Dimensionality Reduction Part 1: PCA and KPCA

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Dimensionality Reduction

- Linear methods
  - **PCA** (Principal Component Analysis)
  - cMDS (Classical Multidimensional Scaling)
- Non-linear methods
  - **KPCA** (Kernel PCA)
  - mMDS (Metric MDS)
  - Isomap
  - LLE (Locally Linear Embedding)
  - t-SNE (t-distributed Stochastic Neighbor Embedding)
  - UMAP (Uniform Manifold Approximation and Projection)

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Principal Component Analysis

- Let X be an $n \times m$ matrix where each row represents a vector in an m-D space
  - X is like a spreadsheet with features in column
- What do we ideally expect to be the "principal components" of X
  1. The components **form a basis**
  2. The components are **orthogonal**
  3. The **first component accounts for the most variation**, the second component accounts for the most variation after removing the first component, and so on

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Principal Component Analysis

- Let X be an $n \times m$ matrix where each row represents a datapoint in an m-D space
  - X represents n datapoints in m-D
- Assume that the rows in X are generated by a random vector $\boldsymbol{X} \in \mathbb{R}^m$
  - Note the difference between $\boldsymbol{X}$ and X
  - The theory of PCA is based on $\boldsymbol{X}$ (and its $m \times m$ covariance matrix M)
- For the first component, we want to find unit vector $u \in \mathbb{R}^m$ such that $\mathrm{var}\left(u^{\mathrm{T}}\boldsymbol{X}\right)$ is maximized

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Principal Component Analysis

- The eigenvector u of the covariance matrix of $\boldsymbol{X}$ with the largest eigenvalue maximizes $\mathrm{var}\left(u^{\mathrm{T}}\boldsymbol{X}\right)$

Let $\boldsymbol{X} \in \mathbb{R}^n$ be a random vector with

- mean $\mu \in \mathbb{R}^n$ and
- covariance matrix $M = \mathbb{E}[(\boldsymbol{X} - \mu)(\boldsymbol{X} - \mu)^{\mathrm{T}}]$

For any $u \in \mathbb{R}^n$, the projection of $u^{\mathrm{T}}\boldsymbol{X}$ has

- $\mathbb{E}[u^{\mathrm{T}}\boldsymbol{X}] = u^{\mathrm{T}}\mu$ and
- $\mathrm{var}\left(u^{\mathrm{T}}\boldsymbol{X}\right) = \mathbb{E}\left[\left(u^{\mathrm{T}}\boldsymbol{X} - u^{\mathrm{T}}\mu\right)^2\right]$

$$= \mathbb{E}[u^{\mathrm{T}}(\boldsymbol{X} - \mu)(\boldsymbol{X} - \mu)^{\mathrm{T}}u] = u^{\mathrm{T}}Mu$$

From min-max theorem, $u^{\mathrm{T}}Mu$ is maximized when u is the eigenvector of M with the largest eigenvalue

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Principal Component Analysis

- Extend to k principal components, we want
  - k-D subspace of $\boldsymbol{X}$ that is defined by orthogonal basis $p_1, \ldots, p_k \in \mathbb{R}^m$ and displacement $p_0 \in \mathbb{R}^m$
  - Distance from $\boldsymbol{X}$ to this subspace is minimized

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- Projection of $\boldsymbol{X}$ onto subspace is $P^{\mathrm{T}}\boldsymbol{X} + \mathrm{p}_{\mathbf{0}}$, where P is matrix whose rows are $p_1, \ldots, p_k$
- Squared distance to subspace is $\mathbb{E}\left\|\boldsymbol{X} - \left(P^{\mathrm{T}}\boldsymbol{X} + p_{\mathbf{0}}\right)\right\|^2$
- By calculus, $\mathrm{p}_{\mathbf{0}} = \mathbb{E}\left\|\boldsymbol{X} - P^{\mathrm{T}}\boldsymbol{X}\right\| = \left(1 - P^{\mathrm{T}}\right)\mu$, hence
  $$\mathbb{E}\left\|\boldsymbol{X} - \left(P^{\mathrm{T}}\boldsymbol{X} + p_{\mathbf{0}}\right)\right\|^2 = \mathbb{E}\|\boldsymbol{X} - \mu\|^2 - \mathbb{E}\left\|P^{\mathrm{T}}(\boldsymbol{X} - \mu)\right\|^2$$
- To maximize that, need to maximize $\mathbb{E}\left\|P^{\mathrm{T}}(\boldsymbol{X} - \mu)\right\|^2 = \mathrm{var}\left(P^{\mathrm{T}}\boldsymbol{X}\right)$
- Finally, same as in previous slide, $p_1, \ldots, p_k$ are eigenvectors of M

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Principal Component Analysis

- If X is normalized (values along each feature deducted by the feature's mean), an unbiased estimator of M can be obtained as

$$M = \frac{1}{n} X^{\mathrm{T}} X \quad \text{(or } M = \frac{1}{n} \sum_i x_i'^{\mathrm{T}} x_i \text{)}$$

- Since SVD of X eigendecomposes $X^{\mathrm{T}} X$
  - We can solve PCA through either
    1. Eigendecompose M, or
    2. Solve SVD for X

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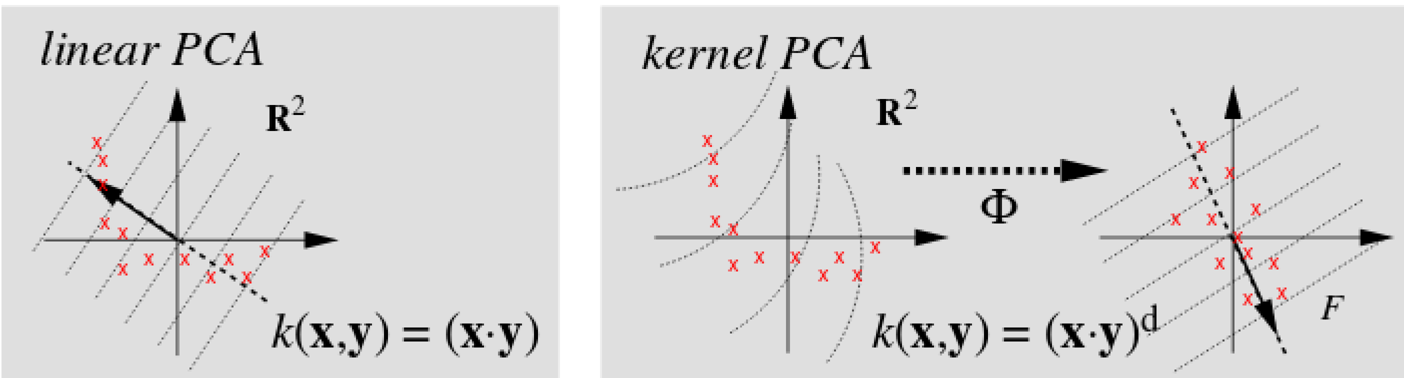
Kernel PCA motivation

- Datapoints that do not lie on a linear manifold in the coordinate space may lie on one after some non-linear transformation ϕ



Scholkopf, Smola, and Muller. Kernel Principal Component Analysis, 1999

- Principal components in the transformed space may be more meaningful in such a case

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Kernel PCA idea

- Extract principal components in a ϕ-mapped feature space:
  1. $x' = \phi(x)$ and $X' = [x_1{}' \quad \ldots \quad x_n{}']^{\mathrm{T}}$
  2. Center X' so that, $\forall i, \sum_i x_1' = 0$
  3. Find covariance matrix, $M' = \frac{1}{n}\sum_i x_i'^{\mathrm{T}} x_i'$
  4. Eigendecompose M'
- But the dimension of x', $\dim(x') \gg n$ (or even ∞)

  ⇒ M' has large (or even ∞) dimensions

  ⇒ Eigendecomposition leads to large number of eigenvectors, each of large (or infinite) dimensions

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Kernel PCA idea foiled

Problem 1: Large number of eigenvectors

- How many eigenvectors are there actually
  - $\mathrm{rank}(M')$, bounded by the number of datapoints
    - Recall that eigenvectors can be expressed as a linear combination of the datapoints by solving the equations $x_i' = \sum_j \langle x_i', u_j \rangle u_j$
      - j is bounded by $\mathrm{rank}(M') \Rightarrow$ may be manageable
      - However, working with the system of equations is hard because $x_i{}'$ and u_j are of…

Problem 2: Large (or ∞) dimensions

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Kernel method

- Do not compute $\phi(x_1), \dots, \phi(x_n)$ or eigenvectors of M'
  - Limit operations in the mapped space to those that involves only the inner products $\langle x_i', x_j' \rangle$
    - Sufficient for finding a relation between the eigenvectors of M' and $\phi(x_1), \dots, \phi(x_n)$
    - Given point x, sufficient for finding the projection of $\phi(x)$ on the eigenvectors of M'
  - Use a function $K(x_i, x_j) = \langle x_i', x_j' \rangle$ (called a kernel function) that does not require computing $\phi(x_i)$ or $\phi(x_j)$
    - More on these functions in later slides

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Relating eigenvector to $x'_1, \ldots, x'_n$

- Relate eigenvectors of M' with $x'_1, \ldots, x'_n$ using a computation that involves only $\langle x'_i, x'_j \rangle$
- Start with the definition of $M' = \frac{1}{n}\left(\sum_{i=1}^{n} x_i'^{\mathrm{T}} x_i'\right)$
  - Solving $M'u = \lambda u$ means $\left(\sum_i x_i'^{\mathrm{T}} x_i'\right)u = n\lambda u$
  - This implies $u = \frac{1}{n\lambda}\sum_i x_i'^{\mathrm{T}} x_i' u$. Since $\overset{\text{Proof later}}{x^{\mathrm{T}}xu = xux^{\mathrm{T}}}$, $u = \frac{1}{n\lambda}\sum_i \overbrace{x_i' u}^{\text{scalar}} x_i'^{\mathrm{T}}$

    Hence can let $u = \sum_{i=1}^{n} \alpha_i x_i'^{\mathrm{T}}$ for $\alpha_i \in \mathbb{R}$
    - $\alpha_1, \ldots, \alpha_n$ **relate eigenvector** u **to** $x'_1, \ldots, x'_n$
- Place $u^{(r)} = \sum_i \alpha_i^{(r)} x_i'^{\mathrm{T}}$ back in $\left(\sum_i x_i'^{\mathrm{T}} x_i'\right)u = n\lambda u$
  - Use superscript r to associate α with its corresponding u and λ

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Solving $\alpha_1, \ldots, \alpha_n$

(Terms in bold cannot be reordered)

System of $\dim(u)$ equations

$$\left(\sum_{i=1}^{n} \boldsymbol{x}_i'^{\mathrm{T}} \boldsymbol{x}_i'\right) \boldsymbol{u}^{(r)} = n\lambda^{(r)} \boldsymbol{u}^{(r)}$$

Replace $\boldsymbol{u}^{(r)}$ with $\sum_j \alpha_j^{(r)} \boldsymbol{x}_j'^{\mathrm{T}}$

$$\left(\sum_{i=1}^{n} \boldsymbol{x}_i'^{\mathrm{T}} \boldsymbol{x}_i'\right) \sum_{j=1}^{n} \alpha_j^{(r)} \boldsymbol{x}_j'^{\mathrm{T}} = n\lambda^{(r)} \sum_{k=1}^{n} \alpha_k^{(r)} \boldsymbol{x}_k'^{\mathrm{T}}$$

Reorder

$$\left(\sum_i \boldsymbol{x}_i'^{\mathrm{T}}\right) \sum_j \overbrace{\boldsymbol{x}_i' \boldsymbol{x}_j'^{\mathrm{T}}}^{\text{scalar}} \alpha_j^{(r)} = n\lambda^{(r)} \sum_k \boldsymbol{x}_k'^{\mathrm{T}} \alpha_k^{(r)}$$

Multiply from the left with $\boldsymbol{x}_l'$ (equation holds for each l)

System of one equation

$$\left(\sum_i \overbrace{\boldsymbol{x}_l' \boldsymbol{x}_i'^{\mathrm{T}}}^{\text{scalar}}\right) \sum_j \boldsymbol{x}_i' \boldsymbol{x}_j'^{\mathrm{T}} \alpha_j^{(r)} = n\lambda^{(r)} \sum_k \underbrace{\boldsymbol{x}_l' \boldsymbol{x}_k'^{T}}_{\text{scalar}} \alpha_k^{(r)}$$

Replace $\boldsymbol{x}_i' \boldsymbol{x}_j'^{\mathrm{T}}$ with the kernel function

$$\sum_i K(x_l, x_i) \sum_j K(x_i, x_j)\, \alpha_j^{(r)} = n\lambda^{(r)} \sum_k K(x_l, x_k)\, \alpha_k^{(r)}$$

Reorder

$$\sum_i \sum_j K(x_l, x_i) K(x_i, x_j)\, \alpha_j^{(r)} = n\lambda^{(r)} \sum_k K(x_l, x_k)\, \alpha_k^{(r)}$$

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Solving $\alpha_1, \dots, \alpha_n$

$$\sum_i \sum_j K(x_l, x_i) K(x_i, x_j)\, \alpha_j^{(r)} = n\lambda^{(r)} \sum_k K(x_l, x_k)\, \alpha_k^{(r)}$$

- **Replace** $K(x_i, x_j)$ **with a matrix** $\boldsymbol{K}$ **where** $k_{ij} = K(x_i, x_j)$ ($\boldsymbol{K}$ is called a kernel matrix)

$$\sum_i \sum_j k_{li} k_{ij}\, \alpha_j^{(r)} = n\lambda^{(r)} \sum_k k_{lk}\, \alpha_k^{(r)}$$

- For each l this gives one single equation with a linear combination of the variables $\alpha_1^{(r)}, \dots, \alpha_n^{(r)}$
  - e.g. $r = 2$

$$\begin{array}{c c c}
 & & \begin{array}{ccc} K_1^{\mathrm{T}} & K_2^{\mathrm{T}} & \\ \downarrow & \downarrow & \end{array} \\
K_r \rightarrow & \begin{bmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} & \begin{bmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}
\end{array}
\begin{bmatrix} \alpha_1^{(r)} \\ \alpha_2^{(r)} \\ \vdots \end{bmatrix} = n\lambda^{(r)} \begin{bmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \alpha_1^{(r)} \\ \alpha_2^{(r)} \\ \vdots \end{bmatrix}$$

$$(k_{21}k_{11} + k_{22}k_{21} + \cdots)\alpha_1^{(r)} + (k_{21}k_{12} + k_{22}k_{22} + \cdots)\alpha_2^{(r)} + \cdots$$
$$= n\lambda^{(r)} \left(k_{21}\alpha_1^{(r)} + k_{21}\alpha_2^{(r)} + \cdots\right)$$

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Solving $\alpha_1, \dots, \alpha_n$

System of one equation

$$\begin{array}{cc} & \\ K_r \rightarrow & \begin{bmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \end{array} \begin{array}{c} \begin{array}{ccc} K_1^{\mathrm{T}} & K_2^{\mathrm{T}} & \\ \downarrow & \downarrow & \end{array} \\ \begin{bmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \end{array} \begin{bmatrix} \alpha_1^{(r)} \\ \alpha_2^{(r)} \\ \vdots \end{bmatrix} = n\lambda^{(r)} \begin{bmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \alpha_1^{(r)} \\ \alpha_2^{(r)} \\ \vdots \end{bmatrix}$$

- Repeat r for 1 to n

System of n equations

$$\begin{bmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \alpha_1^{(r)} \\ \alpha_2^{(r)} \\ \vdots \end{bmatrix} = n\lambda^{(r)} \begin{bmatrix} k_{11} & k_{12} & \cdots \\ k_{21} & k_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \alpha_1^{(r)} \\ \alpha_2^{(r)} \\ \vdots \end{bmatrix}$$

- This in matrix notation is

$$\boldsymbol{K}^2 \boldsymbol{\alpha}^{(r)} = n\lambda^{(r)} \boldsymbol{K} \boldsymbol{\alpha}^{(r)}$$

  - Each $\boldsymbol{\alpha}^{(r)}$ that fulfills the equation relates a eigenvector $\boldsymbol{u}^{(r)}$ of the covariance matrix M' in terms of the data $\boldsymbol{x}_i'$

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Solving $\alpha_1, \dots, \alpha_n$

- Removing $\boldsymbol{K}$ from both sides will only affect the $\boldsymbol{\alpha}^{(r)}$ with zero $\lambda^{(r)}$ (proof omitted), leaving the final form of the eigenvalue system

$$\boldsymbol{K}\boldsymbol{\alpha}^{(r)} = n\lambda^{(r)}\boldsymbol{\alpha}^{(r)}$$

- Since $\|\boldsymbol{u}\| = 1$, we require $n\lambda\boldsymbol{\alpha}^{\mathrm{T}}\boldsymbol{\alpha} = 1 \Rightarrow \|\boldsymbol{\alpha}\|^2 = 1/n\lambda \Rightarrow \|\boldsymbol{\alpha}\| = \sqrt{1/n\lambda}$
  Proof later
- However, $\boldsymbol{\alpha}^*$ from the eigendecomposition of $\boldsymbol{K}$ have unit length and eigenvalue $\lambda^* = n\lambda^{(r)}$
  To correct for this, $\boldsymbol{\alpha}^{(r)} = \dfrac{\boldsymbol{\alpha}^*}{\sqrt{n\lambda^{(r)}}} = \dfrac{\boldsymbol{\alpha}^*}{\sqrt{n\lambda^*/n}} = \dfrac{\boldsymbol{\alpha}^*}{\sqrt{\lambda^*}}$
- Since $\lambda^{(r)} = \lambda^*/n$, the relative importance of the eigenvectors can be determined from λ^*

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Proof for $\|\boldsymbol{u}\| = 1 \Rightarrow n\lambda\boldsymbol{\alpha}^{\mathrm{T}}\boldsymbol{\alpha} = 1$

- Since $\|\boldsymbol{u}\| = 1$

$$\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u} = 1$$

$$\left(\sum_i \alpha_i \boldsymbol{x}_i'^{\mathrm{T}}\right)^{\mathrm{T}}\left(\sum_j \alpha_j \boldsymbol{x}_j'^{\mathrm{T}}\right) = 1$$

$$\sum_i \sum_j \alpha_i \alpha_j \, \boldsymbol{x}_i' \boldsymbol{x}_j'^{\mathrm{T}} = 1$$

$$\sum_i \sum_j \alpha_i K_{ij} \alpha_j = 1$$

- Multiply α_i to $\sum_j K_{ij}\,\alpha_j = n\lambda \sum_k \alpha_k$ gives

$$n\lambda \sum_i \sum_k \alpha_i \alpha_k = \sum_i \sum_j \alpha_i K_{ij}\,\alpha_j$$

$$n\lambda \sum_i \sum_k \alpha_i \alpha_k = 1$$

$$n\lambda\boldsymbol{\alpha}^{\mathrm{T}}\boldsymbol{\alpha} = 1$$

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Proof for $x^{\mathrm{T}}xu = xux^{\mathrm{T}}$

$$(v^{\mathrm{T}}v)u = \begin{pmatrix} v_1v_1 & \cdots & v_1v_n \\ \vdots & \ddots & \vdots \\ v_nv_1 & \cdots & v_nv_n \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}$$

$$= \begin{pmatrix} v_1v_1u_1 + \cdots + v_1v_nu_n \\ \vdots \\ v_nv_1u_1 + \cdots + v_nv_nu_n \end{pmatrix}$$

$$= \begin{pmatrix} (v_1u_1 + \cdots + v_nu_n)v_1 \\ \vdots \\ (v_1u_1 + \cdots + v_nu_n)v_n \end{pmatrix}$$

$$= (v_1u_1 + \cdots + v_nu_n) \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$$

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Projection of $\phi(x)$ on u

- Given a point y, the projection of $\phi(y)$ on the eigenvector $u^{(r)}$ of M' can be computed using $\boldsymbol{\alpha}^{(r)}$ as

$$\phi(y)u^{(r)} = \sum_{i=1}^{n} \alpha_i^{(r)} \phi(y)^{\mathrm{T}} x_i'$$
$$= \sum_i \alpha_i^{(r)} K(y, x_i)$$

- This allows the principal components to be used for clustering the existing datapoints as well as classifying new datapoints into the clusters

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Normalizing M'

- X' has been assumed to be normalized so far
- To normalize a matrix X', subtract every column with the mean of the column:

$$x^* = x' - \frac{1}{n}\sum_{i=1}^{n} x_i'$$

- The corresponding kernel,

$$K^*\left(x_i, x_j\right) = x_i^* x_j^* = \left(x' - \frac{1}{n}\sum_{i=1}^{n} x_i'\right)\left(x' - \frac{1}{n}\sum_{i=1}^{n} x_i'\right)$$

$$= K\left(x_i, x_j\right) - \frac{1}{n}\sum_{k=1}^{n} K(x_i, x_k)$$

$$-\frac{1}{n}\sum_{k=1}^{n} K\left(x_j, x_k\right) + \frac{1}{n^2}\sum_{l,k=1}^{n} K(x_l, x_k)$$

Or in matrix notation

$$\boldsymbol{K}^* = \boldsymbol{K} - 2\mathbf{1}_{1/n}\boldsymbol{K} + \mathbf{1}_{1/n}\boldsymbol{K}\mathbf{1}_{1/n}$$

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