ECON526: Quantitative Economics with Data Science Applications

Applications of Linear Algebra

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Overview

Motivation and Materials

- In this lecture, we will cover some applications of the tools we developed in the previous lecture
- The goal is to build some useful tools to sharpen your intuition on linear algebra and eigenvalues/eigenvectors, and practice some basic coding
- 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)
- Some additional material and references
    - QuantEcon Python
    - QuantEcon DataScience
    - A First Course in Quantitative Economics with Python

Packages

```python
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
```

New Packages for Data Science and ML

```python
import seaborn as sns
import pandas as pd
from sklearn.decomposition import PCA
from sklearn.cluster import KMeans
```

Difference Equations

Linear Difference Equations as Iterative Maps

- Consider $A : \mathbb{R}^N \to \mathbb{R}^N$ as the linear map for the state $x_t \in \mathbb{R}^N$
- An example of a linear difference equation is

$$x_{t+1} = Ax_t$$

where

$$A \equiv \begin{bmatrix} 0.9 & 0.1 \\ 0.5 & 0.8 \end{bmatrix}$$

```python
A = np.array([[0.9, 0.1], [0.5, 0.8]])
x_0 = np.array([1, 1])
x_1 = A @ x_0
print(f"x_1 = {x_1}, x_2 = {A @ x_1}")
```

```
x_1 = [1.  1.3], x_2 = [1.03 1.54]
```

Iterating with $\rho(A) > 1$

Iterate $x_{t+1} = Ax_t$ from x_0 for $t = 100$

```
x_0 = np.array([1, 1])
t = 200
print(f"rho(A) = {np.max(np.abs(eigvals(A)))}")
print(f"x_{t} = {np.linalg.matrix_power(A, t) @ x_0}")
```

```
rho(A) = 1.079128784747792
x_200 = [3406689.32410673 6102361.18640516]
```

- Diverges to $x_\infty = \begin{bmatrix} \infty & \infty \end{bmatrix}^T$
- $\rho = 1 + 0.079$ says in the worst case (i.e., $x_t \propto$ the eigenvector associated with $\lambda = 1.079$ eigenvalue), expands by 7.9% on each iteration

Iterating with $\rho(A) < 1$

```python
A = np.array([[0.6, 0.1], [0.5, 0.8]])
print(f"rho(A) = {np.max(np.abs(eigvals(A)))}")
print(f"x_{t} = {np.linalg.matrix_power(A, t) @ x_0}")
```

```
rho(A) = 0.9449489742783178
x_200 = [6.03450418e-06 2.08159603e-05]
```

- Converges to $x_\infty = \begin{bmatrix} 0 & 0 \end{bmatrix}^T$

Iterating with $\rho(A) = 1$

- To make a matrix that has $\rho(A) = 1$ reverse eigendecomposition!
- Leave previous eigenvectors in Q, change Λ to force $\rho(A)$ directly

```
Q = np.array([[-0.85065081, -0.52573111], [0.52573111, -0.85065081]])
print(f"check orthogonal: dot(x_1,x_2) approx 0: {np.dot(Q[:,0], Q[:,1])}"
Lambda = [1.0, 0.8]  # choosing eigenvalue so max_n|lambda_n| = 1
A = Q @ np.diag(Lambda) @ inv(Q)
print(f"rho(A) = {np.max(np.abs(eigvals(A)))}")
print(f"x_{t} = {np.linalg.matrix_power(A, t) @ x_0}")
```

```
check orthogonal: dot(x_1,x_2) approx 0: -1.9275984594779062e-17
rho(A) = 1.0
x_200 = [ 0.27639321 -0.17082039]
```

Unemployment Dynamics

Dynamics of Employment without Population Growth

- Consider an economy where in a given year $\alpha = 5\%$ of employed workers lose job and $\phi = 10\%$ of unemployed workers find a job
- We start with $E_0 = 900,000$ employed workers, $U_0 = 100,000$ unemployed workers, and no birth or death. Dynamics for the year:

$$E_{t+1} = (1-\alpha)E_t + \phi U_t$$
$$U_{t+1} = \alpha E_t + (1-\phi)U_t$$

- Can write this as a matrix equation

$$\underbrace{\begin{bmatrix} E_{t+1} \\ U_{t+1} \end{bmatrix}}_{X_{t+1}} = \underbrace{\begin{bmatrix} 1-\alpha & \phi \\ \alpha & 1-\phi \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} E_t \\ U_t \end{bmatrix}}_{X_t}$$

Simulating

Simulate by iterating $X_{t+1} = AX_t$ from X_0 until $T = 100$

```
def simulate(A, X_0, T):
    X = np.zeros((2, T+1))
    X[:,0] = X_0
    for t in range(T):
        X[:,t+1] = A @ X[:,t]
    return X
X_0 = np.array([900000, 100000])
A = np.array([[0.95, 0.1], [0.05, 0.9]])
T = 100
X = simulate(A, X_0, T)
print(f"X_{T} = {X[:,T]}")
```

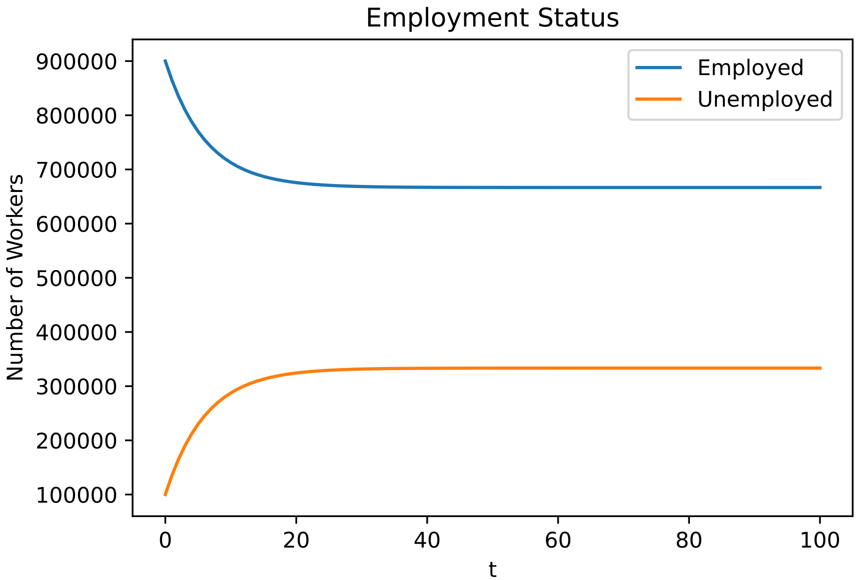


```
X_100 = [666666.6870779  333333.31292209]
```

Plotting Code

```python
fig, ax = plt.subplots(figsize=(6, 4))
ax.plot(range(T+1), X.T, label=["Employed", "Unemployed"])
ax.set(xlabel="t", ylabel="Number of Workers", title="Employment Status")
ax.legend()
plt.show()
```

Dynamics of Unemployment



Convergence to a Longrun Distribution

- Find X_∞ by iterating $X_{t+1} = AX_t$ many times from a X_0?
  - Check if it has converged with $X_\infty \approx AX_\infty$
  - Is X_∞ the same from any X_0? Will discuss "ergodicity" later
- Alternatively, note that this expression is the same as

$$1 \times \bar{X} = A\bar{X}$$

  - i.e, a $\lambda = 1$ where $\bar{X}$ is the corresponding eigenvector of A
  - Is $\lambda = 1$ always an eigenvalue? (yes if all $\sum_{n=1}^{N} A_{ni} = 1$ for all i)
  - Does $\bar{X} = X_\infty$? For any X_0?
  - Multiple eigenvalues with $\lambda = 1 \implies$ multiple $\bar{X}$

Using the First Eigenvector for the Steady State

```python
Lambda, Q = eig(A)
print(f"real eigenvalues = {np.real(Lambda)}")
print(f"eigenvectors are column-by-column in Q =\n{Q}")
print(f"first eigenvalue = 1? {np.isclose(Lambda[0], 1.0)}")
X_bar = Q[:,0] / np.sum(Q[:,0]) * np.sum(X_0)
print(f"X_bar = {X_bar}\nX_{T} = {X[:,T]}")
```

```
real eigenvalues = [1.   0.85]
eigenvectors are column-by-column in Q =
[[ 0.89442719 -0.70710678]
 [ 0.4472136   0.70710678]]
first eigenvalue = 1? True
X_bar = [666666.66666667 333333.33333333]
X_100 = [666666.6870779  333333.31292209]
```

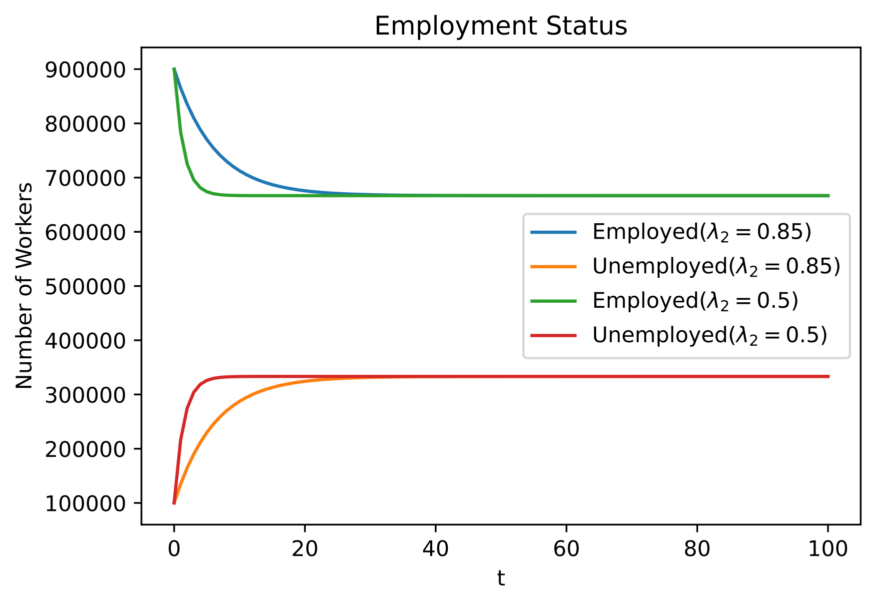
Using the Second Eigenvalue for the Convergence Speed

- The second largest $(\lambda_2 < 1)$ provides information on the speed of convergence
  - 0 is instantaneous convergence here
  - 1 is no convergence here
- Create a new matrix with the same steady state, different speed

```
Lambda_fast = np.array([1.0, 0.5])
A_fast = Q @ np.diag(Lambda_fast) @ inv(Q) # same eigenvectors
X_fast = simulate(A_fast, X_0, T)
print(f"X_{T} = {X_fast[:,T]}")
```

```
X_100 = [666666.66666667 333333.33333334]
```

Dynamics of Unemployment For Difference Convergence Speeds



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
- 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 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 set of features
  - Often uses Singular Value Decomposition (SVD) - a numerically stable generalization of eigendecomposition to non-square matrices.See QuantEcon SVD Notes
  - One of many methods. Many algorithms in ML and econometrics have similar goals but can be non-linear
- Given a matrix $X \in \mathbb{R}^{N \times M}$, can we find a lower-dimensional representation $Z \in \mathbb{R}^{N \times L}$ for $L < M$ that captures the most variation in X?
- The columns of Z are called the principle components of X
- The goal is to invert the X data to find the Z—and provide a mapping to reduce the dimensionality for future data

Decomposing the Data

PCA typically uses SVD in practice - but we will use eigendecomposition (aka spectral decomposition if symmetric) instead

Start by doing a decomposition of the "covariance matrix" of the data, XX^T, and form diagonal Λ as a product of vectors $\sigma \in \mathbb{R}^N$ (the singular values)

$$XX^T = Q\Lambda Q^T = \underbrace{Q\sigma}_{X} \underbrace{\sigma^T Q^T}_{(Q\sigma)^T = X^T}, \quad \text{where } \Lambda \equiv \sigma\sigma^T$$

Hence, denoting the nth column of Q as Q_n, we have

$$X = Q\sigma = Q_1\sigma_1 + Q_2\sigma_2 + ... + Q_M\sigma_M$$

Dimension Reduction

- Assume we sorted so $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_M$. Frequently $\sigma_1 \gg \sigma_M$
- For many problems, the σ_m decay quickly, so we can approximate X with fewer terms by truncating the sum at $L < M$.

$$X \approx Q_1\sigma_1 + Q_2\sigma_2 + ... + Q_L\sigma_L$$

- The eigendecomposition (or SVD) can find the orthogonal 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
- This is useful even if it is not necessary to reduce the dimensionality of the data
    - Many high-dimensional data sources are low-dimensional in the suitable space.
    - This is especially true when models allow for nonlinear transformations (e.g., neural networks, autoencoders, etc.)

Creating a Dataset with Latent Factors

Create a dataset with two latent factors, the first dominating

```
N = 50 # number of observations
L, M = 2, 3 # number of latent and observed factors
Z = np.random.randn(N, L) # latent factors
F = np.array([[1.0, 0.05], # X_1 = Z_1 + 0.05 Z_2
              [2.0, 0.0], # X_2 = 2 Z_1
              [3.0, 0.1]]) # X_3 = 3 Z_1 + 0.1 Z_2
X = Z @ F.T + 0.1 * np.random.randn(N, M) # added noise
```

PCA without any 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

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

```
Singular Values (sqrt eigenvalues):
[29.4181  0.7984  0.6654]
Explained Variance (ordered):
[0.9988 0.0007 0.0005]
```

Dimension Reduction with PCA

```python
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 = -0.9995888625038096
Correlation of Z_2 to Z_hat_2 = 0.5464398297674395
```

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
  - In our process, there are only two latent variables. Why didn't it figure it out?
- How could you have changed the DGP to make this **less** successful?

Present Discounted Values

Geometric Series

- Assume dividends follow $y_{t+1} = G y_t$ for $t = 0, 1, \ldots$ and y_0 is given
- $G > 0$, dividends are discounted at factor $\beta > 1$ then $p_t = \sum_{s=0}^{\infty} \beta^s y_{t+s} = \frac{y_t}{1-\beta G}$
- More generally if $x_{t+1} = A x_t$, $x_t \in \mathbb{R}^N$, $y_t = G x_t$ and $A \in \mathbb{R}^{N \times N}$, then

$$
\begin{aligned}
p_t &= y_t + \beta y_{t+1} + \beta^2 y_{t+2} + \ldots = G x_t + \beta G A x_t + \beta G A A x_t + \ldots \\
&= \sum_{s=0}^{\infty} \beta^s A^s y_t \\
&= G(I - \beta A)^{-1} x_t \quad , \text{ if } \rho(A) < 1/\beta
\end{aligned}
$$

- i.e., spectral radius of A, the maximum scaling, must be less than discounting
- Intuition from univariate: of $G \in \mathbb{R}^{1 \times 1}$ then $\text{eig}(G) = G$, so must have $|\beta G| < 1$

PDV Example

Here is an example with $1 < \rho(A) < 1/\beta$. Try with different A

```
beta = 0.9
A = np.array([[0.85, 0.1], [0.2, 0.9]])
G = np.array([[1.0, 1.0]]) # row vector
x_0 = np.array([1.0, 1.0])
p_t = G @ solve(np.eye(2) - beta * A, x_0)
#p_t = G @ inv(np.eye(2) - beta * A) @ x_0 # alternative
rho_A = np.max(np.abs(np.real(eigvals(A))))
print(f"p_t = {p_t[0]:.4g}, spectral radius = {rho_A:.4g}, 1/beta = {1/beta
```

```
p_t = 24.43, spectral radius = 1.019, 1/beta = 1.111
```

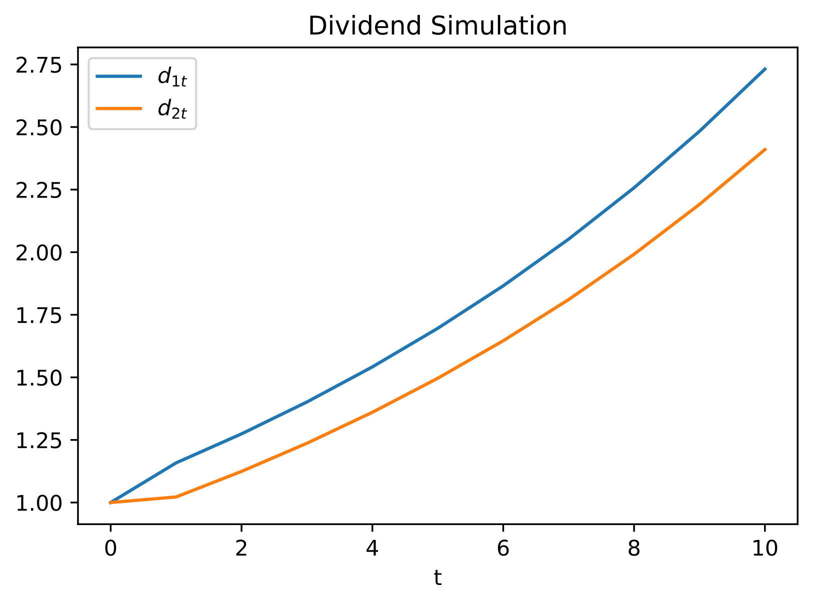
A Portfolio Example

- 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
- Porfolio has $G \equiv \begin{bmatrix} G_1 & G_2 \end{bmatrix}$ shares of each asset and you discount at rate β

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

```
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

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

```
[ 1.10000000e+00 -2.65486732e-09]
```

- The first eigenvector is 1.1, but the second is (numerically) zero!
  - (In fact, I rigged it to be zero by constructing from a Λ, so this is all numerical copy/paste errors)
- Suggests that maybe only one latent factor driving both d_{1t} and d_{2t}?

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

If we stack columns $Q \equiv \begin{bmatrix} q_1 & q_2 \end{bmatrix}$ then,

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

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

```
2.663274500543771e-09
```

Transforming to the Latent State

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

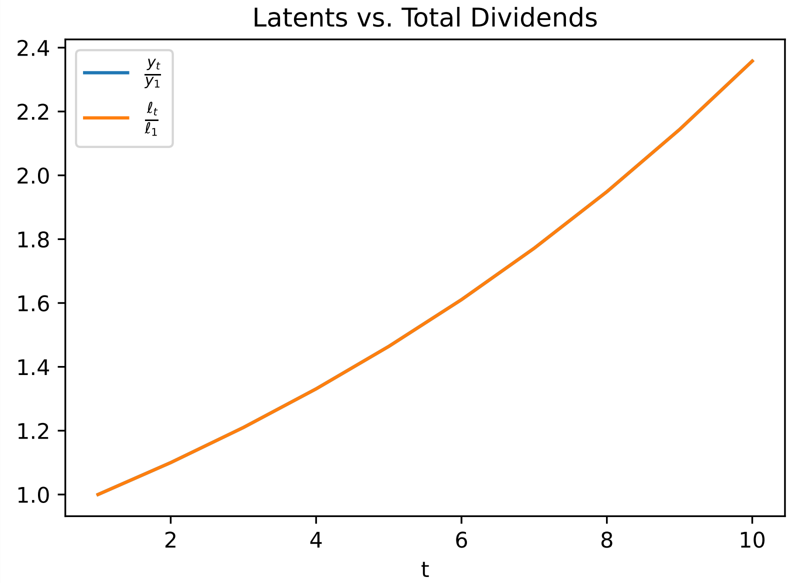
Implementation

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

```
norm = 2.3494410877755447e-10
```

Let's see if these line up perfectly

Total Dividends and the Latent Variable



Discrete Latent Variables

Clustering and 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 lets you take a set of observations with (potentially) variables (i.e., features) and try to assign a discrete latent variable to each observation
  - Sometimes we know the number of groups from theory, usually we do not
  - 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

- Let $X \in \mathbb{R}^{N \times M}$ with $x_1, \ldots x_N \in \mathbb{R}^M$ 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
  - $\mathbf{S} \equiv \{S_1, \ldots, S_K\}$ where each $n = 1, \ldots N$ 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 which 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

- If theory suggests that $n \in S_k$ with similar latent variables should have similar x_n
  - Group observations which are close or similar to each other
  - As always in linear algebra, close suggests using a norm. The euclidean norm in the M dimensional feature space is a good baseline
- The objective of k-means is to choose the partition $\mathbf{S}$ which minimizes the norm between observations within each group (normalized by group size $|S_k|$):

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

- 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

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

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

$$\bar{x}_k \equiv \frac{1}{|S_k|} \sum_{x_n \in S_k} x_n$$

- Careful with using wildly different scales (i.e. $\bar{x}_k$ may be dominated by one feature)

Generating Data with Latent Groups

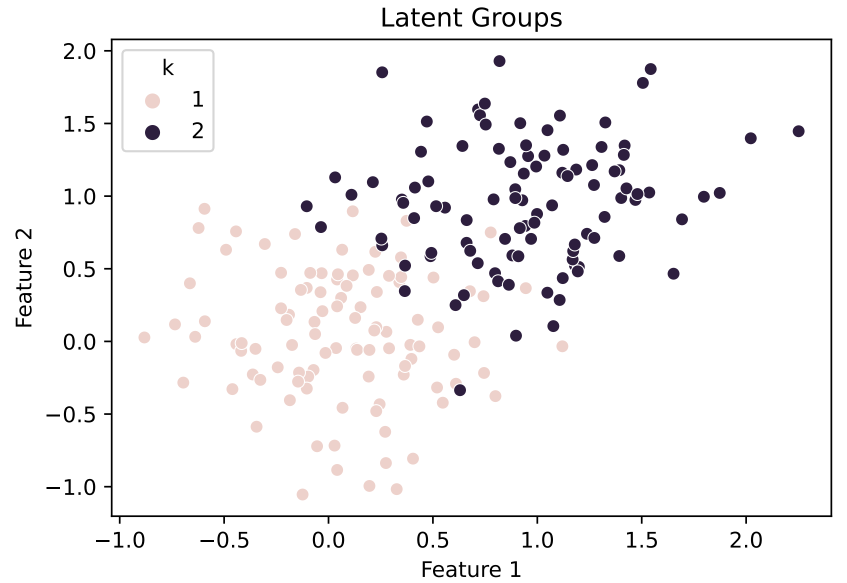
Generate data with 2 features and 2 latent groups and see how k-means does

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

Plotting Code with Seaborn

```python
fig, ax = plt.subplots(figsize=(6, 4))
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()
```

Plot of Features and Latents



k-means to Recover the Latent Groups

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

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

```
Correlation between k and k_hat:0.85
```

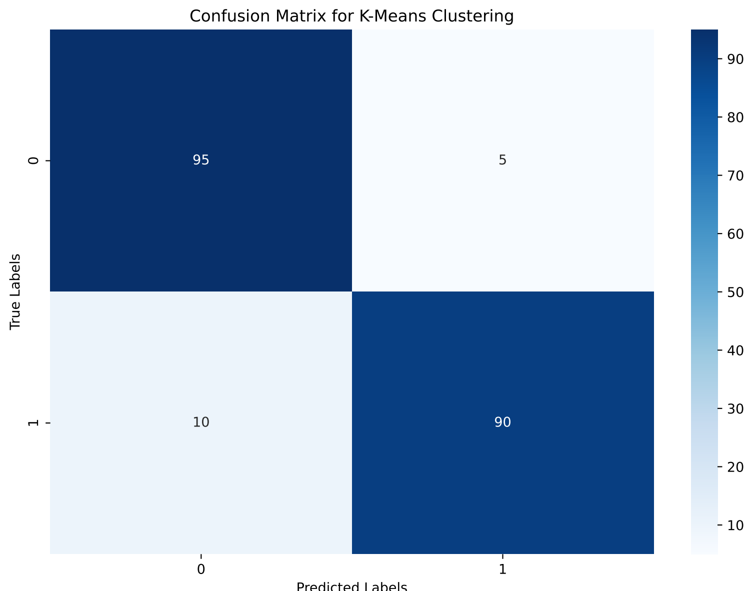
Confusion Matrix

```python
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 for K-Means Clustering')
plt.show()
```

Confusion Matrix



Swap $\hat{k}$ and Compare

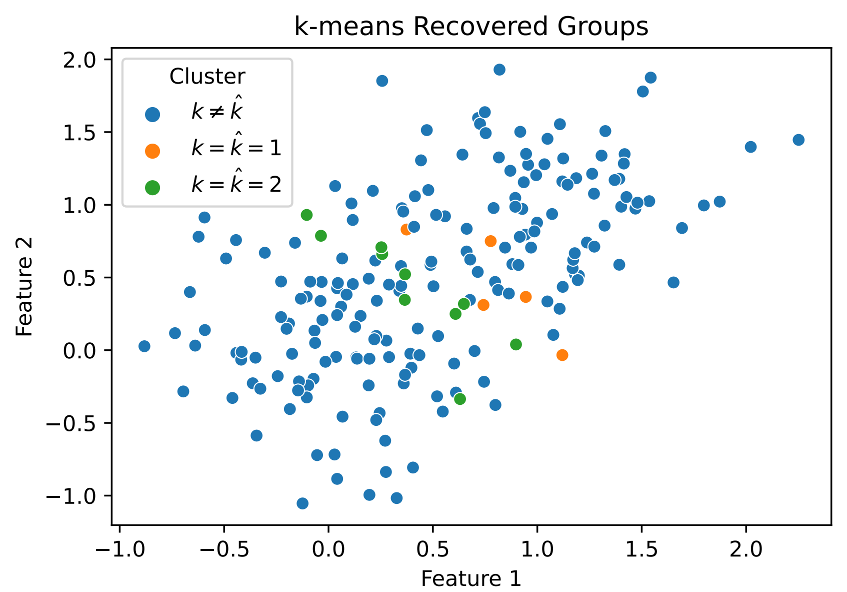
```python
df['k_hat'] = df['k_hat'].replace({1: 2, 2: 1}) # swap for this example
print(f"Correlation now {df['k'].corr(df['k_hat'])}")
df['k_cluster'] = df.apply(lambda x: x['k'] if x['k'] == x['k_hat'] else 3
# Add text to display using latex
df['Cluster'] = df['k_cluster'].replace({1: r'$k=\hat{k}=1$',
                                         2: r'$k=\hat{k}=2$',
                                         3: r'$k \neq \hat{k}$'})
```

```
Correlation now -0.851064496346989
```

Plotting the Uncovered Latent Groups

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

Plotting the Uncovered Latent Groups



(Optional) Matrix Conditioning and Stability

Matrix Conditioning

- Poorly conditioned matrices can lead to inaccurate or wrong solutions
- Tends to happen when matrices are close to singular or when they have very different scales - so there will be times when you need to rescale your problems

```python
eps = 1e-7
A = np.array([[1, 1], [1 + eps, 1]])
print(f"A =\n{A}")
print(f"A^{-1} =\n{inv(A)}")
```

```
A =
[[1.        1.       ]
 [1.0000001 1.       ]]
A^-1 =
[[-9999999.99336215  9999999.99336215]
 [10000000.99336215 -9999999.99336215]]
```

Condition Numbers of Matrices

- $\det(A) \approx 0$ may say it is "almost" singular, but it is not scale-invariant
- cond$(A) \equiv ||A|| \cdot ||A^{-1}||$ where $|| \cdot ||$ is the matrix norm - expensive to calculate in practice. Connected to eigenvalues cond$(A) = |\frac{\lambda_{max}}{\lambda_{min}}|$
- Scale free measure of numerical issues for a variety of matrix operations
- Intuition: if cond$(A) = K$, then $b \to b + \nabla b$ change in b amplifies to a $x \to x + K\nabla b$ error when solving $Ax = b$.
- See Matlab Docs on inv for example, where `inv` is a bad idea due to poor conditioning

```python
print(f"condition(I) = {cond(np.eye(2))}")
print(f"condition(A) = {cond(A)}, condition(A^(-1)) = {cond(inv(A))}")
```

```
condition(I) = 1.0
condition(A) = 40000001.939191714, condition(A^(-1)) = 40000002.00307444
```

Example with Interpolation

- Consider fitting data $x \in \mathbb{R}^{N+1}$ and $y \in \mathbb{R}^{N+1}$ with an N-degree polynomial
- That is, find $c \in \mathbb{R}^{N+1}$ such that

$$
\begin{aligned}
c_0 + c_1 x_1 + c_2 x_1^2 + ... + c_N x_1^N &= y_1 \\
... &= ... \\
c_0 + c_1 x_N + c_2 x_N^2 + ... + c_N x_N^N &= y_N
\end{aligned}
$$

- Which we can then use as $P(x) = \sum_{n=0}^{N} c_n x^n$ to interpolate between the points

Writing as a Linear System

- Define a matrix of all of the powers of the x values

$$A \equiv \begin{bmatrix} 1 & x_0 & x_0^2 & \dots & x_0^N \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_N & x_N^2 & \dots & x_N^N \end{bmatrix}$$

- Then solve for c as the solution to,

$$Ac = y$$

- Which we can solve using our tools. As long as x_n are unique, it is A is invertible
- Let's look at the numerical error here from the interpolation using the inf-norm, i.e., $||x||_\infty = \max_n |x_n|$

Solving an Example

```
N = 5
x = np.linspace(0.0, 10.0, N + 1)
y = np.exp(x)  # example function to interpolate
A = np.array([[x_i**n for n in range(N + 1)] for x_i in x])  # or np.vande
c = solve(A, y)
c_inv = inv(A) @ y
print(f"error = {norm(A @ c - y, np.inf)}, \
error using inv(A) = {norm(A @ c_inv - y, np.inf)}")
print(f"cond(A) = {cond(A)}")
```

```
error = 2.2737367544323206e-11, error using inv(A) = 1.0986695997416973e-0
cond(A) = 564652.321404467
```

Things Getting Poorly Conditioned Quickly

```
N = 10
x = np.linspace(0.0, 10.0, N + 1)
y = np.exp(x)  # example function to interpolate
A = np.array([[x_i**n for n in range(N + 1)] for x_i in x])  # or np.vande
c = solve(A, y)
c_inv = inv(A) @ y # Solving with inv(A) instead of solve(A, y)
print(f"error = {norm(A @ c - y, np.inf)}, \
error using inv(A) = {norm(A @ c_inv - y, np.inf)}")
print(f"cond(A) = {cond(A)}")
```

```
error = 6.348273018375039e-10, error using inv(A) = 4.5510896597988 9e-06
cond(A) = 4462823910804.094
```

Matrix Inverses Fail Completely for $N = 20$

```
N = 20
x = np.linspace(0.0, 10.0, N + 1)
y = np.exp(x)  # example function to interpolate
A = np.array([[x_i**n for n in range(N + 1)] for x_i in x])  # or np.vande
c = solve(A, y)
c_inv = inv(A) @ y # Solving with inv(A) instead of solve(A, y)
print(f"error = {norm(A @ c - y, np.inf)}, \
error using inv(A) = {norm(A @ c_inv - y, np.inf)}")
print(f"cond(A) = {cond(A):.4g}")
```

```
error = 1.9554136088117957e-10, error using inv(A) = 21804.714723170073
cond(A) = 3.325e+24
```

Moral of this Story

- Use `solve`, which is faster and can often solve ill-conditioned problems. Rarely use `inv`, and only when you know the problem is well-conditioned
- Check conditioning of matrices when doing numerical work as an occasional diagnostic, as it is a good indicator of potential problems and collinearity
- For approximation, never use a monomial basis for polynomials
  - Prefer polynomials like Chebyshev, which are designed to be as orthogonal as possible

```
N = 40
x = np.linspace(-1, 1, N+1)  # Or any other range of x values
A = np.array([[np.polynomial.Chebyshev.basis(n)(x_i) for n in range(N+1)]
A_monomial = np.array([[x_i**n for n in range(N + 1)] for x_i in x])  # or
print(f"cond(A) = {cond(A):.4g}, cond(A_monimial) = {cond(A_monomial):.4g}
```

```
cond(A) = 3.64e+09, cond(A_monimial) = 8.903e+17
```