Dynamic Programming

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CS155 Machine Learning and Data Mining

February 27, 2018

Motivation

Much of machine learning is heavily dependent on computational power

Many libraries exist that aim to reduce computational time

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Well-designed algorithms also speed up computation

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- Fibonacci Numbers
- Viterbi Algorithm
- Forward/Backward Algorithm

Aside: why the name 'Dynamic Programming'?

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From Richard Bellman’s autobiography:

I spent the Fall quarter (of 1950) at RAND. My first task was to find a name for multistage decision processes. An interesting question is, ‘Where did the name, dynamic programming, come from?’ The 1950s were not good years for mathematical research. We had a very interesting gentleman in Washington named Wilson. He was Secretary of Defense, and he actually had a pathological fear and hatred of the word, research...His face would suffuse, he would turn red, and he would get violent if people used the term, research, in his presence. You can imagine how he felt, then, about the term, mathematical. The RAND Corporation was employed by the Air Force, and the Air Force had Wilson as its boss, essentially.

Aside: why the name 'Dynamic Programming'?

Hence, I felt I had to do something to shield Wilson and the Air Force from the fact that I was really doing mathematics inside the RAND Corporation. ... I decided therefore to use the word, 'programming.' I wanted to get across the idea that this was dynamic, this was multistage, this was time-varying—I thought, let's kill two birds with one stone. Let's take a word that has an absolutely precise meaning, namely dynamic, in the classical physical sense. It also has a very interesting property as an adjective, and that is it's impossible to use the word, dynamic, in a pejorative sense. Try thinking of some combination that will possibly give it a pejorative meaning. It's impossible. Thus, I thought dynamic programming was a good name. It was something not even a Congressman could object to. So I used it as an umbrella for my activities.

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Optimal substructure is associated with recursion and divide-and-conquer strategies

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Relationship between Optimal Substructure, Overlapping Subproblems, and Dynamic Programming

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- Dynamic programming: store and leverage previous computations to save computation time
  - Would not be helpful for optimal substructure-only case—overkill!
  - With overlapping subproblems: can reduce runtime from exponential to polynomial time

Fibonacci Numbers: An Example

Let's see an example of where the optimal substructure and overlapping subproblems properties are helpful.

Write a function to find the *n*-th Fibonacci number.

$$F_n = F_{n-1} + F_{n-2}$$

where $F_2 = 1$ and $F_1 = 1$

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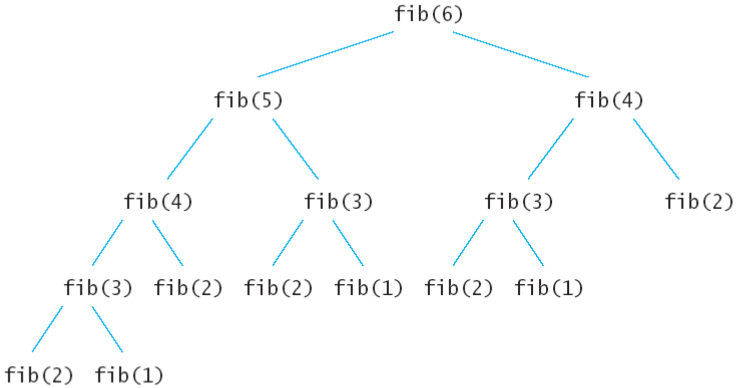
Example

```
def naive_fib(n):
  if n == 1 or n == 2:
    return 1
  else:
    return naive_fib(n-1) + naive_fib(n-2)
```

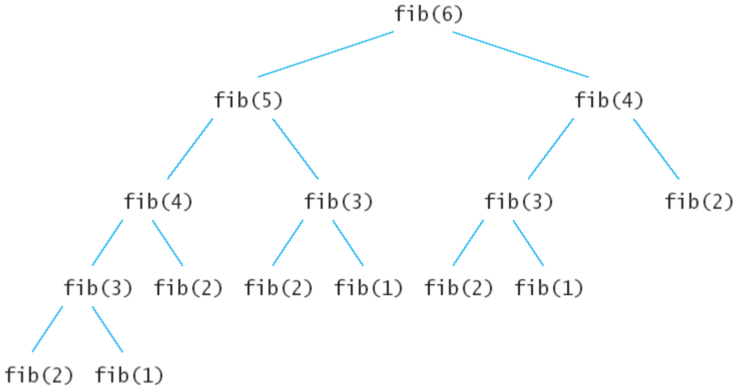
Fibonacci Numbers

How does the computation break down?



Fibonacci Numbers

Optimal substructure? Overlapping subproblems?



Fibonacci Numbers

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- Bottom-up

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Top-down: solve recursively, storing previous computations for later use

Bottom-up: build a table of subproblem results (starting with base cases) that grows until we reach solution

Top-down Fibonacci Numbers

Recursively solve, storing results of subproblems as we go

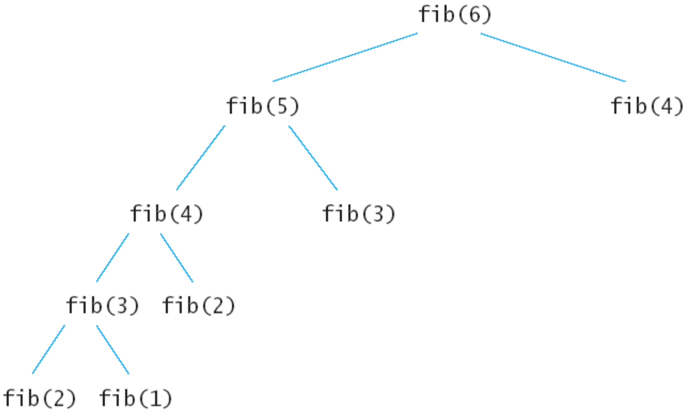
Example

```
table = {}

def top_down_fib(n):
  if n in table:
    return table[n]
  else:
    if n == 1 or n == 2:
      table[n] = 1
    else:
      table[n] = top_down_fib(n-1) + top_down_fib(n-2)
    return table[n]
```

Top-down Fibonacci Numbers

What's the computation path?



Bottom-up Fibonacci Numbers

Build a table of subproblem results, starting from the base cases

Example

```
def bottom_up_fib(n):
  if n == 1 or n == 2:
    return 1
  else:
    table = [0, 1, 1]
    for i in range(3, n+1):
      table.append(table[i-1] + table[i-2])
    return table[n]
```

Bottom-up Fibonacci Numbers

What's the computation path?

fib(1)	fib(2)	fib(3)	fib(4)	fib(5)	fib(6)
1	1	2	3	5	8

What did dynamic programming accomplish here?

Fibonacci Numbers

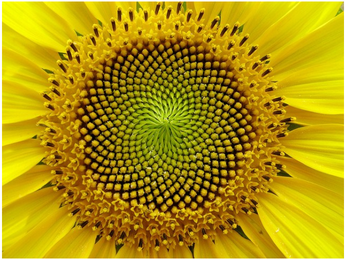
What did dynamic programming accomplish here?

Reduces the number of computations and overall time complexity

$$\mathcal{O}(2^n) \to \mathcal{O}(n)$$

Dramatic speedup, especially for large n

Fun fact: Fibonacci numbers show up in nature!



Reference: Bohannon, John. “Sunflowers Show Complex Fibonacci Sequences.” News from *Science*, 2016, `http://www.sciencemag.org/news/2016/05/sunflowers-show-complex-fibonacci-sequences`.

Hidden Markov Models

Now, let's see how dynamic programming helps us with HMMs

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Recall that with a 1st-order HMM

$$P(\mathbf{x}, \mathbf{y}) = P(End \mid y^M) \prod_{i=1}^{M} P(y^i \mid y^{i-1}) \prod_{i=1}^{M} P(x^i \mid y^i)$$

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- $P(x^i \mid y^i) \rightarrow$ probability of state y^i generating emission x^i
- $P(y^i \mid y^{i-1}) \rightarrow$ probability of state y^{i-1} transitioning to y^i
- $P(y^1 \mid y^0) \rightarrow$ probability of the start state
- $P(End \mid y^M) \rightarrow$ optional

Viterbi Algorithm

$$P(\mathbf{x}, \mathbf{y}) = P(End \mid y^M) \prod_{i=1}^{M} P(y^i \mid y^{i-1}) \prod_{i=1}^{M} P(x^i \mid y^i)$$

Suppose we have a length-M sequence of emissions, $\mathbf{x}$. How can we find the length-M sequence of states, $\mathbf{y}$, for which $P(\mathbf{x}, \mathbf{y})$ is maximized?

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Consider the naive solution:
$\mathbf{y}^* = \arg\max_{\mathbf{y}} \log P(\mathbf{y} \mid \mathbf{x}) = \arg\max_{\mathbf{y}} \log P(\mathbf{x}, \mathbf{y})$.

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This requires evaluating L^M sequences if there are L possible states.

This is too slow. Can we do better?

Dynamic Programming for Viterbi Algorithm

Can we use Dynamic Programming to find the most probable state sequence $\mathbf{y}$? Why?

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To understand this, let's move to a more concrete example

Suppose that $\mathbf{x}$ is a sentence and $\mathbf{y}$ is the corresponding part-of-speech (POS) tag sequence.

$$y^i \in S = \{N = Noun, V = Verb, D = Adverb\}$$

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Find L sequences $\hat{\mathbf{y}}_a^M$ of POS tags maximizing $P(\mathbf{x}, \hat{\mathbf{y}}_a^M)$:

$$\hat{\mathbf{y}}_N^M = y^1 y^2 \ldots y^{M-1} N$$
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Then, $\mathbf{y}^* = \underset{\mathbf{y} = \hat{\mathbf{y}}_a^M, a \in S}{\arg\max} \; P(\mathbf{x}, \mathbf{y})$

Optimal Substructure in Viterbi Algorithm

Problem: Find $\hat{\mathbf{y}}_N^M$, $\hat{\mathbf{y}}_V^M$, and $\hat{\mathbf{y}}_D^M$

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Subproblem: Given a length-$(M-1)$ sentence $\mathbf{x}^{1:M-1}$, find L sequences, $\hat{\mathbf{y}}_a^{M-1}$, of POS tags that maximize $P(\mathbf{x}^{1:M-1}, \hat{\mathbf{y}}_a^{M-1})$, one of each ending in $\{N, V, D\}$:

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How can we use the optimal solution to this subproblem to solve the problem stated above?

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Optimal solutions to subproblems:

$$\left\{\hat{\mathbf{y}}_N^{M-1}, \hat{\mathbf{y}}_V^{M-1}, \hat{\mathbf{y}}_D^{M-1}\right\} = \left\{\hat{\mathbf{y}}_a^{M-1} | a \in S\right\}$$

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Optimal solution to overall problem:

$$\hat{\mathbf{y}}_N^M = \left\{\underset{\mathbf{y} \in \hat{\mathbf{y}}_a^{M-1}, a \in S}{\arg\max} P(\mathbf{x}^{1:M}, \mathbf{y} \oplus N)\right\} \oplus N$$

$$\hat{\mathbf{y}}_V^M = \left\{\underset{\mathbf{y} \in \hat{\mathbf{y}}_a^{M-1}, a \in S}{\arg\max} P(\mathbf{x}^{1:M}, \mathbf{y} \oplus V)\right\} \oplus V$$

$$\hat{\mathbf{y}}_D^M = \left\{\underset{\mathbf{y} \in \hat{\mathbf{y}}_a^{M-1}, a \in S}{\arg\max} P(\mathbf{x}^{1:M}, \mathbf{y} \oplus D)\right\} \oplus D$$

where $\oplus$ is concatenation

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Optimal Substructure in Viterbi Algorithm

Prove optimal substructure by contradiction: suppose that $\hat{\mathbf{y}}_N^M$ was formed using some length-(M - 1) $\mathbf{y} \notin \{\hat{\mathbf{y}}_a^{M-1} | a \in S\}$

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$$P(\mathbf{x}^{1:M}, \mathbf{y}^{1:M}) = P(\mathbf{x}^{1:M-1}, \mathbf{y}^{1:M-1}) P(y^M \mid y^{M-1}) P(x^M \mid y^M)$$

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So, we can replace $\mathbf{y}$ with $\hat{\mathbf{y}}_a^{M-1}$ to get better (i.e. more probable) $\hat{\mathbf{y}}_N^M$.

Overlapping Subproblems in Viterbi Algorithm

Our problem has the optimal substructure property. We can also see that it has the overlapping subproblems property:

$$\hat{\mathbf{y}}_N^M = \left\{ \underset{\mathbf{y}=\hat{\mathbf{y}}_a^{M-1}, a \in S}{\arg\max} \; P(\mathbf{x}^{1:M}, \mathbf{y} \oplus N) \right\} \oplus N$$

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Use a bottom-up approach. Build a table of solutions to the suproblems. Extend the table until we have $\hat{\mathbf{y}}_N^M$, $\hat{\mathbf{y}}_V^M$, $\hat{\mathbf{y}}_D^M$.

Dynamic Programming in Viterbi Algorithm

Now we understand why we can use dynamic programming for this problem. But how do we do it?

Use a bottom-up approach. Build a table of solutions to the suproblems. Extend the table until we have $\hat{\mathbf{y}}_N^M$, $\hat{\mathbf{y}}_V^M$, $\hat{\mathbf{y}}_D^M$.

How do we start?

$$\hat{\mathbf{y}}_N^1 = N$$
$$\hat{\mathbf{y}}_V^1 = V$$
$$\hat{\mathbf{y}}_D^1 = D$$

Dynamic Programming in Viterbi Algorithm

a is some part of speech, $a \in S = \{N, V, D\}$

$$\begin{aligned}
\hat{\mathbf{y}}^i_a &= \left\{ \operatorname*{arg\,max}_{\mathbf{y}=\hat{\mathbf{y}}^{i-1}_a, a \in S} P(\mathbf{x}^{1:i}, \mathbf{y} \oplus a) \right\} \oplus a \\
&= \left\{ \operatorname*{arg\,max}_{\mathbf{y}=\hat{\mathbf{y}}^{i-1}_a, a \in S} P(\mathbf{x}^{1:i-1}, \mathbf{y}) P(y^i = a \mid y^{i-1}) P(x^i \mid y^i = a) \right\} \oplus a
\end{aligned}$$

Dynamic Programming in Viterbi Algorithm

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\end{aligned}$$

	1	2	...	M-1	M
N	N	VN	...	...N	...VN
V	V	VV	...	...V	...DV
D	D	ND	...	...D	...DD

Applications of the Viterbi Algorithm

- Computational linguistics, natural language processing
  - Part-of-speech tagging

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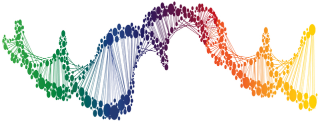
- Bioinformatics
  - Genome sequencing, modeling families of proteins



Computing Marginal Probabilities: Forward/Backward Algorithm

Now let's shift gears and talk about the Forward/Backward Algorithm

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For unsupervised training of HMMs, we need to be able to compute the terms,

$$P(y^i = z \mid \mathbf{x}) \text{ and } P(y^i = b, y^{i-1} = a \mid \mathbf{x})$$

Computing Marginal Probabilities: Forward/Backward Algorithm

Now let's shift gears and talk about the Forward/Backward Algorithm

For unsupervised training of HMMs, we need to be able to compute the terms,

$$P(y^i = z \mid \mathbf{x}) \text{ and } P(y^i = b, y^{i-1} = a \mid \mathbf{x})$$

These expressions can be written in terms of $\alpha_a(i)$ and $\beta_b(i)$:

$$\alpha_a(i) \propto P(\mathbf{x}^{1:i}, y^i = a)$$
$$\beta_b(i) \propto P(\mathbf{x}^{i+1:M} \mid y^i = b)$$

Forward Algorithm

Problem: Compute $\alpha_a(i) \propto P(\mathbf{x}^{1:i}, y^i = a)$ for all a, i.

Forward Algorithm

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Naive solution: sum over all possible sequences $\mathbf{y}^{1:i-1}$:

$$\alpha_a(i) \propto \sum_{\mathbf{y}^{1:i-1}} P(\mathbf{x}^{1:i}, y^i = a, \mathbf{y}^{1:i-1})$$

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$$\alpha_a(i) \propto \sum_{\mathbf{y}^{1:i-1}} P(\mathbf{x}^{1:i}, y^i = a, \mathbf{y}^{1:i-1})$$

This is too slow. Can we apply dynamic programming here? Yes!

Let's see how the $\alpha_a(i)$ terms exhibit optimal substructure and overlapping subproblems.

Optimal Substructure in Forward Algorithm

First, let's see how to build $\alpha_a(i)$ from $\alpha_a(i-1)$

Recall: $y^i \in S = \{N, V, D\}$

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$$= \sum_{a' \in S} P(\mathbf{x}^{1:i-1}, y^{i-1} = a') P(y^i = a \mid y^{i-1} = a') P(x^i \mid y^i = a)$$

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First, let's see how to build $\alpha_a(i)$ from $\alpha_a(i-1)$

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$$\begin{aligned}
\alpha_a(i) \propto P(\mathbf{x}^{1:i}, y^i = a) &= \sum_{a' \in S} P(\mathbf{x}^{1:i}, y^i = a, y^{i-1} = a') \\
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&\propto \sum_{a' \in S} \alpha_{a'}(i-1) P(y^i = a \mid y^{i-1} = a') P(x^i \mid y^i = a)
\end{aligned}$$

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$$\propto \sum_{a' \in S} \alpha_{a'}(i-1) P(y^i = a \mid y^{i-1} = a') P(x^i \mid y^i = a)$$
$$\alpha_a(i) = \sum_{a' \in S} \alpha_{a'}(i-1) P(y^i = a \mid y^{i-1} = a') P(x^i \mid y^i = a)$$

Optimal Substructure in Forward Algorithm

Remember: $\alpha_a(i-1) \propto P(\mathbf{x}^{1:i-1}, y^{i-1} = a)$

'Optimal' solutions for the subproblems:

$$\alpha_N(i) = P(x^i \mid y^i = N) \sum_{a \in S} \alpha_a(i-1) P(y^i = N \mid y^{i-1} = a)$$
$$\alpha_V(i) = P(x^i \mid y^i = V) \sum_{a \in S} \alpha_a(i-1) P(y^i = V \mid y^{i-1} = a)$$
$$\alpha_D(i) = P(x^i \mid y^i = D) \sum_{a \in S} \alpha_a(i-1) P(y^i = D \mid y^{i-1} = a)$$

Overlapping Subproblems in Forward Algorithm

Remember: $\alpha_a(i-1) \propto P(\mathbf{x}^{1:i-1}, y^{i-1} = a)$

As in the Viterbi Algorithm, we can see the overlapping subproblems here as well:

$$\alpha_N(i) = P(x^i \mid y^i = N) \sum_{a \in S} \alpha_a(i-1) P(y^i = N \mid y^{i-1} = a)$$

$$\alpha_V(i) = P(x^i \mid y^i = V) \sum_{a \in S} \alpha_a(i-1) P(y^i = V \mid y^{i-1} = a)$$

$$\alpha_D(i) = P(x^i \mid y^i = D) \sum_{a \in S} \alpha_a(i-1) P(y^i = D \mid y^{i-1} = a)$$

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How do we start?

$$\alpha_N(1) = P(x^{1:1}, y^1 = N) = P(x^1 \mid y^1 = N)P(y^1 = N \mid y^0)$$
$$\alpha_V(1) = P(x^{1:1}, y^1 = V) = P(x^1 \mid y^1 = V)P(y^1 = V \mid y^0)$$
$$\alpha_D(1) = P(x^{1:1}, y^1 = D) = P(x^1 \mid y^1 = D)P(y^1 = D \mid y^0)$$

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Proceed from here using the equations from the previous page

Backward Algorithm

Problem: Compute $\beta_b(i) \propto P(\mathbf{x}^{i+1:M} \mid \mathbf{y}^i = b)$ for all b, i.

Backward Algorithm

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This is too slow. Can we apply dynamic programming here? Yes!

Let's see how the $\beta_b(i)$ terms exhibit optimal substructure and overlapping subproblems.

Optimal Substructure in Backward Algorithm

Remember: $\beta_b(i+1) \propto P(\mathbf{x}^{i+2:M} \mid y^{i+1} = b)$

Similarly to the $\alpha_a(i)$ values, we can also recursively define $\beta_b(i)$:

$$\beta_b(i) = \sum_{b' \in S} \beta_{b'}(i+1) P(y^{i+1} = b' \mid y^i = b) P(x^{i+1} \mid y^{i+1} = b')$$

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'Optimal' solutions for the subproblems:

$$\beta_N(i) = \sum_{b \in S} \beta_b(i+1) P(y^{i+1} = b \mid y^i = N) P(x^{i+1} \mid y^{i+1} = b)$$

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$$\beta_D(i) = \sum_{b \in S} \beta_b(i+1) P(y^{i+1} = b \mid y^i = D) P(x^{i+1} \mid y^{i+1} = b)$$

Overlapping Subproblems in Backward Algorithm

Remember: $\beta_b(i+1) \propto P(\mathbf{x}^{i+2:M} \mid y^{i+1} = b)$

As in the Viterbi and forward algorithms, we can see the overlapping subproblems property:

$$\beta_N(i) = \sum_{b \in S} \beta_b(i+1) P(y^{i+1} = b \mid y^i = N) P(x^{i+1} \mid y^{i+1} = b)$$

$$\beta_V(i) = \sum_{b \in S} \beta_b(i+1) P(y^{i+1} = b \mid y^i = V) P(x^{i+1} \mid y^{i+1} = b)$$

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Again, use a bottom-up approach. Build a table of solutions to subproblems, i.e. a table of $\beta_b(i)$ values for all b, i

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How do we start?

$$\beta_N(M) = P(\mathbf{x}^{M+1:M} \mid y^M = N) = 1$$
$$\beta_V(M) = P(\mathbf{x}^{M+1:M} \mid y^M = V) = 1$$
$$\beta_D(M) = P(\mathbf{x}^{M+1:M} \mid y^M = D) = 1$$

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$$\beta_D(M) = P(\mathbf{x}^{M+1:M} \mid y^M = D) = 1$$

Initialize as 1, then proceed **backward** using the equations from the previous slides

Thanks for joining!

Questions?