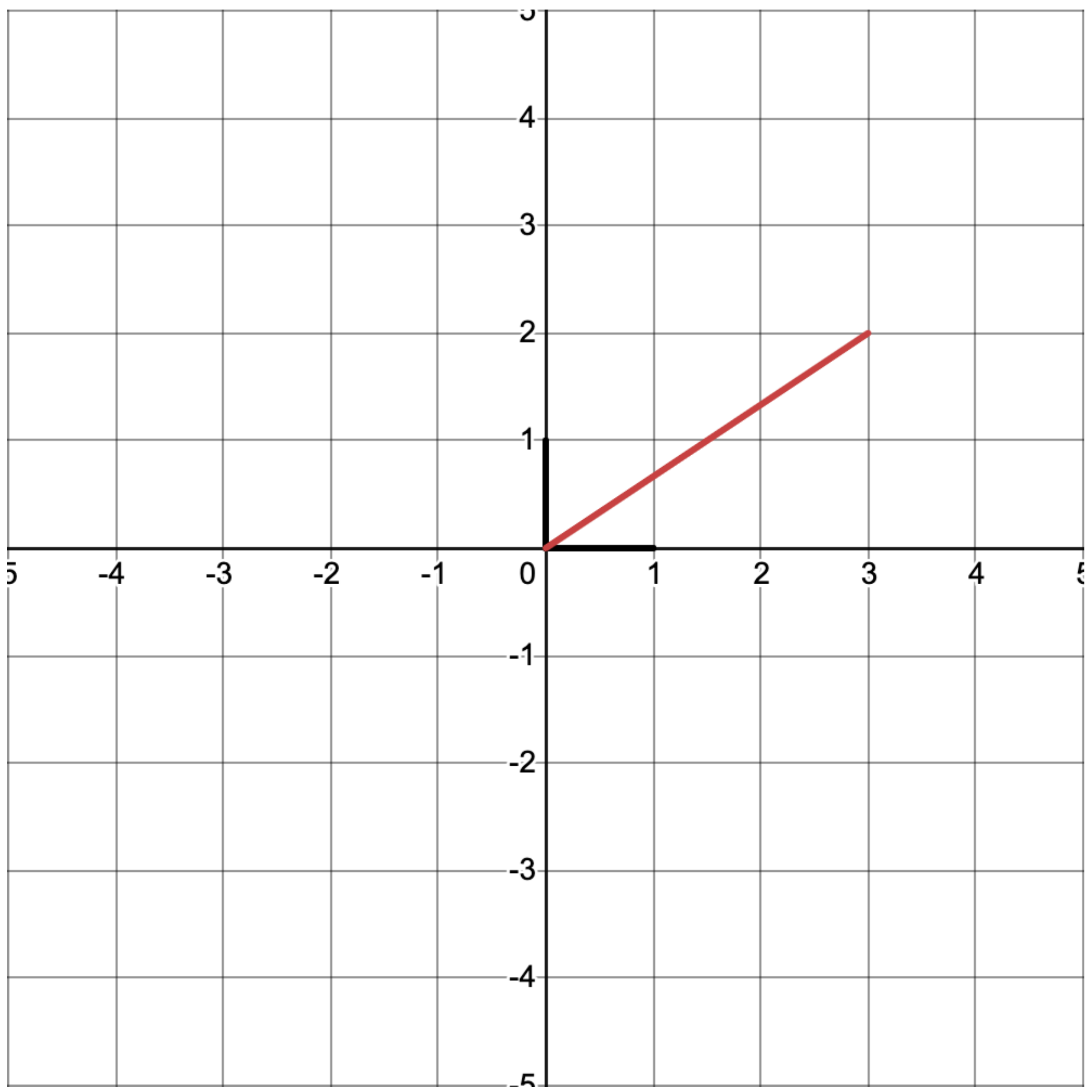
Week 6: SVD & PCA

Index

Change of Basis

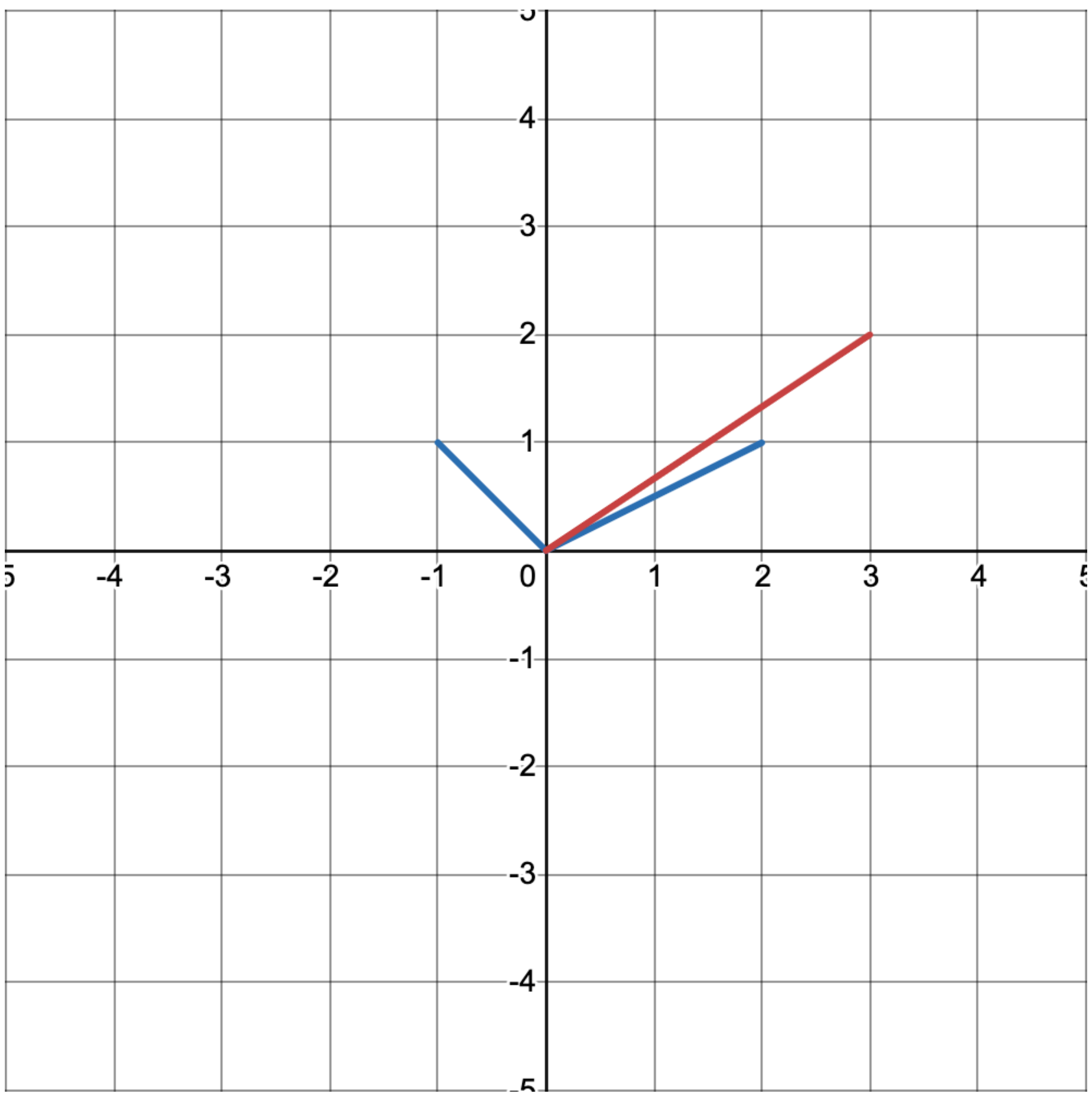


Standard Basis

$$\mathbb{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \mathbb{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\mathbb{x} = 3\begin{bmatrix} 1 \\ 0 \end{bmatrix} + 2\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

Change of Basis



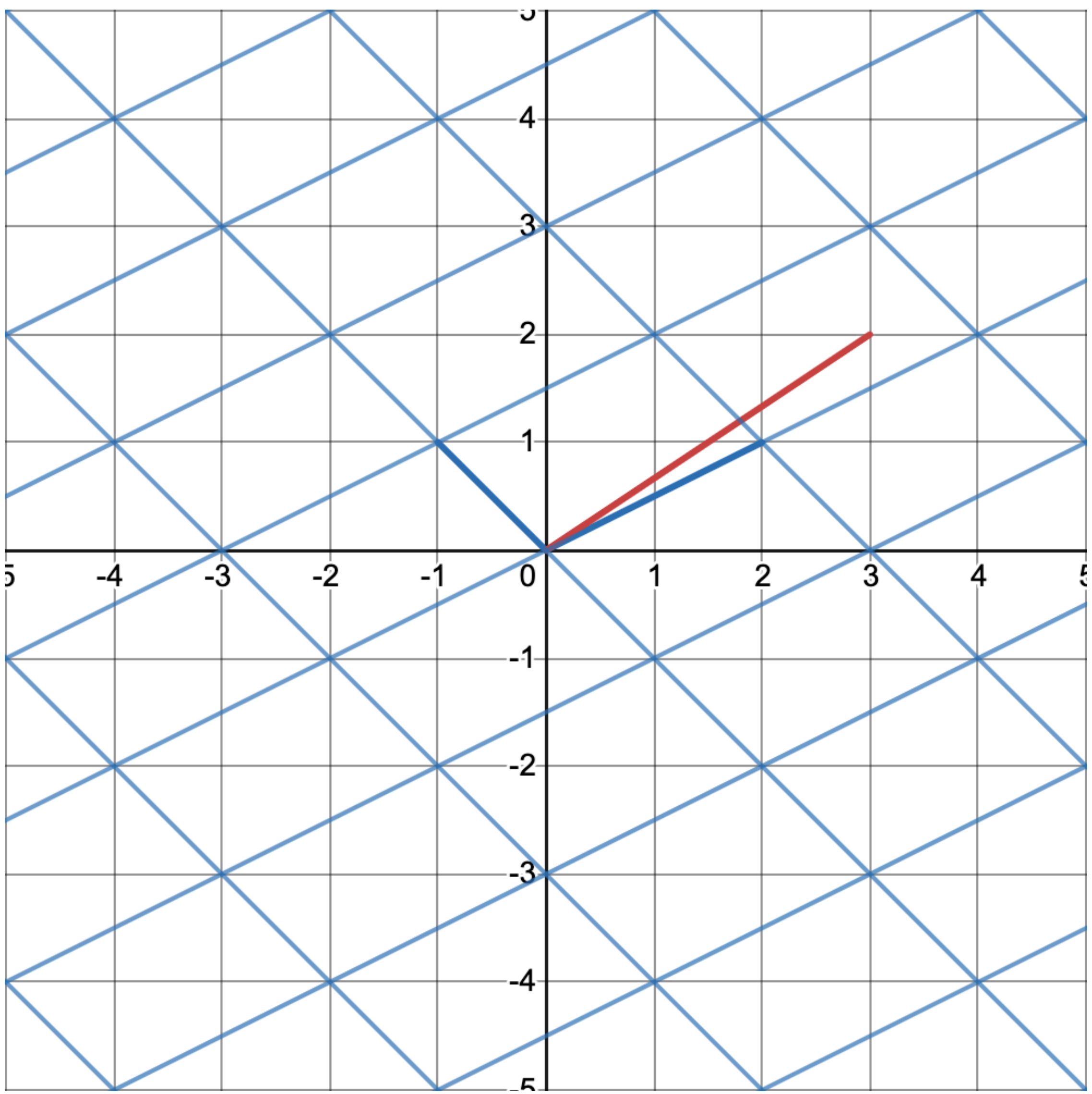
New Basis

$\mathbb{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $\quad$ $\mathbb{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

$\Downarrow$

$\mathbb{b}_1 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$ $\quad$ $\mathbb{b}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$

Change of Basis



New Basis

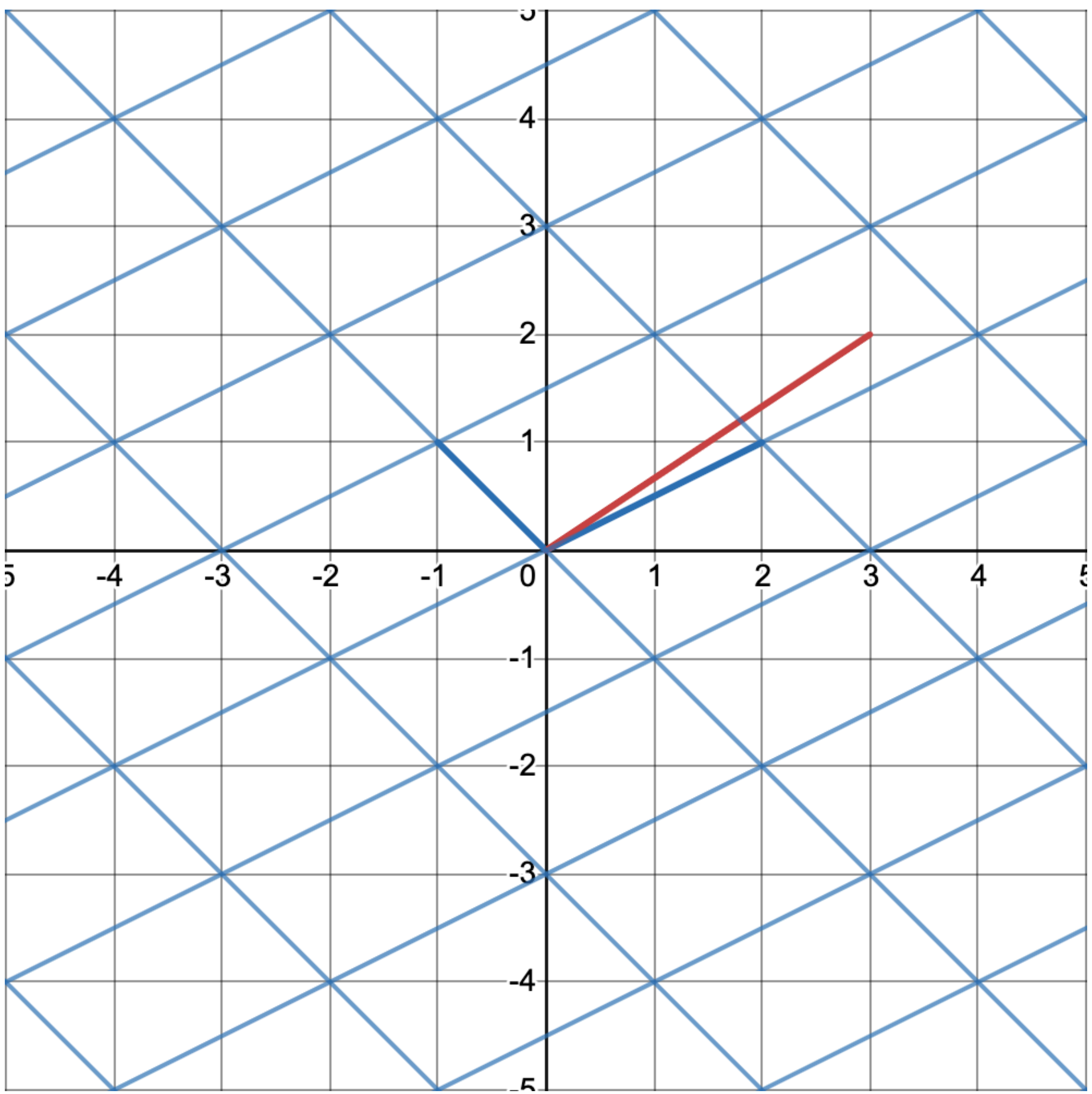
$$\mathbb{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \mathbb{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\Downarrow$$

$$\mathbb{b}_1 = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \qquad \mathbb{b}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$\mathbb{x} = \begin{bmatrix} 3 \\ 2 \end{bmatrix} \Rightarrow \mathbb{x}' = \begin{bmatrix} ? \\ ? \end{bmatrix}$$

Change of Basis



New Basis

$$\mathbb{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \mathbb{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

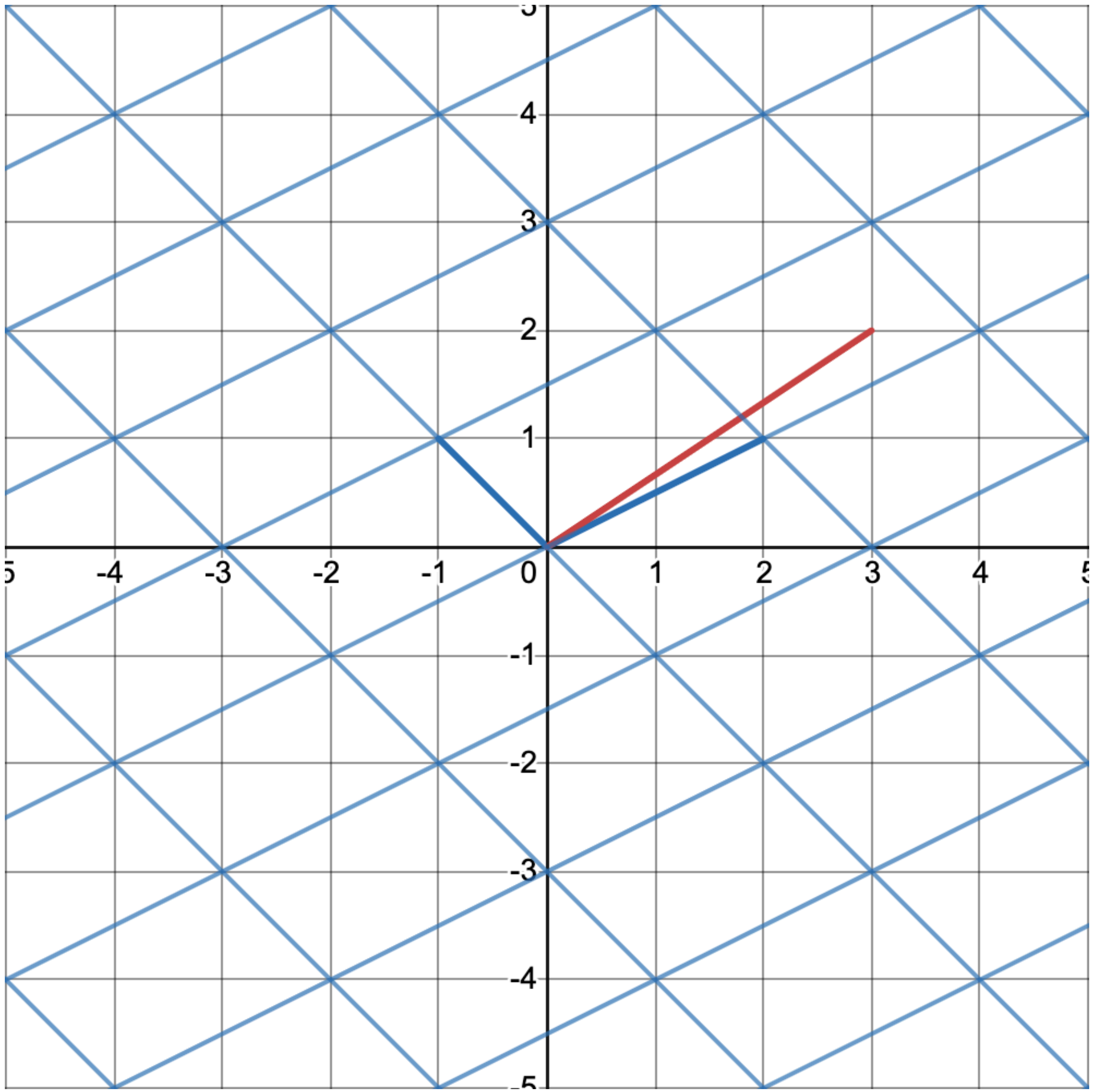
$$\Downarrow$$

$$\mathbb{b}_1 = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \qquad \mathbb{b}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

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

Transition Matrix $P_{B \to S} = P$

Change of Basis



New Basis

$$\mathbb{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \mathbb{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

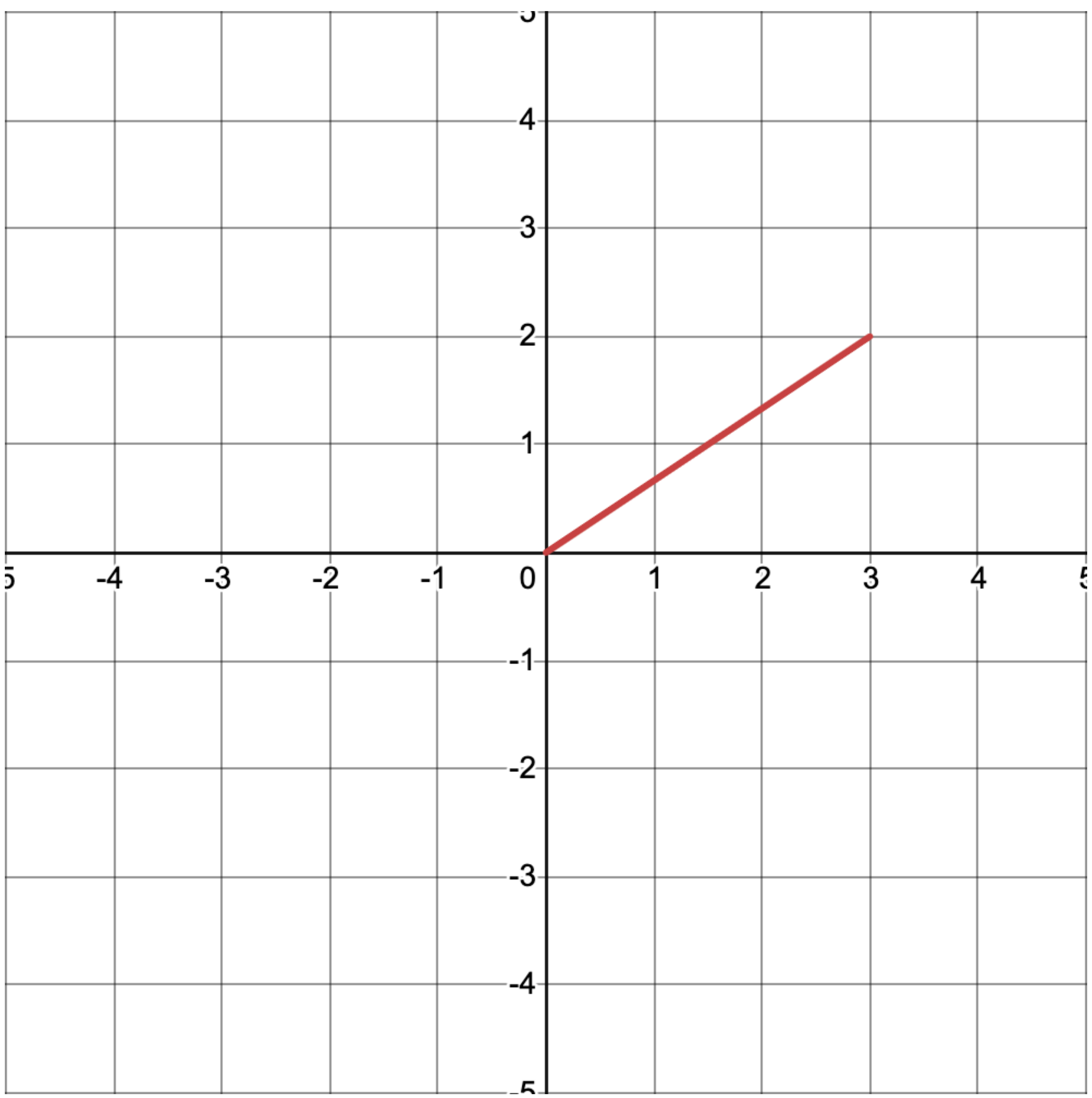
$$\Downarrow$$

$$\mathbb{b}_1 = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \qquad \mathbb{b}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$\mathbb{x}' = \boxed{\begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix}^{-1}} \begin{bmatrix} 3 \\ 2 \end{bmatrix} = \begin{bmatrix} 5/3 \\ 1/3 \end{bmatrix}$$

Transition Matrix $P_{S \to B} = P^{-1}$

Matrix Transformation with New Coordinates



Matrix Transformation

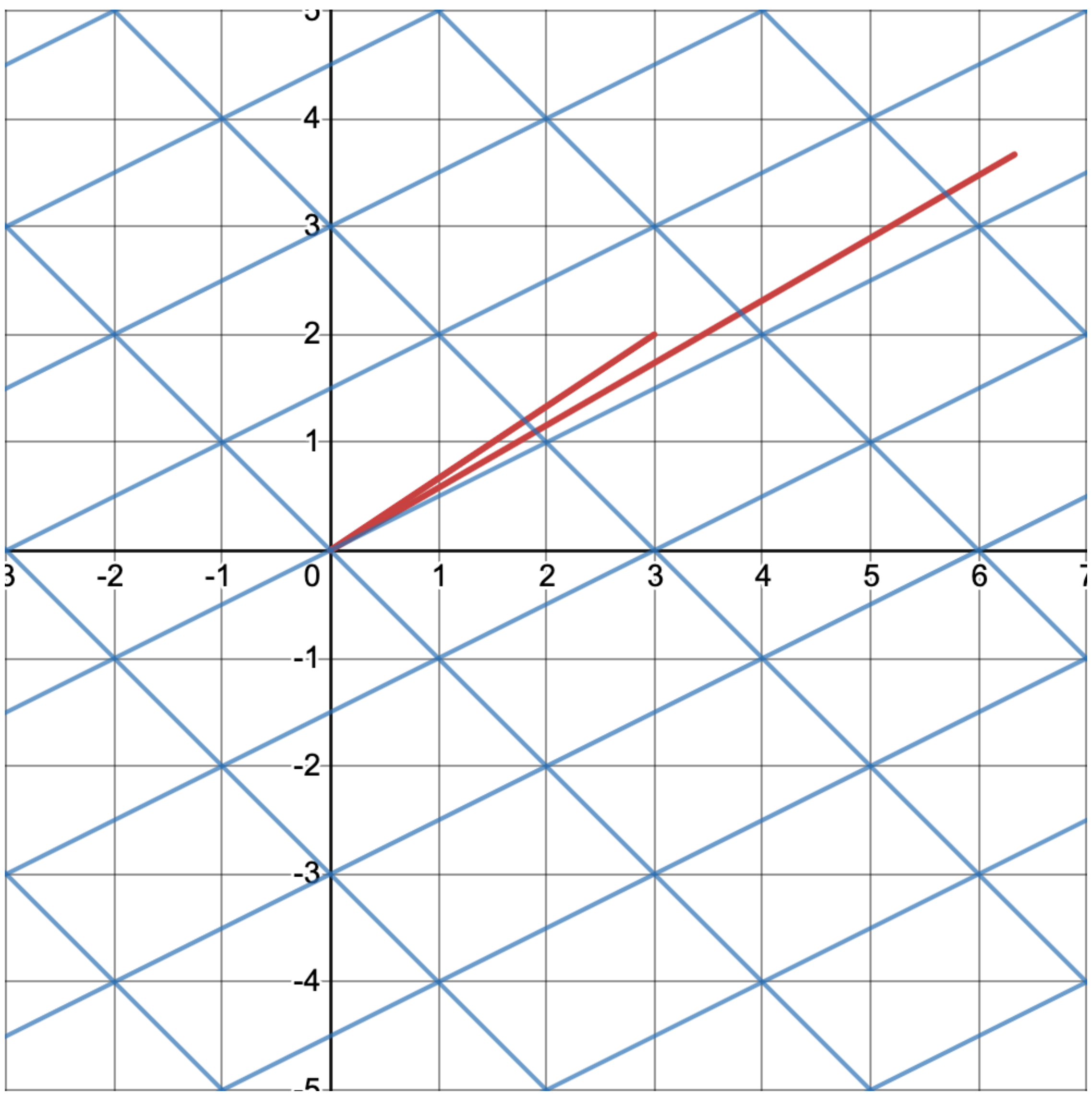
$$A = \begin{bmatrix} 5/3 & 2/3 \\ 1/3 & 4/3 \end{bmatrix}$$

$$A\mathbb{x} = ?$$

Standard Coordinates 상의 선형 변환 A는

New Coordinates에서 어떠한 변환으로 나타날까?

Matrix Transformation with New Coordinates



Matrix Transformation

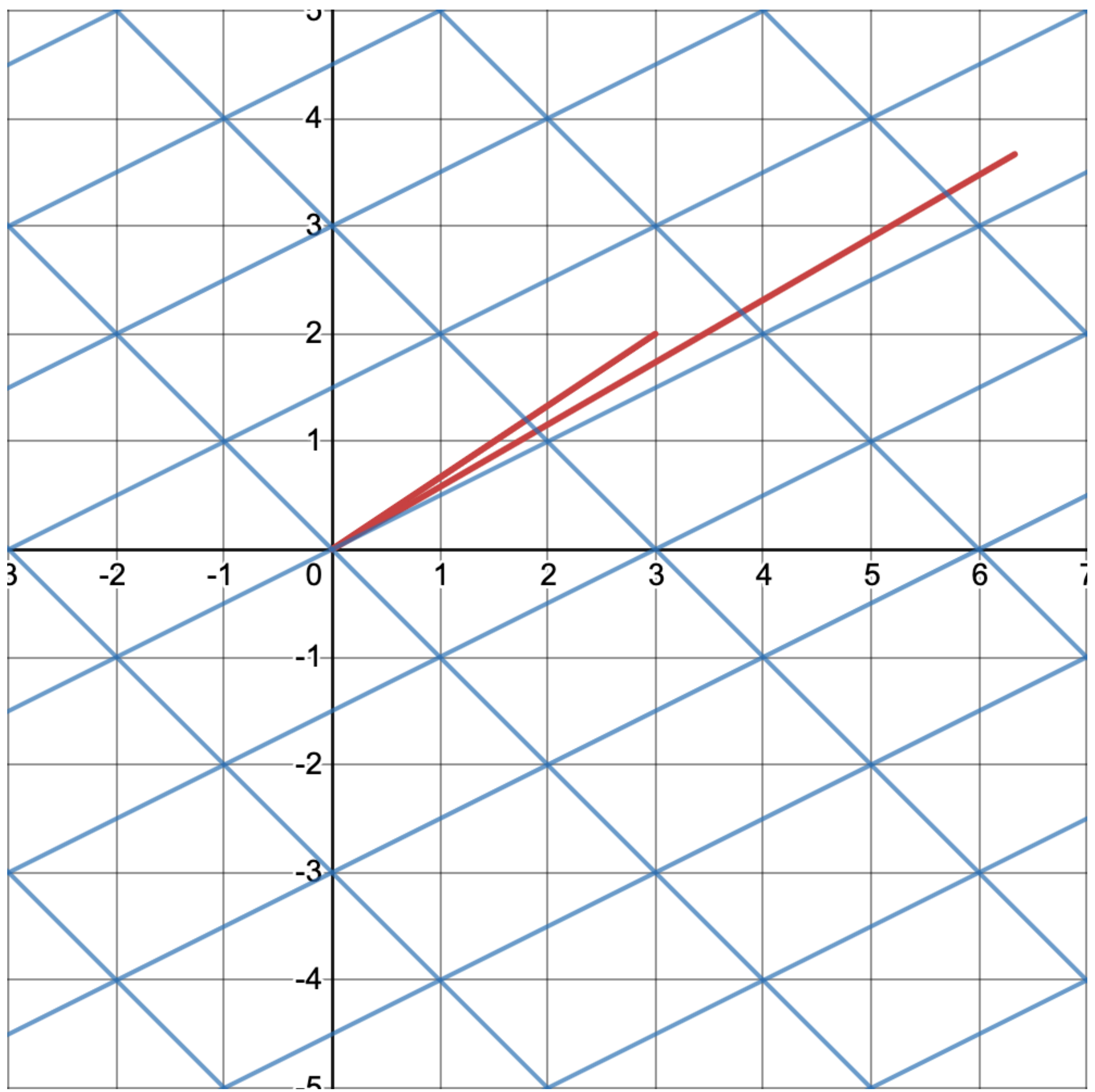
$$A = \begin{bmatrix} 5/3 & 2/3 \\ 1/3 & 4/3 \end{bmatrix}$$

$$\underbrace{\begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix}^{-1}}_{P^{-1}} \underbrace{\color{red}{\begin{bmatrix} 3 \\ 2 \end{bmatrix}}}_{\color{red}{\mathbb{x}}} = A\color{red}{\mathbb{x}}$$

$$\underbrace{\begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}}_{C} \underbrace{\begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix}}_{P^{-1}} \underbrace{\color{red}{\begin{bmatrix} 3 \\ 2 \end{bmatrix}}}_{\color{red}{\mathbb{x}}} = A\color{red}{\mathbb{x}}$$

$$\underbrace{\begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix}}_{P} \underbrace{\begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}}_{C} \underbrace{\begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix}^{-1}}_{P^{-1}} \underbrace{\color{red}{\begin{bmatrix} 3 \\ 2 \end{bmatrix}}}_{\color{red}{\mathbb{x}}} = A\color{red}{\mathbb{x}}$$

Matrix Transformation with New Coordinates



Matrix Transformation

$$A = \begin{bmatrix} 5/3 & 2/3 \\ 1/3 & 4/3 \end{bmatrix}$$

$$\underset{P}{\begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix}} \underset{C}{\begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}} \underset{P^{-1}}{\begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix}^{-1}} \underset{\mathbb{x}}{\begin{bmatrix} 3 \\ 2 \end{bmatrix}} = A\mathbb{x}$$

$$C = P^{-1}AP = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}$$

Standard Coordinates 상의 선형변환 A는

New Coordinates에서의 선형변환 C와 같다.

Diagonalization

$$A = PDP^{-1}$$

만약 C가 Diagonal Matrix라면?

Standard Coordinates 상의 선형변환 A는

New Coordinates에서의 **Stretching**과 같다!

Diagonalization

$$A = PDP^{-1}$$

만약 C가 Diagonal Matrix라면?

Standard Coordinates 상의 선형변환 A는

New Coordinates에서의 **Stretching**과 같다!

$$AP = PD$$

$$[A\mathbb{p}_1 \quad A\mathbb{p}_2 \quad \cdots \quad A\mathbb{p}_n] = [d_1\mathbb{p}_1 \quad d_2\mathbb{p}_2 \quad \cdots \quad d_n\mathbb{p}_n]$$

$d_1, d_2, \dots, d_n$: A의 Eigenvalue

$\mathbb{p}_1, \mathbb{p}_2, \dots, \mathbb{p}_n$: A의 Eigenvector

Standard Coordinates 상의 선형변환 A는

A의 Eigenvector를 Basis로 갖는 New Coordinates에서의

A의 Eigenvalue만큼의 **Stretching**과 같다!

Spectral Decomposition / Eigenvalue Decomposition

Singular Value Decomposition

A가 *Square Matrix*가 아니라면?

$$A = U\Sigma V^T$$

$A_{m\times n}\ (m > n)$

$\mathrm{rank}(A) = k$

A^TA의 Eigenvector

$$\begin{bmatrix} \mathbb{u}_1 & \mathbb{u}_2 & \cdots & \mathbb{u}_m \end{bmatrix} \begin{bmatrix} \sqrt{\lambda_1} & 0 & \cdots & 0 \\ 0 & \sqrt{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{\lambda_n} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} \mathbb{v}_1^T \\ \mathbb{v}_2^T \\ \vdots \\ \mathbb{v}_n^T \end{bmatrix}$$

AA^T의 Eigenvector

AA^T or A^TA의 Eigenvalue

$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq \lambda_{k+1} = \cdots = \lambda_n = 0$

Singular Value Decomposition

$$A = U\Sigma V^T$$

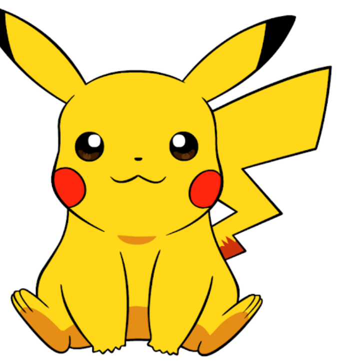
n차원의 Standard Coordinates를
$A^T A$의 Eigenvector를 Basis로 갖는 n차원의 New Coordinates로 변환

$A^T A$의 Eigenvector를 Basis로 갖는 n차원의 New Coordinates상의 벡터를
m차원으로 $A^T A$의 Eigenvalue 만큼 Stretching

m차원의 New Coordinates를 m차원의 Standard Coordinates로 변환

Singular Value Decomposition

```r
library(EBImage)

pika = readImage('pika.png')

display(pika, method='raster')

dim(pika) # [1] 512 504   3

img_comp = function(img, rank){
  matrix = imageData(img)

  r = svd(matrix[,,1])
  g = svd(matrix[,,2])
  b = svd(matrix[,,3])

  r_svd = r$u[,1:rank] %*% diag(r$d[1:rank]) %*% t(r$v[,1:rank])
  g_svd = g$u[,1:rank] %*% diag(g$d[1:rank]) %*% t(g$v[,1:rank])
  b_svd = b$u[,1:rank] %*% diag(b$d[1:rank]) %*% t(b$v[,1:rank])

  matrix = rgbImage(r_svd, g_svd, b_svd)
  display(matrix, method='raster', all=TRUE)
}

img_comp(pika, rank)
```

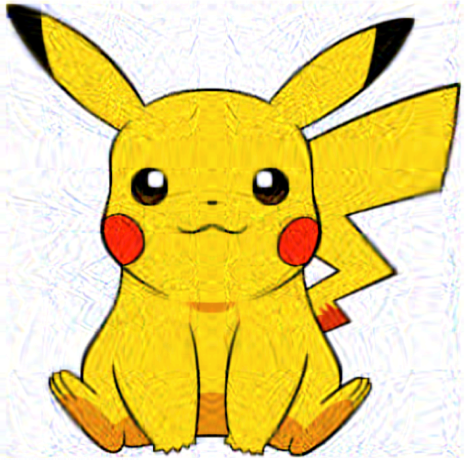


$$
\begin{aligned}
A_r &= U_r \Sigma_r V_r^T \\
&= \begin{bmatrix} \mathbb{u}_1 & \mathbb{u}_2 & \cdots & \mathbb{u}_r \end{bmatrix} \begin{bmatrix} \sigma_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_r \end{bmatrix} \begin{bmatrix} \mathbb{v}_1^T \\ \mathbb{v}_2^T \\ \vdots \\ \mathbb{v}_r^T \end{bmatrix} \\
&= \sigma_1 \mathbb{u}_1 \mathbb{v}_1 + \sigma_2 \mathbb{u}_2 \mathbb{v}_2 + \cdots + \sigma_r \mathbb{u}_r \mathbb{v}_r
\end{aligned}
$$

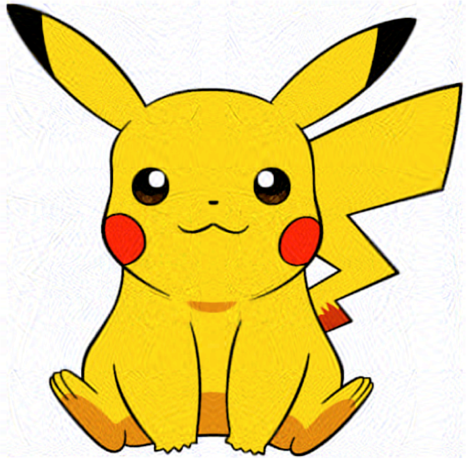
Singular Value Decomposition

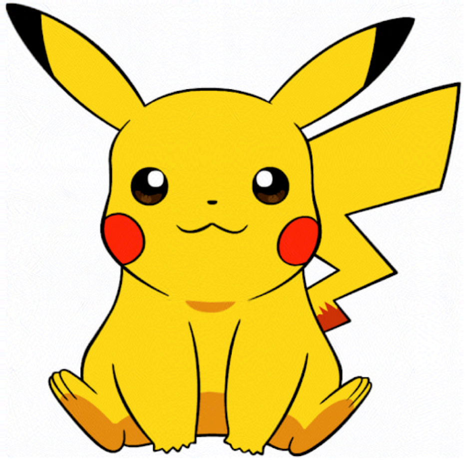
Rank 10

Rank 50

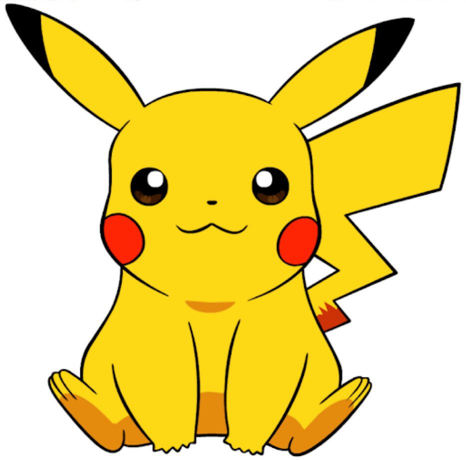


Rank 100





Rank 200



Original

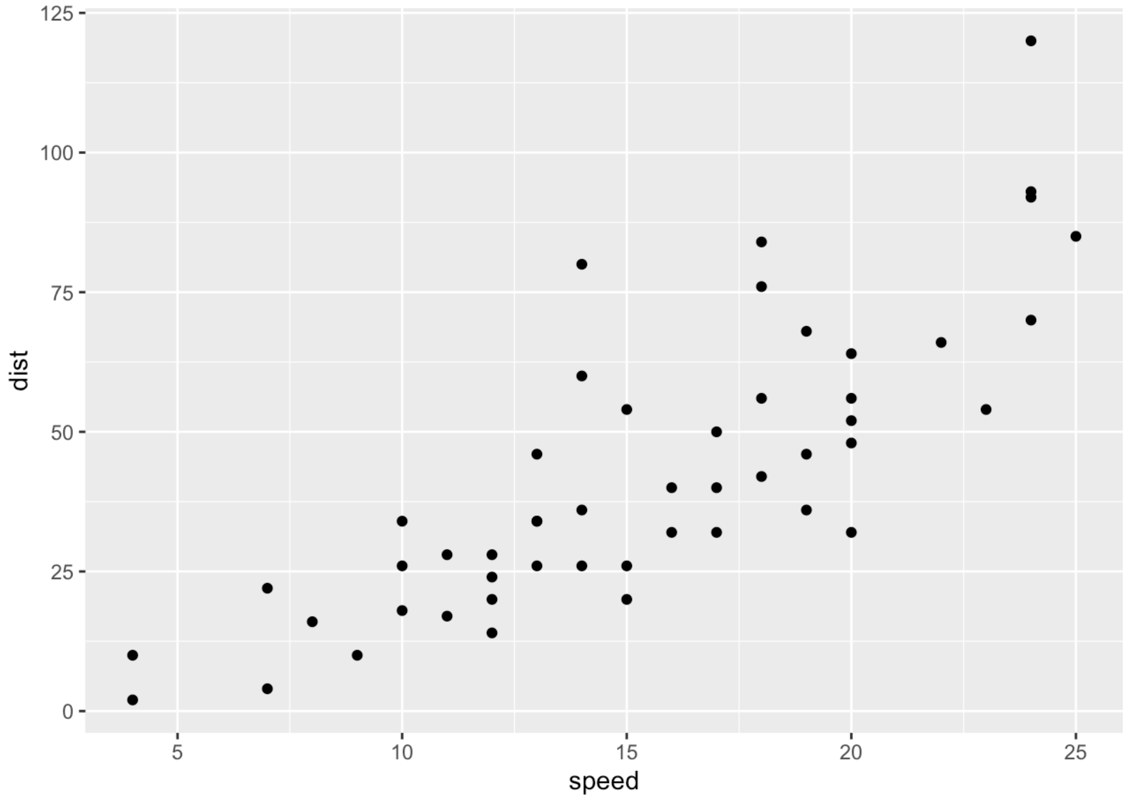
Principal Component Analysis

데이터를 어떠한 축에 투영시킴으로써 차원을 축소하는 방법

Assumption

1. 데이터가 선형 관계에 있다.
2. Scaled된 데이터를 사용한다.

다음과 같은 2차원의 데이터를 1차원으로 축소해보자!



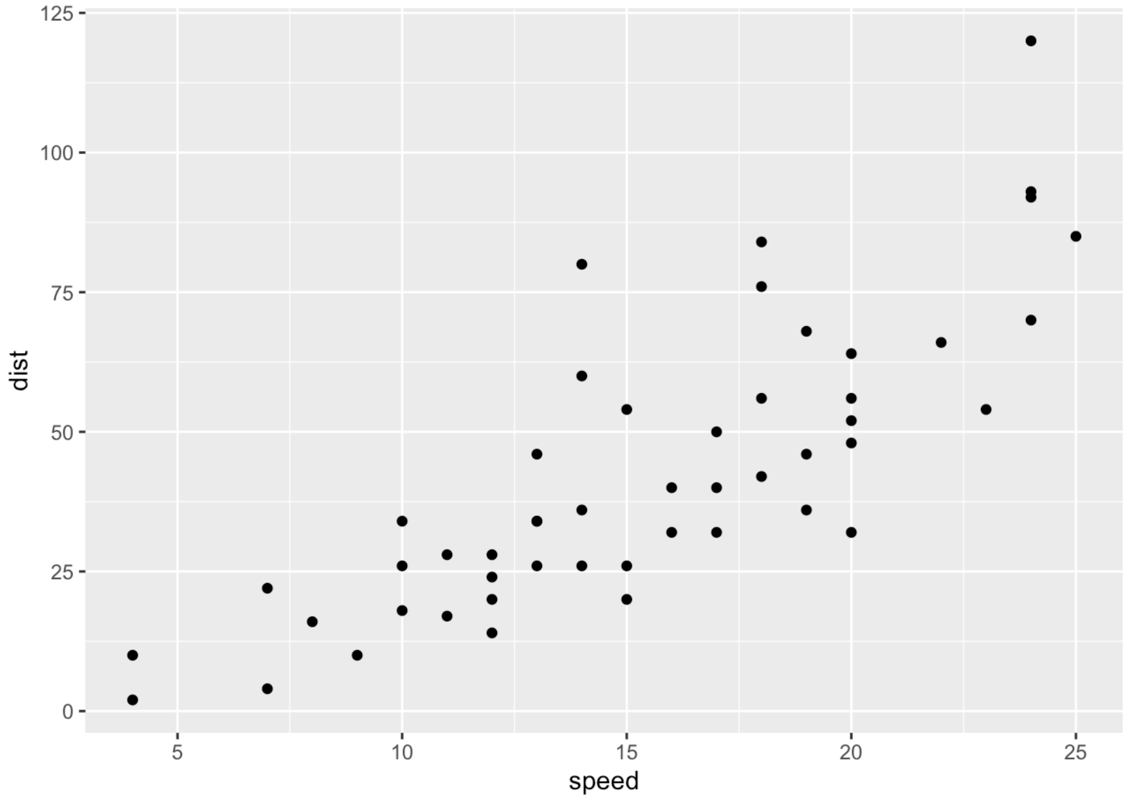
Principal Component Analysis

데이터를 어떠한 축에 투영시킴으로써 차원을 축소하는 방법

- 투영 이후 데이터의 분산이 최대화 되는 축
- 기존 데이터와 투영된 데이터 사이의
  평균제곱거리를 최소화하는 축

⇒ 데이터의 *Covariance Matrix*의 Eigenvalue가
가장 큰 Eigenvector가 Span하는 Line에
데이터를 투영했을 때 데이터의 분산이 최대화 된다.

가장 큰 Eigenvalue를 갖는 Eigenvector에 투영하자!



Principal Component Analysis

Covariance Matrix의 Eigenvalue와 Eigenvector를 구해야 한다!

Covariance Matrix

$$X = \begin{bmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \cdots & x_{mn} \end{bmatrix}$$

$$A = \begin{bmatrix} x_{11} - \mu_1 & \cdots & x_{1n} - \mu_n \\ \vdots & \ddots & \vdots \\ x_{m1} - \mu_1 & \cdots & x_{mn} - \mu_n \end{bmatrix}$$

$$S = \frac{A^T A}{n-1}$$

$A^T A$의 Eigenvalue & Eigenvector?

1. 직접 계산하거나
2. SVD를 활용 $A = U\Sigma V^T$

V의 Column Vector = $A^T A$의 Eigenvector

Principal Component Analysis

Covariance Matrix의 Eigenvalue와 Eigenvector를 구해야 한다!

```r
A = cars %>%
  mutate(speed=speed-mean(speed), dist=dist-mean(dist)) %>%
  as.matrix

S = t(A) %*% A / (nrow(A)-1)

eigen(S)

# eigen() decomposition
# $values
# [1] 682.528426   9.491574

# $vectors
#            [,1]       [,2]
# [1,] 0.1656479 -0.9861850
# [2,] 0.9861850  0.1656479

svd(A)$v

#             [,1]       [,2]
# [1,] -0.1656479 -0.9861850
# [2,] -0.9861850  0.1656479
```

$A^T A$의 Eigenvalue & Eigenvector?

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svd(A)$v

#             [,1]       [,2]
# [1,] -0.1656479 -0.9861850
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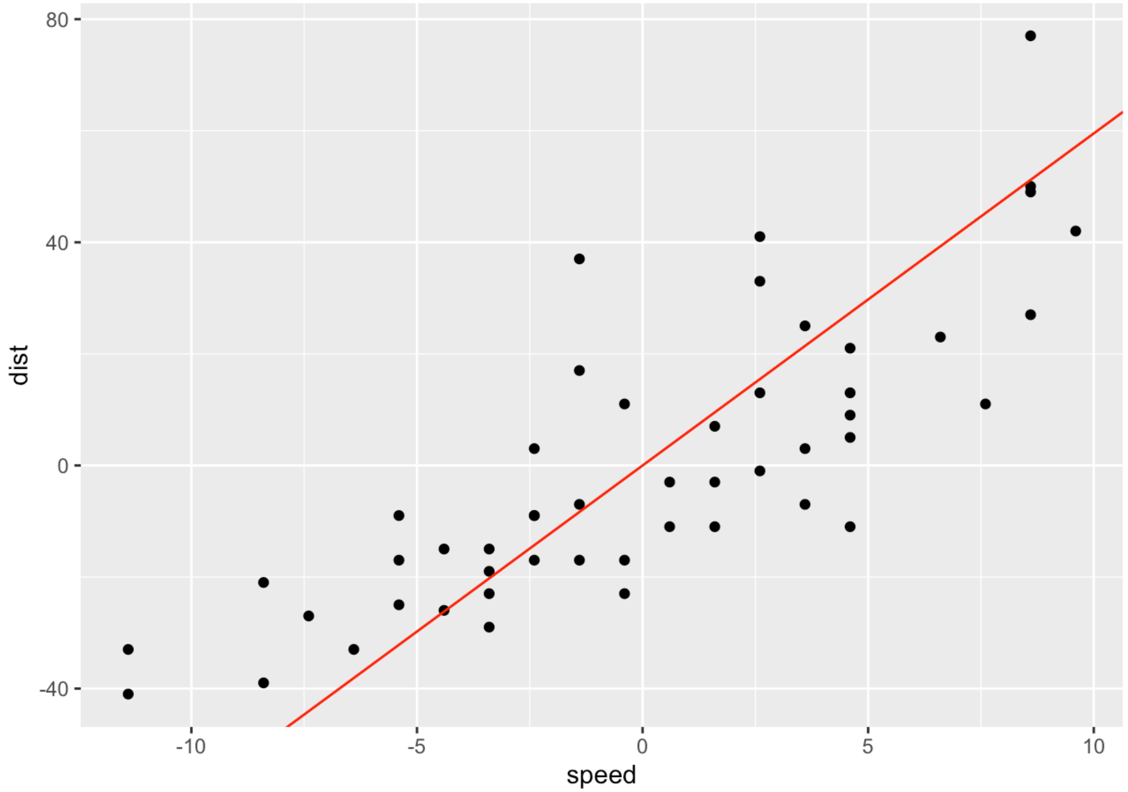
```



Principal Component Analysis

데이터를 어떠한 축에 투영시킴으로써 차원을 축소하는 방법

```
eigen_vector = as.matrix(c(0.1656479, 0.9861850))

PCA = as.data.frame((A %*% eigen_vector) %*% t(eigen_vector))

PCA %>%
  ggplot(aes(V1, V2)) + geom_point() +
  geom_segment(aes(x=0, y=0, xend=0.1656479*50, yend=0.9861850*50), color='red', arrow=arrow())
```