Nearest Neighbor Complexity and Boolean Circuits

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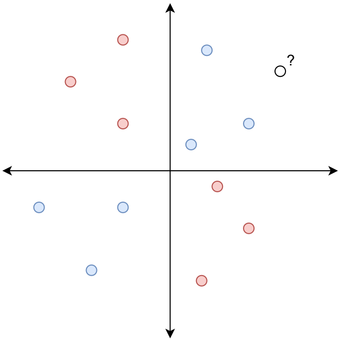
Nearest neighbor complexity

Convex polytopes

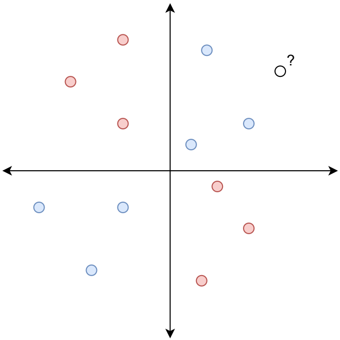
Boolean circuits

Open questions

How to color the "?" point?



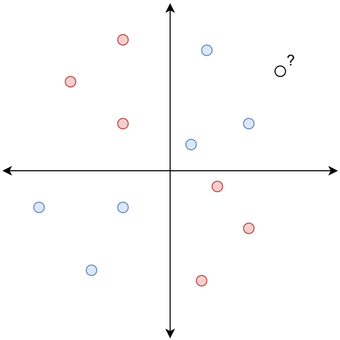
How to color the “?” point?



Nearest neighbor rule (informal)

Just **copy the color** of the **closest point**

How to color the "?" point?



Definition (Nearest neighbor rule)

Let $S \subseteq X$ be a set of labelled **anchors**.

- On input $\vec{q} \in X$
- Compute $\vec{q}$'s **nearest neighbor** in S,

$$\vec{p^*} = \arg\min_{\vec{p} \in S} \{\mathrm{dist}(\vec{p}, \vec{q})\}$$

- Return (the label of) $\vec{p^*}$

Nearest neighbors

Historical context*

- Known as early as 10'th century (Alhazen 965-1040)
- Often regarded as Ockham's razor (Ockham 1287-1347)
- Modern formulation due to Fix and Hodges [1952]

*[Pelillo, 2014]

Nearest neighbors

Main areas of study

- Nearest neighbors **as a learning algorithm**
  - Cover and Hart [1967]: The NN rule has **asymptotically optimal error**
- Nearest neighbors **as a data structure** (given anchors $S \subseteq \{0,1\}^d$)
  - **Brute force:** $O(d|S|)$ query time and $O(1)$ space
  - **Precompute everything:** $O(1)$ query time and $O(|S|2^d)$ space
  - **Curse of dimensionality:** "**sub-linear** query time $\implies$ **exponential** space"
- ϵ**-approximate nearest neighbors**
  - Indyk and Motwani [1998]: $O(d\log(|S|)/\epsilon^2)$ query time and $|S|^{O(\log(1/\epsilon)/\epsilon^2)}$ space

New ideas

Recently, more focus on ***representational complexity***

"How many anchors do we need to (exactly) represent a given function?"

- Introduced by Hajnal, Liu, and Turán [2022]
- Adds to the study of **Boolean function complexity** (e.g. [Kilic et al., 2023])
- Connections to **tropical** (min-plus) mathematics

"Nearest" with respect to...

For $\vec{x}, \vec{y} \in \mathbb{R}^n$, let Δ denote the **squared Euclidean distance**

$$\Delta(\vec{x}, \vec{y}) := ||\vec{x} - \vec{y}||_2^2$$

> If $\vec{x}, \vec{y} \in \{0, 1\}^n$, then Δ is equal to the **Hamming distance** $\sum_{i=1}^{n} |x_i - y_i|$

Representations

A **Nearest Neighbor (NN)** representation of $f : \{0,1\}^n \to \{0,1\}$ consists of "positive" and "negative" **anchors** $P, N \subseteq \mathbb{R}^n$ such that

- $f(\vec{x}) = 1$ if there exists a $\vec{p} \in P$ with $\Delta(\vec{x}, \vec{p}) < \Delta(\vec{x}, \vec{q})$ for all $\vec{q} \in N$.
- $f(\vec{x}) = 0$ if there exists a $\vec{q} \in N$ with $\Delta(\vec{x}, \vec{q}) < \Delta(\vec{x}, \vec{p})$ for all $\vec{p} \in P$.

Complexity classes

- Let NN also refer to the **class** of **polynomial size** NN **representations**:

$$f : \{0,1\}^n \to \{0,1\} \in \text{NN} \iff f \text{ has a } \mathrm{poly}(n)\text{-anchor NN rep.}$$

- Let HNN be the same class, where **anchors are Boolean** (i.e., $P, N \subseteq \{0,1\}^n$).

Some questions

What is the expressive power of nearest neighbors?

1. Which functions have "small" NN representations?
2. Does NN have a significant advantage over HNN?
3. How does NN relate to **other complexity classes** (e.g., circuits, decision trees)?

Question 1

Which functions have "small" NN *representations?**

*Every Boolean function has a "trivial" representation with 2^n anchors.

Example (threshold functions)

Definition

THR is the class of **threshold functions**. A function $f : \{0,1\}^n \to \{0,1\} \in$ THR if

$$f(x_1, \cdots, x_n) = 1 \iff a_1 x_1 + \cdots + a_n x_n \geq a_0$$

for some coefficients $a_i \in \mathbb{R}$.

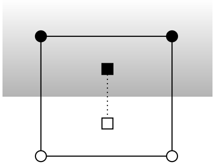
Example (threshold functions)

Theorem

THR = ***two-anchor*** NN.

Proof.

Both are equivalent to **half-space containment** □



Question 2

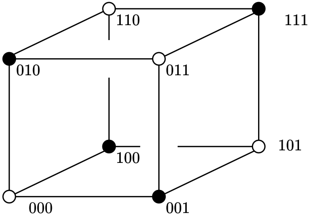
Does NN *have a significant advantage over* HNN*?*

Example (parity)

Definition

The XOR function is defined by

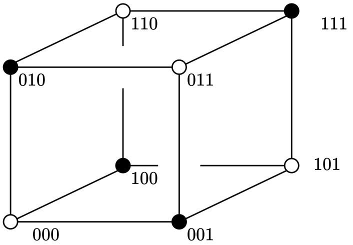
$$\text{XOR}(x_1, \cdots, x_n) = \sum_{i=1}^{n} x_i \mod 2$$



Example (parity)

Theorem (Hajnal et al. [2022])

$$\mathsf{NN}(\mathsf{XOR}) \leq n + 1$$



Example (parity)

Proof.

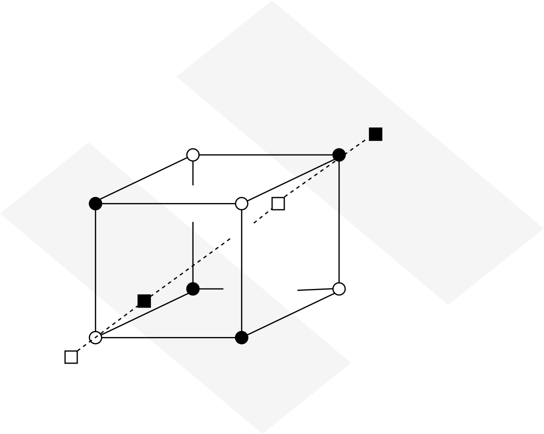
Let $\vec{p}_\ell = \left(\frac{\ell}{n}, \cdots, \frac{\ell}{n}\right)$

- $P = \{\vec{p}_i \mid i \text{ odd}\}$
- $N = \{\vec{p}_i \mid i \text{ even}\}$

If $\sum_i x_i = w$, then for all $\ell \neq w$,

$$||\vec{x} - \vec{p}_w||_2 < ||\vec{x} - \vec{p}_\ell||_2$$

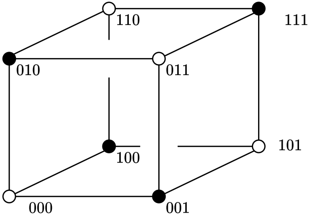
□



Example (parity)

Theorem (Hajnal et al. [2022])

$$\mathsf{HNN}(\mathsf{XOR}) = 2^n$$



Proof.

1. Suppose $\vec{x}$ is not an anchor.
2. It's neighbors have **opposite parity**, so they can't be anchors either.
3. And so on... $\Rightarrow\!\Leftarrow$

□

Question 3

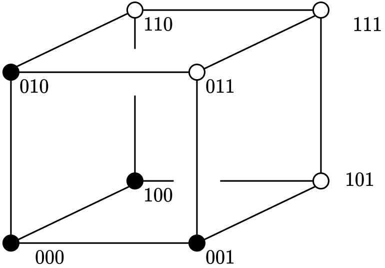
How does NN *relate to* ***other complexity classes****?*

Example (majority)

Definition

The **majority** function is defined by

$$\mathrm{MAJ}(x_1, \cdots, x_n) = 1 \iff \sum_{i=1}^{n} x_i \geq \frac{n}{2}$$



Example (majority)

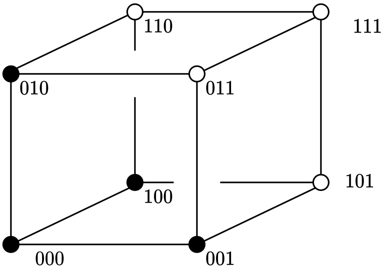
Theorem (Hajnal et al. [2022])

*For all **odd** $n > 0$,*

$$\text{HNN}(\text{MAJ}) = 2$$

Proof.

Take $P = \{1^n\}$, $N = \{0^n\}$. □

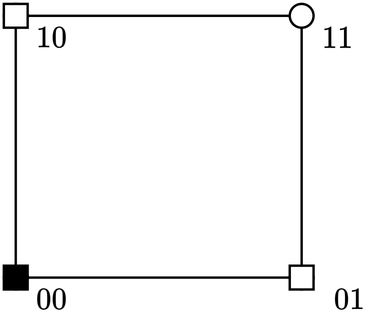


Example (majority)

Theorem

For all ***even*** $n > 0$,

$$\mathsf{HNN}(\mathsf{MAJ}) = \frac{n}{2} + 2$$



Example (majority)

Definition

AC^0 is the class of **small*** circuits with AND, OR, and NOT gates.

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* i.e., depth $O(1)$ and size $\mathrm{poly}(n)$

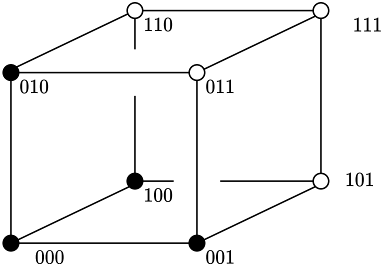
Example (majority)

Theorem (Hastad [1986])

$$\mathrm{MAJ} \notin \mathrm{AC}^0$$

Corollary

$$\mathrm{HNN} \not\subset \mathrm{AC}^0$$



Nearest neighbor complexity

Convex polytopes

Boolean circuits

Open questions

Nearest neighbor complexity

Convex polytopes

MAJ for even n

Boolean circuits

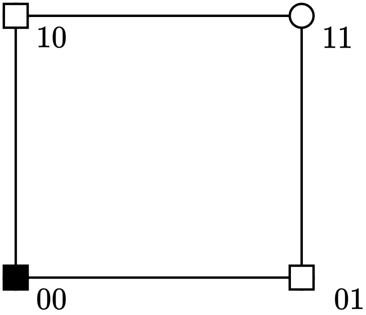
Open questions

Even majority

Theorem (DiCicco et al. [2024])

*For all **even** $n > 0$,*

$$\mathsf{HNN}(\mathsf{MAJ}) = \frac{n}{2} + 2$$



Proof (lower bound)

Let $P \cup N$ be an HNN representation of MAJ for even n.

Claim

For each $\vec{x} \in \{0,1\}^n$ with $|\vec{x}| = n/2$, there is a $\vec{p} \in P$ with $\vec{p} \neq \vec{1}$ with $\vec{x} \leq \vec{p}$.*

* in coordinate-wise order

Proof (claim)

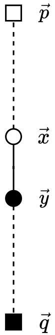
Proof of Claim.

- Let $\vec{p} \in P$ be nearest to $\vec{x}$ with $x_i = 1$ but $p_i = 0$.
- Let $\vec{y} = \vec{x} - \vec{e_i}$ and let $\vec{q} \in N$ be nearest to $\vec{y}$. Then,

$$\Delta(\vec{x},\vec{p}) = \Delta(\vec{y},\vec{p}) + 1 \qquad > \Delta(\vec{y},\vec{q}) + 1$$

$$\text{But } \Delta(\vec{x},\vec{p}) < \Delta(\vec{x},\vec{q}) \qquad \leq \Delta(\vec{y},\vec{q}) + 1$$

$\Longleftarrow\!\!\!\!\!\!\times\!\!\!\!\!\!\Longrightarrow$

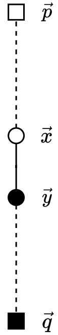


Proof (claim)

Proof of Claim.

- So $\vec{x} \leq \vec{p}$.
- (Similarly, $\vec{q} \leq \vec{y}$.)
- Finally, $|\vec{y}| = n/2 - 1$ implies $\Delta(\vec{x}, \vec{p}) < n/2$ and $\vec{p} \neq \vec{1}$.

□



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- Now assume $|P \cup N| \leq n/2 + 1$
- Since N cannot be empty, $|P| \leq n/2$
- Construct $\vec{x} \in \{0,1\}^n$ which contradicts the claim:
  - For each $\vec{p} \in P$ find some i where $p_i = 0$, and set $x_i = 1$.

$\square$

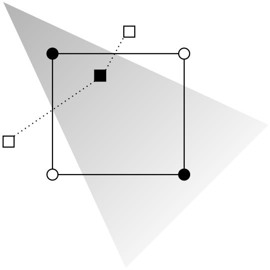
Observation 1

Theorem

Convex polytopes *with* m *faces have* $m+1$ *anchor* NN *representations.*

Proof.

Place one positive anchor $\vec{p}$ inside the polytope, and **reflect** $\vec{p}$ over each face. $\square$



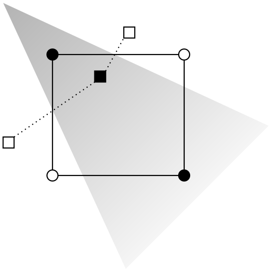
Observation 1

Theorem

$$\mathsf{AND} \circ \mathsf{THR} \subseteq \mathsf{NN}$$

Corollary

Any CNF formula with m clauses has an $m+1$-anchor NN representation



Also holds for $\mathsf{OR} \circ \mathsf{THR}$ and DNFs!

Observation 2

Definition

The **components** of $f : \{0,1\}^n \to \{0,1\}$ are the **connected components** of $f^{-1}(1)$ in the **Hamming cube graph**.

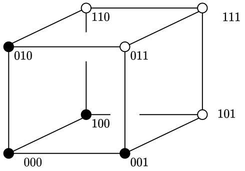


Figure: One component

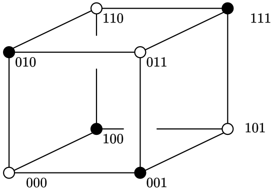
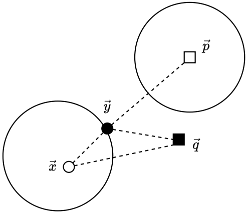


Figure: Four components

Observation 2

Theorem

If f has m components, then any HNN representation of f has at least m positive anchors.



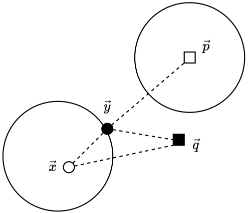
Observation 2

Proof.

- Suppose a component C contains no anchors.
- Let $\vec{p} \in P$ be nearest to $\vec{x} \in C$

  $\implies \vec{p}$ is in a different component
- Let $\vec{y} \in f^{-1}(0)$ lie on the **shortest** $\vec{x} \to \vec{p}$ **path** and let $\vec{q} \in N$ be nearest to $\vec{y}$
- $\triangle$ inequality $\implies \Delta(\vec{x}, \vec{p}) > \Delta(\vec{x}, \vec{q}) \;\not\Longleftrightarrow$

$\square$



Observation 2

Lemma

There exists a CNF with $m = \Theta(n)$ *clauses and* $2^{\Omega(m)}$ *components*

Corollary

There exists a CNF with $\Theta(n)$ *clauses with no* $\text{poly}(n)$*-size* HNN *representation*

Summary

- Every CNF has a polynomial size NN representation
- There exists a CNF with no polynomial-size HNN representation

Nearest neighbor complexity

Convex polytopes

Boolean circuits

Open questions

Connections to circuits

Questions

- What circuit classes **contain** NN?
  - Can a **depth-two circuit** compute NN?
- What circuit classes are **contained in** NN?
  - Can NN help us prove **circuit lower bounds**?

Nearest neighbor complexity

Convex polytopes

Boolean circuits

- Circuits computing nearest neighbors
- Min-plus polynomial threshold functions
- Sub-functions

Open questions

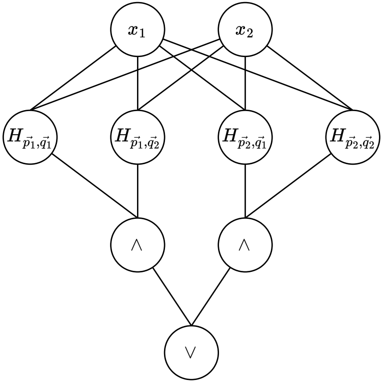
Nearest neighbors in depth three

Definition

$\mathsf{OR} \circ \mathsf{AND} \circ \mathsf{THR}$ is the class of **depth-three** circuits with a **polynomial** number of **threshold gates** at level one, **conjunctions** at level two, and a **disjunction** at the output.

Theorem (Murphy [1990])

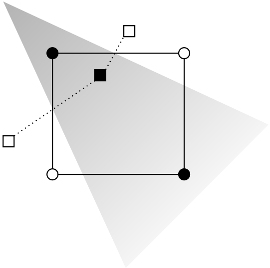
$$\mathsf{NN} \subseteq \mathsf{OR} \circ \mathsf{AND} \circ \mathsf{THR}$$



Nearest neighbors in depth three

Recall that AND $\circ$ THR $\subseteq$ NN, so

AND $\circ$ THR $\subseteq$ NN $\subseteq$ OR $\circ$ AND $\circ$ THR



Equivalently,

Convex polytopes* $\subseteq$ NN $\subseteq$ **unions** of convex polytopes*

*with $\mathrm{poly}(n)$ faces

Nearest neighbors in depth two

*What about **Boolean** anchors?*

Theorem

$$\mathsf{HNN} \subseteq \mathsf{THR} \circ \mathsf{MAJ}$$

MAJ (the class) is just THR with $\mathrm{poly}(n)$-bounded coefficients

Nearest neighbor complexity

Convex polytopes

Boolean circuits

- Circuits computing nearest neighbors
- Min-plus polynomial threshold functions
- Sub-functions

Open questions

Definition (Hansen and Podolskii [2015])

A **min-plus polynomial threshold function (mpPTF)** is an expression*

$$\min_{i \leq \ell_1}(L_i(\vec{x})) \leq \min_{j \leq \ell_2}(R_j(\vec{x}))$$

where $\{L_1, \cdots, L_{\ell_1}\} \cup \{R_1, \cdots, R_{\ell_2}\}$ are **integer linear forms**.

- The number of **terms** in an mpPTF is equal to $\ell_1 + \ell_2$,
- The **maximum weight** is equal to the largest absolute value of a coefficient.

*we interpret as a Boolean function equal to 1 iff the inequality holds

Min-plus polynomial threshold functions

Definition

- mpPTF(∞) is the class of mpPTFs with $\mathrm{poly}(n)$ terms and unbounded weight.
- mpPTF($\mathrm{poly}(n)$) is the same class with $\mathrm{poly}(n)$-bounded maximum weight.

Observation 3

Observation

The distance from $\vec{x} \in \{0,1\}^n$ to an anchor $\vec{p} \in \mathbb{R}^n$ is a **linear form**:

$$\begin{aligned}\Delta(\vec{x},\vec{p}) = \sum_i (x_i - p_i)^2 &= \sum_i \left[x_i^2 - 2p_i x_i + p_i^2\right] \\ &= \sum_i \left[(1-2p_i)x_i + p_i^2\right] \\ &= \langle \vec{1} - 2\vec{p}, \vec{x}\rangle + ||\vec{p}||_2^2.\end{aligned}$$

Observation 3

Lemma

- $\mathsf{NN} \subseteq \mathsf{mpPTF}(\infty)$
- $\mathsf{HNN} \subseteq \mathsf{mpPTF}(\mathrm{poly}(n))$

Proof.

$$\text{The nearest anchor to } \vec{x} \text{ is positive} \iff \min_{\vec{p}\in P}(\Delta(\vec{x},\vec{p})) \leq \min_{\vec{q}\in N}(\Delta(\vec{x},\vec{q}))$$

□

What about the converse?

Lemma (Hansen and Podolskii [2015])

$$\mathsf{XOR} \in \mathsf{mpPTF}(\mathrm{poly}(n))$$

What about the converse?

Proof.

Take the mpPTF

$$\min \{L_0(\vec{x}), L_2(\vec{x}), \cdots\} \leq \min \{L_1(\vec{x}), L_3(\vec{x}), \cdots\}$$

where $L_i(\vec{x}) = i^2 - 2i \cdot (\sum_{i=1}^{n} x_i)$.

Suppose $\sum_{i=1}^{n} x_i = \ell$ and let $k \neq \ell$.

- $L_\ell(\vec{x}) = -\ell^2$
- $L_k(\vec{x}) = k^2 - 2k\ell = (k - \ell)^2 - \ell^2$

□

What about the converse?

Corollary

$$\mathsf{HNN} \subsetneq \mathsf{mpPTF}(\mathrm{poly}(n))$$

Proof.

We proved before that $\mathsf{XOR} \notin \mathsf{HNN}$. □

What about the unbounded case?

Conjecture

$$\mathsf{NN} \subsetneq \mathsf{mpPTF}(\infty)$$

Outline

Suppose we want to prove $\mathsf{mpPTF}(\infty) \subseteq \mathsf{NN}$

Given an mpPTF

$$\min_{i \le \ell_1}(L_i(\vec{x})) \le \min_{j \le \ell_2}(R_j(\vec{x}))$$

If we can construct **anchors** $P = \{\vec{p}_1, \cdots, \vec{p}_{\ell_1}\}$ where

$$\Delta(\vec{x}, \vec{p}_i) = L_i(\vec{x})$$

(similarly $N = \{\vec{q}_1, \cdots, \vec{q}_{\ell_2}\}$) **then we are done.**

Idea 1

1. The distance from $\vec{x}$ to the all-zero anchor $\vec{0}$ is

$$\Delta(\vec{x}, \vec{0}) = x_1 + x_2 + \cdots + x_n$$

2. If we restrict the input space by **identifying** $x_1 = x_2$, then

$$\Delta(\vec{x}, \vec{0}) = 2x_1 + x_3 + \cdots + x_n$$

3. $\implies$ We can **control coefficients** by identifying input variables!

Idea 2

1. The distance from $\vec{x}$ to the all-zero anchor $\vec{0}$ is

$$\Delta(\vec{x}, \vec{0}) = x_1 + x_2 + \cdots + x_n$$

2. Let $\vec{x^*} = (\vec{x}, 1)$. Then,

$$\Delta(\vec{x^*}, \vec{0}) = x_1 + x_2 + \cdots + x_n + 1$$

3. $\implies$ We can **introduce constant terms** by adding constant variables!

Sub-functions

Definition

A **subfunction** of $g(x_1, \cdots, x_n)$ is obtained by **fixing input variables** as follows:

- Identification of variables (e.g., $x_1 = x_2$)
- Assigning variables to constants (e.g., $x_1 = 0$).

Example

Subfunctions of $x_1 + \cdots + x_n$ **introduce coefficients** and **constant terms**:

$x_1 = x_2$ and $x_3 = \cdots = x_n = 1$ yields $2x_1 + (n-2)$

Closure

Definition

Let $\mathcal{C}$ be a collection of functions.

The **closure** $\overline{\mathcal{C}}$ is the collection of **sub-functions** of elements of $\mathcal{C}$ obtained by identifying/assigning **polynomially-many variables***

This is quite natural: Circuit classes are **already closed** under this operation.

*with respect to the **input dimension of the sub-function**

Nearest neighbors vs. mpPTFs

Theorem

- $\overline{\mathsf{NN}} = \mathsf{mpPTF}(\infty)$
- $\overline{\mathsf{HNN}} = \mathsf{mpPTF}(\mathrm{poly}(n))$

Proof.

$\langle$ Apply Ideas 1 and 2 $\rangle$ □

Corollary 1 (HNN)

Corollary

$$\text{HNN} \not\subset \text{MAJ} \circ \text{MAJ}$$

Proof Sketch.

There exists a function f ($\text{OMB} \circ \text{AND}_2$) where

- $f \in \text{mpPTF}(\mathrm{poly}(n))$ by Hansen and Podolskii [2015], but
- $f \notin \text{MAJ} \circ \text{MAJ}$ by Buhrman et al. [2007]

□

Corollary 2 (NN)

Corollary

$$\mathsf{NN} \not\supset \mathsf{AND} \circ \mathsf{OR} \circ \mathsf{AND}_2$$

Proof Sketch.

There exists a function f where

- $f \notin \mathsf{mpPTF}(\infty)$ by Hansen and Podolskii [2015], but
- $f \in \mathsf{AND} \circ \mathsf{OR} \circ \mathsf{AND}_2$ by Hajnal et al. [1993]

□

Summary

- $\overline{\mathsf{NN}} = \mathsf{mpPTF}(\infty)$
- $\overline{\mathsf{HNN}} = \mathsf{mpPTF}(\mathrm{poly}(n))$
- $\implies$ known results about mpPTF also apply to nearest neighbors

More results

- The **more general** k**-nearest neighbors rule** has the same (closure) relationship with a **more general version of** mpPTF, based on expressions

  The k'th smallest value in $\{L_i(\vec{x})\} \leq$ The k'th smallest value in $\{R_i(\vec{x})\}$

- When $k = O(1)$, $\overline{\text{kNN}} = \overline{\text{NN}}$
- When $k = O(n)$, $\overline{\text{kNN}}$ contains SYM $\circ$ MAJ and ELDL

Nearest neighbor complexity

Convex polytopes

Boolean circuits

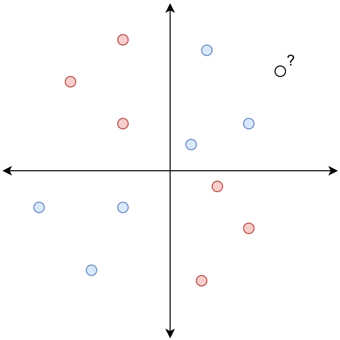
Open questions

Open questions

Open questions

- Does $\mathsf{NN} = \overline{\mathsf{NN}}$?
  - Is there $f \in \mathsf{mpPTF}(\infty)$ but $f \notin \mathsf{NN}$?
- How does **bit-complexity** effect the expressiveness of NN?
  - Kilic et al. [2023]: Can we represent THR with only $\log(n)$ bits per coordinate?
- What about **approximate representations**?

Thank you



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