



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

```
1 import numpy as np
2 import matplotlib.pyplot as plt
3 import scipy
4 from numpy.linalg import cond, matrix_rank, norm
5 from scipy.linalg import inv, solve, det, eig, lu, eigvals
6 from scipy.linalg import solve_triangular, eigvalsh, cholesky
7 import seaborn as sns
8 import pandas as pd
9 from sklearn.decomposition import PCA
10 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 $\mathbf{X} \in \mathbb{R}^{N \times M}$, can we find a lower-dimensional representation $\mathbf{Z} \in \mathbb{R}^{N \times L}$ for $L < M$ that captures the most variation in \mathbf{X} ?
- The goal is to invert the \mathbf{X} data to find the \mathbf{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 $\mathbf{X} \in \mathbb{R}^{N \times M}$ is:

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

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

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

$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_M$:

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

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

- $u_m \in \mathbb{R}^N$ is the m -th column of U and $v_m \in \mathbb{R}^M$ is the m th 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.

Interpreting Rank

- Intuition: rank r if it can be decomposed into the sum of r rank-1 matrices
 - Alternatively, can interpret rank of an $N \times M$ matrix is 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., $\text{rank}(X) = L < M$) 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 \mathbf{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

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

```
1 N = 50 # number of observations
2 L, M = 2, 3 # number of latent and observed factors
3 Z = np.random.randn(N, L) # latent factors
4 F = np.array([[1.0, 0.05], # X_1 = Z_1 + 0.05 Z_2
5               [2.0, 0.0], # X_2 = 2 Z_1
6               [3.0, 0.1]]) # X_3 = 3 Z_1 + 0.1 Z_2
7 X = Z @ F.T + 0.1 * np.random.randn(N, M) # added noise
8 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

```
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):

[26.0863 0.8233 0.6916]

Explained Variance (ordered):

[0.9983 0.001 0.0007]

Dimension Reduction with PCA

```
1  pca = PCA(n_components=2) # one less, and correctly specified
2  Z_hat = pca.fit_transform(X) # transformed by dropping last factor
3  # Scale and sign may not match due to indeterminacy
4  print(f"Correlation of Z_1 to Z_hat_1 = {np.corrcoef(Z.T, Z_hat.T)[0,2]}")
5  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 $\{x_1, \dots, x_N\}$

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

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 $\|\hat{x} - x\|_2^2$.

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

- 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

- Let $\mathbf{X} \in \mathbb{R}^{N \times M}$ with $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^M$ the individual observations
- Assume that each \mathbf{x}_n has a latent discrete $k \in \{1, \dots, K\}$ then we can assign each observation to one group
 - $\mathbf{S} \equiv \{S_1, \dots, S_K\}$ 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 \mathbf{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 $\mathbf{n} \in \mathcal{S}_k$ with should have similar \mathbf{x}_n
 - Group observations that 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
- Objective function of k-means: choose the partition \mathbf{S} which minimizes the norm between observations within each group
 - Normalize by group size $|\mathcal{S}_k|$ 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

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

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

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

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

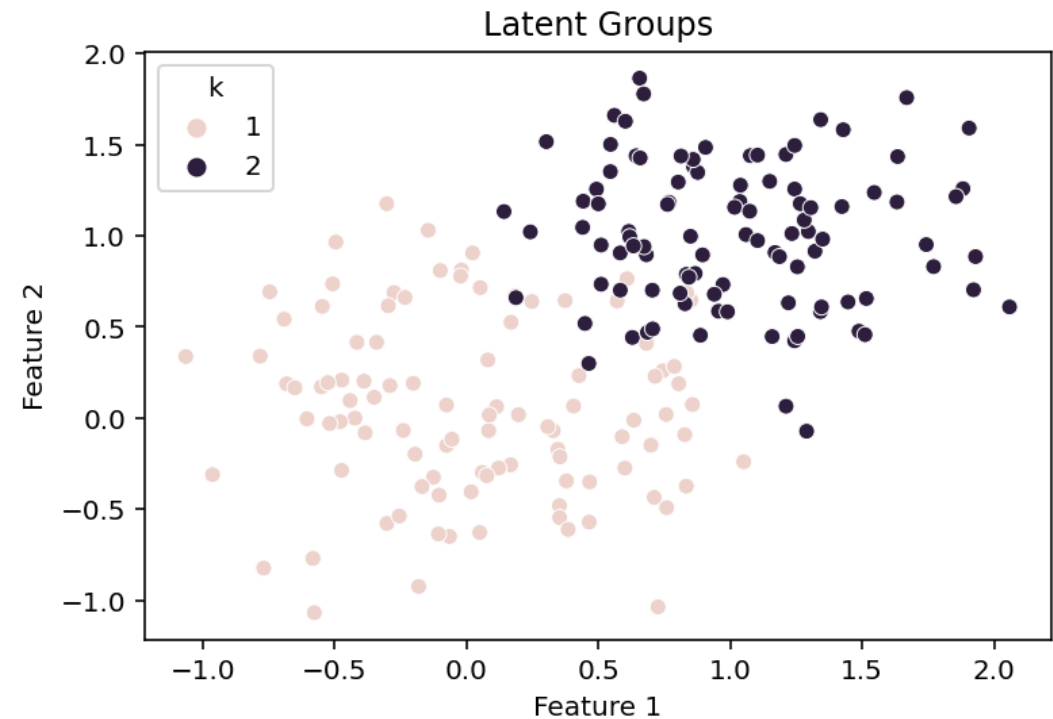
Generating Data with Latent Groups

- 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

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



k-means to Recover the Latent Groups

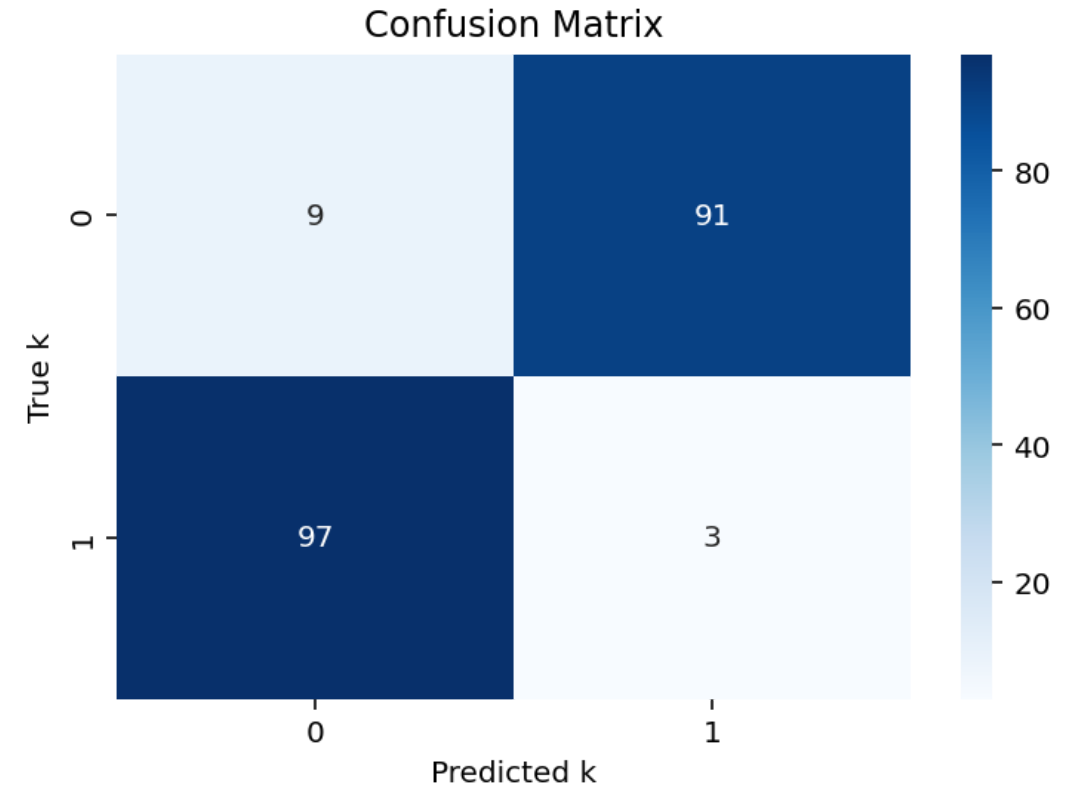
- Run k-means with 2 clusters and check the results
- If correlation is close to 1 then successfully recovered the latent groups
- If the correlation is close to -1 then it was successful. The latent groups \hat{k} numbers are ordered arbitrarily, just as k was

```
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:-0.88

Confusion Matrix

```
1 from sklearn.metrics import confusion_matrix
2
3 # compute confusion matrix
4 cm = confusion_matrix(df["k"], df["k_hat"])
5
6 # plot confusion matrix
7 sns.heatmap(cm, annot=True, cmap='Blues')
8 plt.xlabel('Predicted k')
9 plt.ylabel('True k')
10 plt.title('Confusion Matrix')
11 plt.show()
```



Potentially Swap \hat{k} and Compare

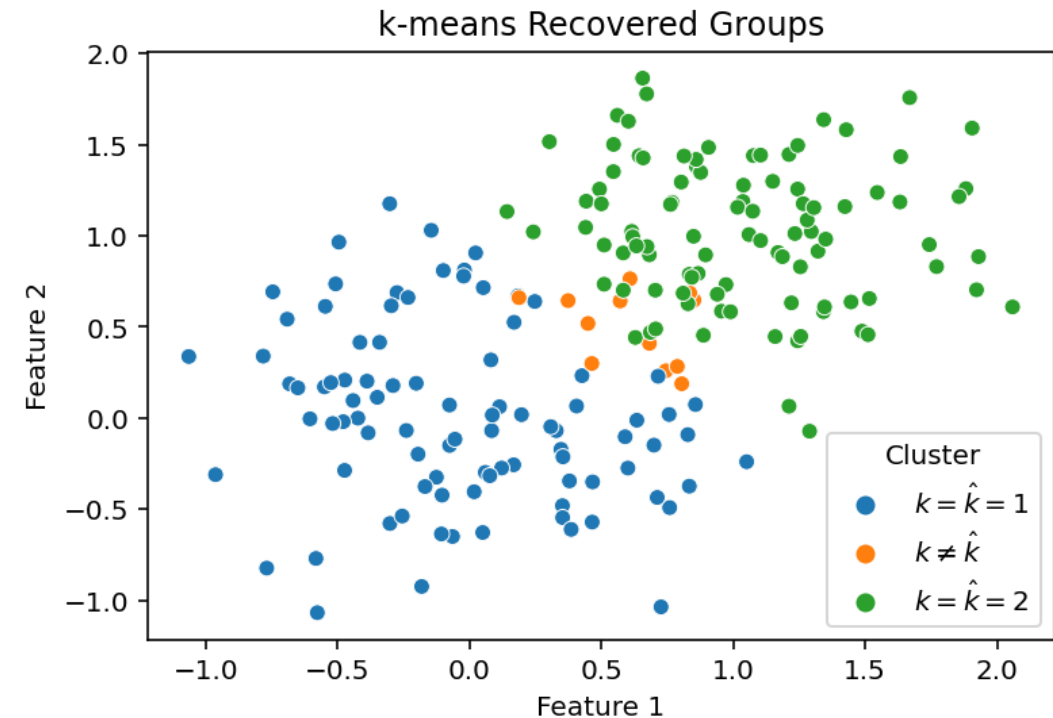
Label ordering arbitrary, so “confusion matrix might require reordering to compare

```
1 if df['k'].corr(df['k_hat']) < 0.5:
2     df['k_hat'] = df['k_hat'].replace({1: 2, 2: 1})
3     print(f"Correlation now {df['k'].corr(df['k_hat'])}")
4
5 df['Cluster'] = df.apply(lambda x: rf"$k=\hat{{{k}}}={{{{{x['k']:.0g}}}}} $"
6                         if x['k'] == x['k_hat'] else r'$k \neq \hat{k}$ ',
7                         axis=1)
```

Correlation now 0.8815882896709472

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
```

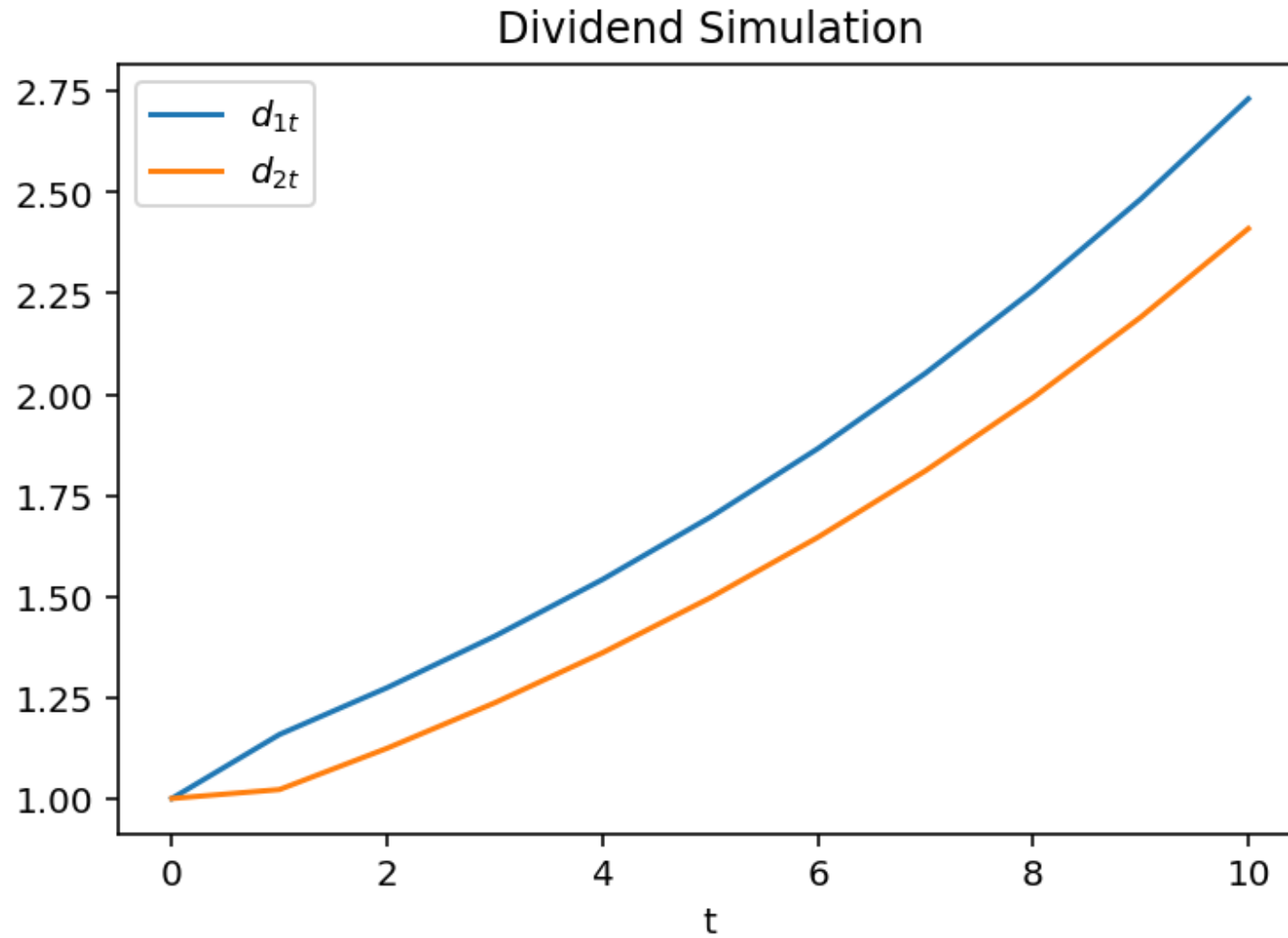

A Portfolio Example

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

```
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 -2.65486733e-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,

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

```
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

- 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

```
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 = 2.3494410875961204e-10

Let's see if these line up perfectly

Total Dividends and the Latent Variable

