No Free Lunch

Summer Lecture Series 2002

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Overview

- “The Original” NFL Theorem
- An improved NFL Theorem
- NFL Assumptions
  - Objective Functions
  - Performance Measures
  - Optimization Scenarios
- NFL Implications

General Randomized Search Heuristics

Search in some search space X for points rated by a function f.

Black Box Scenario:

- no direct access to f
- no a priori knowledge
- only way to learn about f is sampling

Assumption: The heuristic is complete.

Optimizing an Arbitrary Function

What is an arbitrary function?

- $f : X \rightarrow Y$

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- X discrete

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Optimizing an Arbitrary Function

What is an arbitrary function?

- $f : X \to Y$
- X discrete
- Y discrete
- X finite
- Y finite
- no function “more likely” than any other

Performance Measures

- function evaluations matter
- success measured in function values found

Performance Measures

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- performance measured in function val. found
- re-evaluations easy to avoid

Performance Measures

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- performance measured in function val. found
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Consider algorithm A on function f and ignore re-evaluations.

Performance Measures (continued)

Consider algorithm's trace
$T(A, f, t) =< (x_1, f(x_1)), (x_2, (f(x_2)), \ldots, (x_t, f(x_t)) >$.

Performance Measures (continued)

Consider algorithm's trace
$T(A, f, t) =< (x_1, f(x_1)), (x_2, (f(x_2)), \ldots, (x_t, f(x_t)) >$.

Measure performance based on performance vector
$V(T(A, f, t)) =< f(x_1), f(x_2), \ldots, f(x_t) >$.

Performance Measures (continued)

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$V(T(A, f, t)) =< f(x_1), f(x_2), \ldots, f(x_t) >$.

Performance measure
$M : \{V(T(A, f, t)) \mid A, f, t\} \rightarrow \mathbb{R}$

Performance Measures (continued)

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Global performance measure

$$\left(\sum_{f \in Y^X} M\left(V(T(A, f, |X|))\right) \right) / |Y|^{|X|}$$

The No Free Lunch Theorem

No Free Lunch Theorem:

For all finite sets X, Y

and for all global performance measures,

all search algorithms perform equal.

Proving the NFL Theorem (I)

First step: Consider only deterministic search algorithms.

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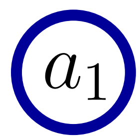

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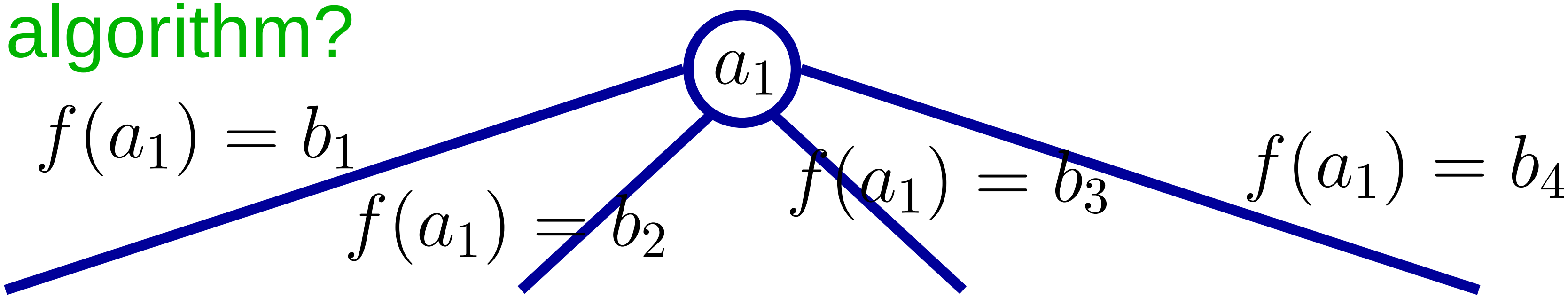

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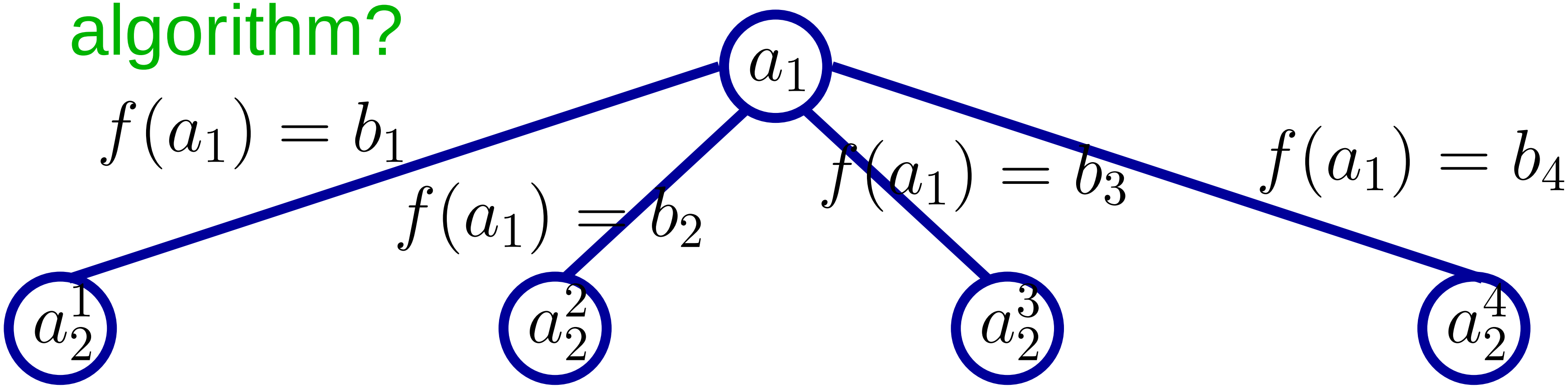

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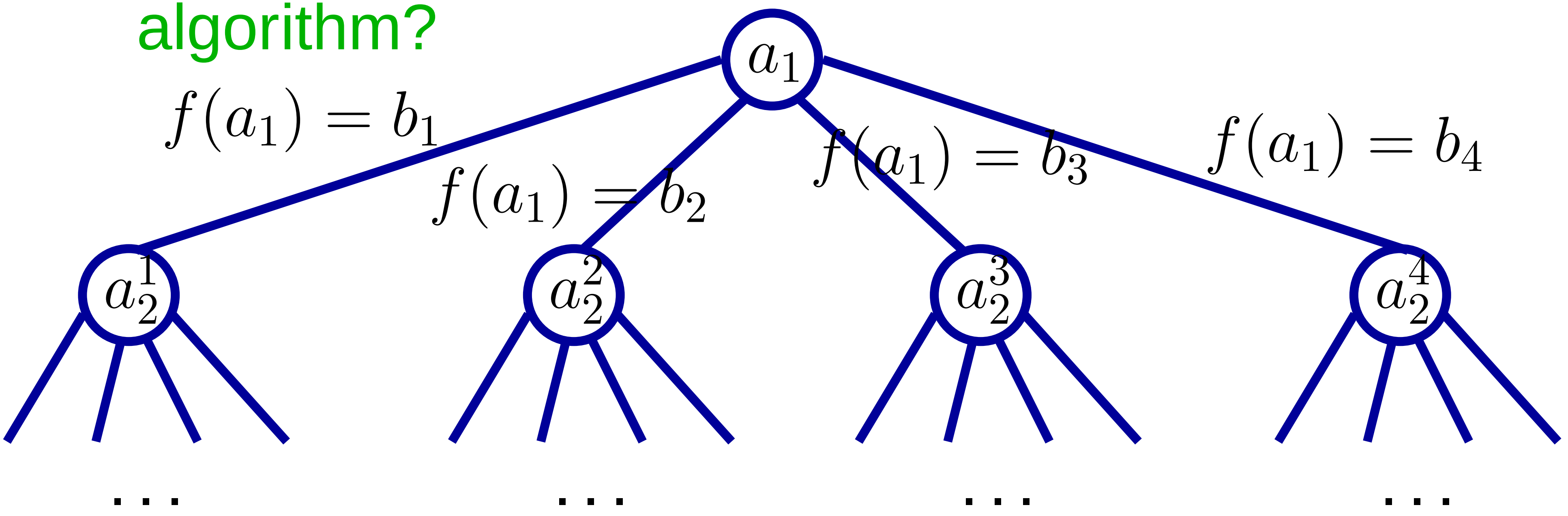

Proving the NFL Theorem (II)

Consider a fixed search algorithm A.

Claim:

$$\forall f, g: \; V(T(A, f, |X|)) = V(T(A, g, |X|)) \Rightarrow f = g$$

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Proof:

$$f: \quad (a_1, f(a_1))$$

$$g: \quad (a_1, g(a_1))$$

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Proof:

$$\begin{array}{lll} f: & (a_1, f(a_1)), & (a_2, f(a_2)) \\ g: & (a_1, g(a_1) = f(a_1)), & (a_2, g(a_2)) \end{array}$$

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$$\begin{array}{lllll} f: & (a_1, f(a_1)), & (a_2, f(a_2)), & & (a_3, f(a_3)), \ldots \\ g: & (a_1, f(a_1)), & (a_2, g(a_2) = f(a_2)), & & (a_3, g(a_3)), \ldots \end{array}$$

$\square$

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Proof:

$$\left|\left\{f \mid f \in Y^X\right\}\right| = |Y|^{|X|}$$

$$\forall f, g \in Y^X :$$
$$f \neq g \Rightarrow V(T(A, f, |X|)) \neq V(T(A, g, |X|))$$

□

Proving the NFL Theorem (IV)

Conclusion:

$$\forall A, B: \quad \{V(T(A, f, |X|)) \mid f \in Y^X\} = \{V(T(B, f, |X|)) \mid f \in Y^X\}$$

Conclusion:

For all finite sets X, Y,
and for all global performance measures,

all deterministic search algorithms perform equal.

Proving the NFL Theorem (V)

X, Y finite $\Rightarrow Y^X$ finite $\Rightarrow$ number of essentially different deterministic search algorithms finite

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Proving the NFL Theorem (V)

X, Y finite $\Rightarrow Y^X$ finite $\Rightarrow$ number of essentially different deterministic search algorithms finite

$\Rightarrow$ "randomized search algo." $=$ "prob. dist. over essentially different deterministic search algo."

$\Rightarrow$ "performance of randomized search algorithm" $=$ "weighted sum of the performance of some deterministic search algorithms"

$\Rightarrow$ For all finite sets X, Y, and for all global performance measures, all search algorithms perform equal.

Overview

- “The Original” NFL Theorem √
- An improved NFL Theorem
- NFL Assumptions
  - Objective Functions
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Improved NFL (I)

NFL theorems do not only hold for global measures considering all possible functions.

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Permutations of functions:

Definition: $\sigma \in \text{Perm}(X)\colon \sigma f(x) := f(\sigma^{-1}(x))$

Definition: $\mathcal{F} \subseteq Y^X$ closed under permutations
$\Leftrightarrow \forall f \in \mathcal{F}\colon \forall \sigma \in \text{Perm}(X)\colon \sigma f \in \mathcal{F}$

Definition: performance measure global on $\mathcal{F}$
$\Leftrightarrow \left(\sum_{f \in \mathcal{F}} M(V(A, f, |X|)) \right) / |\mathcal{F}|$

Improved NFL (II)

Improved NFL Theorem:

For all finite sets X, Y,
for all sets $\mathcal{F} \subseteq Y^X$ closed under permutations,
and for all performance measures global on $\mathcal{F}$,
all search algorithms perform equal.

Improved NFL (II)

Improved NFL Theorem:

For all finite sets X, Y,
for all sets $\mathcal{F} \subseteq Y^X$ closed under permutations,
and for all performance measures global on $\mathcal{F}$,
all search algorithms perform equal.

Proof:

$$\forall f \in Y^X : \forall A, B : \exists \sigma \in \text{Perm}(X) :$$
$$V(A, f, |X|) = V(B, \sigma f, |X|)$$

□

Improved NFL (III)

NFL theorems do not hold for performance measures global on arbitrary $\mathcal{F}$.

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NFL theorems do not hold for performance measures global on arbitrary $\mathcal{F}$.

Improved NFL Theorem:

For all finite sets X, Y,
for all sets $\mathcal{F} \subseteq Y^X$,
all search algorithms perform equal
for all performance measures global on $\mathcal{F}$,

if and only if $\mathcal{F}$ is closed under permutations.

Improved NFL (IV)

Proof: by contradiction

X, Y, algorithm A fixed
$\mathcal{F} \subseteq Y^X$ not closed under permutations

$f \in \mathcal{F}$, $\sigma \in$ Perm(X), $\sigma f \notin \mathcal{F}$

Define M: $M(V) = \begin{cases} 1 & \text{if } V = V(T(A, f, |X|)) \\ 0 & \text{otherwise} \end{cases}$

Improved NFL (V)

Obvious: $\sum_{g \in \mathcal{F}} M(V(T(A, g, |X|))) = 1$

We assume NFL holds for $\mathcal{F}$.

Thus for all search algorithms B:

$$\sum_{g \in \mathcal{F}} M(V(T(B, g, |X|))) = 1$$

There is an algorithm C such that

$V(T(C, \sigma f, |X|)) = V(T(A, f, |X|))$.

$\sigma f \notin \mathcal{F} \Rightarrow \sum_{g \in \mathcal{F}} M(V(T(C, g, |X|))) = 0$

contradiction

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NFL Assumptions — Objective Functions

Original NFL: all functions

Example: Assume $X = \{0,1\}^{40}, Y = \{0,1\}^{8}$.
Assume objective function f is coded in at most 1 giga byte of RAM.

Only $100 \cdot \frac{1024^8 \cdot 8}{(2^8)^{2^{40}}} \% < 10^{-8,796,093,022,120} \%$ of all functions possible.

Most functions can neither be represented nor evaluated.

NFL Assumptions — Objective Functions

Improved NFL:

$\mathcal{F} \subseteq Y^X$ closed under permutations

Claim:

fraction of non-empty $\mathcal{F}$ closed under permutations:

$$\frac{2^{\binom{|X|+|Y|-1}{|X|}} - 1}{2^{|Y|^{|X|}} - 1}$$

Sets with NFL results exponentially small fraction.

NFL Assumptions — Objective Functions

The number of sets closed under permutations:

Definition: For $f : X \rightarrow Y$: histogram $h_f : Y \rightarrow \mathbb{N}_0$ with $h_f(y) = |\{x \in X \mid f(x) = y\}|$

Observation: "$f \sim g \Leftrightarrow h_f = h_g$" defines equivalence relation

Definition: basis class B_f: equivalence class of f

NFL Assumptions — Objective Functions

The number of sets closed under permutations:

Claim: There are $\binom{|X|+|Y|-1}{|X|}$ pairwise disjoint basis classes.

Proof: basis class "$\triangleq$" histogram

$$\left| \begin{array}{c} 1 \\ n_1 \end{array} \right| \begin{array}{c} 2 \\ n_2 \end{array} \left| \begin{array}{c} 3 \\ n_3 \end{array} \right| \begin{array}{c} \ldots \\ \ldots \end{array} \left| \begin{array}{c} |Y|-1 \\ n_{|Y|-1} \end{array} \right| \begin{array}{c} |Y| \\ n_{|Y|} \end{array} \Bigg| \text{ with } \sum_{i=1}^{|Y|} n_i = |X|$$

Think of each image is a ball:
Pick pos. of $|X|$ balls from $|X| + |Y| - 1$ pos.

NFL Assumptions — Objective Functions

The number of sets closed under permutations:

Claim: $f \sim g \Leftrightarrow \exists \sigma \in \text{Perm}(X) : \sigma f = g$

Proof:

"$\Rightarrow$": Define σ.

"$\Leftarrow$": histogram permutation-invariant

$\square$

NFL Assumptions — Objective Functions

The number of sets closed under permutations:

Claim: $\forall \mathcal{F} \subseteq Y^X$ closed under permutation:
$\mathcal{F}$ is union of basis classes

Proof:
For $f \in \mathcal{F}$ consider $F_f := B_f \cap \mathcal{F}$.

Observations:

$$\bigcup_{f \in \mathcal{F}} F_f = \mathcal{F} \qquad F_f \subseteq B_f \qquad B_f \subseteq F_f$$

□

NFL Assumptions — Objective Functions

The number of sets closed under permutations:

Claim:
fraction of non-empty $\mathcal{F}$ closed under permutations:

$$\frac{2^{\binom{|X|+|Y|-1}{|X|}} - 1}{2^{|Y|^{|X|}} - 1}$$

Proof: number of non-empty unions of basis classes: $2^{\text{number of basis classes}} - 1$
number of all non-empty sets: $2^{\text{number of functions}} - 1$

□

NFL Assumptions — Objective Functions

Definition: neighborhood $N\colon X \times X \to \{\text{true}, \text{false}\}$

Definition: neighborhood N non-trivial $\Leftrightarrow$
$\exists x_1, x_2, x_3, x_4 \in X :$
$(x_1 \neq x_2 \wedge N(x_1, x_2) = \text{true}) \wedge$
$(x_3 \neq x_4 \wedge N(x_3, x_4) = \text{false})$

Observation:
Any non-trivial neighborhood is not invariant under permutations.

NFL Assumptions — Objective Functions

Let $\mathcal{F} \subseteq Y^X$ be the set of “possible functions”.

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Conclusion:

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NFL results do not hold.

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Conclusion:

For $\mathcal{F}$ with a bounded number of local optima
NFL results do not hold.

NFL Assumptions — Performance Measures

Randomized search heuristics do re-evaluate.

Re-evaluations do influence the computation time.

NFL results have limited implications for consideration of computation time.

NFL Assumptions — Optimization Scenarios

Black Box Optimization:

Randomized search heuristic has to work for all $f \in \mathcal{F}$, where $\mathcal{F} \subseteq Y^X$ is complexity restricted.

Possible complexity restrictions:

- evaluation time restricted
- representation size restricted
- Kolmogoroff complexity restricted

The ANFL Theorem

The Almost No Free Lunch Theorem:

$X = \{0,1\}^n$, $Y = \{0,1,\dots,N-1\}$, $f\colon X \to Y$,
A a randomized search algorithm

$|\{f^*\colon \{0,1\}^n \to \{0,1,\dots,N\} \mid f^*$ agrees with f on $\geq 2^n - 2^{n/3}$ inputs and A finds the max. of f^* within $2^{n/3}$ steps with prob. $\leq 2^{-n/3}\ \}| \geq N^{2^{n/3}-1}$.

For exp. many functions $f^*\colon C(f^*) = C(f) + O(n)$

where C is evaluation time, circuit representation size, or Kolmogoroff complexity

Proof of the ANFL Theorem (I)

A: randomized search algorithm

$f:\{0,1\}^n \to \{0,1,\ldots,N-1\}$: function,
such that A is efficient on f

Consider first $2^{n/3}$ steps of A on f.

$q(x) = \text{Prob}(A \text{ visits } x \text{ in the first } 2^{n/3} \text{ steps})$

$$\sum_{x\in\{0,1\}^n} q(x)$$

Proof of the ANFL Theorem (I)

A: randomized search algorithm

$f: \{0,1\}^n \to \{0,1,\ldots,N-1\}$: function,
such that A is efficient on f

Consider first $2^{n/3}$ steps of A on f.

$q(x) =$ Prob(A visits x in the first $2^{n/3}$ steps)

$$\sum_{x \in \{0,1\}^n} q(x) \leq 2^{n/3}$$

Proof of the ANFL Theorem (II)

Definition for $b \in \{0,1\}^{2n/3}$:

$$S_b := \{x \in \{0,1\}^n \mid \forall i \in \{1,2,\ldots,2n/3\}\colon x_i = b_i\}$$

Observations:

- $\forall b \in \{0,1\}^{2n/3}\colon\ |S_b| = 2^{n/3}$
- $\left|\left\{S_b \mid b \in \{0,1\}^{2n/3}\right\}\right| = 2^{2n/3}$
- $\forall b \neq b' \in \{0,1\}^{2n/3}\colon S_b \cap S_{b'} = \emptyset$

Proof of the ANFL Theorem (III)

Definition:

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Proof of the ANFL Theorem (III)

Definition:

$q^*(b) :=$ Prob$($$A$ visits S_b in the first $2^{n/3}$ steps$)$

Obvious: $q^*(b) \leq \sum_{x \in S_b} q(x)$

Conclusion: $\exists b^*: q^*(b^*) \leq \frac{2^{n/3}}{2^{2n/3}} = 2^{-n/3}$

Proof of the ANFL Theorem (III)

Definition:

$f^*: \{0,1\}^n \longrightarrow \mathbb{R}$ with

- $\forall x \notin S_{b^*}: f^*(x) = f(x)$
- $\exists x^* \in S_{b^*}: f^*(x^*) = N$

Proof of the ANFL Theorem (III)

Definition:

$f^*: \{0,1\}^n \to \mathbb{R}$ with

- $\forall x \notin S_{b^*}: f^*(x) = f(x)$
- $\exists x^* \in S_{b^*}: f^*(x^*) = N$

Observations:

- There are at least $N^{2^{n/3}} - 1$ such f^*.
- Prob(A optimizes f^* in $\leq 2^{n/3}$ steps) $\leq 2^{-n/3}$

Proof of the ANFL Theorem (III)

Problem: Almost all such f^* are hard to represent and evaluate.

Solution:

$$f^*_{x^*,c}(x) = \begin{cases} f(x) & x \notin S_{b^*} \\ N & x = x^* \\ c & \text{otherwise} \end{cases}$$

There are $N \cdot 2^{n/3}$ such functions $f^*_{x^*,c}$. $\square$

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- NFL has little impact on research.

NFL Implications

- The (improved) NFL is a valid theorem.
- Be careful with claims like “algorithm A is better than algorithm B”.
- If someone claims “In my application domain NFL results do not hold” he or she is prob. right.
- When measuring computation time, NFL is not helpful.
- NFL has little impact on research.
- The ANFL Theorem restricts what can be achieved.

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