi_{11},\phi_{21},\ldots,\phi_{p1}} \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j1} x_{ij} \right)^2 \text{ s.t. } \sum_{j=1}^{p} \phi_{j1}^2 = 1$$

Maximize variance but subject to normalization constraint.

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  Maximize variance but subject to normalization constraint.

- **The second transformation, ϕ_2 is obtained similarly with the added constraint that ϕ_2 is orthogonal to ϕ_1**

- **Taken together $[\phi_1, \phi_2]$ define a pair of linear transformations of the data into 2 dimensional space**

$$Z_{n\times 2} = X_{n\times p}[\phi_1, \phi_2]_{p\times 2}$$

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- Each of the columns of the Z matrix are called Principal components.
- The units of the PCs are meaningless.
- In practice we may also scale X_j to have unit variance.
- In general if variables X_j are measured in different units(e.g., miles vs. liters vs. dollars), variables should be scaled to have unit variance.

HOW MANY PRINCIPAL COMPONENTS ?

- How many PCs should we consider in post-hoc analysis?
- One result of PCA is a measure of the variance to each PC relative to the total variance of the dataset.
- We can calculate the percentage of variance explained for the m-th PC:

$$PVE_m = \frac{\sum_{i=1}^{n} z_{im}^2}{\sum_{j=1}^{p} \sum_{i=1}^{n} x_{ij}^2}$$

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