HGEN 48860 HW4 Lin Yu

Condition Number = 
$$\frac{|\Delta y/y|}{|\Delta x/x|} = \frac{|xf'(x)|}{|f(x)|} = |\frac{\pi \cos x}{\sin x}| = |\pi \cdot \cot(x)|$$

when  $x = n\pi$ , the condition number might go to infinity.

$$P = (St)^{ns} \cdot (rt)^{nc}$$

$$\begin{aligned} \log P &= (Ns. \log |St) + Nc. \log Yt \\ &= n_s. \log 3 (\frac{1}{4} - \frac{4}{4}e^{-\frac{43t}{3}}) + n_c. \log (\frac{1}{4} + \frac{3}{4}e^{-\frac{43t}{3}}) \\ &= n_s. \log 3 + n_s. \log (\frac{1}{4} - \frac{1}{4}e^{-\frac{4}{3}t}) + n_c. \log (\frac{1}{4} + \frac{3}{4}e^{-\frac{4}{3}t}) \end{aligned}$$

$$\frac{\partial \log P}{\partial t} = 5 \cdot (\frac{1}{4} - \frac{1}{4}e^{-\frac{1}{3}t})^{-1} \cdot \frac{1}{4} \cdot e^{-\frac{1}{3}t} \cdot (-\frac{1}{3}) + 25 \cdot (\frac{1}{4} + \frac{2}{4}e^{-\frac{1}{3}t})^{-1} \cdot \frac{2}{4} \cdot e^{-\frac{1}{3}t}$$

Use Newton Method on computer for the rest part.

as we can't solve 
$$\frac{2\log p}{2t} = 0$$
 analytically.

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3. (a)
$$\frac{\partial f}{\partial x} = bx^{2} - bx - by \cdot (x - y - 1) - bxy \cdot 1$$

$$= bx^{2} - bx - 12xy + by^{2} + by$$

$$\frac{\partial f}{\partial y} = -bx (x - y - 1) - bxy \cdot (-1)$$

$$= -bx^{2} + bxy + bx + bxy$$

$$= -bx^{3} + bx + 12xy$$
For critical points, 
$$\frac{\partial f}{\partial x} = 0 \text{ and } \frac{\partial f}{\partial y} = 0$$

$$\begin{cases}
bx^{2} - bx - 12xy + by^{2} + by = 0 \\
-bx^{3} + bx + 12xy = 0
\end{cases}$$

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x = 0 \\
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 $Hf((-1,-1)) = \begin{pmatrix} -b & b \\ b & -12 \end{pmatrix}$ 

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4. As A is non real symmetric matrix, A has an orthonormal leigenbasis and all eigenvalues are real.

let  $\lambda_1, \lambda_2, \dots \lambda_n$  be A's eigenvalues,  $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$  and  $\nu_1, \dots \nu_n$  are their corresponding eigenvectors, and  $||\nu_1||^2 = 1$  for  $\tilde{\tau} = 1, \tilde{\sigma}, \dots n$ 

 $v_1^T A v_2 \geqslant \min_{x \in IR^n} f(x)$ ,  $v_n^T A v_n \leq \max_{x \in IR^n} f(x) \Rightarrow \lambda_1 \leq \min_{x \in IR^n} f(x)$  ||x|| = 1  $\lambda_1 \leq \min_{x \in IR^n} f(x)$  ||x|| = 1  $\lambda_1 \leq \min_{x \in IR^n} f(x)$ ||x|| = 1  $\lambda_1 \leq \min_{x \in IR^n} f(x)$ 

Given  $x \in \mathbb{R}^n$ , ||x|| = 1,  $x = \sum_{i=1}^n \partial_i V_i$   $\sum_{i=1}^n \partial_i^2 = 1$ .

 $f(x) = x^{T} A x = \langle x, A x \rangle = \langle \sum_{i=1}^{n} a_{i} V_{i}, A \sum_{i=1}^{n} a_{i} V_{i} \rangle$   $= \langle \sum_{i=1}^{n} a_{i} V_{i}, \sum_{i=1}^{n} a_{i} \lambda_{i} V_{i} \rangle = \sum_{i=1}^{n} \lambda_{i} \cdot a_{i}^{2}$ 

 $f(x) \le \sum_{i=1}^{n} \lambda_n di^2 = \lambda_n \quad \text{for } \forall x \in \mathbb{R}^n \quad ||x|| = 1$ 

f(x) > \( \frac{1}{2} \lambda\_1 \alpha\_1^2 = \lambda\_2 \), for any x ∈ \( \text{R}^h \), ||x||=1

Thus, min  $f(x) = \lambda_1$ , max  $f(x) = \lambda_2$  for  $x \in \mathbb{R}^n$ , ||x|| = 1.

# Scanned with CamScanner

## $\text{Lin}_{\text{Yu}}$ HW4

April 21, 2024

```
[1]: import numpy as np
from scipy.optimize import newton
import matplotlib.pyplot as plt
```

#### 1 Problem 2

Part B

```
[2]: \#(b)
     # Log-likelihood derivatives
     def log_likelihood_prime(t, nS=5, nC=25):
         """Calculates the first derivative of the log-likelihood function with \sqcup
      ⇔respect to t."""
         # Compute st and rt
         st = 3 * (0.25 - 0.25 * np.exp(-4 * t / 3))
         rt = 0.25 + 0.75 * np.exp(-4 * t / 3)
         # Compute derivatives of st and rt with respect to t
         dst_dt = 1 * np.exp(-4 * t / 3) # Corrected to match the explanation above
         drt_dt = -1 * np.exp(-4 * t / 3) # As you originally had, aligning with
      →the negative exponential derivative
         \# Log-likelihood derivative calculation
         return nS * (dst_dt / st) + nC * (drt_dt / rt)
     def log_likelihood_double_prime(t, nS=5, nC=25):
         """Calculates the second derivative of the log-likelihood function with \sqcup
      ⇔respect to t."""
         # Compute st and rt
         st = 3 * (0.25 - 0.25 * np.exp(-4 * t / 3))
         rt = 0.25 + 0.75 * np.exp(-4 * t / 3)
         # Compute derivatives of st and rt with respect to t
         dst_dt = 1 * np.exp(-4 * t / 3)
         drt_dt = -1 * np.exp(-4 * t / 3)
```

```
# Compute second derivatives of st and rt with respect to t
        d2st_dt2 = -4/3 * dst_dt
        d2rt_dt2 = -4/3 * drt_dt
         # Log-likelihood second derivative calculation
        return nS * (-dst_dt**2 / st**2 + d2st_dt2 / st) + nC * (-drt_dt**2 / rt**2_
      →+ d2rt dt2 / rt)
[3]: initial t = 0.5
     # Use scipy.optimize.newton to find the root of the first derivative (extremum,
     →of the log-likelihood)
     t_estimated = newton(log_likelihood_prime, initial_t,_

¬fprime=log_likelihood_double_prime, args=(5, 25))
     print(f"Given ns=5, nc=25, the estimated divergence time t: {t_estimated:.4f}")
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel_5337/3037943102.py:7:
    RuntimeWarning: overflow encountered in exp
      st = 3 * (0.25 - 0.25 * np.exp(-4 * t / 3))
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel_5337/3037943102.py:8:
    RuntimeWarning: overflow encountered in exp
      rt = 0.25 + 0.75 * np.exp(-4 * t / 3)
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel 5337/3037943102.py:11
    : RuntimeWarning: overflow encountered in exp
      dst_dt = 1 * np.exp(-4 * t / 3) # Corrected to match the explanation above
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel_5337/3037943102.py:12
    : RuntimeWarning: overflow encountered in exp
      drt_dt = -1 * np.exp(-4 * t / 3) # As you originally had, aligning with the
    negative exponential derivative
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel_5337/3037943102.py:15
    : RuntimeWarning: invalid value encountered in scalar divide
      return nS * (dst_dt / st) + nC * (drt_dt / rt)
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel_5337/3037943102.py:20
    : RuntimeWarning: overflow encountered in exp
      st = 3 * (0.25 - 0.25 * np.exp(-4 * t / 3))
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel_5337/3037943102.py:21
    : RuntimeWarning: overflow encountered in exp
      rt = 0.25 + 0.75 * np.exp(-4 * t / 3)
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel_5337/3037943102.py:24
    : RuntimeWarning: overflow encountered in exp
      dst_dt = 1 * np.exp(-4 * t / 3)
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel_5337/3037943102.py:25
    : RuntimeWarning: overflow encountered in exp
      drt_dt = -1 * np.exp(-4 * t / 3)
    /var/folders/t2/7mtp11ks3nnd016dwsngd1680000gn/T/ipykernel 5337/3037943102.py:32
    : RuntimeWarning: invalid value encountered in scalar divide
      return nS * (-dst_dt**2 / st**2 + d2st_dt2 / st) + nC * (-drt_dt**2 / rt**2 +
```

RuntimeError

Cell In[3], line 4

```
1 initial_t = 0.5
           3 # Use scipy.optimize.newton to find the root of the first derivative
      →(extremum of the log-likelihood)
      ----> 4 t_estimated =_
       anewton(log_likelihood_prime, initial_t, fprime=log_likelihood_double_prime, a 'gs=(5, 25))
            6 print(f"Given ns=5, nc=25, the estimated divergence time t: {t estimate}:

  .4f}")
     File ~/opt/anaconda3/lib/python3.9/site-packages/scipy/optimize/_zeros_py.py:
       →381, in newton(func, x0, fprime, args, tol, maxiter, fprime2, x1, rtol, u

¬full_output, disp)
          378 if disp:
                 msg = ("Failed to converge after %d iterations, value is %s."
          379
          380
                         % (itr + 1, p))
                 raise RuntimeError(msg)
          383 return _results_select(full_output, (p, funcalls, itr + 1, _ECONVERR))
     RuntimeError: Failed to converge after 50 iterations, value is nan.
[4]: | initial_t = 10
     # Use scipy.optimize.newton to find the root of the first derivative (extremum_
     ⇔of the log-likelihood)
     t_estimated = newton(log_likelihood_prime, initial_t,_

¬fprime=log_likelihood_double_prime, args=(5, 25))
     print(f"Given ns=5, nc=25, the estimated divergence time t: {t_estimated:.4f}")
     RuntimeError
                                                Traceback (most recent call last)
     Cell In[4], line 4
           1 initial_t = 10
           3 # Use scipy.optimize.newton to find the root of the first derivative
      ⇔(extremum of the log-likelihood)
      ----> 4 t_estimated =_
       newton(log_likelihood_prime, initial_t, fprime=log_likelihood_double_prime, a 'gs=(5, 25))
            6 print(f"Given ns=5, nc=25, the estimated divergence time t: {t_estimate}:
       File ~/opt/anaconda3/lib/python3.9/site-packages/scipy/optimize/_zeros_py.py:
       →381, in newton(func, x0, fprime, args, tol, maxiter, fprime2, x1, rtol, u

¬full_output, disp)
```

Traceback (most recent call last)

```
378 if disp:
379 msg = ("Failed to converge after %d iterations, value is %s."
380 % (itr + 1, p))
--> 381 raise RuntimeError(msg)
383 return _results_select(full_output, (p, funcalls, itr + 1, _ECONVERR))

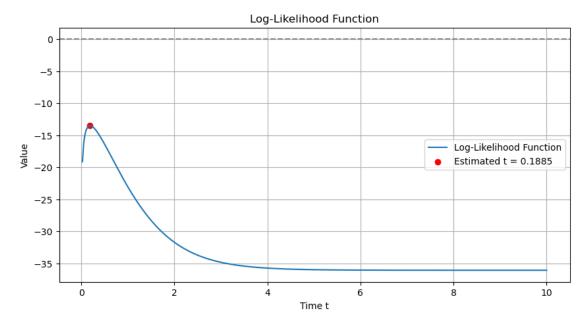
RuntimeError: Failed to converge after 50 iterations, value is 47.5000063138963
```

Given ns=5, nc=25, the estimated divergence time t: 0.1885

Part C

The second derivative of the log\_likelihood function at time t: 0.18848582121067955 is -130.666666666666

```
[7]: \#(c)
     def log_likelihood(t, nS=5, nC=25):
         """Calculates the log-likelihood function of t."""
         # Compute st and rt,
         st = 3 * (0.25 - 0.25 * np.exp(-4 * t / 3))
         rt = 0.25 + 0.75 * np.exp(-4 * t / 3)
         if st <= 0 or rt <= 0:</pre>
             return np.nan # Return NaN if st or rt is non-positive, to avoid
      → taking log of non-positive numbers
         return nS * np.log(st) + nC * np.log(rt)
     t_values = np.linspace(0, 10, 400)
     function_values = [log_likelihood(t, 5, 25) for t in t_values]
     estimated_y = log_likelihood(t_estimated, 5, 25) # Calculate log-likelihood at_
      \hookrightarrow estimated t
     # Plot the log-likelihood function
     plt.figure(figsize=(10, 5))
```



As demonstrated, the solution where the derivative of the log-likelihood function equals zero is **0.1885**. Importantly, the outcome of Newton's method is highly sensitive to the initial guess provided. Since the second derivative at this point is negative, we can conclude that it represents a local **maximum** for the parameters  $n_{C} = 5$  and  $n_{C} = 25$ . This conclusion is corroborated by the plot of the log-likelihood function.

### 2 Problem 3

```
[8]: # (b)

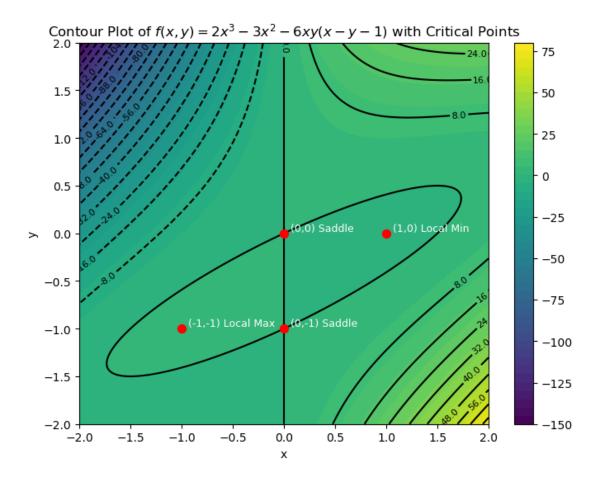
def is_positive_definite_eigen(matrix):
    # Compute the eigenvalues
    eigenvalues = np.linalg.eigvals(matrix)
    # Check if all eigenvalues are greater than zero
```

```
if (np.all(eigenvalues > 0)):
              return("The Hessian matrix is positive definite")
          elif (np.all(eigenvalues < 0)):</pre>
              return("The Hessian matrix is negative definite")
          else:
              return("The Hessian matrix is indefinite")
      Hf = np.array([[-6, 6],
                     [6, 0]]
      print("Critial point: (0,0)")
      is_positive_definite_eigen(Hf)
     Critial point: (0,0)
 [8]: 'The Hessian matrix is indefinite'
 [9]: # (-1,-1)
      Hf = np.array([[-6, 6],
                     [6, -12]])
      print("Critial point: (-1,-1)")
      is_positive_definite_eigen(Hf)
     Critial point: (-1,-1)
 [9]: 'The Hessian matrix is negative definite'
[10]: \# (0,-1)
      print("Critial point: (0,-1)")
      Hf = np.array([[6, -6]],
                     [-6, 0]]
      is_positive_definite_eigen(Hf)
     Critial point: (0,-1)
[10]: 'The Hessian matrix is indefinite'
[11]: # (1,0)
      print("Critial point: (1,0)")
      Hf = np.array([[6, -6]],
                     [-6, 12]]
      is_positive_definite_eigen(Hf)
     Critial point: (1,0)
```

[11]: 'The Hessian matrix is positive definite'

After evaluating the Hessian matrices at three critical points—(0,0), (-1,-1), (0,-1), and (1,0)—we find that both (0,0) and (0,-1) are saddle points, while (1,0) is a local minimum and (-1,-1) is a local maximum for the function.

```
[12]: # (c)
      # Define the function f(x, y)
      def f(x, y):
          return 2*x**3 - 3*x**2 - 6*x*y*(x - y - 1)
      # Create a grid of x and y values
      x = np.linspace(-2, 2, 1000)
      y = np.linspace(-2, 2, 1000)
      X, Y = np.meshgrid(x, y)
      Z = f(X, Y)
      # Create a contour plot with labels for better visibility of critical points
      plt.figure(figsize=(8, 6))
      contours = plt.contour(X, Y, Z, levels=30, colors='black')
      plt.clabel(contours, inline=True, fontsize=8, fmt='%1.1f')
      contourf = plt.contourf(X, Y, Z, levels=50, cmap='viridis')
      plt.colorbar(contourf)
      # Annotating the critical points
      critical_points = [(0, 0), (0, -1), (1, 0), (-1, -1)]
      cp_labels = ['(0,0) Saddle', '(0,-1) Saddle', '(1,0) Local Min', '(-1,-1) Local__
       -Max']
      for i, (x, y) in enumerate(critical_points):
          plt.scatter(x, y, color='red', s=50, zorder=5) # Mark critical points
          plt.text(x, y, ' ' + cp_labels[i], color='white', fontsize=9, ha='left',
       ⇔va='bottom')
      plt.title('Contour Plot of f(x, y) = 2x^3 - 3x^2 - 6xy(x - y - 1) with
       ⇔Critical Points')
      plt.xlabel('x')
      plt.ylabel('y')
      plt.show()
```



```
for start in starting_points:
    result_f = minimize(f, start)
    result_neg_f = minimize(neg_f, start)
    results_f.append((start, result_f.fun, result_f.x))
    results_neg_f.append((start, -result_neg_f.fun, result_neg_f.x))
# Display results
for start, min_f, point_f in results_f:
    print(f"Starting Point: {start} -> Minimum of f: {min_f}, at point:
 →{point f}")
    print( )
for start, min_neg_f, point_neg_f in results_neg_f:
    print(f"Starting Point: {start} -> Minimum of -f: {min_neg_f}, at point:

√{point_neg_f}")

    print( )
Starting Point: (0, 0) -> Minimum of f: 0.0, at point: [0. 0.]
Starting Point: (1, 0) \rightarrow Minimum of f: -1.0, at point: [1.0.]
Starting Point: (-1, 1) -> Minimum of f: -5550808007.577093, at point:
[-861.53969642 574.69313094]
Starting Point: (0.5, -0.5) -> Minimum of f: -0.99999999999212, at point: [
9.99999800e-01 -4.47909316e-08]
Starting Point: (-0.5, 0.5) -> Minimum of f: -5476568621.81335, at point:
[-877.53376092 548.64611174]
Starting Point: (0, 0) -> Minimum of -f: 0.0, at point: [0. 0.]
Starting Point: (1, 0) -> Minimum of -f: -1.0, at point: [1. 0.]
Starting Point: (-1, 1) -> Minimum of -f: 5606573018.859791, at point:
[1228.29292677 1410.53354554]
Starting Point: (0.5, -0.5) -> Minimum of -f: 3210706.0018725474, at point: [
5.00030823e-01 -1.03474000e+03]
Starting Point: (-0.5, 0.5) -> Minimum of -f: 14994354.946734795, at point: [
37.13467489 277.26325098]
```

As seen from the results above, different starting points yield varying minima for f and -f. This variation is attributed to the nature of the algorithms used in scipy.optimize.minimize (such as 'BFGS', 'Nelder-Mead', 'L-BFGS-B', etc.), which are local optimization methods. These algorithms

efficiently find a local minimum near the initial starting point but do not guarantee the discovery of the global minimum unless the function is convex, which is not applicable in this case.

### 3 Dynamic Programming

 $\hookrightarrow$  (seq2[j-1], seq1[i-1]).

return score\_matrix

 $\hookrightarrow$  of -1.

```
[14]: from Bio.Align.substitution matrices import load
      # Load the BLOSUM62 substitution matrix
      blosum62 = load("BLOSUM62")
[15]: import numpy as np
      def initialize_score_matrix(seq1, seq2, gap_penalty):
          '''Initialize the first row and column of score matrix'''
          m, n = len(seq1), len(seq2)
          score_matrix = np.zeros((m+1, n+1))
          # Initialize first row and column
          for i in range(1, m+1):
              score_matrix[i][0] = i * gap_penalty
          for j in range(1, n+1):
              score_matrix[0][j] = j * gap_penalty
          return score_matrix
[16]: def fill_score_matrix(seq1, seq2, score_matrix, gap_penalty):
          """Fill the rest of matrix from top to bottom and left to right with
       ⇒blosum62 matrix"""
          m, n = len(seq1), len(seq2)
          for i in range(1, m+1):
              for j in range(1, n+1):
                  match\_score = blosum62.get((seq1[i-1], seq2[j-1]), blosum62.
       \rightarrowget((seq2[j-1], seq1[i-1]), -1))
                   # Calculate the match score between amino acids at current_
       \rightarrowpositions i and j in seq1 and seq2
                   # Fetch the score directly from the BLOSUM62 matrix using the tuple_
       \hookrightarrow (seq1[i-1], seq2[j-1]).
```

# If the tuple is not found, try with the reversed tuple\_

diagonal = score\_matrix[i-1][j-1] + match\_score
delete = score\_matrix[i-1][j] + gap\_penalty
insert = score\_matrix[i][j-1] + gap\_penalty

score\_matrix[i][j] = max(diagonal, delete, insert)

# If neither tuple exists in the matrix, default to a penalty score\_

```
[17]: def traceback(sequence1, sequence2, scoring_matrix, penalty_for_gap):
          Perform the traceback step in sequence alignment using dynamic programming.
          Constructs the alignment by navigating from the bottom-right to the \Box
       \hookrightarrow top-left of the scoring matrix.
          sequence1: First sequence being aligned
          sequence2: Second sequence being aligned
          scoring_matrix: Matrix with computed scores for alignments
          penalty_for_gap: Penalty score used for gaps in the alignment (deletion or_{\sqcup}
       \hookrightarrow insertion)
          .....
          aligned_seq1, aligned_seq2 = "", ""
          index1, index2 = len(sequence1), len(sequence2)
          # Trace back from the bottom-right of the matrix to the top-left
          while index1 > 0 and index2 > 0:
              current score = scoring matrix[index1][index2]
              diagonal_score = scoring_matrix[index1-1][index2-1]
              left_score = scoring_matrix[index1][index2-1]
              up_score = scoring_matrix[index1-1][index2]
              # Check if the current cell was filled from the diagonal cell
              if current_score == diagonal_score + blosum62.get((sequence1[index1-1],__

¬sequence2[index2-1]), blosum62.get((sequence2[index2-1],
□
       ⇔sequence1[index1-1]), -1)):
                  aligned_seq1 += sequence1[index1-1]
                  aligned_seq2 += sequence2[index2-1]
                  index1 -= 1
                  index2 -= 1
              # Check if the current cell was filled from the left cell
              elif current_score == up_score + penalty_for_gap:
                  aligned_seq1 += sequence1[index1-1]
                  aligned_seq2 += '-'
                  index1 -= 1
              # Otherwise, the current cell was filled from the upper cell
              else:
                  aligned_seq1 += '-'
                  aligned_seq2 += sequence2[index2-1]
                  index2 -= 1
          # Finish tracing back to the top of the matrix if there are remaining.
       ⇔characters in sequence1
          while index1 > 0:
              aligned_seq1 += sequence1[index1-1]
              aligned_seq2 += '-'
```

```
index1 -= 1
# Finish tracing back to the left of the matrix if there are remaining
characters in sequence2
while index2 > 0:
    aligned_seq1 += '-'
    aligned_seq2 += sequence2[index2-1]
    index2 -= 1

# Return aligned sequences in the correct order (they are built backwards)
return aligned_seq1[::-1], aligned_seq2[::-1]
```

```
[19]: def align_sequences(seq1, seq2, gap_penalty=-2):
    """

Aligns two biological sequences using dynamic programming with the BLOSUM62_

substitution matrix.

seq1: First sequence (string of amino acids) to align
seq2: Second sequence (string of amino acids) to align
gap_penalty: Penalty score for introducing a gap in alignment (default is_

-2)

"""

# Initialize the score matrix with base values for the first row and column
score_matrix = initialize_score_matrix(seq1, seq2, gap_penalty)

# Fill the rest of the score matrix based on sequence comparison and gap_

-penalties
score_matrix = fill_score_matrix(seq1, seq2, score_matrix, gap_penalty)

# Perform traceback to construct the optimal alignment from the score matrix
print(traceback(seq1, seq2, score_matrix, gap_penalty))
```

```
[21]: Sequence_1="PWAGAWHHEE"
Sequence_2="CAWDEAE"
align_sequences(Sequence_1, Sequence_2, gap_penalty=-2)
```

('PWAGAWHHE-E', '--C-AW-DEAE')