ECON526: Quantitative Economics with Data Science Applications

Latent Variables and Introduction to Unsupervised Learning

Jesse Perla

jesse.perla@ubc.ca

University of British Columbia

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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
  - $\rightarrow$ May allow mapping data into a lower-dimensional, uncorrelated features
  - $\rightarrow$ Uses Singular Value Decomposition (SVD) - a generalization of eigendecomposition to non-square matrices
- 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 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 $X \in \mathbb{R}^{N \times M}$ is:

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

- The diagonal elements of $\Sigma \in \mathbb{R}^{N \times M}$ are singular values, and there are zeros everywhere else. If $M < N$ then there M singular values $(\sigma_1, \ldots \sigma_M)$
  - → Those singular values are also the square roots of the eigenvalues of XX^T (or X^TX)
  - → The number of non-zero singular values is the rank of the matrix X
- $U \in \mathbb{R}^{N \times N}$ and $V \in \mathbb{R}^{M \times M}$ are orthogonal matrices
  - → 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 $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_M$:

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

Note that

- $u_m \in \mathbb{R}^N$ 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 $N \times M$ matrix but you can show that it is rank-1. i.e., you can decompose it into the product of two vectors.

Interpretation the Scatter (Covariance) Matrix

- Assuming the data has been de-meaned already, $\boldsymbol{X}^\top \boldsymbol{X}$ is the covariance matrix, otherwise it is called a scatter matrix
- The covariance matrix, $\boldsymbol{X}^\top \boldsymbol{X}$ is a $M \times M$ matrix where

$$[\boldsymbol{X}^\top \boldsymbol{X}]_{ij} = \sum_{k=1}^{N} x_{ki} x_{kj}$$

- Calculates an expression related to the the covariance between features
- The eigenvectors of this tell you along which directions is there the most variation

Interpretation of the Gram Matrix

- The Gramian is $\boldsymbol{X}\boldsymbol{X}^\top$ is a $N \times N$ matrix where

$$[\boldsymbol{X}\boldsymbol{X}^\top]_{ij} = \boldsymbol{x}_i^\top \boldsymbol{x}_j$$

- i.e., each element measures the similarity between features of the $\boldsymbol{i}$th and $\boldsymbol{j}$th observations
- Inner products are a classic way to measure similarity

  $\longrightarrow$ If $\boldsymbol{x}_i^T \boldsymbol{x}_j$ is large, then the $\boldsymbol{i}$th and $\boldsymbol{j}$th observations are similar, and it is maximized if equal.

  $\longrightarrow$ If $\boldsymbol{x}_i^T \boldsymbol{x}_j$ is zero then the features are as different as possible
- This is important in what are called ``Kernel methods” which form approximations by comparing the similarity of observations

Interpreting Rank

- Intuition: rank r if it can be decomposed into the sum of r rank-1 matrices

  $\rightarrow$ Alternatively, can interpret rank of an $N \times M$ matrix is $\mathbf{3}$ if can find a $A \in \mathbb{R}^{N \times 3}$ and $B \in \mathbb{R}^{3 \times M}$ such that $X = AB$

- Remember: this works for **any** matrix $X \in \mathbb{R}^{N \times M}$

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 $L < M$.

$$X \approx \sum_{m=1}^{L} \sigma_m u_m v_m^T$$

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

PCA as an Optimal Dimension Reduction

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

See here for some intuition on this as an optimization problem.

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
print(f"Z is {Z.shape}, X is {X.shape}")
```

```
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

```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):
[26.0863  0.8233  0.6916]
Explained Variance (ordered):
[0.9983 0.001  0.0007]
```

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 = -0.9991910948940889
Correlation of Z_2 to Z_hat_2 = -0.1894085947160488
```

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
  - → Function f, the encoder, maps X to a latent space Z, which may be lower-dimensional
  - → Function g, the decoder, maps points in the latent space Z back to X
  - → θ_e and θ_d are parameters for f and g which we are trying to find
- Then the goal is to find the θ_e and θ_d parameters for our encoder, f, and decoder, g, where for as many X as possible we have

$$g(f(x;\theta_e);\theta_d) \approx x$$

- 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

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

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

$$\min_{\theta_e,\theta_d} \frac{1}{N}\sum_{n=1}^{N}||g(f(x_n;\theta_e);\theta_d) - x_n||_2^2$$

PCA as a Linear Auto-Encoder

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

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

- In more advanced machine learning examples, intuition seems to come up frequently. Related to embeddings, which come up with NLP, networks, etc.

Connection to PCA

- From a SVD of $X = U\Sigma V^T$ where V are the eigenvectors. Assuming Σ is sorted largest to smallest.
  - → If we are using L components, then we truncate by taking the first L columns of V and Σ
  - → Then let $W^\top = \Sigma_{1:L} V_{1:L}^\top$
- With this, $f(x) = W^\top x$ is an low-dimensional approximation to x that minimizes the reconstruction error

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

- 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
  - $\rightarrow$ $\mathbf{S} \equiv \{S_1, \ldots, S_K\}$ 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 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

- Consider if the $n \in S_k$ with should have similar x_n
  - $\longrightarrow$ Group observations that are close or similar to each other
  - $\longrightarrow$ 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 $\mathbf{S}$ which minimizes the norm between observations within each group
  - $\longrightarrow$ Normalize by group size $|S_k|$ to avoid distorting the objective function due to different group sizes

Formal Optimization Problem

- Formally,

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

- 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

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

- Avoid different scales so $\bar{x}_k$ isn't dominated by one feature

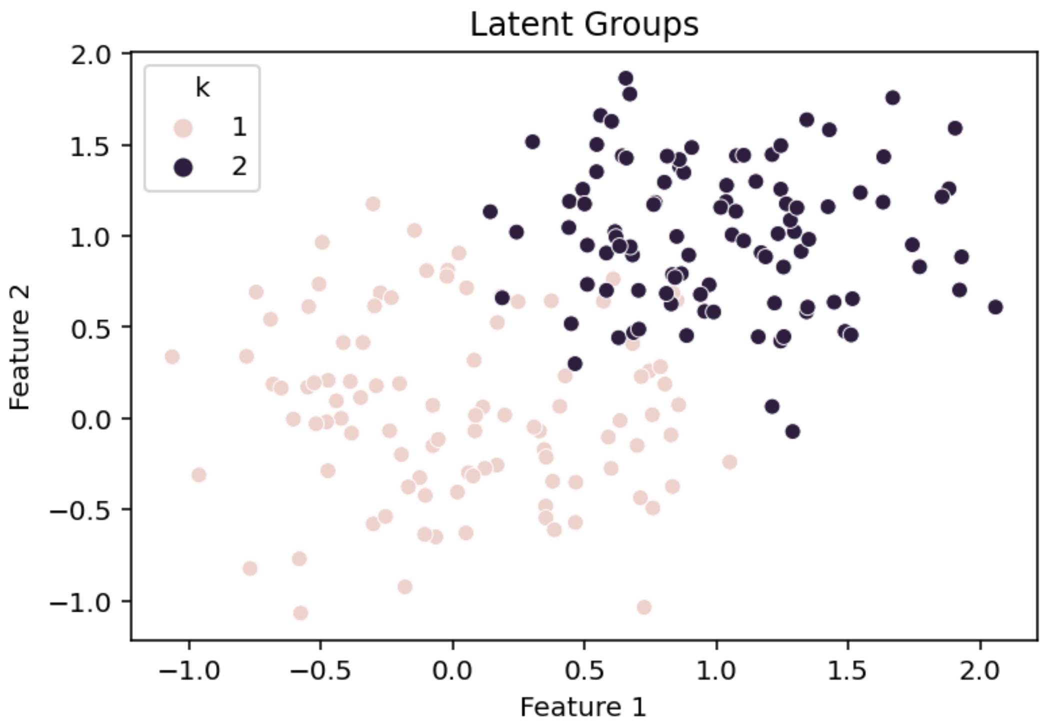
Generating Data with Latent Groups

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

```
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()
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

```
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}")
```

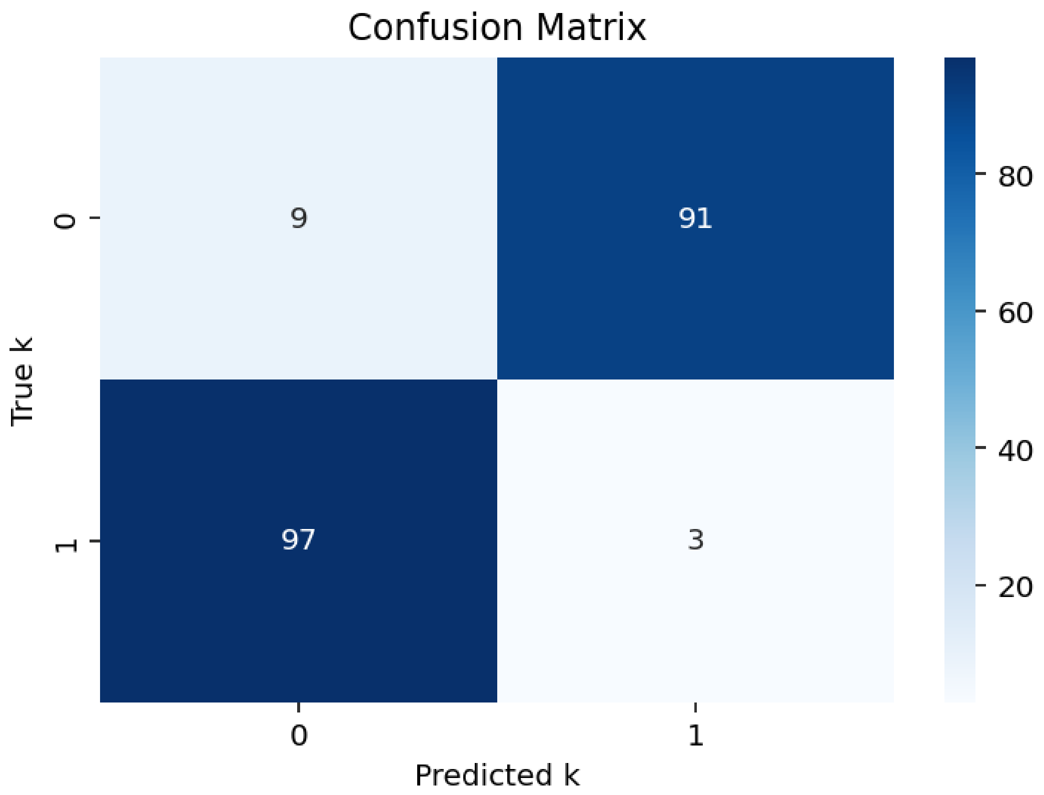
```
Correlation between k and k_hat:-0.88
```

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

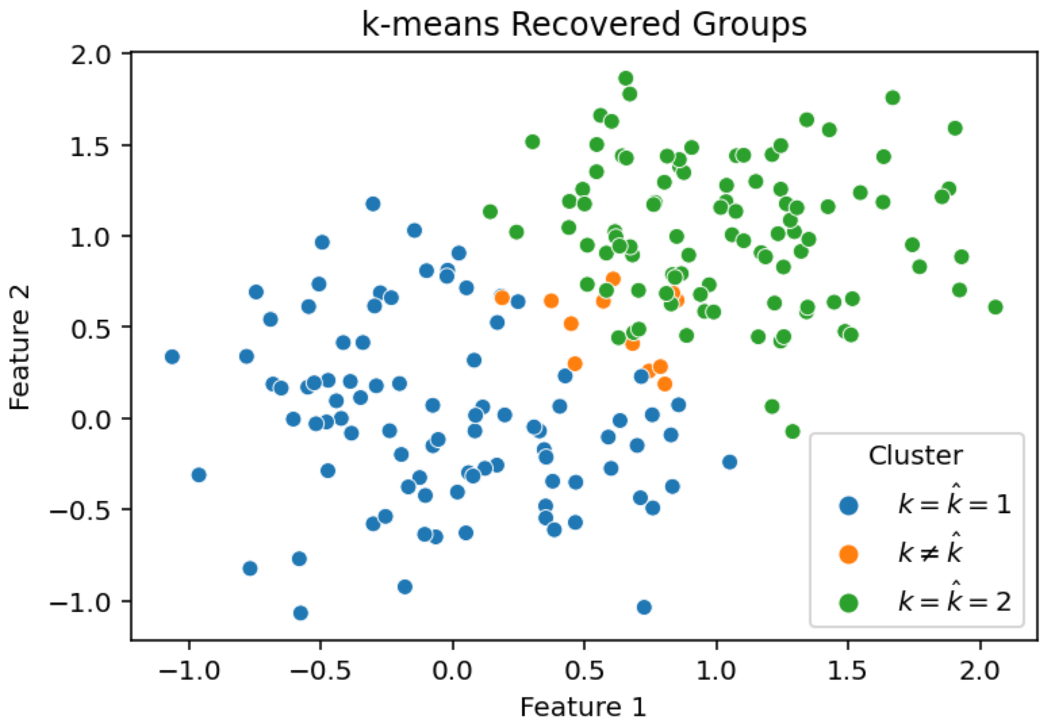
```
if df['k'].corr(df['k_hat']) < 0.5:
  df['k_hat'] = df['k_hat'].replace({1: 2, 2: 1})
  print(f"Correlation now {df['k'].corr(df['k_hat'])}")

df['Cluster'] = df.apply(lambda x: rf"$k=\hat{{k}}={{{x['k']:.0g}}}$"
                          if x['k'] == x['k_hat'] else r'$k \neq \hat{k}$',
                          axis=1)
```

```
Correlation now 0.8815882896709472
```

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 Groups")
plt.show()
```



(Optional) Factors within a Portfolio Model

Simulation

In the previous lecture we introduced code for simulation

```
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
```

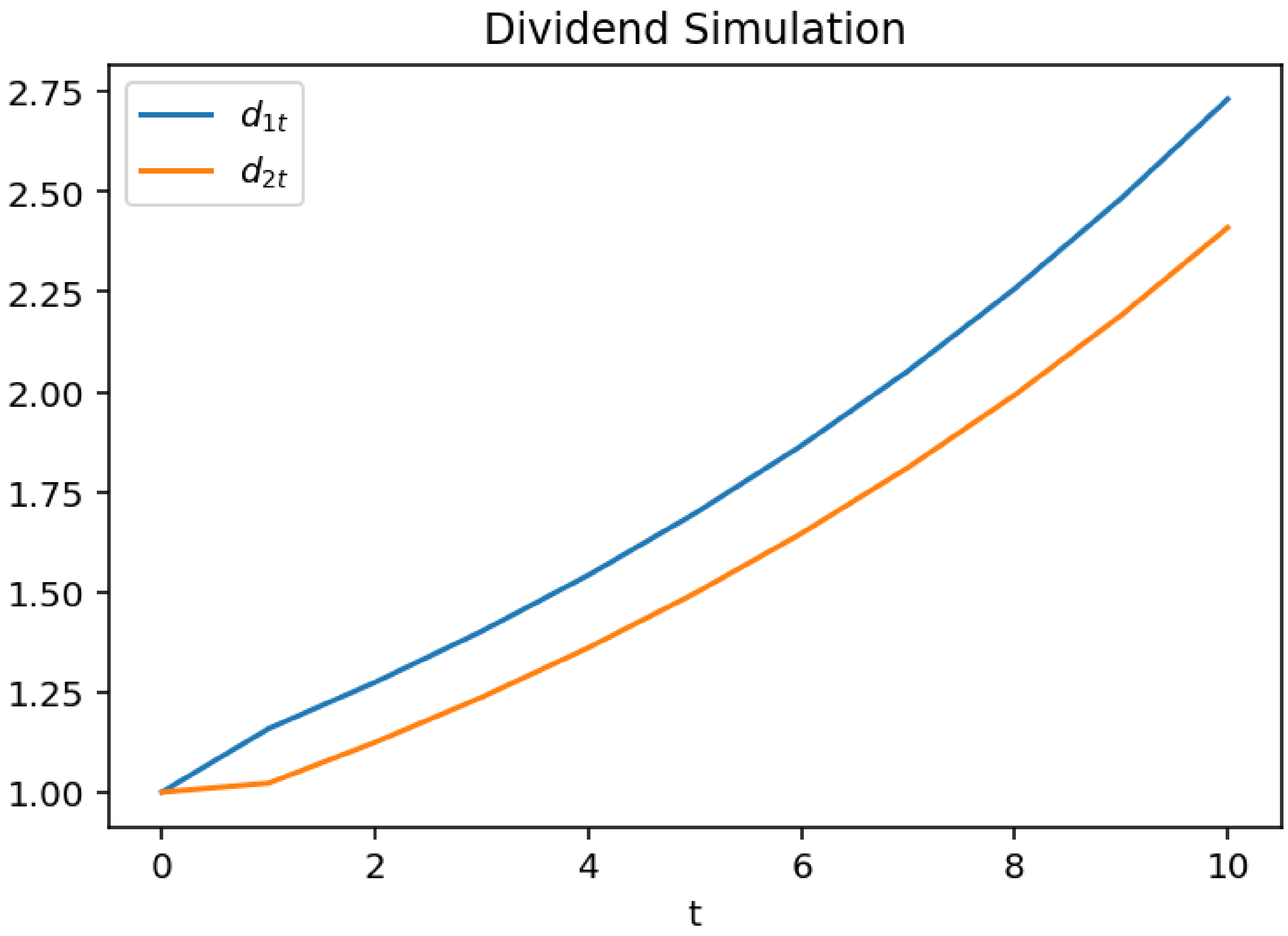
A Portfolio Example

- 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
- Portfolio 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} 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

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

```
[ 1.10000000e+00 -2.65486733e-09]
```

- The first eigenvector is 1.1, but the second is very close to 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}?
- 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,

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

```
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 $\boldsymbol{d}_0$ to ℓ_0 using $\boldsymbol{q}_1^{-1}$
  - → 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 $\boldsymbol{q}_1$
  - → Checking if it aligns with the $\boldsymbol{d}_t$

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 = 2.3494410875961204e-10
```

Let's see if these line up perfectly

Total Dividends and the Latent Variable