Algorithms for Data Science

CSOR W4246

Eleni Drinea
Computer Science Department

Columbia University

The dynamic programming principle; segmented least squares

Outline

1. Segmented least squares
   - An exponential recursive algorithm

2. A Dynamic Programming (DP) solution
   - A quadratic iterative algorithm
   - Applying the DP principle

Today

1. Segmented least squares
   - An exponential recursive algorithm
2. A Dynamic Programming (DP) solution
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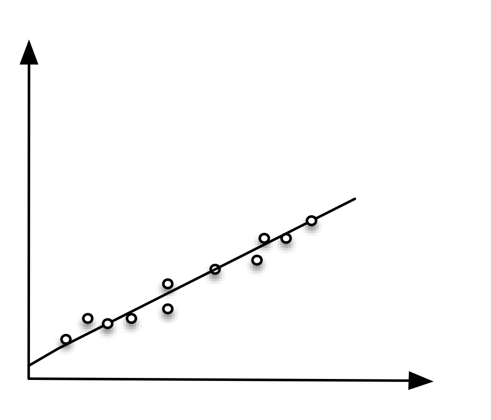
Linear least squares fitting

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



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 error

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

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

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

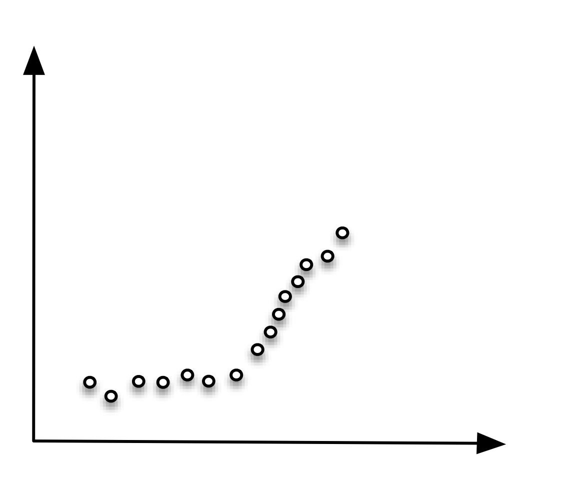
satisfies

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

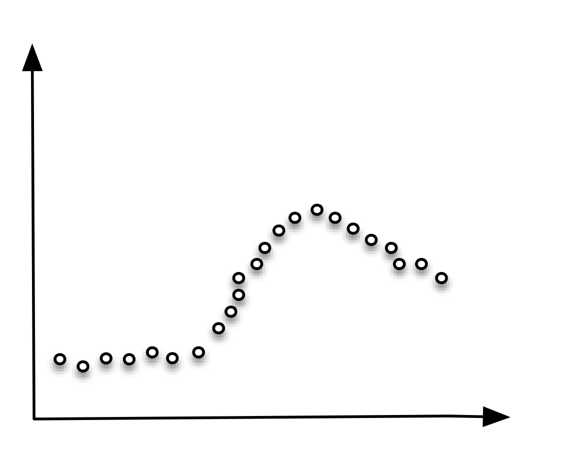
$$b = \frac{\sum_i y_i - a \sum_i x_i}{n} \tag{4}$$

How fast can we compute a, b?

What if the data changes direction?



What if the data changes direction more than once?



How to detect change in the data

- Any single line would have large error.
- **Idea 1:** hardcode number of lines to 2 (or some *fixed* m).
  - Fails for the dataset on the last slide.
- **Idea 2:** pass an *arbitrary set* of lines through the points and seek the set of lines that minimizes the error.
  - Trivial solution: have a different line pass through each pair of consecutive points in P.
- **Idea 3:** fit the points well, using as few lines as possible.
  - Trade-off between complexity and error of the model

Formalizing the problem

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 the input.
- 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

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

Segmented least squares

This problem is an instance of change detection in data mining and statistics.

Input: A set P of n data points $p_i = (x_i, y_i)$ as before.

Output: A segmentation $\mathcal{A}^* = \{S_1, S_2, \ldots, S_{m_{\mathcal{A}^*}}\}$ of P whose cost

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

is minimum.

A brute force approach

We can find the optimal partition (that is, the one incurring the minimum cost) by exhaustive search.

- Enumerate every possible partition (segmentation) and compute its cost.
- Output the one that incurs the minimum cost.

$\triangle$ $\Omega(2^n)$ partitions

A crucial observation regarding the last data point

Consider the last point p_n in the data set.

- p_n belongs to a single segment in the optimal partition.
- That segment starts at an earlier point p_i, for some $1 \leq i \leq n$.

This suggests a recursive solution: **if** we knew where the last segment starts, then we could remove it and recursively solve the problem on the remaining points $\{p_1, \ldots, p_{i-1}\}$.

A recursive approach

- Let $OPT(j)$ = minimum cost of a partition of the points $p_1, \ldots, p_j$.
- Then, if the last segment of the optimal partition is $\{p_i, \ldots, p_n\}$, the cost of the optimal solution is

$$OPT(n) = err(L, \{p_i, \ldots, p_n\}) + C + OPT(i-1).$$

- But we don't know where the last segment starts! *How do we find the point p_i?*
- Set

$$OPT(n) = \min_{1 \leq i \leq n} \Big\{ err(L, \{p_i, \ldots, p_n\}) + C + OPT(i-1) \Big\}.$$

A recurrence for the optimal solution

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

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

If we apply 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!).*

Exponential-time recursion

Notation: $T(n)$ = time to compute $OPT(n)$, that is, the cost of the optimal partition for n points.

Then

$$T(n) \geq T(n-1) + T(n-2).$$

- Can show that $T(n) \geq F_n$, the n-th Fibonacci number (by strong induction on n).
- From optional problem 6a in Homework 1, $F_n = \Omega(2^{n/2})$.
- Hence $T(n) = \Omega(2^{n/2})$.

$\Rightarrow$ The recursive algorithm requires $\Omega(2^{n/2})$ time.

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Are we really that far from an efficient solution?

Recall Fibonacci problem from HW1: exponential recursive algorithm, polynomial iterative solution

How?

1. Overlapping subproblems: spectacular redundancy in computations of recursion tree
2. Easy-to-compute recurrence for combining the smaller subproblems: $F_n = F_{n-1} + F_{n-2}$
3. Iterative, bottom-up computations: we computed and stored the subproblems from smallest (F_0, F_1) to largest (F_n), iteratively.
4. Small number of subproblems: only solved $n - 1$ subproblems.

Elements of DP in segmented least squares

Our problem exhibits similar properties.

1. Overlapping subproblems
2. Easy-to-compute recurrence for combining optimal solutions to smaller subproblems into the optimal solution of a larger subproblem (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

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

- 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, with the subproblem of size 0 being the smallest and the subproblem of size n the largest.

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

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

- Boundary conditions: $OPT(0) = 0$.
- Segment $p_k, \ldots, p_j$ appears in the optimal solution only if the minimum in the expression above is achieved for $i = k$.

An iterative algorithm for segmented least squares

Let M be an array of 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 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.