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Subject: Gene Alignment Project

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1 Attachment, 39.1 KB



CS 312 : Project 5 Duane Johnson

Methods

Pseudo-code for Scoring Algorithm

```
Input: sequence A of size n, sequence B of size m
Output: an integer value indicating edit distance

Create a cost array of size n
Initialize the cost array with increments of size IndelCost (5)

Loop from 1..b
costBelow <- cost[0] + IndelCost
```

```
op from 1..b

costBelow <- cost[0] + IndelCost

Loop from 1..a

diagonalCost <- cost[a - 1] + (A[a] == B[b] ? MatchCost : SubstCost)

costHere <- MIN(cost[a] + IndelCost, costBelow + IndelCost, diagonalCost)

cost[a - 1] <- costBelow

costBelow <- costHere
```

Pseudo-code for Alignment Algorithm

```
Input: sequence A of size n, sequence B of size m
Output: console gets a list of aligned pairs, with a description of action taken to get there
```

Create a *cost* array of size n x m Initialize the first row and first column of *cost* array to increments of size IndelCost (5)

```
Loop from 1..b
Loop from 1..a
diagonal <- cost[a - 1][b - 1] + (A[a] == B[b] ? MatchCost : SubstCost)
cost[a][b] <- MIN(diagonal, cost[a][b - 1] + IndelCost, cost[a - 1][b] + IndelCost)
```

Display the results by backtracking from cost[n][m] to cost[0][0]

How Alignment / Extraction Works

The alignment algorithm works by considering all possible actions in each step (cell) along the way and caching the results in an n x m matrix. The action that is chosen (Match/Subst/Indel) is an optimal path from the start to the current location in the matrix, therefore future computations can rely on sub-problems to reduce computational load.

The results of the alignment are displayed by backtracking through the cached results and finding the minimum path again. Depending on which branch of the 3-way branches leads to a minimal cost, the branch is chosen and the operation (Match/Subst/Indel) is displayed.

Proof of Algorithm Complexity

```
Scoring Algorithm:
```

Space complexity is O(n) because the cost array is reused. Time complexity is O(n*m):

Consider array lookups and data assignments as O(1) operations;

outer loop is n, inner loop is m;

therefore, the algorithm is O(n*m) because the time depends only on the loops

Extraction Algorithm

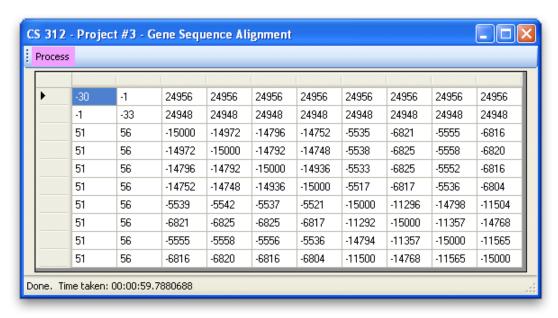
Space complexity is $O(n^*m)$ because the cached results are needed in step 2 Time complexity is $O(n^*m)$:

Just like the scoring algorithm above, but multiplied by a constant of 2;

the constant is simply due to retracing our steps to display the alignment information

Results

Screenshot of 10x10 Scoring Matrix



Alignment of Taxa 3 and Taxa 4

Whew... it's a long one. Here ya go... source code is at the end.

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Source Code

```
private int Score(GeneSequence seqA, GeneSequence seqB)
  int maxA = Math.Min(seqA.Sequence.Length, MaxCharactersToAlign);
  int maxB = Math.Min(seqB.Sequence.Length, MaxCharactersToAlign);
  int a, b;
  int[] cost = new int[maxA];
  int costBelow = 0, costHere = 0;
  // Cost of first cell depends on match or not
  cost[0] = seqA.Sequence[0] == seqB.Sequence[0] ? MatchCost : SubstCost;
  // Initialize the cost array by computing the first column
  for (a = 1; a < maxA; a++) cost[a] = cost[a - 1] + IndelCost;
  for (b = 1; b < maxB; b++)
  {
    // Before the inner loop, calculate the bottom row's cost
    costBelow = cost[0] + IndelCost;
    for (a = 1; a < maxA; a++)
       bool isMatching = seqA.Sequence[a] == seqB.Sequence[b];
      int diagonal = cost[a - 1] + (isMatching ? MatchCost : SubstCost);
       int left = cost[a] + IndelCost;
       int below = costBelow + IndelCost;
       costHere = Math.Min(diagonal, Math.Min(left, below));
       // Prepare for the next column, using an N-space cost array
       cost[a - 1] = costBelow;
      // The next row up will use a "cost below" of whatever the cost is here
       costBelow = costHere;
    }
  //Console.WriteLine("Cost is " + costHere);
  return costHere;
}
private void showCost(int[] cost, int max, int column)
  Console.WriteLine("Cost at column " + column.ToString());
  for (int i = 0; i < max; i++)
    Console.WriteLine(i.ToString() + ": " + cost[i].ToString());
}
private void Extract(GeneSequence seqA, GeneSequence seqB)
  int maxA = Math.Min(seqA.Sequence.Length, MaxCharactersToAlign);
  int maxB = Math.Min(seqB.Sequence.Length, MaxCharactersToAlign);
  int a, b;
  int[][] cost = new int[maxA + 1][];;
  for (a = 0; a < maxA + 1; a++)
    cost[a] = new int[maxB + 1];
  // Initialize sequence A column of insertions
```

```
for (a = 0; a < maxA + 1; a++)
     cost[a][0] = a * IndelCost;
   // Initialize sequence B row of insertions
   for (b = 0; b < maxB + 1; b++)
     cost[0][b] = b * IndelCost;
   // Calculate the Cost matrix
   for (b = 1; b < maxB + 1; b++)
   {
     for (a = 1; a < maxA + 1; a++)
        bool isMatching = seqA.Sequence[a - 1] == seqB.Sequence[b - 1];
       int diagonal = cost[a - 1][b - 1] + (isMatching ? MatchCost : SubstCost);
       int left = cost[a][b - 1] + IndelCost;
       int below = cost[a - 1][b] + IndelCost;
       // Use the min path, wherever it leads us
       cost[a][b] = Math.Min(diagonal, Math.Min(left, below));
   }
   Console.WriteLine("{0} x {0} cost array", maxA + 1, maxB + 1);
   // Display the results of the alignment in the console
   int pathA = maxA, pathB = maxB;
   while (pathA > 0 \&\& pathB > 0)
   {
     int diagonal = cost[pathA - 1][pathB - 1];
     int left = cost[pathA][pathB - 1];
     int below = cost[pathA - 1][pathB];
     char charA = seqA.Sequence[pathA - 1];
     char charB = seqB.Sequence[pathB - 1];
     if (diagonal <= left && diagonal <= below)
     {
        Console.Write(charA.ToString() + " " + charB.ToString());
       if (charA == charB)
          Console.WriteLine(" Match");
       }
       else
          Console.WriteLine(" Subst");
       }
       pathA--;
       pathB--;
     else if (left <= diagonal && left <= below)
        Console.WriteLine(charA.ToString() + " - Indel");
       pathB--;
     else // min is below
        Console.WriteLine("-" + charB.ToString() + " Indel");
       pathA--;
     }
  }
}
```