

ECON526: Quantitative Economics with Data Science Applications

Latent Variables and Introduction to Unsupervised Learning

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Overview



Motivation and Materials

- In this lecture, we will continue with some applications of the tools we developed in the previous lectures
- We introduce scikit-learn, a package for old-school (i.e. not deep learning or neural networks) ML and data analysis
 - → Introduces "unsupervised learning" (i.e., tools to interpret data structure without any forecasts/predictions)



Packages

```
import numpy as np
import matplotlib.pyplot as plt
import scipy
from numpy.linalg import cond, matrix_rank, norm
from scipy.linalg import inv, solve, det, eig, lu, eigvals
from scipy.linalg import solve_triangular, eigvalsh, cholesky
import seaborn as sns
import pandas as pd
from sklearn.decomposition import PCA
from sklearn.cluster import KMeans
```



Latent Variables



Features, Labels, and Latents

- Data science and ML often use different terminology than economists:
 - → **Features** are economists **explanatory or independent variables**. They have the key source of variation to make predictions and conduct counterfactuals
 - → Labels correspond to economists observables or dependent variables
 - → Latent Variables are unobserved variables, typically sources of heterogeneity or which may drive both the dependent and independent variables
- Economists will use theory and experience to transform data (i.e., what ML people call "feature engineering") for better explanatory power or map to theoretical models



Unsupervised Learning

- ML refers to methods using only features as unsupervised learning. The structure of the underlying data can teach you about its data generating process
- **Key:** uncover and interpret latent variables using statistics coupled with assumptions from economic theory. There is theory beyond all interpretation



Principle Components



Principle Components and Factor Analysis

- Another application of eigenvalues is dimension reduction, which simplifies features by uncovering latent variables. Unsupervised
- One technique is Principle Components Analysis (PCA), which uncovers latent variables that capture the primary directions of variation in the underlying data
 - → May allow mapping data into a lower-dimensional, uncorrelated features
 - → Uses Singular Value Decomposition (SVD) a generalization of eigendecomposition to non-square matrices
- Given a matrix $X \in \mathbb{R}^{N imes M}$, can we find a lower-dimensional representation $Z \in \mathbb{R}^{N imes L}$ for L < M that captures the most variation in X?
- The goal is to invert the X data to find the Z-and provide a mapping to reduce the dimensionality for future data.



Singular Value Decomposition

- Many applications of SVD (e.g., least squares, checking rank), in part because
 it is especially "numerically stable" (i.e., not sensitive to the roundoff errors we
 talked about previously)
- One application is to find the latent variables in PCA
- PCA can be interpreted with an eigendecomposition, but can be more confusing than just using the SVD directly.



SVD

An SVD for any $X \in \mathbb{R}^{N imes M}$ is:

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

- The diagonal elements of $\Sigma \in \mathbb{R}^{N imes M}$ are singular values, and there are zeros everywhere else. If M < N then there M singular values $(\sigma_1, \ldots \sigma_M)$
 - ightarrow Those singular values are also the square roots of the eigenvalues of XX^T (or X^TX)
 - ightarrow The number of non-zero singular values is the rank of the matrix X
- ullet $U \in \mathbb{R}^{N imes N}$ and $V \in \mathbb{R}^{M imes M}$ are orthogonal matrices
 - ightarrow U is eigenvectors of XX^T and V is eigenvectors of X^TX



Decomposing the Data

A key result is that we can decompose the data into a sum of outer products of the eigenvectors and singular values. Assume ordered so that

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_M$$
:

$$X = U \Sigma V^T = \sum_{m=1}^M \sigma_m u_m v_m^T$$

Where here we assumed that the $\mathrm{rank}(X) \leq M$ and

- $ullet u_m \in \mathbb{R}^N$ is the m-th column of U and $v_m \in \mathbb{R}^M$ is the mth column of V
- So $u_m v_m^T$ is an N imes M matrix but you can show that it is rank-1. i.e., you can decompose it into the product of two vectors.



Interpreting Rank

- Intuition: rank r if it can be decomposed into the sum of r rank-1 matrices
 - o Alternatively, can interpret rank of an N imes M matrix is 3 if can find a $A\in\mathbb{R}^{N imes 3}$ and $B\in\mathbb{R}^{3 imes M}$ such that X=AB
- ullet Remember: this works for **any** matrix $X \in \mathbb{R}^{N imes M}$



Dimension Reduction

• Frequently $\sigma_1\gg\sigma_M$ and the σ_m may decay quickly, so we can approximate X with fewer terms by truncating the sum at L < M.

$$Xpprox \sum_{m=1}^{L}\sigma_{m}u_{m}v_{m}^{T}$$

• Note that if the data is actually lower-dimensional in a suitable space (e.g., ${\rm rank}(X)=L< M$) then $\sigma_m=0$ for $L< m\leq M$, so the truncated sum is exact



PCA as an Optimal Dimension Reduction

- ullet Can prove that if we truncate at L < M, this is the best rank L approximation to X according to some formal criteria.
 - → Intuitively, finds directions of the data that capture the most variation in the covariance matrix
 - → Can prove it is the solution to the optimization problem to explain the most variation in the data with the lowest dimensionality



Creating a Dataset with Latent Factors

Create a dataset with two latent factors, the first dominating

Z is (50, 2), X is (50, 3)



PCA Without Dimension Reduction

- See QuantEcon SVD for coding yourself. We will use the sklearn package
- The explained variance is the fraction of the variance explained by each factor

```
1 pca = PCA(n_components=3)
2 pca.fit(X)
3 with np.printoptions(precision=4, suppress=True, threshold=5):
4  print(f"Singular Values (sqrt eigenvalues):\n{pca.singular_values_}")
5  print(f"Explained Variance (ordered):\n{pca.explained_variance_ratio_}")

Singular Values (sqrt eigenvalues):
[29.3117  0.8639  0.7378]
Explained Variance (ordered):
[0.9985  0.0009  0.0006]
```



Dimension Reduction with PCA

```
pca = PCA(n_components=2) # one less, and correctly specified

Z_hat = pca.fit_transform(X) # transformed by dropping last factor

Scale and sign may not match due to indeterminacy

print(f"Correlation of Z_1 to Z_hat_1 = {np.corrcoef(Z.T, Z_hat.T)[0,2]}")

print(f"Correlation of Z_2 to Z_hat_2 = {np.corrcoef(Z.T, Z_hat.T)[1,3]}")
```

Correlation of Z_1 to $Z_{hat_1} = 0.9995222995521564$ Correlation of Z_2 to $Z_{hat_2} = -0.5347669077019769$



Interpreting the Results

- The first factor in the decomposition is nearly perfectly (positive or negatively) correlated with the more important latent factor
 - → The sign could have gone either way. The key is the shared information
 - → How could you have known the sign is indeterminate?
- The 2nd factor has a good but not great correlation with the 2nd latent. Why?
- The variance decomposition that gave a 3rd factor with non-zero variance
 - → We only had two latent variables. Why didn't it figure it out?
- How could you have changed the DGP to make this less successful?



Warning

- We have just scratched the surface to build some intuition.
- Many missing details and caveats (e.g., you may want to rescale your data, make sure everything is demeaned if implementing yourself, etc.)
- Read up on the documentation and theory before using in practice
- Many generalizations exist which are more appropriate in particular settings



Auto-Encoders



Auto-Encoders and Dimensionality Reduction

- General class of problems which they call auto-encoders in ML/data science
 - ightarrow Function f, the encoder, maps X to a latent space Z, which may be lower-dimensional
 - ightarrow Function g, the decoder, maps points in the latent space Z back to X
 - ightarrow $heta_e$ and $heta_d$ are parameters for f and g which we are trying to find
- Then the goal is to find the $heta_e$ and $heta_d$ parameters for our encoder, f, and decoder, g, where for as many X as possible we have

$$g(f(x; heta_e); heta_d) pprox x$$

• The $z=f(x;\theta_e)$ may be lower-dimensional, but may be useful regardless



Optimization Problem for an Auto-encoder

• If we had a distribution for x then can solve

$$\min_{ heta_e, heta_d} \mathbb{E} ||g(f(x; heta_e); heta_d) - x||_2^2$$

• But typically in practice we replace expectation with empirical distribution $\{x_1, \dots x_N\}$

$$\min_{ heta_e, heta_d} rac{1}{N} \sum_{n=1}^N ||g(f(x_n; heta_e); heta_d) - x_n||_2^2$$



PCA as a Linear Auto-Encoder

• Let $f(x)=W^Tx$ and g(z)=Wz where $W\in\mathbb{R}^{M imes L}$. If $\hat{x}pprox WW^Tx$, "reconstruction error" is $||\hat{x}-x||_2^2$.

$$\min_{W} rac{1}{N} \sum_{n=1}^{N} ||W \overbrace{W^T x_n}^{z_n = f(x_n;W)} - x_n||_2^2, \quad ext{with } W^T W = I$$

- ullet Can show gives equivalent to PCA! For fixed L latent space size, W are the first L columns of V from the SVD (sorted by size of singular values)
- In more advanced machine learning examples, intuition seems to come up frequently. Related to embeddings, which come up with NLP, networks, etc.



Discrete Latent Variables



Discrete Latent Variables

- PCA was a way to uncover continuous latent variables or find low-dimensional continuous approximations
- But latent variables may be discrete (e.g., types of people, firms)
- Hidden discrete variables require assigning observations to groups



Clustering

- Clustering lets you take a set of observations with (potentially) variables (i.e., features) and try to assign a discrete latent variable to each observation
 - → Theory may or may not help us know the number of groups
 - → While some are statistical and probabilistic, most methods assign a single latent type rather than a distribution
 - → Choosing the number of groups to assign to is a challenge that requires theory and regularization - which we will avoid here
 - → Instead, just as with PCA we will choose the number of groups ad-hoc rather than in a disciplined way



Partitioning Sets

- ullet Let $X \in \mathbb{R}^{N imes M}$ with $x_1, \dots x_N \in \mathbb{R}^M$ the individual observations
- Assume that each x_n has a latent discrete $k \in \{1, \ldots K\}$ then we can assign each observation to one group
 - $ightarrow \mathbf{S} \equiv \{S_1, \dots, S_K\}$ where each $n=1,\dots N$ is in exactly one S_k (i.e. a partition)
- The goal is to find the partition which is the most likely to assign each x_n the correct latent variable k
- An alternative interpretation is to think of this as a dimension-reduction technique that reduces complicated data into a low-dimensional discrete variable
- In economics, we will sometimes cluster on some observations to reduce the dimension, then leave others continuous



k-means Clustering

- ullet Consider if the $n \in S_k$ with should have similar x_n
 - → Group observations that are close or similar to each other
 - ightharpoonup As always in linear algebra, close suggests using a norm. The Euclidean norm in the M dimensional feature space is a good baseline
- Objective function of k-means: choose the partition ${\bf S}$ which minimizes the norm between observations within each group
 - ightarrow Normalize by group size $|S_k|$ to avoid distorting the objective function due to different group sizes



Formal Optimization Problem

Formally,

$$\min_{\mathbf{S}} \sum_{k=1}^K rac{1}{|S_k|} \sum_{x_n, x_{n'} \in S_k} ||x_n - x_{n'}||_2^2$$

ullet Using standard Euclidean norm between two elements in S_k

$$||x_n-x_{n'}||_2^2=\sum_{m=1}^M(x_{nm}-x_{n'm})^2$$



k-means Objective Function

• Can prove that the previous objective is equivalent to minimizing the sum of the squared distances from the group k's mean

$$\min_{\mathbf{S}} \sum_{k=1}^K \sum_{n \in S_k} ||x_n - ar{x}_k||_2^2$$

ullet Where the mean of group k is standard, and across all m features

$$ar{x}_k \equiv rac{1}{|S_k|} \sum_{x_n \in S_k} x_n$$

ullet Avoid different scales so $ar{x}_k$ isn't dominated by one feature



Generating Data with Latent Groups

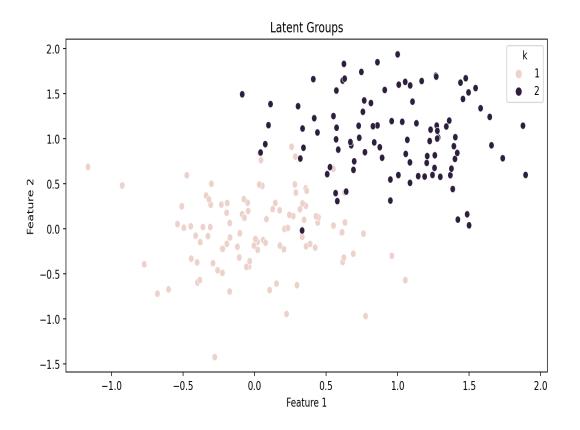
- Generate data with 2 features and 2 latent groups and see how k-means does
- First, put the data in a dataframe

```
1 mu_1 = np.array([0.0, 0.0]) # mean of k=1
2 mu_2 = np.array([1.0, 1.0]) # mean of k=2
3 sigma = np.array([[0.2, 0], [0, 0.2]]) # use same variance
4 N = 100 # observations
5 X_1 = np.random.multivariate_normal(mu_1, sigma, N)
6 X_2 = np.random.multivariate_normal(mu_2, sigma, N)
7 df_1 = pd.DataFrame({"f1": X_1[:, 0], "f2": X_1[:, 1], "k": 1})
8 df_2 = pd.DataFrame({"f1": X_2[:, 0], "f2": X_2[:, 1], "k": 2})
9 df = pd.concat([df_1, df_2], ignore_index=True)
```



Plotting Code with Seaborn

```
fig, ax = plt.subplots()
sns.scatterplot(data=df, x="f1", y="f2",
hue="k", ax=ax)
ax.set(xlabel="Feature 1", ylabel="Feature 2",
title="Latent Groups")
plt.show()
```





k-means to Recover the Latent Groups

- Run k-means with 2 clusters and check the results
- If correlation is close to 1 then successfully recovered the latent groups
- If the correlation is close to -1 then it was successful. The latent groups \hat{k} numbers are ordered arbitrarily, just as k was

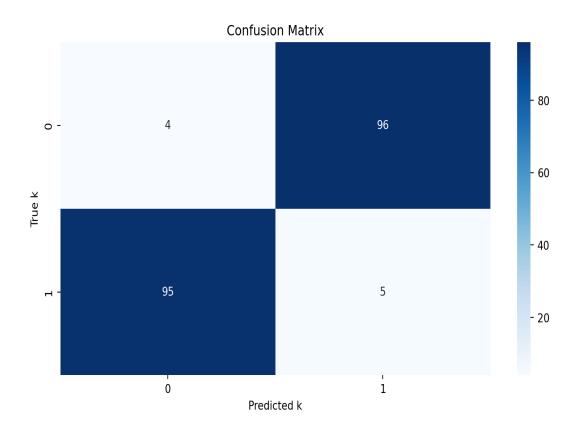
```
1 kmeans = KMeans(n_clusters=2, random_state=0)
2 k_hat = kmeans.fit_predict(df[["f1", "f2"]])
3 df["k_hat"] = k_hat + 1
4 corr = df["k"].corr(df["k_hat"])
5 print(f"Correlation between k and k_hat:{corr:.2f}")
```

Correlation between k and k_hat:-0.91



Confusion Matrix

```
from sklearn.metrics import confusion_matrix
# compute confusion matrix
cm = confusion_matrix(df["k"], df["k_hat"])
# plot confusion matrix
sns.heatmap(cm, annot=True, cmap='Blues')
plt.xlabel('Predicted k')
plt.ylabel('True k')
plt.title('Confusion Matrix')
plt.show()
```





Potentially Swap \hat{k} and Compare

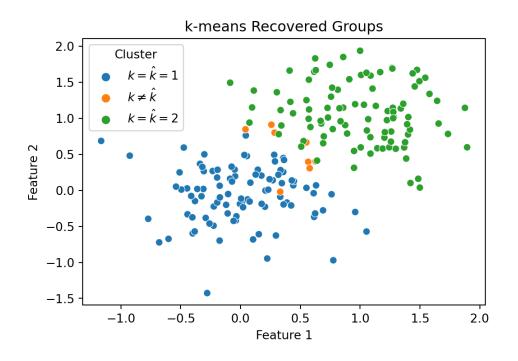
Label ordering arbitary, so "confusion matrix might require reordering to compare

Correlation now 0.9100455034127839



Plotting the Uncovered Latent Groups

```
1 fig, ax = plt.subplots(figsize=(6, 4))
2 sns.scatterplot(data=df, x="f1", y="f2",
3 hue="Cluster", ax=ax)
4 ax.set(xlabel="Feature 1", ylabel="Feature 2",\
5 title="k-means Recovered Groups")
6 plt.show()
```





(Optional) Factors within a Portfolio Model



Simulation

In the previous lecture we introduced code for simulation

```
1 def simulate(A, X_0, T):
2     X = np.zeros((2, T+1))
3     X[:,0] = X_0
4     for t in range(T):
5         X[:,t+1] = A @ X[:,t]
6     return X
```



A Portfolio Example

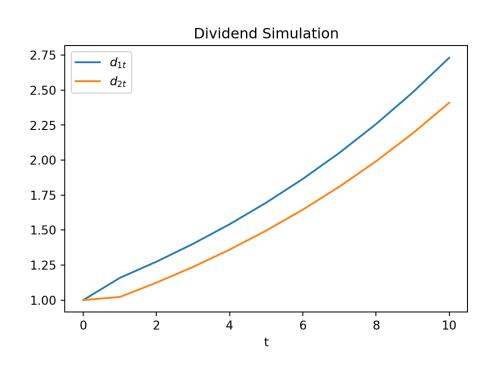
- ullet Two assets pay dividends $d_t \equiv \begin{bmatrix} d_{1t} & d_{2t} \end{bmatrix}^T$ following $d_{t+1} = A\,d_t$ from d_0
- ullet Portfolio has $G\equiv [G_1\quad G_2]$ shares of each asset and you discount at rate eta

```
1 A = np.array([[0.6619469, 0.49646018],[0.5840708, 0.4380531]])
2 G = np.array([[10.0, 4.0]])
3 d_0 = np.array([1.0, 1.0])
4 T, beta = 10, 0.9
5 p_0 = G @ solve(np.eye(2) - beta * A, d_0)
6 d = simulate(A, d_0, T)
7 y = G @ d # total dividends from portfolio
8 print(f"Portfolio value at t=0 is {p_0[0]:.5g}, total dividends at time {T} is {y[0,T]:.5g}")
```

Portfolio value at t=0 is 1424.5, total dividends at time 10 is 36.955



Dividends Seem to Grow at a Similar Rate?





Digging Deeper

Let's do an eigendecomposition to analyze the factors

```
1 Lambda, Q = eig(A)
2 print(np.real(Lambda))
```

- 1.10000000e+00 -2.65486732e-09]
- The first eigenvector is 1.1, but the second is very close to zero!
 - \rightarrow (In fact, I rigged it to be zero by constructing from a Λ , so this is all numerical copy/paste errors)
- ullet Suggests that maybe only one latent factor driving both d_{1t} and d_{2t} ?
- Of course, you may have noticed that the columns in the matrix looked collinear, which was another clue.



Evolution Matrix is Very Simple with $\lambda_2=0$

If we stack columns $Q \equiv [q_1 \quad q_2]$ then,

$$A = Q \Lambda Q^{-1} = Q egin{bmatrix} \lambda_1 & 0 \ 0 & 0 \end{bmatrix} Q^{-1} = \lambda_1 q_1 q_1^{-1}$$

```
1 lambda_1 = np.real(Lambda[0])
2 q_1 = np.reshape(Q[:,0], (2,1))
3 q_1_inv = np.reshape(inv(Q)[0,:], (1,2))
4 norm(A - lambda_1 * q_1 @ q_1_inv) # pretty close to zero!
```

2.663274500543771e-09



Transforming to the Latent State

- ullet Recall: $A=Q\Lambda Q^{-1}$ can be interpreted as:
 - → Transformation to latent space, scaling, transform back
- We can demonstrate this in our example:
 - ightarrow Transforming d_0 to ℓ_0 using q_1^{-1}
 - ightarrow Evolving ℓ_t from ℓ_0 with $\ell_{t+1} = \lambda_1 \ell_t$, or $\ell_t = \lambda_1^t \ell_0$
 - ightarrow Transforming back with q_1
 - ightarrow Checking if it aligns with the d_t



Implementation

```
1 l_0 = lambda_1 * q_1_inv @ d_0 # latent space
2 l = l_0 * np.power(lambda_1, np.arange(0, T)) # powers
3 d_hat = q_1 * l # back to original space
4 # Missing d_0 since doing A * d_0 iterations
5 print(f"norm = {norm(d[:,1:] - d_hat)}")
6 y_hat = G @ d_hat
```

norm = 2.3494410877755447e-10

Let's see if these line up perfectly



Total Dividends and the Latent Variable

