Principal Component Analysis (PCA)

Shusen Wang

Some Statistical Concepts

Mean and Variance (Scalar)

- Let X be a random scalar variable and $p(\cdot)$ be the probability density function (PDF).
- **Mean**: $\mu = \mathbb{E}[X] = \int x \cdot p(x)\, dx.$
- **Variance**: $\sigma^2 = \mathbb{E}[(X - \mu)^2] = \int (x - \mu)^2 \cdot p(x)\, dx.$

- Let $x_1, \cdots, x_n$ be independently drawn observations of X.
- **Sample mean**: $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$.
- **Sample variance**: $\hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{\mu})^2.$

Mean and Covariance (Vector)

- Let X be a random vector variable and $p(\cdot)$ be the probability density function (PDF).
- **Mean**: $\boldsymbol{\mu} = \mathbb{E}[X] = \int \mathbf{x} \cdot\ p(\mathbf{x})\, d\mathbf{x}\ \in\ \mathbb{R}^d$.
- **Covariance**: $\mathbf{C} = \mathbb{E}[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T] \in\ \mathbb{R}^{d \times d}$.

- Let $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d$ be independently drawn observations of X.
- **Sample mean**: $\hat{\boldsymbol{\mu}} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i \in\ \mathbb{R}^d$.
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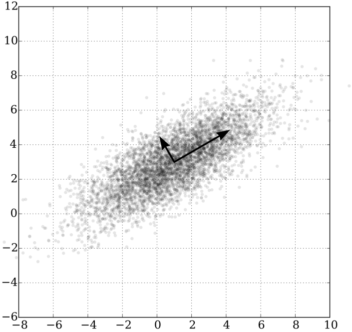
Principal Component Analysis (PCA)

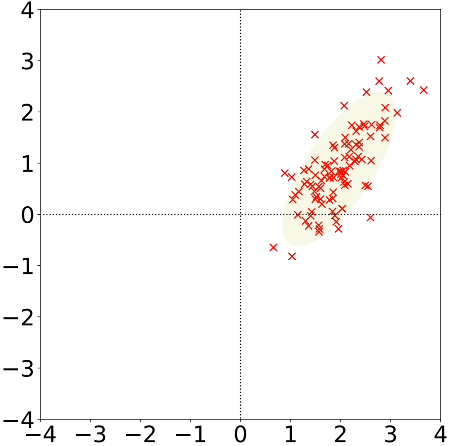
PCA Explained

- Transforms the data to a new coordinate system.
  - The greatest variance lie on the first coordinate (called the 1st principal component).
  - The 2nd greatest variance on the second coordinate, and so on…



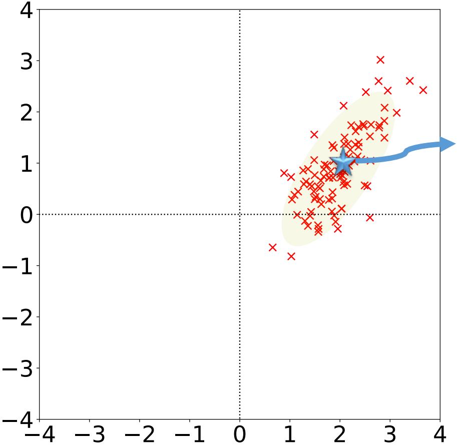
PCA Explained

The original data.



PCA Explained

Step 1: subtract the mean



- **Sample mean:** $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$

PCA Explained

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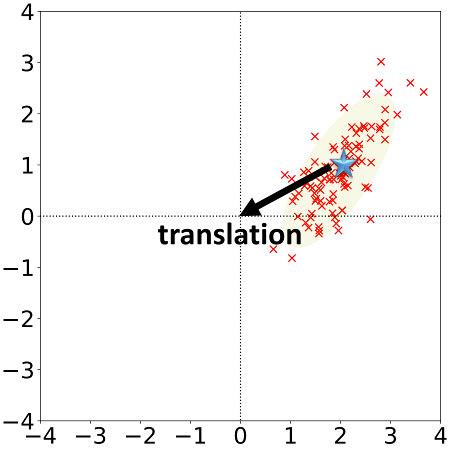

- Sample mean: $\hat{\boldsymbol{\mu}} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$
- **Translation**: $\mathbf{x}_i' = \mathbf{x}_i - \hat{\boldsymbol{\mu}}$

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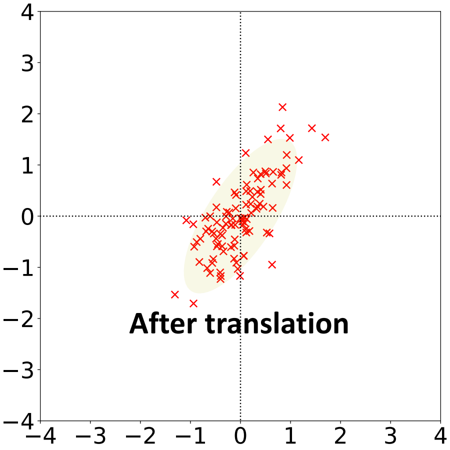

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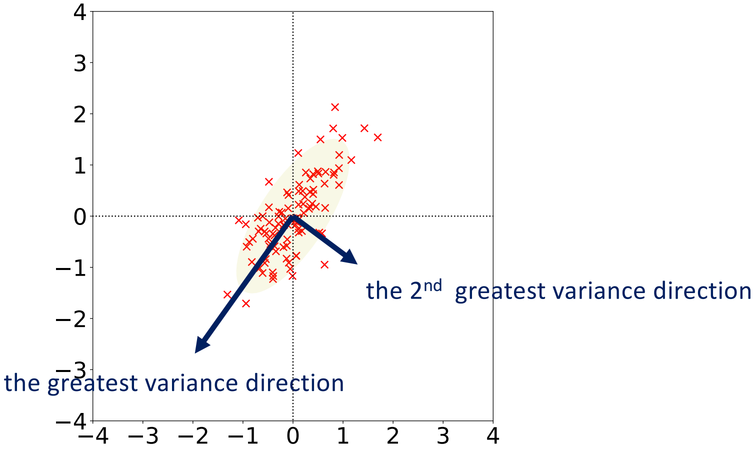
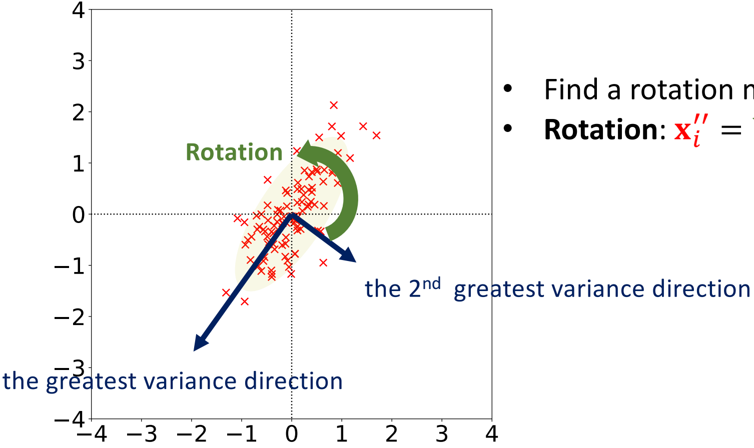
PCA Explained

Step 2: rotation



PCA Explained

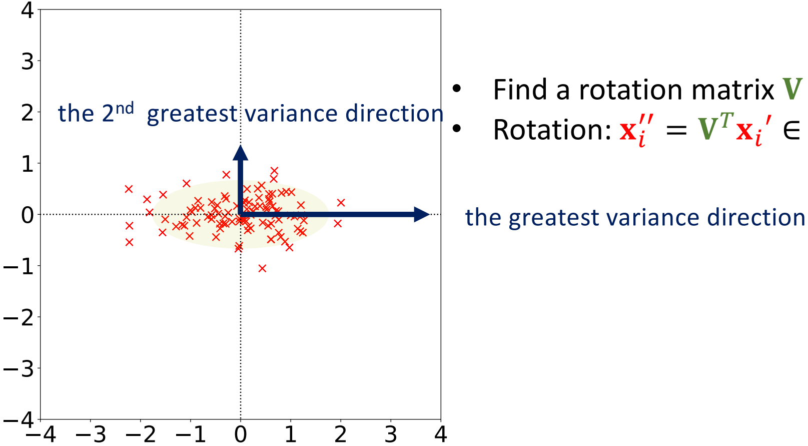
Step 2: rotation



- Find a rotation matrix $\mathbf{V} \in \mathbb{R}^{d\times d}$
- **Rotation**: $\mathbf{x}_i'' = \mathbf{V}^T \mathbf{x}_i' \in \mathbb{R}^d$

PCA Explained

The result



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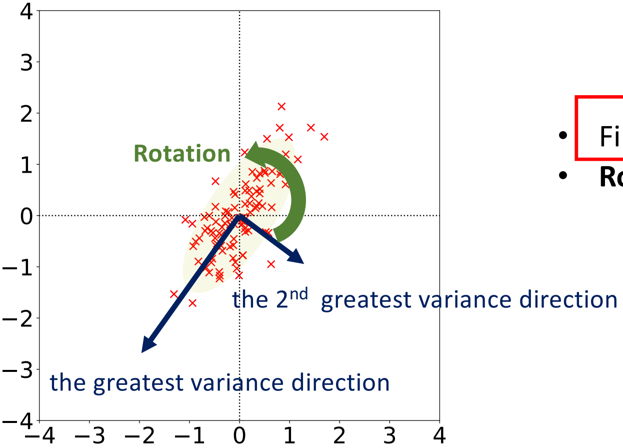

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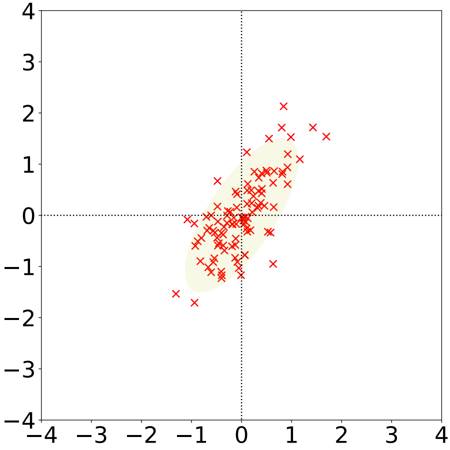

- $\mathbf{X}' \in \mathbb{R}^{n \times d}$: the stack of $\mathbf{x}'_1, \cdots, \mathbf{x}'_n$.

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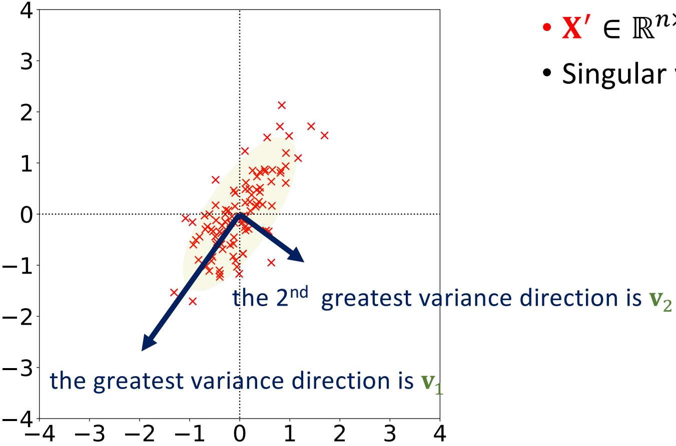

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$$\mathbf{X}' = \sum_{j=1}^{d} \sigma_j \, \mathbf{u}_j \, \mathbf{v}_j^T .$$

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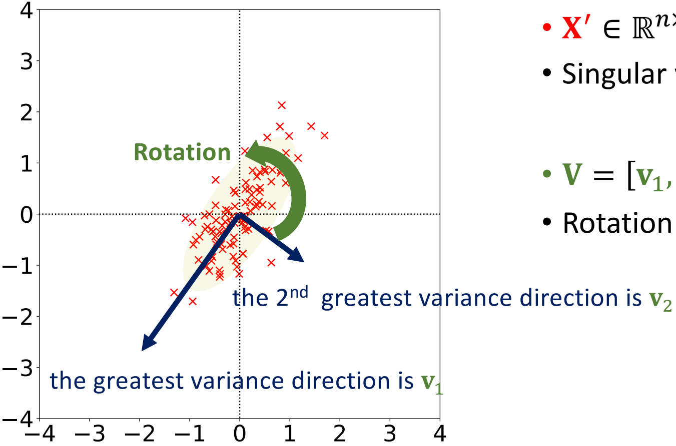

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- $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_d] \in \mathbb{R}^{d \times d}$.
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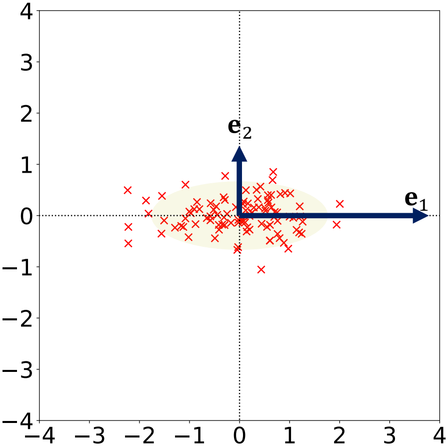

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- $\mathbf{X}'' \in \mathbb{R}^{n \times d}$: the stack of $\mathbf{x}_1'', \cdots, \mathbf{x}_n''$.
- Its right singular vectors are the standard basis: $\mathbf{e}_1, \cdots, \mathbf{e}_d$.

The Procedure of PCA (Recap)

1. Input: data $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d$ and target rank k ($\leq d$).
2. Subtract the mean: $\hat{\boldsymbol{\mu}} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$ and $\mathbf{x}_i' = \mathbf{x}_i - \hat{\boldsymbol{\mu}}$.
   - Obtain matrix $\mathbf{X}' \in \mathbb{R}^{n \times d}$: the stack of $\mathbf{x}_1', \cdots, \mathbf{x}_n'$.

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   - Obtain matrix $\mathbf{X}' \in \mathbb{R}^{n \times d}$: the stack of $\mathbf{x}_1', \cdots, \mathbf{x}_n'$.
3. Find the rotation matrix $\mathbf{V}_k = [\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_k] \in \mathbb{R}^{d \times k}$
   - Truncated SVD: $\mathbf{X}_k' = \sum_{j=1}^{k} \sigma_j \, \mathbf{u}_j \, \mathbf{v}_j^T$.

Question: Why setting a target rank $k \leq d$? Why not using $k = d$?

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- $\mathbf{v}_1$ is the greatest variance direction, $\mathbf{v}_2$ is the 2nd greatest, and so on.
- Only the top variance directions are interesting.
  - The top ones are features.
  - The bottom ones are noise.
- For visualization, we set $k = 2$ or 3.

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4. Rotation (and dimensionality reduction):
   - $\mathbf{x}_i'' = \mathbf{V}_k^T \, \mathbf{x}_i{}' \in \mathbb{R}^k$, for $i = 1$ to n, are the outputs.

Dimensionality reduction: $\mathbf{x}_i \in \mathbb{R}^d \longrightarrow \mathbf{x}_i'' \in \mathbb{R}^k$

Why is $\mathbf{v}_1$ the Greatest Variance Direction?

- The rows of $\mathbf{X}' \in \mathbb{R}^{n \times d}$ have zero mean.
  - $\mathbf{x}_i' = \mathbf{x}_i - \widehat{\boldsymbol{\mu}}$ is the result of translation (Step 1 of PCA).
- The sample covariance matrix of $\mathbf{x}_1, \cdots, \mathbf{x}_n \in \mathbb{R}^d$ is:
  - $\widehat{\mathbf{C}} = \frac{1}{n-1} \sum_{i=1}^{n} (\mathbf{x}_i - \overline{\boldsymbol{\mu}})(\mathbf{x}_i - \overline{\boldsymbol{\mu}})^T \in \mathbb{R}^{d \times d}$.

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- $\mathbf{X}' = \sum_{j=1}^{d} \sigma_j \, \mathbf{u}_j \, \mathbf{v}_j^T$
  - $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_d$.

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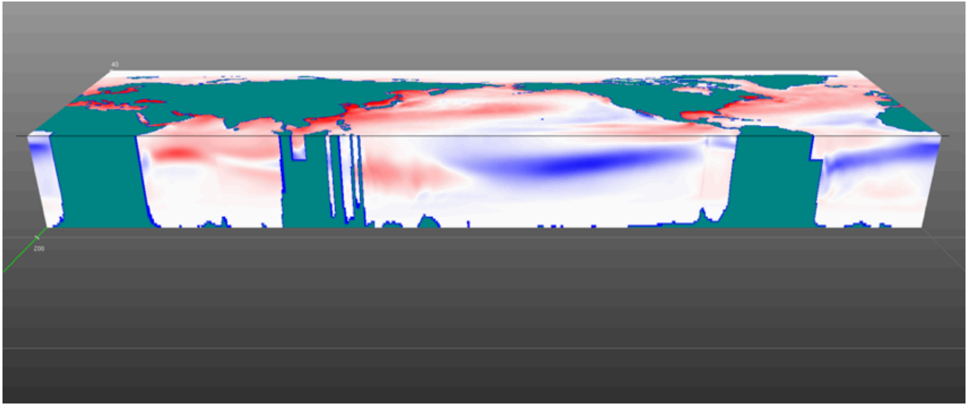
  - $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_d$.
- $\mathbf{v}_1 = \mathrm{argmax}_{\mathbf{v}} \; \mathbf{v}^T \, \hat{\mathbf{C}} \, \mathbf{v}$.

PCA: A Real-World Example

Ocean Temperature Data



ocean temperatures taken 1979—2011 at 6 hour intervals

Ocean Temperature Data

- Just keep the surface temperature
- Shape: $n \times d_1 \times d_2$ (oder-3 tensor)
  - $n = 4 \times 365 \times 32 = 46{,}720$ (4 measurements per day)
  - $d_1 = 2 \times 360 = 720$ (2 measurement per degree of longitude)
  - $d_2 = 2 \times 180 = 360$ (2 measurement per degree of latitude)

- Reshape the tensor to a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$
  - Temporal dimension: $n = 46{,}720$
  - Spatial dimension: $d = d_1 d_2 = 259{,}200$

Compute the Top $k = 4$ Principal Components

- Ocean temperature data: $\mathbf{X} \in \mathbb{R}^{n \times d}$
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- Treat each row as a sample.
- The result of PCA is $n \times 4$ matrix.

- Treat each column as a sample.
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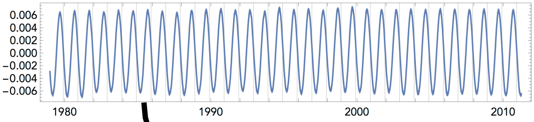
The first principal component ($n \times 1$)



One of the n time points

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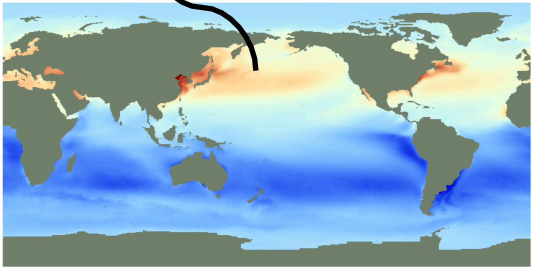
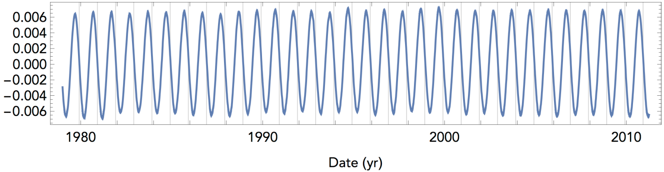
The first principal component ($d \times 1$)

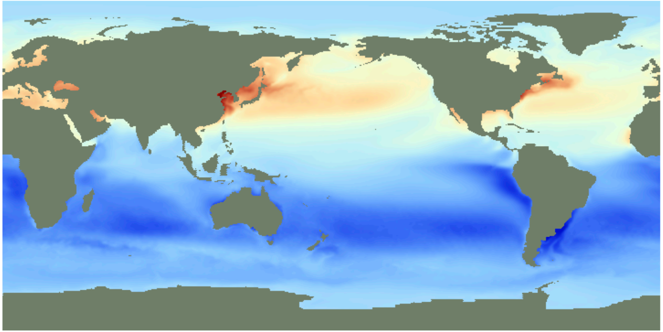
One of the d locations (color indicates value)



The 1st Principal Components

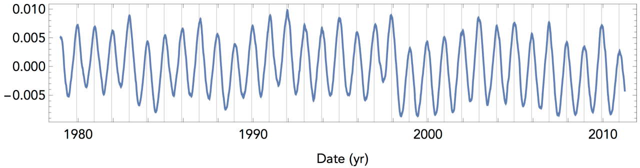
Annual cycle

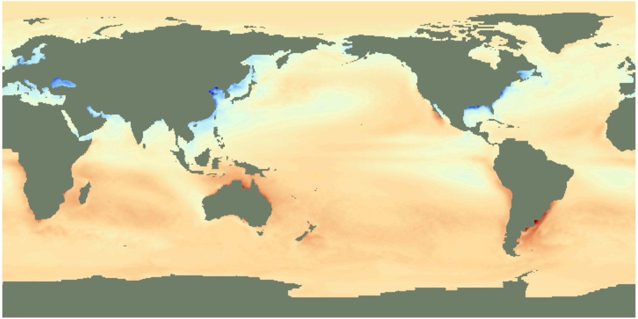




The 2nd Principal Components

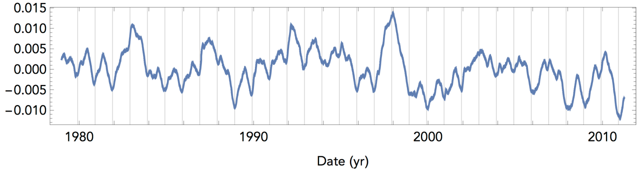
Annual cycle

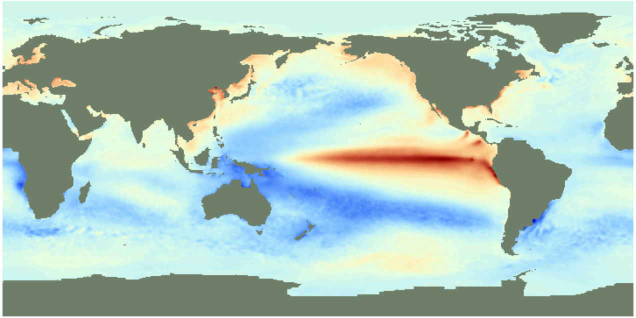




The 3rd Principal Components

El Nino





The 4th Principal Components

La Nina