Enumeration and stratifiaction of Boolean functions by canalizing depth

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My talk in one slide

Background

A Boolean function is canalizing if some variable can determine the output.

If that variable doesn't take its "canalizing input", the output is a function on $n-1$ variables:

$$g(\hat{x}_i) = g(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)\,.$$

We ask if it too is canalizing, and so on.

The nested canalizing functions (NCFs) are those that are "fully recursively canalizing."

NCFs are well-understood. They decompose nicely into "extended monomial layers" and have been enumerated. (Murrugarra et al., 2013)

Our contribution

Every Boolean function has a well-defined canalizing depth, k.

This allows us to decompose every Boolean function into extended monomial layers and a core polynomial.

This extends work by Murrugarra et al. on the *algebraic structure* of NCFs.

We derive enumeration formulas for "k-canalizing functions," which generalize known enumeration results for both canalizing functions and NCFs.

Canalizing & nested canalizing functions

Definition

A Boolean function $f\colon \mathbb{F}_2^n \to \mathbb{F}_2$ is canalizing if there exists a variable x_i, a Boolean function $g(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$, and $a, b \in \mathbb{F}_2$ such that

$$f(x_1, \dots, x_n) = \begin{cases} b & x_i = a, \\ g \not\equiv b & x_i \neq a. \end{cases}$$

In this case, x_i is a canalizing variable, the input a is the canalizing input, and the output value b when $x_i = a$ is the corresponding canalized output.

Definition

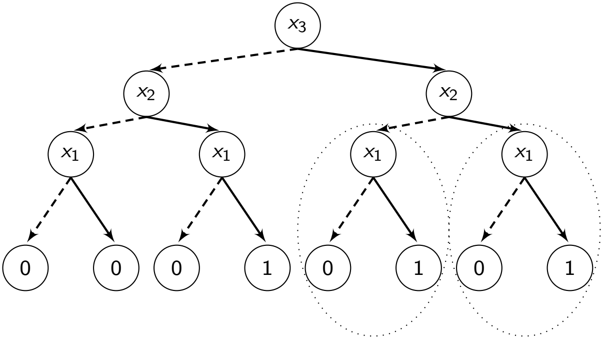
A function $f\colon \mathbb{F}_2^n \to \mathbb{F}_2$ is nested canalizing w.r.t. $\sigma \in \mathfrak{S}_n$, inputs a_i and outputs b_i, for $i = 1, 2, \dots, n$, if it can be represented as:

$$f(x_1, \dots, x_n) = \begin{cases} b_1 & x_{\sigma(1)} = a_1, \\ b_2 & x_{\sigma(1)} \neq a_1, x_{\sigma(2)} = a_2, \\ b_3 & x_{\sigma(1)} \neq a_1, x_{\sigma(2)} \neq a_2, x_{\sigma(3)} = a_3, \\ \vdots & \vdots \\ b_n & x_{\sigma(1)} \neq a_1, \dots, x_{\sigma(n-1)} \neq a_{n-1}, x_{\sigma(n)} = a_n, \\ \overline{b_n} & x_{\sigma(1)} \neq a_1, \dots, x_{\sigma(n-1)} \neq a_{n-1}, x_{\sigma(n)} \neq a_n. \end{cases}$$

Binary decision tree

A Boolean function can be evaluated using a binary decision tree and a fixed variable order.

For example, consider $f(x_1, x_2, x_3) = x_1x_2x_3 + x_1x_2 + x_1x_3$, with respect to variable order $x_3 < x_2 < x_1$.



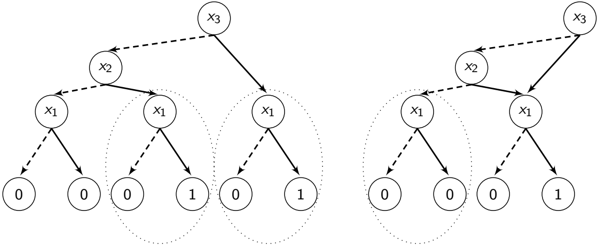
Binary decision diagram (BDD)

Reduction rules

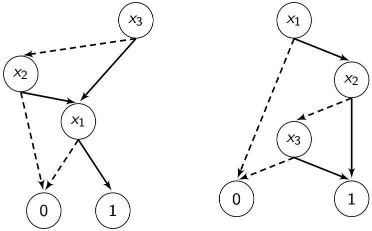
We can reduce the binary decision tree to a BDD by applying the following rules:

(i) Merge identical substructures that have the same parent node, and then eliminate that node.

(ii) Merge identical substructures that have different parents.



Average path length (APL) of BDDs



$$APL_f^{x_3<x_2<x_1} = (2 \cdot 6 + 3 \cdot 2)/8 = \frac{9}{4}$$

$$APL_f^{x_1<x_2<x_3} = (1 \cdot 4 + 2 \cdot 2 + 3 \cdot 2)/8 = \frac{7}{4}$$

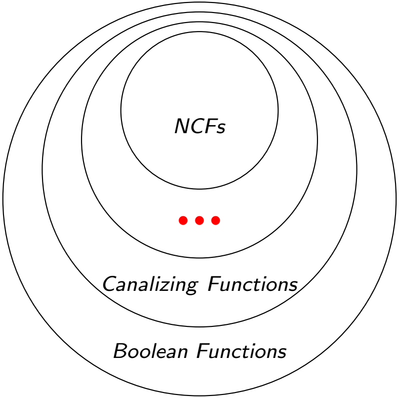
Theorem (Jarrah et al., 2007)

The n-variable Boolean functions with no ficticious variables that have minimum APL $(2 - \frac{1}{2^{n-1}})$ are precisely the nested canalizing functions.

Remark

The n-variable parity function (and its negation) has maximum APL of n.

A cartoon of all 2^{2^n} Boolean functions on n variables.



Not quite nested canalizing

Many functions are canalizing, but not nested canalizing.

For example, in a Boolean model of the *lac* operon by Robeva/Davies (2013):

$$f_L(t+1) = \overline{G_e} \wedge [(L \wedge \overline{E}) \vee (L_e \wedge E)] .$$

This means "*internal lactose (L) will be present the following timestep if there is no external glucose (G_e), and at least one of the following holds*":

- internal lactose is present, but the enzyme β-galactosidase (E) that breaks it down is absent;
- external lactose (L_e) is available *and* the *lac* permease transporter protein (E) is present.

Note: $\overline{G_e}$ is canalizing because it acts as a "shut-down" switch: if $G_e = 1$, then $f_L = 0$ regardless of the other variables. Thus,

$$f_L(G_e, L_e, L, E) = \begin{cases} 0 & G_e = 1, \\ (L \wedge \overline{E}) \vee (L_e \wedge E) & G_e \neq 0. \end{cases}$$

The function $g = (L_e \wedge E) \vee (L \wedge \overline{E})$ is not canalizing, and so f_L is canalizing but not nested canalizing.

k-canalizing functions

Definition

A Boolean function $f(x_1, \ldots, x_n)$ is k-canalizing, where $0 \leq k \leq n$, w.r.t. $\sigma \in \mathfrak{S}_n$, inputs a_i, and outputs b_i, for $1 \leq i \leq k$, if

$$f(x_1, \ldots, x_n) = \begin{cases} b_1 & x_{\sigma(1)} = a_1, \\ b_2 & x_{\sigma(1)} \neq a_1, x_{\sigma(2)} = a_2, \\ b_3 & x_{\sigma(1)} \neq a_1, x_{\sigma(2)} \neq a_2, x_{\sigma(3)} = a_3, \\ \vdots & \vdots \\ b_k & x_{\sigma(1)} \neq a_1, \ldots, x_{\sigma(k-1)} \neq a_{k-1}, x_{\sigma(k)} = a_k, \\ g \not\equiv b_k & x_{\sigma(1)} \neq a_1, \ldots, x_{\sigma(k-1)} \neq a_{k-1}, x_{\sigma(k)} \neq a_k. \end{cases}$$

where $g = g(x_{\sigma(k+1)}, \ldots, x_{\sigma(n)})$. When g is non-canalizing, k is the canalizing depth of f. If g is non-constant, it is the core function of f, denoted f_C.

Remark

Since $g \not\equiv b_k$, a function f that is k-canalizing with respect to $\sigma \in \mathfrak{S}_n$, inputs a_i and outputs b_i is essential in each $x_{\sigma(i)}$ for $i = 1, \ldots, k$.

k-canalizing functions

Example

The Boolean function $f(x, y, z, w) = xy(z + w)$ has canalizing depth 2 and core function $f_C = z + w$.

$$f(x,y,z,w) = \begin{cases} 0 & x = 0 \\ 0 & x \neq 0,\ y = 0 \\ z + w & x \neq 0,\ y \neq 0 \end{cases}$$

Remarks

In our framework, if we consider the set of all Boolean functions on n variables, then:

- The canalizing depth of a k-canalizing function is at least k.
- A non-canalizing function has canalizing depth 0, and if it is non-constant, then $f_C = f$.
- Every Boolean function is 0-canalizing.
- 1-canalizing means "canalizing."
- n-canalizing means "nested canalizing."
- If f has canalizing depth k and g is constant, then f has $n - k$ fictitious variables, and is an NCF its k essential variables.

Polynomial form

The set of Boolean functions on n variables is isomorphic to the quotient ring

$$R := \mathbb{F}_2[x_1, \ldots, x_n]/I, \qquad \text{where} \quad I = \langle x_i^2 - x_i : 1 \leq i \leq n \rangle .$$

Thus, a Boolean function f can be uniquely expressed as a square-free polynomial – its "algebraic normal form."

Lemma (Murrugarra et al., 2013)

$f(x_1, \ldots, x_n)$ is canalizing in x_i, with input a_i and output b_i, iff for some polynomial $g \not\equiv 0$,

$$f = (x_i + a_i)g(\hat{x}_i) + b_i \, .$$

Theorem

$f(x_1, \ldots, x_n)$ is k-canalizing, w.r.t. $\sigma \in \mathfrak{S}_n$, inputs a_i and outputs b_i, for $1 \leq i \leq k$, iff it has polynomial form

$$f(x_1, \ldots, x_n) = (x_{\sigma(1)} + a_1)g(\hat{x}_i) + b_1 \, ,$$

where

$$g(\hat{x}_i) = (x_{\sigma(2)} + a_2)\Big[\ldots \big[(x_{\sigma(k-1)} + a_{k-1})[(x_{\sigma(k)} + a_k)\bar{g} + \Delta b_{k-1}] + \Delta b_{k-2} \big] \ldots \Big] + \Delta b_1$$

for some polynomial $\bar{g} = \bar{g}(x_{\sigma(k+1)}, \ldots, x_{\sigma(n)}) \not\equiv 0$, where $\Delta b_i := b_{i+1} - b_i = b_{i+1} + b_i$.

Extended monomial layers

Definition

A Boolean function $M(x_1, \dots, x_m)$ is an extended monomial in variables $x_1, \dots, x_m$ if

$$M(x_1, \dots, x_m) = \prod_{i=1}^{m} (x_i + a_i),$$

where $a_i \in \mathbb{F}_2$ for each $i = 1, \dots, m$.

(Murrugarra et al., 2013)

A function $f(x_1, \dots, x_n)$ is an NCF iff

$$f(x_1, \dots, x_n) = M_1(M_2(\cdots(M_{r-1}(M_r + 1) + 1)\cdots) + 1) + b$$

for extended monomials M_i with disjoint supports, and $b \in \mathbb{F}_2$.

Special case of this: all variables are canalizing iff $f = M(x_1, \dots, x_n) + b$, where M is an extended monomial in all variables.

Extended monomial layers & core polynomials

Not only can NCFs be written in disjoint extended monomial layers, but so can all Boolean functions.

Theorem

Every Boolean function $f(x_1, \ldots, x_n) \not\equiv 0$ can be uniquely written as

$$f(x_1, \ldots, x_n) = M_1(M_2(\cdots(M_{r-1}(M_r p_C + 1) + 1)\cdots) + 1) + b, \tag{1}$$

where each $M_i = \prod_{j=1}^{k_i}(x_{i_j} + a_{i_j})$ is a nonconstant extended monomial, $p_C \not\equiv 0$ is the core polynomial of f, and $k = \sum k_i$ is the canalizing depth. Each x_i appears in exactly one of $\{M_1, \ldots, M_r, p_C\}$, and the only restrictions on Eq. (1) are the following "exceptional cases":

(i) If $p_C \equiv 1$ and $r \neq 1$, then $k_r \geq 2$;

(ii) If $p_C \equiv 1$ and $r = 1$ and $k_1 = 1$, then $b = 0$;

When f is non-canalizing, then $p_C = f$.

Example

The Boolean function $f(x_1, \ldots, x_7) = x_1\overline{x_2}(x_3x_4(x_5 + x_6 + x_7 + 1) + 1)$ has canalizing depth 4. With respect to the permutation $\sigma = 1, 2, 3, 4$, its canalizing inputs are $(a_i)_{i=1}^4 = (0, 1, 0, 0)$, outputs $(b_i)_{i=1}^4 = (0, 0, 1, 1)$ and the core polynomial is $p_C = x_5 + x_6 + x_7 + 1$.

Extended monomial layers & core polynomials

Let's take a look at the last example a little more closely.

Example

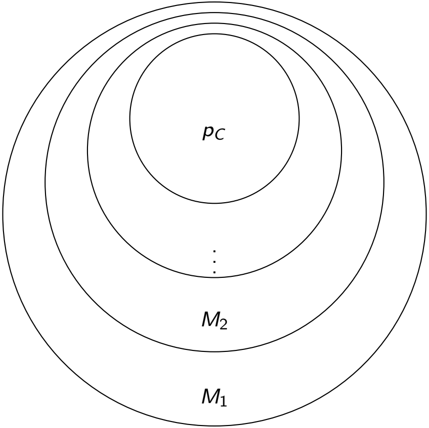
The Boolean function $f(x_1, \ldots, x_7) = x_1\overline{x_2}(x_3x_4(x_5 + x_6 + x_7 + 1) + 1)$ has canalizing depth 4. With respect to the permutation $\sigma = 1, 2, 3, 4$, its canalizing inputs are $(a_i)_{i=1}^4 = (0, 1, 0, 0)$, outputs $(b_i)_{i=1}^4 = (0, 0, 1, 1)$ and the core polynomial is $p_C = x_5 + x_6 + x_7 + 1$.

$$f(x_1, \ldots, x_7) = \begin{cases} 0 & x_1 = 0 \\ 0 & x_1 \neq 0, x_2 = 1 \\ 1 & x_1 \neq 0, x_2 \neq 1, x_3 = 0 \\ 1 & x_1 \neq 0, x_2 \neq 1, x_3 \neq 0, x_4 = 0 \\ x_5 + x_6 + x_7 & x_1 \neq 0, x_2 \neq 1, x_3 \neq 0, x_4 \neq 0 \end{cases}$$

There are 2^{2^n} Boolean functions on n variables. Each one has a unique well-defined:

- canalizing depth,
- extended monomial layers structure,
- core polynomial.

A cartoon of an arbitrary Boolean function



Enumeration

Prior results

- *Just/Shmulevich/Konvalina, 2004*: The number C_n of canalizing Boolean functions on $n \geq 0$ variables is

$$C_n = 2((-1)^n - n - 1) + \sum_{k=1}^{n} (-1)^{k+1} \binom{n}{k} 2^{k+1} 2^{2^{n-k}}.$$

- *Murrugarra et al., 2013*: The number of NCFs on n variables is:

$$B(n,n) = 2^{n+1} \sum_{r=1}^{n-1} \sum_{\substack{k_1+\ldots+k_r=n \\ k_i \geq 1,\ k_r \geq 2}} \binom{n}{k_1, \ldots, k_r},$$

where $\binom{n}{k_1,\ldots,k_r} = \frac{n!}{k_1!k_2!\ldots k_r!}$.

Theorem

The number of Boolean functions on n variables with canalizing depth k is

$$B(n,k) = \binom{n}{k} \left[B(k,k) + B^*(n-k,0) \cdot 2^{k+1} \sum \binom{k}{k_1, \ldots, k_r} \right],$$

where the sum is taken over all *compositions of* k.

An example: $n = 4$

There are $2^{2^4} = 65536$ Boolean functions on 4 variables.

The number of functions with canalizing depth exactly k, for $k = 1, 2, 3, 4$ is

$$
\begin{aligned}
B(4,4) &= \binom{4}{4}(736 + 0) = 736 \\
B(4,3) &= \binom{4}{3}(64 + 0) = 256 \\
B(4,2) &= \binom{4}{2}(8 + 2 \cdot 8 \cdot 3) = 336. \\
B(4,1) &= \binom{4}{1}(2 + 136 \cdot 4 \cdot 1) = 2184.
\end{aligned}
$$

Summing these yields the total number of canalizing functions on 4 variables,

$$C_4 = 3512 = 736 + 256 + 336 + 2184 = B(4,4) + B(4,3) + B(4,2) + B(4,1).$$

Thus, there are $B(4,0) = 65536 - 3512 = 62024$ non-canalizing functions on four variables, including the two constant functions.

Average path length of k-canalizing functions

Recall that the APL an n-variable function is:

- minimized for the NCFs (i.e., n-canalizing functions); APL$= 2 - \frac{1}{2^{n-1}}$.
- maximized for Par and 1+Par (which are 0-canalizing); APL$= n$.

Theorem (H.)

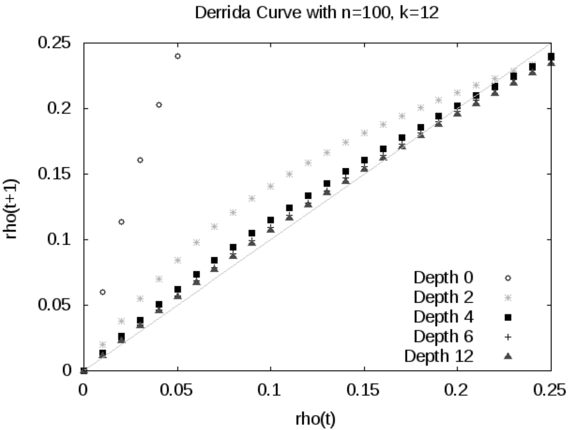
If f is k-canalizing ($k \geq 1$) on n variables, then the APL of its BDD is:

$$2 - \frac{1}{2^{k-1}} \leq APL_f \leq 2 - \frac{1}{2^{k-1}} + \frac{n-k}{2^k}$$

Network dynamics of k-canalizing functions

Graph dynamical systems built with k-canalizing functions are more stable than random networks.

Moreover, the stability increases with k. This can be measured using a Derrida plot.



Current and future research

In the future, we plan to:

- derive asymptotics for the number of n-variables Boolean functions of canalizing depth k, as n and k grow large;
- investigate well-known Boolean network models and compute the canalizing depth of the proposed functions;
- design reverse-engineering algorithms for Boolean networks models from partial data using k-canalizing functions;
- investigate whether the set of k-canalizing functions that fit the model space has an inherent algebraic structure (e.g., toric variety?);
- extend the results from this talk from Boolean to multi-state functions.

Open-ended questions for NDSSL: In GDS theory, many computationally hard algorithms become tractable for special classes of functions and/or graphs, such as

- bounded tree width
- k-symmetric functions

I'm particularly interested in discussing with you whether anything can be said about these problems for k-canalizing functions.

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