# CS621/CSL611 Quantum Computing For Computer Scientists

Quantum Search

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### **Quantum Search**

Grover's Algorithm

#### **Problem Statement**

- Given an unordered array of m elements, find a particular element.
- Classically, in the worst case, this takes *m* queries.
- On average, we will find the desired element in m/2 queries.

#### Can we do better?

- Lov Grover's search algorithm does the job in  $\sqrt{m}$  queries.
- Grover's algorithm has many applications to database theory and other areas.

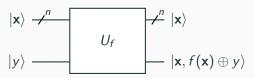
#### **Problem Definition**

- Let us look at the search problem from the point of view of functions.
- **Given:** A function  $f: \{0,1\}^n \to \{0,1\}: \exists \mathbf{x_0} \in \{0,1\}^n$

$$f(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} = \mathbf{x_0}, \\ 0, & \text{if } \mathbf{x} \neq \mathbf{x_0}. \end{cases}$$

- Goal: To find x<sub>0</sub>
- Worst case effort:
  - Classical Search: 2<sup>n</sup> evaluations of f
  - **Grover's Search:**  $\sqrt{2^n} = 2^{\frac{n}{2}}$  evaluations of f

$$|\mathbf{x},y\rangle \xrightarrow{U_f} |\mathbf{x},f(\mathbf{x})\oplus y\rangle$$



## Example (For n = 2, if f "picks out" 10, then $U_f$ is) 00, 1 01, 0 01, 1 10, 0 10, 1 11, 0 00, 0 00, 0 00, 1 01, 0 01, 1 **10**, **0** 10, 1 **11**, **0** 11, 1

• Find  $U_f$ , if f "picks out" 11.

```
00, 0 00, 1 01, 0 01, 1 10, 0 10, 1 11, 0 11, 1

00, 0

00, 1

01, 0

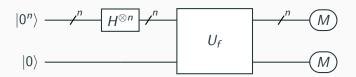
01, 1

10, 0

10, 1

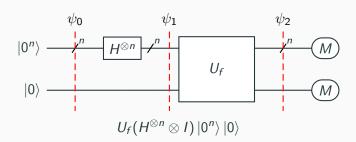
11, 0

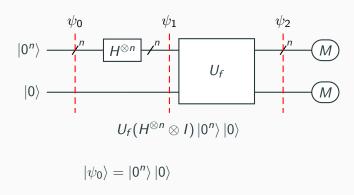
11, 1
```

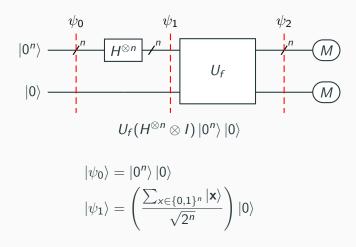


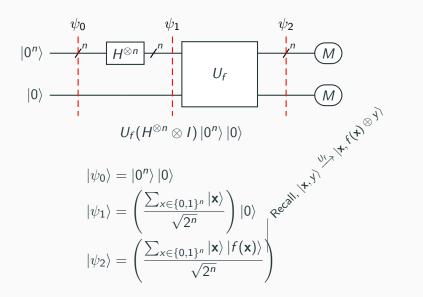
- Try placing  $|x\rangle$  into a superposition of all possible strings
- Then evaluate  $U_f$
- In terms of matrices this becomes

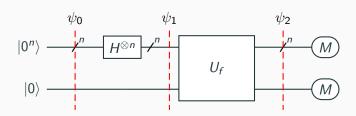
$$U_f(H^{\otimes n} \otimes I) |0^n\rangle |0\rangle$$





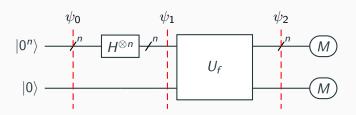






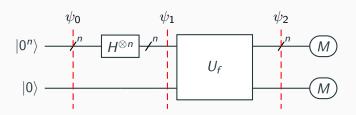
$$\ket{\psi_2} = \left(rac{\sum_{\mathbf{x} \in \{0,1\}^n} \ket{\mathbf{x}}\ket{f(\mathbf{x})}}{\sqrt{2^n}}
ight)$$

- Measuring the top qubits will, with equal probability, give one of the 2<sup>n</sup> binary strings
- Measuring the bottom qubit will give
  - $|0\rangle$  with probability  $\frac{2^n-1}{2^n}$
  - $|1\rangle$  with probability  $\frac{1}{2^n} \implies$  the top qubit will reveal  $x_0$ ? How?



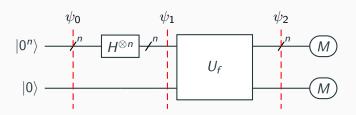
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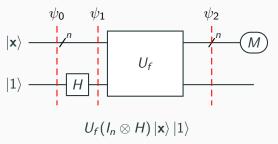
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- Measuring the bottom qubit will give
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  - $|1\rangle$  with probability  $\frac{1}{2^n}$   $\Longrightarrow$  the top qubit will reveal  $x_0$ ? How?

- Trick-1: Phase Inversion:
  - Changes the phase of the desired state
- Trick-2: Inversion About The Mean/Average:
  - This is a way of boosting the separation of the phases.

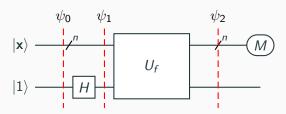
#### Idea

Take  $U_f$  and place the bottom qubit in the superposition  $\frac{|0\rangle-|1\rangle}{\sqrt{2}}$ 

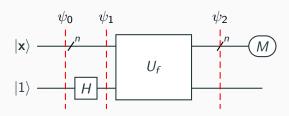
• Corresponding quantum circuit for an arbitrary x



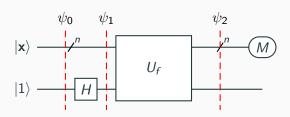
• Note: Phase inversion, by construction, is a unitary operation.



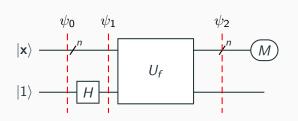
$$\left|\psi_{0}\right\rangle =\left|\mathbf{x}\right\rangle \left|1\right\rangle$$



$$\begin{split} |\psi_0\rangle &= |\mathbf{x}\rangle\,|1\rangle \\ |\psi_1\rangle &= |\mathbf{x}\rangle\left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) = \left(\frac{|\mathbf{x}\rangle\,|0\rangle - |\mathbf{x}\rangle\,|1\rangle}{\sqrt{2}}\right) \end{split}$$



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#### **Effect of Phase Inversion**

• Let  $|\mathbf{x}\rangle$  start in a equal superposition of four different states:

$$|\mathbf{x}\rangle 
ightarrow \left[rac{1}{2},rac{1}{2},rac{1}{2},rac{1}{2}
ight]^T$$

- Let f be the function that uniformly chooses "10"
- After phase inversion state looks like:

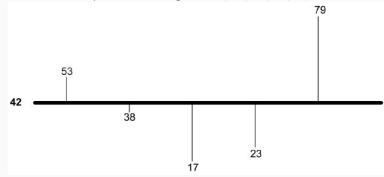
$$\left[\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right]^T$$

- Measurement does not help since  $\left|\frac{1}{2}\right|^2 = \left|-\frac{1}{2}\right|^2 = \frac{1}{4}$
- Implication: Just separating phases is not enough

#### What next?

- Boosting Phase Separation between desired binary string from the other binary strings
- Inversion About The Mean/Average
- A way of boosting the separation of the phases.
- How? Let us see an example

• Consider a sequence of integers: 53, 38, 17, 23, and 79.



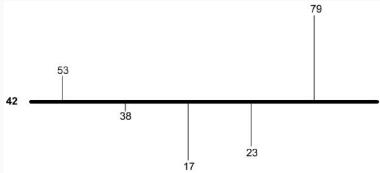
#### Interpreting the Average

Average is a = 42

The average is the number such that the *sum of the lengths of* the lines above the average is the same as the *sum of the lengths* of the lines below.

## **Inversion About The Mean/Average**

• Consider a sequence of integers: 53, 38, 17, 23, and 79.

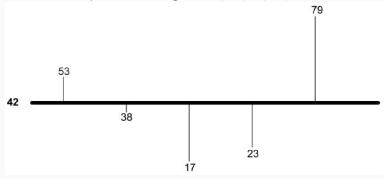


#### **Target**

#### **Change The Sequence**

- Invert elements around the average
  - $\bullet \ \ \, \mathsf{Above} \leftrightarrow \mathsf{Below}$
  - Absolute distance of from average is preserved

• Consider a sequence of integers: 53, 38, 17, 23, and 79.

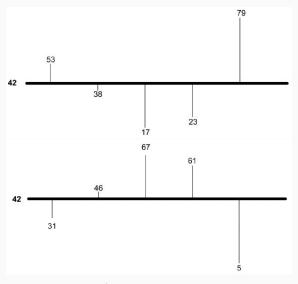


**Example** 
$$(v' = a + (a - v) \implies v' = -v + 2a)$$

53 (Above) 
$$\to$$
 31 (Below) [ $a + (a - 53) = 31$ ]

38 (Below) 
$$\rightarrow$$
 46 (Above) [ $a + (a - 38) = 46$ ]

## Inversion About The Mean/Average



$$\{53, 38, 17, 23, 79\} \xrightarrow{\mathsf{Average, a}} \{31, 46, 67, 61, 5\}$$

#### **Exercise**

• Consider the following numbers: 5, 38, 62, 58, 21, and 35. Invert these numbers around their mean.

#### **Unitary Matrix For Inversion About The Mean**

- Continuing with the example:  $V = [53, 38, 17, 23, 79]^T$
- Consider the following operation: AV

$$\begin{bmatrix} \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \end{bmatrix} \begin{bmatrix} 53 \\ 38 \\ 17 \\ 23 \\ 42 \\ 42 \end{bmatrix}$$

- So matrix A finds the average of a sequence.
- In terms of matrices, the formula v' = -v + 2a becomes

$$V' = -V + 2AV = (-I + 2A)V$$

#### **Unitary Matrix For Inversion About The Mean**

$$(-I+2A) = \begin{bmatrix} \left(-1+\frac{2}{5}\right) & \frac{2}{5} & \frac{2}{5} & \frac{2}{5} & \frac{2}{5} \\ \frac{2}{5} & \left(-1+\frac{2}{5}\right) & \frac{2}{5} & \frac{2}{5} & \frac{2}{5} \\ \frac{2}{5} & \frac{2}{5} & \left(-1+\frac{2}{5}\right) & \frac{2}{5} & \frac{2}{5} \\ \frac{2}{5} & \frac{2}{5} & \frac{2}{5} & \left(-1+\frac{2}{5}\right) & \frac{2}{5} \\ \frac{2}{5} & \frac{2}{5} & \frac{2}{5} & \frac{2}{5} & \left(-1+\frac{2}{5}\right) \end{bmatrix}$$

In our case:

$$(-I + 2A)[53, 38, 17, 23, 79]^T = [31, 46, 67, 61, 5]^T$$

#### **Generalization for 2**<sup>n</sup> **Numbers**

$$A = \begin{bmatrix} \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} \\ \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} \\ \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} \\ \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} \\ \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} & \frac{1}{2^n} \end{bmatrix}$$

(-I + 2A)

$$\begin{bmatrix} \left(-1+\frac{2}{2^{n}}\right) & \frac{2}{2^{n}} & \frac{2}{2^{n}} & \frac{2}{2^{n}} & \frac{2}{2^{n}} \\ \frac{2}{2^{n}} & \left(-1+\frac{2}{2^{n}}\right) & \frac{2}{2^{n}} & \frac{2}{2^{n}} & \frac{2}{2^{n}} \\ \frac{2}{2^{n}} & \frac{2}{2^{n}} & \left(-1+\frac{2}{2^{n}}\right) & \frac{2}{2^{n}} & \frac{2}{2^{n}} \\ \frac{2}{2^{n}} & \frac{2}{2^{n}} & \frac{2}{2^{n}} & \left(-1+\frac{2}{2^{n}}\right) & \frac{2}{2^{n}} \\ \frac{2}{2^{n}} & \frac{2}{2^{n}} & \frac{2}{2^{n}} & \frac{2}{2^{n}} & \left(-1+\frac{2}{2^{n}}\right) \end{bmatrix}$$

#### **Exercise**

• Prove that -I + 2A is a unitary matrix.

#### Combining Trick-1 and Trick-2

- When considered separately, phase inversion and inversion about the mean are each innocuous operations.
- However, when combined, they are a very powerful operation that separates the amplitude of the desired state from those of all the other states.
- Let us do an example to understand this interplay of Trick-1 and Trick-2

- Consider the vector  $[10, 10, 10, 10, 10]^T$ .
- Target the fourth element:
- State after phase inversion:

```
[ \quad , \quad , \quad , \quad ]
```

- Average is:
- State after inversion about mean:

```
[ \qquad , \qquad , \qquad , \qquad ]
```

 The difference between the fourth element and all the others is: • State after phase inversion:

```
[\phantom{a},\phantom{a},\phantom{a},\phantom{a},\phantom{a}]
```

- Average is:
- State after inversion about mean:

```
[\phantom{a},\phantom{a},\phantom{a},\phantom{a},\phantom{a}]
```

 The difference between the fourth element and all the others is:

- **Step 1.** Start with a state  $|0^n\rangle$
- Step 2. Apply  $H^{\otimes n} |0^n\rangle$
- **Step 3.** Repeat  $\sqrt{2^n}$  times:
  - **Step 3a.** Apply the phase inversion operation:

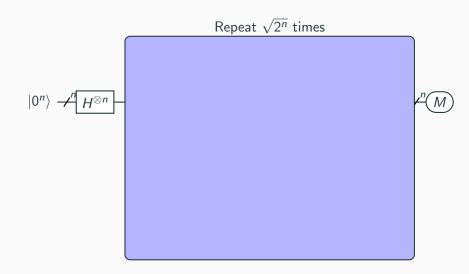
$$U_f(I \otimes H)$$

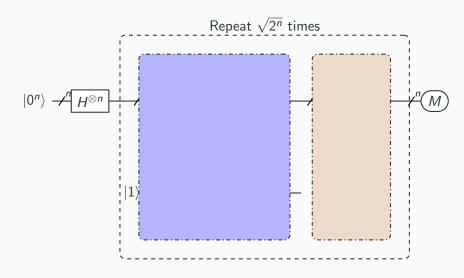
• **Step 3b.** Apply the inversion about the mean operation:

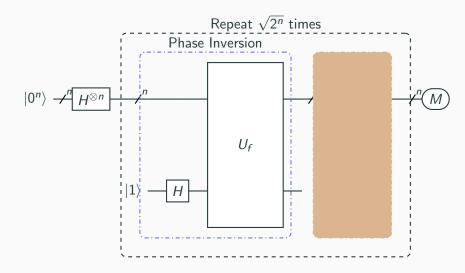
$$-1 + 2A$$

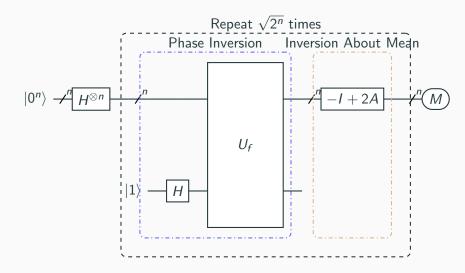
• Step 4. Measure the qubits

# **Grover's Algorithm**









- Let f be a function that picks out the string "101".
- Initial state:

$$|\phi_1\rangle = \left[ \overbrace{1}^{000}, \overbrace{0}^{001}, \overbrace{0}^{010}, \overbrace{0}^{011}, \overbrace{0}^{100}, \overbrace{0}^{101}, \overbrace{0}^{110}, \overbrace{0}^{111}, \overbrace{0}^{111} \right]^T$$

After H<sup>⊗n</sup>

$$|\phi_2\rangle = \left[ \overbrace{\frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}} \right]^T$$

After Phase Inversion

$$|\phi_{3a}\rangle = \left[ \overbrace{\frac{1}{\sqrt{8}}}^{000}, \overbrace{\frac{1}{\sqrt{8}}}^{001}, \overbrace{\frac{1}{\sqrt{8}}}^{010}, \overbrace{\frac{1}{\sqrt{8}}}^{011}, \overbrace{\frac{1}{\sqrt{8}}}^{100}, \overbrace{\frac{1}{\sqrt{8}}}^{101}, \overbrace{\frac{1}{\sqrt{8}}}^{110}, \overbrace{\frac{1}{\sqrt{8}}}^{111} \right]^{T}$$

• Average of the numbers:

• Calculating the inversion about the mean:

For, 
$$\frac{1}{\sqrt{8}}$$
,  $-v + 2a =$ 

For, 
$$-\frac{1}{\sqrt{8}}$$
,  $-v + 2a =$ 

After this step,

$$|\phi_{3b}\rangle = \begin{bmatrix} 000 & 001 & 010 & 011 & 100 & 101 & 111 \\ 000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^T$$

• Repeating... After phase inversion:

$$|\phi_{3a}\rangle = \left[ \overbrace{\phantom{a}}^{000}, \overbrace{\phantom{a}}^{001}, \overbrace{\phantom{a}}^{010}, \overbrace{\phantom{a}}^{011}, \overbrace{\phantom{a}}^{100}, \overbrace{\phantom{a}}^{101}, \overbrace{\phantom{a}}^{110}, \overbrace{\phantom{a}}^{111} \right]^T$$

• Average of the numbers:

• Calculating the inversion about the mean:

For, Case 
$$-1:, -v + 2a =$$

For, Case 
$$-2:, -v + 2a =$$

After this step,

$$|\phi_{3b}\rangle = \left[ \overbrace{\phantom{a}}^{000}, \overbrace{\phantom{a}}^{001}, \overbrace{\phantom{a}}^{010}, \overbrace{\phantom{a}}^{011}, \overbrace{\phantom{a}}^{100}, \overbrace{\phantom{a}}^{101}, \overbrace{\phantom{a}}^{110}, \overbrace{\phantom{a}}^{111} \right]^T$$

• What are the number values of the numbers in  $|\phi_{3b}\rangle$ ?

$$Case - 1:$$
,  $Case - 2:$ 

• Let us square the numbers in  $|\phi_{3b}\rangle$  to get the probabilities.

$$Case - 1$$
: ,  $Case - 2$ :

• Most probable state after measurement:

$$|\phi_4\rangle = \left[ \overbrace{0}^{000}, \overbrace{0}^{001}, \overbrace{0}^{010}, \overbrace{0}^{011}, \overbrace{0}^{100}, \overbrace{1}^{101}, \overbrace{0}^{110}, \overbrace{0}^{111} \right]^T$$

#### **Exercise**

• Write a program in your favorite programming language to do a similar analysis for the case where n=4 and f chooses the "1101" string?

#### Verdict

- A classical algorithm will search an unordered array of size n
  in n steps.
- Grover's algorithm will take time  $\sqrt{n}$ .
- This is what is referred to as a quadratic speedup.

## What happens if we repeat beyond $\sqrt{n}$

- The phase difference will degrade.
- The overcooking effect<sup>1</sup>!
- Let us look at Bernstein's Indocrypt 2021 Example to see a demonstration of this effect.

<sup>&</sup>lt;sup>1</sup>Proof makes use of geometry. Needs another view of the systems

#### **Quantum Search**

Grover's Search Demo

Adapted from Bernstein's Invited Talk at Indocrypt 2021

## Grover's algorithm

Assume: unique  $s \in \{0, 1\}^n$  has f(s) = 0.

Goal: Figure out s.

Non-quantum algorithm to find s: compute f for many inputs, hope to find output 0. Success probability is very low until #tries approaches  $2^n$ .

## Grover's algorithm

Assume: unique  $s \in \{0, 1\}^n$ has f(s) = 0.

Goal: Figure out s.

Non-quantum algorithm to find s: compute f for many inputs. hope to find output 0. Success probability is very low

until #tries approaches  $2^n$ . Grover's algorithm takes only  $2^{n/2}$ quantum evaluations of f.

e.g.  $2^{64}$  instead of  $2^{128}$ .

Start from uniform superposition over n-bit strings u: each  $a_u = 1$ .

Start from uniform superposition over *n*-bit strings *u*: each  $a_u = 1$ .

Step 1: Set  $a \leftarrow b$  where  $b_{\mu} = -a_{\mu}$  if f(u) = 0,

 $b_{\mu} = a_{\mu}$  otherwise. This is fast if f is fast. over *n*-bit strings *u*: each  $a_u = 1$ .

Start from uniform superposition

Step 1: Set  $a \leftarrow b$  where  $b_{\mu} = -a_{\mu}$  if f(u) = 0,

 $b_{ii} = a_{ii}$  otherwise.

This is fast if f is fast.

This is also fast.

Step 2: "Grover diffusion". Negate a around its average. over *n*-bit strings u: each  $a_u = 1$ . Step 1: Set  $a \leftarrow b$  where

Start from uniform superposition

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This is also fast.

Repeat Step 1 + Step 2 about  $0.58 \cdot 2^{0.5n}$  times.

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Negate *a* around its average.

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Repeat Step 1 + Step 2about  $0.58 \cdot 2^{0.5n}$  times.

Measure the n qubits.

With high probability this finds s.

for an example with n = 12after 0 steps: 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after Step 1: 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after Step 1 + Step 2: 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after Step 1 + Step 2 + Step 1: 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $2 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $3 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $4 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $5 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $6 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $7 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $8 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $9 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $10 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $11 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $12 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $13 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $14 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $15 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $16 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5

Normalized graph of  $u \mapsto a_u$ 

-1.0

for an example with n = 12after  $17 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $18 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5

Normalized graph of  $u \mapsto a_u$ 

-1.0

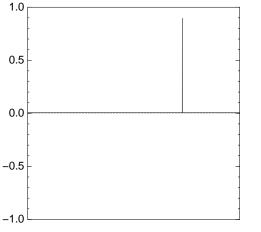
for an example with n = 12after  $19 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $20 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $25 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $30 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

Normalized graph of  $u \mapsto a_u$  for an example with n = 12 after  $35 \times (\text{Step } 1 + \text{Step } 2)$ :

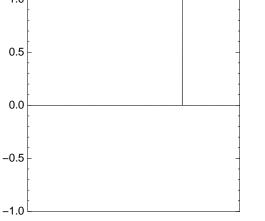


Good moment to stop, measure.

for an example with n = 12after  $40 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5 -1.0

for an example with n = 12after  $45 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

Normalized graph of  $u \mapsto a_u$  for an example with n = 12 after  $50 \times (\text{Step } 1 + \text{Step } 2)$ :



Traditional stopping point.

for an example with n = 12after  $60 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5 -1.0

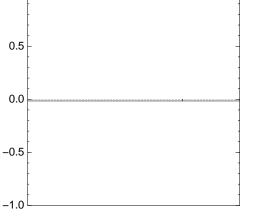
for an example with n = 12after  $70 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $80 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12after  $90 \times (Step 1 + Step 2)$ : 1.0 0.5 0.0 -0.5-1.0

for an example with n = 12 after  $100 \times (\text{Step } 1 + \text{Step } 2)$ :

Normalized graph of  $u \mapsto a_u$ 



Very bad stopping point.