Singular Value Decomsition

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Definition of Matrix

Define an $m \times n$ matrix $\mathbf{A}$

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{i1} & a_{i2} & \dots & a_{in} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix} = (a_{ij}) = \begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \\ \vdots \\ \mathbf{R}_m \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{C}_1 & \mathbf{C}_2 & \dots & \mathbf{C}_n \end{pmatrix}$$

where

$$\mathbf{R}_i = i\text{-th } 1 \times n \text{ row vector, } i = 1, \dots, m$$

$$\mathbf{C}_j = j\text{-th } m \times 1 \text{ column vector, } j = 1, \dots, n$$

Spectral Decomposition

Each symmetric matrix $\mathbf{A}(p \times p)$ can be written as

$$\mathbf{A} = \mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Gamma}^T = \sum_{j=1}^{p} \lambda_j \gamma_j \gamma_j^T$$

where

$$\mathbf{\Lambda} = \mathrm{diag}\{\lambda_1, \ldots, \lambda_p\} = \begin{pmatrix} \lambda_1 & 0 & \ldots & 0 \\ 0 & \lambda_2 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & \lambda_p \end{pmatrix} : p \times p$$

where

$$\mathbf{\Gamma} = (\gamma_1, \gamma_2, \ldots, \gamma_p) : p \times p$$

where is an orthogonal matrix consisting of the eigenvectors γ_j of $\mathbf{A}$.

Spectral Decomposition

Let $\mathbf{A}$ be $p \times p$ symmetric matrix of rank r, $(r \leq p)$. Then there exists $p \times p$ orthogonal matrix $\mathbf{\Gamma}$ so that $\mathbf{\Gamma}^T\mathbf{\Gamma} = \mathbf{I}_p$ and

$$\mathbf{A} = \mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Gamma}^T = \mathbf{\Gamma}\begin{pmatrix} \mathbf{\Lambda}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}\mathbf{\Gamma}^T = \mathbf{\Gamma}_1\mathbf{\Lambda}_1\mathbf{\Gamma}_1^T$$

where letting δ_i = i-th eigenvalue, $i = 1, \ldots, r$

$$\mathbf{\Gamma} = (\mathbf{\Gamma}_1, \mathbf{\Gamma}_0): \quad \mathbf{\Gamma}_1 : p \times r, \quad \mathbf{\Gamma}_0 : p \times (p-r)$$

$$\mathbf{\Lambda}_1 = \mathrm{diag}\{\lambda_1, \ldots, \lambda_r\} = \begin{pmatrix} \lambda_1 & 0 & \ldots & 0 \\ 0 & \lambda_2 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & \lambda_r \end{pmatrix} : r \times r.$$

$\mathbf{\Gamma}_1^T\mathbf{\Gamma}_1 = \mathbf{I}_r$, $\mathbf{\Gamma}_1^T\mathbf{\Gamma}_0 = \mathbf{0}$, $\mathbf{\Gamma}_1^T\mathbf{\Gamma}_0 = \mathbf{0}$ and

$$\begin{aligned}
\mathbf{A}^2 &= \mathbf{A}^T\mathbf{A} = \mathbf{A}\mathbf{A}^T \\
&= (\mathbf{\Gamma}_1\mathbf{\Lambda}_1\mathbf{\Gamma}_1^T)^T\mathbf{\Gamma}_1\mathbf{\Lambda}_1\mathbf{\Gamma}_1^T = \mathbf{\Gamma}_1\mathbf{\Lambda}_1\mathbf{\Gamma}_1^T\mathbf{\Gamma}_1\mathbf{\Lambda}_1\mathbf{\Gamma}_1^T \\
&= \mathbf{\Gamma}_1\mathbf{\Lambda}_1^2\mathbf{\Gamma}_1^T.
\end{aligned}$$

Let γ_i be i-th $p \times 1$ column vector of $\mathbf{\Gamma}$. Then

$$\gamma_i^T\gamma_j = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j. \end{cases}$$

Thus

$$
\begin{aligned}
\mathbf{A} &= \mathbf{\Gamma}_1\mathbf{\Lambda}_1\mathbf{\Gamma}_1^T = \sum_{i=1}^{r} \lambda_i \gamma_i \gamma_i^T \\
\mathbf{A}^T\mathbf{A} &= \mathbf{\Gamma}_1\mathbf{\Lambda}_1^2\mathbf{\Gamma}_1^T = \sum_{i=1}^{r} \lambda_i^2 \gamma_i \gamma_i^T \\
\mathbf{A}\mathbf{A}^T &= \mathbf{\Gamma}_1\mathbf{\Lambda}_1^2\mathbf{\Gamma}_1^T = \sum_{i=1}^{r} \lambda_i^2 \gamma_i \gamma_i^T \\
\gamma_k^T\mathbf{A} &= \lambda_k \gamma_k^T \gamma_k \gamma_k^T = \lambda_k \gamma_k^T \\
\mathbf{A}\gamma_k &= \lambda_k \gamma_k \gamma_k^T \gamma_k = \lambda_k \gamma_k .
\end{aligned}
$$

Spectral Decomposition

Remark 1

Let $\mathbf{\Gamma}$ be an orthogonal matrix so that $\mathbf{\Gamma}^T\mathbf{\Gamma} = \mathbf{I}$. Then

$$\det(\mathbf{\Gamma}) = |\mathbf{\Gamma}| = 1.$$

Remark 2

Let $\mathbf{A}$ be $p \times p$ symmetric matrix of full rank. Then, by the Spectral Decomposition,

$$\begin{aligned}
\det(\mathbf{A}) &= |\mathbf{A}| = |\mathbf{\Gamma}||\mathbf{\Lambda}||\mathbf{\Gamma}^T| \\
&= |\mathbf{\Lambda}| = \begin{vmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \lambda_p \end{vmatrix} = \prod_{i=1}^{p} \lambda_i
\end{aligned}$$

Remark 3

Let $\mathbf{A}$ be $p \times p$ symmetric matrix of full rank. Then, by the Spectral Decomposition,

$$\mathbf{A}^{\alpha} = (\boldsymbol{\Gamma}\boldsymbol{\Lambda}\boldsymbol{\Gamma}^{T})(\boldsymbol{\Gamma}\boldsymbol{\Lambda}\boldsymbol{\Gamma}^{T})\dots(\boldsymbol{\Gamma}\boldsymbol{\Lambda}\boldsymbol{\Gamma}^{T}) = \boldsymbol{\Gamma}\boldsymbol{\Lambda}^{\alpha}\boldsymbol{\Gamma}^{T} \qquad \text{for some } \alpha \in \mathbb{R}$$

In particular, a covariance matrix Σ can be written by

$$\Sigma = \boldsymbol{\Gamma}\boldsymbol{\Lambda}\boldsymbol{\Gamma}^{T} = \sum_{i=1}^{r} \lambda_i \gamma_i \gamma_i^{T}$$

then

$$\Sigma^{-1} = \boldsymbol{\Gamma}\boldsymbol{\Lambda}^{-1}\boldsymbol{\Gamma}^{T} = \sum_{i=1}^{r} \lambda_i^{-1} \gamma_i \gamma_i^{T}$$

$$\Sigma^{-1/2} = \boldsymbol{\Gamma}\boldsymbol{\Lambda}^{-1/2}\boldsymbol{\Gamma}^{T} = \sum_{i=1}^{r} \lambda_i^{-1/2} \gamma_i \gamma_i^{T}$$

Singular value Decomposition: General-version

- Any arbitrary matrix $\mathbf{A}(n \times p)$ with rank r can be decomposed as

$$\mathbf{A} = \mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Delta}^T = \sum_{j=1}^{r} \lambda_j \gamma_j \delta_j^T$$

  where $\mathbf{\Gamma}(n \times r)$ and $\mathbf{\Delta}(p \times r)$.

- Both $\mathbf{\Gamma}$ and $\mathbf{\Delta}$ are column orthogonal, i.e., $\mathbf{\Gamma}^T\mathbf{\Gamma} = \mathbf{\Delta}^T\mathbf{\Delta} = \mathbf{I}_r$ and $\mathbf{\Lambda} = \mathrm{diag}\left(\lambda_1, \ldots, \lambda_r\right),\ \lambda_j > 0$.
- The values $\lambda_1, \ldots, \lambda_r$ are the non-zero eigenvalues of the matrices $\mathbf{A}\mathbf{A}^T$ and $\mathbf{A}^T\mathbf{A}$.
- $\mathbf{\Gamma}$ and $\mathbf{\Delta}$ consist of the corresponding r eigenvectors of theses matrices.

Singular Value Decomposition: General-version

Thus

$$
\begin{aligned}
\mathbf{A} &= \mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Delta}^T = \sum_{j=1}^{r} \lambda_j \gamma_j \delta_j^T \\
\mathbf{A}^T\mathbf{A} &= \mathbf{\Delta}\mathbf{\Lambda}^2\mathbf{\Delta}^T = \sum_{j=1}^{r} \lambda_j^2 \delta_j \delta_j^T \\
\mathbf{A}\mathbf{A}^T &= \mathbf{\Gamma}\mathbf{\Lambda}^2\mathbf{\Gamma}^T = \sum_{j=1}^{r} \lambda_j^2 \gamma_j \gamma_j^T \\
\gamma_k^T\mathbf{A} &= \gamma_k^T\mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Delta}^T = \lambda_k \delta_k^T \\
\mathbf{A}\delta_k &= \mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Delta}^T\delta_k = \lambda_k \gamma_k.
\end{aligned}
$$

Singular Value Decomposition: General-version

G-inverse (Generalized inverse) matrix $\mathbf{A}^-$

$$\mathbf{A} = \mathbf{\Gamma\Lambda\Delta}^T = \sum_{j=1}^{r} \lambda_j \gamma_j \delta_j^T$$

Define

$$\mathbf{A}^- = \mathbf{\Delta\Lambda}^{-1}\mathbf{\Gamma}^T = \sum_{j=1}^{r} \lambda_j^{-1} \delta_j \gamma_j^T$$

Then

$$\mathbf{AA}^-\mathbf{A} = \mathbf{\Gamma\Lambda\Delta}^T\mathbf{\Delta\Lambda}^{-1}\mathbf{\Gamma}^T\mathbf{\Gamma\Lambda\Delta}^T = \mathbf{\Gamma\Lambda\Delta}^T = \sum_{j=1}^{r} \lambda_j \gamma_j \delta_j^T = \mathbf{A}$$

Singular value Decomposition: Another-version

- Any arbitrary matrix $\mathbf{A}(n \times p)$ with rank r can be decomposed as

$$\mathbf{A} = \mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Delta}^T = \sum_{j=1}^{r} \lambda_j^{1/2} \gamma_j \delta_j^T$$

  where $\mathbf{\Gamma}(n \times r)$ and $\mathbf{\Delta}(p \times r)$.
- Both $\mathbf{\Gamma}$ and $\mathbf{\Delta}$ are column orthogonal, i.e., $\mathbf{\Gamma}^T\mathbf{\Gamma} = \mathbf{\Delta}^T\mathbf{\Delta} = \mathbf{I}_r$ and $\mathbf{\Lambda} = \mathrm{diag}\left(\lambda_1^{1/2}, \ldots, \lambda_r^{1/2}\right),\ \lambda_j^{1/2} > 0$.
- The values $\lambda_1, \ldots, \lambda_r$ are the non-zero eigenvalues of the matrices $\mathbf{A}\mathbf{A}^T$ and $\mathbf{A}^T\mathbf{A}$.
- $\mathbf{\Gamma}$ and $\mathbf{\Delta}$ consist of the corresponding r eigenvectors of theses matrices.

- A quadratic form $Q(x)$ is defined to be

$$Q(x) \;=\; x^T \mathbf{A} x = \sum_{i=1}^{p}\sum_{j=1}^{p} a_{ij} x_i x_j$$

for a symmetric matrix $\mathbf{A}(p \times p)$ and a vector $x \in \mathbb{R}^p$

-

$$\begin{aligned} Q(x) &> 0 \qquad \text{for all } x \neq 0\text{: Positive definite} \\ Q(x) &\geq 0 \qquad \text{for all } x \neq 0\text{: Positive semidefinite} \end{aligned}$$

- **A** is called **positive definite(semidefinite)** if the corresponding quadratic form $Q(\cdot)$ is positive definite(semidefinite).
- Notation: $\mathbf{A} > 0 (\geq 0)$

Quadratic Forms

Proposition 1

If $\mathbf{A}$ is symmetric and $Q(x) = x^T\mathbf{A}x$ is the corresponding quadratic form, then there exists a transformation $y = \mathbf{\Gamma}^T x$ such that

$$Q(x) = x^T\mathbf{A}x = \sum_{i=1}^{p} \lambda_i y_i^2$$

where λ_i's are the eigenvalues of $\mathbf{A}$.

Proposition 2

$\mathbf{A} > 0$ if and only of all $\lambda_i > 0,\ i = 1, \ldots, p$

Corollary 1

If $\mathbf{A} > 0$, then $\mathbf{A}^{-1}$ exists and $|\mathbf{A}| > 0$.

Proposition 3

- If $\mathbf{A}$ and $\mathbf{B}$ are symmetric and $\mathbf{B} > 0$, then the maximum of $\frac{x^T\mathbf{A}x}{x^T\mathbf{B}x}$ is given by the largest eigenvalues of $\mathbf{B}^{-1}\mathbf{A}$.
- More generally,

$$\max \frac{x^T\mathbf{A}x}{x^T\mathbf{B}x} = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p = \min \frac{x^T\mathbf{A}x}{x^T\mathbf{B}x}$$

  where $\lambda_1, \ldots, \lambda_p$ denote the eigenvalues of $\mathbf{B}^{-1}\mathbf{A}$.
- The vector which maximizes(minimizes) $\frac{x^T\mathbf{A}x}{x^T\mathbf{B}x}$ is the eigenvector of $\mathbf{B}^{-1}\mathbf{A}$ which corresponds to the largest(smallest) eigenvalue of $\mathbf{B}^{-1}\mathbf{A}$.
- If $x^T\mathbf{B}x = 1$, then

$$\max x^T\mathbf{A}x = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p = \min x^T\mathbf{A}x$$

Partitioned Matrices

Note

Let $\mathbf{A}(n \times p)$ and $\mathbf{B}(p \times n)$ be any two matrices and $n \geq p$. Then

$$\begin{vmatrix} -\lambda \mathbf{I}_n & -\mathbf{A} \\ \mathbf{B} & \mathbf{I}_p \end{vmatrix} = (-\lambda)^{n-p} |\mathbf{BA} - \lambda \mathbf{I}_n| = |\mathbf{AB} - \lambda \mathbf{I}_n|$$

Proposition 4

For $\mathbf{A}(n \times p)$ and $\mathbf{B}(p \times n)$, the non-zero eigenvalues of $\mathbf{AB}$ and $\mathbf{BA}$ are the same and have the same multiplicity. If x is an eigenvector of $\mathbf{AB}$ for an eigenvalues $\lambda \neq 0$, then $y = \mathbf{B}x$ is an eigenvector of $\mathbf{BA}$.

Corollary 2

For $\mathbf{A}(n \times p)$, $\mathbf{B}(q \times n)$, $a(p \times 1)$ and $b(q \times 1)$,

$$\operatorname{rank}(\mathbf{A}ab\mathbf{B}) \leq 1$$

The non-zero eigenvalue, if it exists, equals $b^T \mathbf{BA}a$ with eigenvector $\mathbf{A}a$

Geometrical Aspects

Note

- $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k$ are **mutually orthogonal** if and only if $\mathbf{x}_i^T \mathbf{x}_j = 0$ for all i, j.
- In that case, $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k)$ has **rank** k, and $\mathbf{X}^T\mathbf{X}$ is a diagonal matrix with $\mathbf{x}_i^T\mathbf{x}_i$ in the i-th diagonal position.
- Let's consider bivariate data $(x_i, y_i), i = 1, \ldots, n$, and let $\tilde{x}_i = x_i - \bar{\mathbf{x}}$ and $\tilde{y}_i = y_i - \bar{\mathbf{y}}$. Then the **correlation between x and y** is

$$\frac{\sum_{i=1}^n (x_i - \bar{\mathbf{x}}_i)(y_i - \bar{\mathbf{y}}_i)}{\sqrt{\sum_{i=1}^n (x_i - \bar{\mathbf{x}}_i)^2 \sum_{i=1}^n (y_i - \bar{\mathbf{x}}_i)^2}} = \frac{\tilde{\mathbf{x}}^T\tilde{\mathbf{y}}}{||\tilde{\mathbf{x}}||||\tilde{\mathbf{y}}||} = \cos(\theta)$$

where θ is the angle between the deviation vectors $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{y}}$.

Rotations

For two dimensions, the clockwise rotation can be expressed:

$$\begin{aligned}\mathbf{y} &= \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ &= \mathbf{\Gamma} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \mathbf{\Gamma x}\end{aligned}$$

the counter-clockwise rotation can be expressed

$$\begin{aligned}\mathbf{y} &= \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ &= \mathbf{\Gamma}^T \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \mathbf{\Gamma}^T \mathbf{x}\end{aligned}$$

Definition

Consider an $n \times p$ matrix $\mathbf{X}$.

$$\begin{aligned}
\mathcal{C}(\mathbf{X}) &= \{x \in \mathbb{R}^n \,|\, \exists a \in \mathbb{R}^p \text{ so that } \mathbf{X}a = x\} \subseteq \mathbb{R}^n \\
&= \text{the } \textbf{column(range) space} \text{ of } \mathbf{X} \\
\mathcal{N}(\mathbf{X}) &= \{y \in \mathbb{R}^p \,|\, \mathbf{X}y = 0\} \subseteq \mathbb{R}^p \\
&= \text{the } \textbf{null space} \text{ of } \mathbf{X} \\
\mathcal{R}(\mathbf{X}) &= \{z \in \mathbb{R}^p \,|\, \exists b \in \mathbb{R}^n \text{ so that } \mathbf{X}^T b = z\} \subseteq \mathbb{R}^p \\
&= \text{the } \textbf{row space} \text{ of } \mathbf{X} \\
&= \mathcal{C}(\mathbf{X}^T) = \text{the } \textbf{column space} \text{ of } \mathbf{X}^T
\end{aligned}$$

Consider an $n \times p$ matrix $\mathbf{X}$ with $\text{rank}(\mathbf{X}) = r$

Spaces by Singular Value Decomposition: General-version

$$
\begin{aligned}
\mathbf{X} &= \mathbf{\Gamma\Lambda\Delta}^T = \sum_{j=1}^{r} \lambda_j \gamma_j \delta_j^T \\
\mathcal{C}(\mathbf{X}) &= \{\gamma_1, \gamma_2, \ldots, \gamma_r\} \\
\mathcal{N}(\mathbf{X}) &= \{\delta_{r+1}, \delta_{r+2}, \ldots, \delta_p\} \\
\mathcal{R}(\mathbf{X}) &= \{\delta_1, \delta_2, \ldots, \delta_r\}
\end{aligned}
$$

Column, Row and Null Spaces

Note 1: Let X be $n \times p$ matrix. Then

$$\begin{aligned} \mathcal{N}(\mathbf{X}) &= \mathcal{C}(\mathbf{X}^T)^\perp = \mathcal{R}(\mathbf{X})^\perp \\ \mathcal{N}(\mathbf{X})^\perp &= \mathcal{C}(\mathbf{X}^T) = \mathcal{R}(\mathbf{X}) \end{aligned}$$

Note 2: Let X be $n \times p$ matrix. Then

$$\mathcal{C}(\mathbf{X}^T\mathbf{X}) = \mathcal{C}(\mathbf{X}^T) = \mathcal{R}(\mathbf{X})$$

Note 3: Let X be $n \times p$ matrix. Then

- $\dim(\mathcal{C}(\mathbf{X})) = \dim(\mathcal{R}(\mathbf{X})) = \text{rank}(\mathbf{X}) = \text{rank}(\mathbf{X}^T) = \text{rank}(\mathbf{X}^T\mathbf{X}) = r \leq \min(n, p)$
- $\mathbf{X}^T\mathbf{X}$ has full rank (is nonsingular) if and only if **X** has full column rank (**X** has linearly independent columns).

Example: arbitrary 3×4 matrix A

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 5 & 1 \\ 2 & 2 & 10 & 6 \\ 3 & 4 & 15 & 1 \end{pmatrix} = \sum_{i=1}^{3} \lambda_i \gamma_i \delta_i^T = \lambda_1 \gamma_1 \delta_1^T + \lambda_2 \gamma_2 \delta_2^T + \lambda_3 \gamma_3 \delta_3^T$$

$$= 20.15 \begin{pmatrix} -0.274 \\ -0.568 \\ -0.776 \end{pmatrix} (-0.186, -0.238, -0.927, -0.221)$$

$$+4.40 \begin{pmatrix} -0.072 \\ 0.817 \\ -0.572 \end{pmatrix} (-0.035, -0.182, -0.177, 0.967)$$

$$+0.69 \begin{pmatrix} -0.959 \\ 0.101 \\ 0.265 \end{pmatrix} (0.053, -0.954, 0.265, -0.129)$$

Example: arbitrary 3×4 matrix A

The eigenvalues and eigenvectors by Singular Value Decomposition are given by

$$\lambda_1 = 20.15 \qquad \lambda_2 = 4.40 \qquad \lambda_3 = 0.69$$

$$\gamma_1 = \begin{pmatrix} -0.274 \\ -0.568 \\ -0.776 \end{pmatrix} \quad \gamma_2 = \begin{pmatrix} -0.072 \\ 0.817 \\ -0.572 \end{pmatrix} \quad \gamma_3 = \begin{pmatrix} -0.959 \\ 0.101 \\ 0.265 \end{pmatrix}$$

$$\delta_1 = \begin{pmatrix} -0.186 \\ -0.238 \\ -0.927 \\ -0.221 \end{pmatrix} \quad \delta_2 = \begin{pmatrix} -0.035 \\ -0.182 \\ -0.177 \\ 0.967 \end{pmatrix} \quad \delta_3 = \begin{pmatrix} 0.053 \\ -0.954 \\ 0.265 \\ -0.129 \end{pmatrix}$$