Analysis of Algorithms, I
CSOR W4231.002

Eleni Drinea
Computer Science Department

Columbia University

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Outline

Today

Review of the last lecture

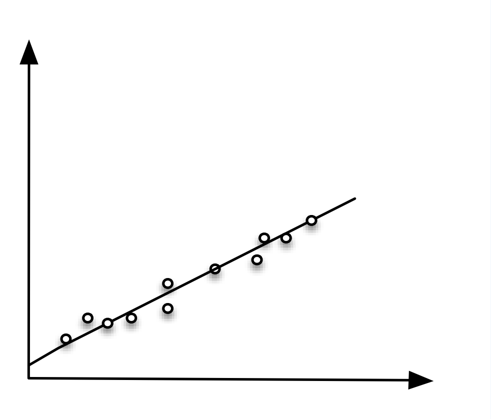
Dynamic Programming

- The problem: data segmentation
- A mathematical formulation of the problem
- An exponential-time brute-force approach
- A recurrence for the optimal cost
- An exponential-time recursive algorithm for the optimal cost

Today

Linear least squares fitting

A foundational problem in statistics: find a line of *best fit* through some data points.



A first problem: **linear** least squares fitting

Input: a set P of n data points (x_1, y_1), (x_2, y_2), ..., (x_n, y_n); we assume $x_1 < x_2 < \ldots < x_n$.

Output: the line L defined as $y = ax + b$ that minimizes the *sum of the vertical distances of the points from the line*:

$$err(L, P) = \sum_{i=1}^{n} (y_i - ax_i - b)^2 \tag{1}$$

Linear least squares fitting: solution

Given a set P of data points, we can use calculus to show that the line L given by $y = ax + b$ that minimizes

$$err(L,P) = \sum_{i=1}^{n} (y_i - ax_i - b)^2 \tag{2}$$

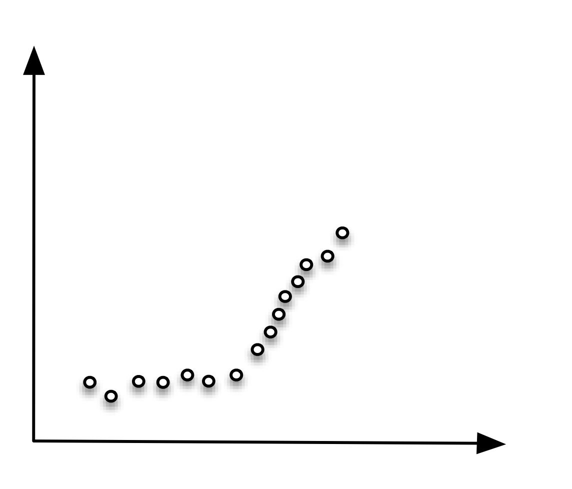
satisfies

$$a = \frac{n\sum_i x_i y_i - (\sum_i x_i)(\sum_i y_i)}{n\sum_i x_i^2 - (\sum_i x_i)^2} \tag{3}$$

$$b = \frac{\sum_i y_i - a\sum_i x_i}{n} \tag{4}$$

How fast can we compute a, b?

What if the data changes direction?



Formalizing Segmented Least Squares

Input: data set $P = \{p_1, \ldots, p_n\}$ of points on the plane.

- A segment $S = \{p_i, p_{i+1}, \ldots, p_j\}$ is a contiguous subset of P.
- Let $\mathcal{A}$ be a partition of P into $m_{\mathcal{A}}$ segments $S_1, S_2, \ldots, S_{m_{\mathcal{A}}}$.
  For every segment S_k, use (2), (3), (4) to compute a line L_k that minimizes $err(L_k, S_k)$.
- Let $C > 0$ be a fixed multiplier. The cost of partition $\mathcal{A}$ is

$$\sum_{S_k \in \mathcal{A}} err(L_k, S_k) + m_{\mathcal{A}} \cdot C$$

Output: a partition of minimum cost, and its cost.

A recurrence for the optimal solution

Notation: let $e_{i,j} = err(L, \{p_i, \ldots, p_j\})$, for $1 \leq i \leq j \leq n$.

- $OPT(n) = \min_{1 \leq i \leq n} \left\{ e_{i,n} + C + OPT(i-1) \right\}$.
- Applying the above expression recursively to remove the last segment, we obtain the recurrence

$$OPT(j) = \min_{1 \leq i \leq j} \left\{ e_{i,j} + C + OPT(i-1) \right\} \tag{5}$$

Remark 1.

1. *We can precompute and store all $e_{i,j}$ using equations* (2), (3), (4) *in $O(n^3)$ time. Can be improved to $O(n^2)$.*
2. *The natural recursive algorithm arising from recurrence* (5) *is* **not** *efficient (think about its recursion tree!).*

Elements of DP in segmented least squares

1. Overlapping subproblems
2. An easy-to-compute recurrence (5) for combining solutions to the smaller subproblems into a solution to a larger subproblem in $O(n)$ time (once smaller subproblems have been solved).
3. Iterative, bottom-up computations: compute the subproblems from smallest (0 points) to largest (n points), iteratively.
4. Small number of subproblems: we only need to solve n subproblems.

A dynamic programming approach

$$OPT(j) = \min_{1 \leq i \leq j} \left\{ e_{i,j} + C + OPT(i-1) \right\}$$

- The optimal solution to the subproblem on $p_1, \ldots, p_j$ contains optimal solutions to smaller subproblems.
- Recurrence 5 provides an **ordering** of the subproblems from **smaller to larger**: the subproblem of size 0 is the smallest, the subproblem of size n is the largest.
- Boundary condition: $OPT(0) = 0$.

⇒ There are $n+1$ subproblems in total. Solving the j-th subproblem requires $\Theta(j) = O(n)$ time.

⇒ The overall running time is $O(n^2)$.

- Segment $p_k, \ldots, p_j$ appears in the optimal solution when the minimum in the expression above is achieved for $i = k$.

An iterative algorithm for segmented least squares

Let M be an array with n entries such that

$$M[i] = \text{cost of optimal partition of the first } i \text{ data points}$$

`SegmentedLS`(n, P)
  $M[0] = 0$
  for all pairs $i \leq j$ **do**
    Compute $e_{i,j}$ for segment $p_i, \ldots, p_j$ using (2), (3), (4)
  end for
  for $j = 1$ to n **do**
    $M[j] = \min_{1 \leq i \leq j} \{e_{i,j} + C + M[i-1]\}$
  end for
  Return $M[n]$

Running time: time required to fill in dynamic programming array M is $O(n^3) + O(n^2)$. Can be brought down to $O(n^2)$.

Reconstructing an optimal segmentation

We can reconstruct the optimal partition recursively, using array M and error matrix e.

```
OPTSegmentation(j)
  if (j == 0) then return
  else  // find the first point of the segment where p_j belongs
      Find 1 ≤ i ≤ j such that M[j] = e_{i,j} + C + M[i − 1]
      OPTSegmentation(i − 1)
      Output segment {p_i, ..., p_j}
  end if
```

- Initial call: `OPTSegmentation`(n)
- *Running time?*

Obtaining efficient algorithms using DP

1. Optimal substructure: the optimal solution to the problem contains optimal solutions to the subproblems.
2. A recurrence for the overall optimal solution in terms of optimal solutions to appropriate subproblems. The recurrence should provide a natural ordering of the subproblems from smaller to larger and require polynomial work for combining solutions to the subproblems.
3. Iterative, bottom-up computation of subproblems, from smaller to larger.
4. Small number of subproblems (polynomial in n).

Dynamic programming vs Divide & Conquer

- They both combine solutions to subproblems to generate the overall solution.
- However, divide and conquer starts with a large problem and divides it into small pieces.
- While dynamic programming works from the bottom up, solving the smallest subproblems first and building optimal solutions to steadily larger problems.

Today

String similarity

This problem arises when comparing strings.

Example: consider an online dictionary.

- **Input:** a word, e.g., "ocurrance"
- **Output:** *did you mean* "occurrence" *?*

Similarity: intuitively, two words are similar if we can "almost" line them up by using gaps and mismatches.

Aligning strings using gaps and mismatches

We can align “ocurrance” and “occurrence” using

- one gap and one mismatch

o	c	–	u	r	r	a	n	c	e
o	c	c	u	r	r	e	n	c	e

- or, three gaps

o	–	c	u	r	r	–	a	n	c	e
o	c	c	u	r	r	e	–	n	c	e

Strings in biology

- Similarity of english words is rather intuitive.
- Determining similarity of biological strings is a central computational problem for molecular biologists.
  - Chromosomes again: an organism's genome consists of chromosomes (giant linear DNA molecules)
  - We may think of a chromosome as an enormous linear tape containing a string over the alphabet $\{A, C, G, T\}$.
  - The string encodes instructions for building protein molecules.

Why similarity?

Why are we interested in similarity of biological strings?

- Roughly speaking, the sequence of symbols in an organism's genome determines the properties of the organism.
- So similarity can guide decisions about biological experiments.

How do we define similarity between two strings?

Similarity based on the notion of "lining up" two strings

Informally, an alignment between two strings tells us which pairs of positions will be lined up with one another.

Example: $X = \mathrm{GCAT}$, $Y = \mathrm{CATG}$

x_1	x_2	x_3	x_4	
G	C	A	T	-
-	C	A	T	G
	y_1	y_2	y_3	y_4

The set of pairs $\{(2,1),(3,2),(4,3)\}$ is an **alignment** of X, Y: these are the pairs of positions in X, Y that are **matched**.

Definition of alignment of two strings

An alignment L of $X = x_1 \dots x_m$, $Y = y_1 \dots y_n$ is a set of **ordered** pairs of indices (i, j) with $i \in [1, m]$, $j \in [1, n]$ such that the following two properties hold:

P1. every $i \in [1, m]$, $j \in [1, n]$ appears at most once in L;

P2. pairs do not *cross*: if $(i, j), (i', j') \in L$ and $i < i'$, then $j < j'$.

Example: $X = \text{GCAT}$, $Y = \text{CATG}$

x_1	x_2	x_3	x_4	
G	C	A	T	-
-	C	A	T	G
	y_1	y_2	y_3	y_4

1. $\{(2, 1), (3, 2), (4, 3)\}$ is an alignment; but
2. $\{(2, 1), (3, 2), (4, 3), (1, 4)\}$ is **not** an alignment (violates P2).

Cost of an alignment

Let L be an alignment of $X = x_1 \dots x_m$, $Y = y_1 \dots y_n$.

1. Gap penalty δ: there is a cost δ for every position of X and Y that is not matched.
2. Mismatch cost: there is a cost α_{pq} for every pair of alphabet symbols p, q that are matched in L.
   - So every pair $(i, j) \in L$ incurs a cost of $\alpha_{x_i y_j}$.
   - **Assumption:** $\alpha_{pp} = 0$ (matching a symbol with itself incurs no cost).

The cost of alignment L is the sum of all the gap and the mismatch costs.

Cost of alignment in symbols

In symbols, given alignment L, let

- $X_i^L = 1$ if position i of X is not matched (gap),
- $Y_j^L = 1$ if position j of Y is not matched (gap).

Then the cost of alignment L is given by

$$cost(L) = \sum_{1 \leq i \leq m} X_i^L \delta \;+\; \sum_{1 \leq j \leq n} Y_j^L \delta \;+\; \sum_{(i,j) \in L} \alpha_{x_i y_j}$$

Examples

Example 1.

Let L_1 be the alignment shown below.

x_1	x_2		x_3	x_4	x_5	x_6	x_7	x_8	x_9
o	c	-	u	r	r	a	n	c	e
o	c	c	u	r	r	e	n	c	e
y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8	y_9	y_{10}

$L_1 = \{(1,1),(2,2),(3,4),(4,5),(5,6),(6,7),(7,8),(8,9),(9,10)\}$

$cost(L_1) = \delta + \alpha_{ae}$ (This is $Y_3^{L_1} + \alpha_{x_6 y_7}$.)

Example 2.

Let L_2 be the alignment shown below.

x_1		x_2	x_3	x_4	x_5		x_6	x_7	x_8	x_9
o	-	c	u	r	r	-	a	n	c	e
o	c	c	u	r	r	e	-	n	c	e

$L_1 = \{(1,1),(2,3),(3,4),(4,5),(5,6),(7,8),(8,9),(9,10)\}$

$cost(L_2) = 3\delta$ (This is $X_6^{L_2} + Y_2^{L_2} + Y_7^{L_2}$.)

Example 3.

Let L_3, L_4 be the alignments shown below.

x_1	x_2	x_3	x_4
G	C	A	T
C	A	T	G
y_1	y_2	y_3	y_4

x_1	x_2	x_3	x_4	
G	C	A	T	-
-	C	A	T	G
	y_1	y_2	y_3	y_4

$L_3 = \{(1,1),(2,2),(3,3),(4,4)\}$

$cost(L_3) = \alpha_{\mathrm{GC}} + \alpha_{\mathrm{CA}} + \alpha_{\mathrm{AT}} + \alpha_{\mathrm{TG}}$

$L_4 = \{(2,1),(3,2),(4,3)\}$

$cost(L_4) = 2\delta$

The sequence alignment problem

Input:

- **two** strings X, Y consisting of m, n symbols respectively; each symbol is from some alphabet Σ
- the gap penalty δ
- the mismatch costs $\{\alpha_{pq}\}$ for every pair $(p, q) \in \Sigma^2$

Output: the **minimum** cost to align X and Y, and an optimal alignment.

Towards a recursive solution

Claim 1.

Let L be the optimal alignment. Then either

1. *the last two symbols x_m, y_n of X, Y are matched in L, hence the pair $(m, n) \in L$; or*
2. *x_m, y_n are not matched in L, hence $(m, n) \notin L$.*
   In this case, at least one of x_m, y_n is not matched in L, hence at least one of m, n does not appear in L.

Proof of Claim 1

By contradiction.

Suppose $(m, n) \notin L$ but x_m and y_n are **both** matched in L. That is,

1. x_m is matched with y_j for some $j < n$, hence $(m, j) \in L$;
2. y_n is matched with x_i for some $i < m$, hence $(i, n) \in L$.

Since pairs (i, n) and (m, j) cross, L is not an alignment.

Rewriting Claim 1

The following equivalent way of stating Claim 1 will allow us to easily derive a recurrence.

Fact 4.

In an optimal alignment L, at least one of the following is true

1. $(m, n) \in L$*; or*
2. x_m *is not matched; or*
3. y_n *is not matched.*

The subproblems for sequence alignment

Let

$OPT(i,j) =$ minimum cost of an alignment between $x_1 \dots x_i$, $y_1 \dots y_j$

We want $OPT(m,n)$. From Fact 4,

1. If $(m,n) \in L$, we pay $\alpha_{x_m y_n} + OPT(m-1, n-1)$.
2. If x_m is not matched, we pay $\delta + OPT(m-1, n)$.
3. If y_n is not matched, we pay $\delta + OPT(m, n-1)$.

How do we decide which of the three to use for $OPT(m,n)$*?*

The recurrence for the sequence alignment problem

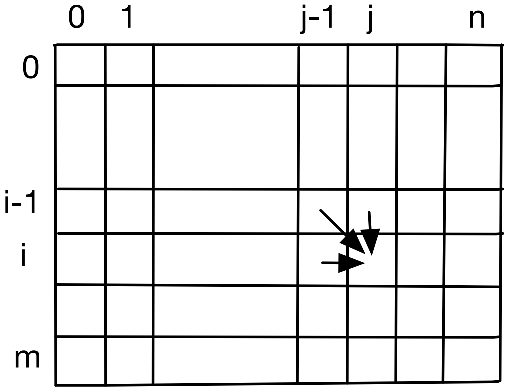
$$OPT(i,j) = \begin{cases} j\delta & \text{, if } i = 0 \\ \min \begin{cases} \alpha_{x_i y_j} + OPT(i-1, j-1) \\ \delta + OPT(i-1, j) \\ \delta + OPT(i, j-1) \end{cases} & \text{, if } i, j \geq 1 \\ i\delta & \text{, if } j = 0 \end{cases}$$

Remarks

- Boundary cases: $OPT(0, j) = j\delta$ and $OPT(i, 0) = i\delta$.
- Pair (i, j) appears in the optimal alignment for subproblem $x_1 \dots x_i, y_1 \dots y_j$ if and only if the minimum is achieved by the first of the three values inside the min computation.

Computing the cost of the optimal alignment

- M is an $(m+1) \times (n+1)$ dynamic programming table.
- Fill in M so that all subproblems needed for entry $M[i, j]$ have already been computed when we compute $M[i, j]$ (e.g., column-by-column).



Pseudocode

```
SequenceAlignment(X, Y)
   Initialize M[i, 0] to iδ
   Initialize M[0, j] to jδ
   for j = 1 to n do
      for i = 1 to m do
         M[i, j] = min{α_{x_i y_j} + M[i − 1, j − 1],
                       δ + M[i − 1, j], δ + M[i, j − 1]}
      end for
   end for
   return M[m, n]
```

Running time?

Reconstructing the optimal alignment

Given M, we can reconstruct the optimal alignment as follows.

TraceAlignment(i, j)
    if $i == 0$ or $j == 0$ **then** return
    else
        if $M[i, j] == \alpha_{x_i y_j} + M[i-1, j-1]$ **then**
            TraceAlignment$(i-1, j-1)$
            Output (i, j),
        else
            if $M[i, j] == \delta + M[i-1, j]$ **then** TraceAlignment$(i-1, j)$
            else TraceAlignment$(i, j-1)$
            end if
        end if
    end if

Initial call: TraceAlignment(m, n)
Running time?

Resources used by dynamic programming algorithm

- Time: $O(mn)$
- Space: $O(mn)$
  - English words: $m, n \leq 10$
  - Computational biology: $m = n = 100000$
    - Time: 10 billions ops
    - Space: 10GB table!
- *Can we avoid using quadratic space while maintaining quadratic running time?*

Using only $O(m + n)$ space

1. First, suppose we are only interested in the **cost** of the optimal alignment.
   Easy: keep a table M with 2 columns, hence $2(m + 1)$ entries.

2. *What if we want the optimal alignment too?*
   - No longer possible in $O(n + m)$ time.

Today

Graphs

Definition 5.

A directed graph consists of a finite set of vertices V and a set of directed edges E. A directed edge is an ordered pair of vertices (u, v).

- In mathematical terms, a directed graph $G = (V, E)$ is just a binary relation $E \subseteq V \times V$ on a finite set V.
- An undirected graph is the special case of a directed graph where $(u, v) \in E$ if and only if $(v, u) \in E$. In this case, an edge may be indicated as the unordered pair $\{u, v\}$.
- Notational convention: $|V| = n, |E| = m$

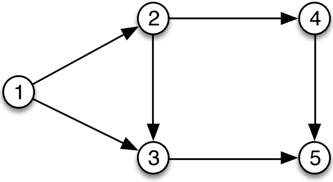
Node degrees

- Degree of a vertex v in an undirected graph: the number of edges incident to v.
- In-degree of a vertex v in a directed graph: the number of edges entering v.
- Out-degree of a vertex v in a directed graph: the number of edges leaving v.

Example graphs

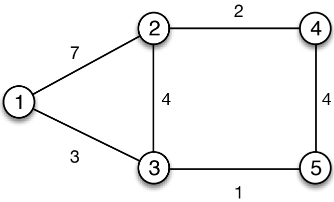
Circles denote vertices (nodes).
Lines denote edges connecting vertices.
Arrows on lines indicate the direction along which the edge may be traversed.

A directed, unweighted graph G
(default edge weight w(e) = 1)



indegree(1) = 0   outdegree(1) = 2
indegree(3) = 2   outdegree(3) = 1

An undirected, weighted graph G'



degree(1) = 2
degree(3) = 3

Examples of graphs (networks)

- **Transportation** networks: e.g., nodes are cities, edges (potentially weighted) are highways connecting the cities
  - *Can we reach a city j from a city i?*
  - *If* **yes**, *what is the shortest (or cheapest) path?*
- **Information** networks: e.g., we can model the World Wide Web as a directed graph
- **Wireless** networks: nodes are devices sitting at locations in physical space and there is an edge from u to v if v is close enough to u to hear from it.
- **Social** networks: nodes are people, edges represent friendship
- **Dependency** networks: e.g., given a list of functions in a large program, find an order to test the functions.

Useful definitions

- A **path** is a sequence of vertices $(x_1, x_2, \ldots, x_n)$ such that consecutive vertices are adjacent (edge $(x_i, x_i + 1) \in E$ for all $1 \leq i \leq n - 1$).
  Example: $(1, 2, 3, 2, 4)$ in G' is a path.
- A path is **simple** when all vertices are distinct.
  Example: $(1, 2, 4)$ in G' is a simple path.
- A **cycle** is a simple path that ends where it starts, that is, $x_n = x_1$.
  Example: $(1, 2, 3, 1)$ in G' is a cycle.
- The **distance** from u to v is the length of the *shortest* path from u to v.
  Example: the distance from 1 to 4 in G is 2.

Useful definitions (cont'd)

- An undirected graph is **connected** when there is a path between every pair of vertices.
  Example: G' is connected.
- The **connected component** of a node u is the set of all nodes in the graph reachable by a path from u.
  Example: the connected component of node 1 in G' is $\{1, 2, 3, 4, 5\}$.
- A directed graph is **strongly connected** if for every pair of vertices u, v, there is a path from u to v and from v to u.
- The **strongly connected component** of a node u in a directed graph is the set of nodes v in the graph such that there is a path from u to v and from v to u.
  Example: the strongly connected component of node 1 in G is $\{1\}$.

Trees and tree properties

Definition 6.

A tree is a connected acyclic graph (undirected graphs). Or;
A rooted graph such that there is a unique path from the root to any other vertex (all graphs).

Example: G is a (directed) tree.

It is the most widely used special type of graph: it is the minimal connected graph.

Lemma 7.

Let G be an undirected graph. Any two of the following properties imply the third property, and that G is a tree.

1. *G is connected;*
2. *G is acyclic;*
3. $|E| = |V| - 1$.

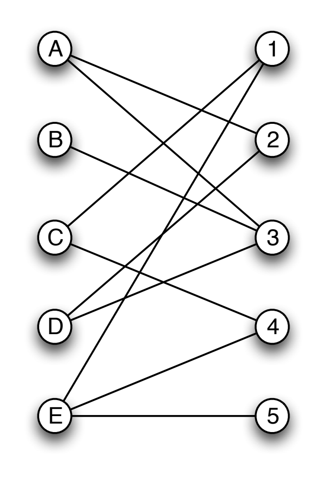
Matchings and bipartite graphs

Bipartite graphs: vertices can be split into two subsets such that there are no edges between vertices in the same subset.

- Applications: social networks, coding theory
- **Notation:** $G = (X \cup Y, E)$, where $X \cup Y$ is the set of vertices in G and every edge in E has one endpoint in X and one endpoint in Y.

Example: suppose there are 5 people and 5 jobs and certain people qualify for certain jobs.

Example of bipartite graph



Goal: find a one-to-one **matching** (also called, a perfect matching) of people to jobs, if one exists.

Degree theorem

Theorem 8.

In any graph, the sum of the degrees of all vertices is equal to twice the number of the edges.

Proof.

Every edge is incident to two vertices, thus contributes twice to the total sum of the degrees. (Summing the degrees of all vertices simply counts all instances of some edge being incident to some vertex.) □