

Predicting the Integer Decomposition Property via Machine Learning

Brian Davis

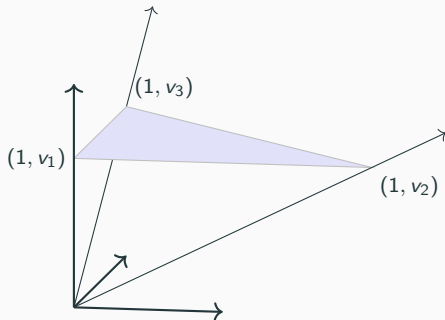
2 Aug 2018

University of Kentucky

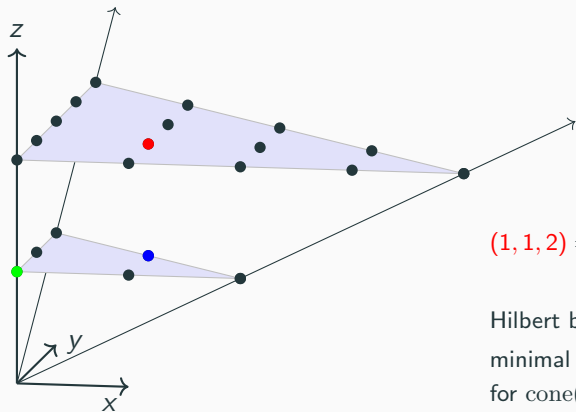
Hilbert Basics

Cone over a lattice simplex

$$\mathbf{v} = \{v_1, \dots, v_{d+1}\} \subset \mathbb{Z}^d \quad \text{cone}(\mathbf{v}) = \mathbb{R}_{\geq 0} \langle (1, v_1), \dots, (1, v_{d+1}) \rangle \subset \mathbb{R}^{d+1}$$



Hilbert basis = additively minimal lattice points



$$(1, 1, 2) = (0, 0, 1) + (1, 1, 1)$$

Hilbert basis $\text{HB}(\mathbf{v})$:
minimal additive generating set
for $\text{cone}(\mathbf{v}) \cap \mathbb{Z}^{d+1}$

The Integer Decomposition Property (IDP)

We say that the simplex with vertices $\{v_1, \dots, v_{d+1}\}$ has the **Integer Decomposition Property (IDP)** if for all elements z of the Hilbert basis $\text{HB}(\mathbf{v})$,

$$\text{height}(z) := z_0$$

is equal to 1.

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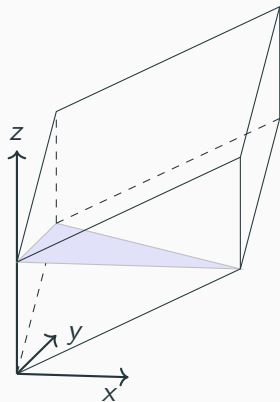
PROPOSED SOLUTION:

Consider IIDP to be a 0/1 function and approximate it with an easily evaluated function $\widehat{\text{IIDP}}$.

Apply $\widehat{\text{IIDP}}$ to very large test set to get likely IDP candidates, then validate candidates with Normaliz.

An intermediate step

The fundamental parallelepiped



The fundamental parallelepiped Π is the set

$$\left\{ \sum_{i=1}^{d+1} \gamma_i (\mathbf{1}, \mathbf{v}_i) : 0 \leq \gamma_i < 1 \right\}$$

FACT:

$\text{HB}(\mathbf{v})$ is the union of $\{(\mathbf{1}, \mathbf{v}_1), \dots, (\mathbf{1}, \mathbf{v}_{d+1})\}$
and the additively minimal elements of

$$\Pi \cap \mathbb{Z}^{d+1}$$

Partition the fundamental parallelepiped

Map $z \in \Pi$ to $\{0, \dots, n-1\}^{d+1}$

by

$$z \mapsto ([n \gamma_1], \dots, [n \gamma_{d+1}])$$

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$$z \mapsto (\lfloor n \gamma_1 \rfloor, \dots, \lfloor n \gamma_{d+1} \rfloor)$$

EX: $n = d = 2$

$$z = \frac{3}{4}(1, v_1) + \frac{2}{4}(1, v_2) + \frac{3}{4}(1, v_3)$$

$$\begin{aligned} z \mapsto & \left(\left\lfloor 2 \cdot \frac{3}{4} \right\rfloor, \left\lfloor 2 \cdot \frac{2}{4} \right\rfloor, \left\lfloor 2 \cdot \frac{3}{4} \right\rfloor \right) \\ & = (1, 1, 1) \in \{0, 1\}^3 \end{aligned}$$

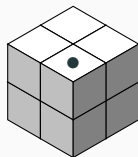
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Record the box containing z



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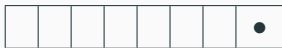
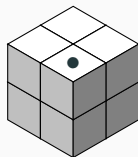
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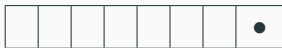
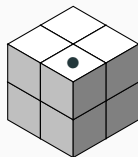
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$$(0, 0, 0, 0, 0, 0, 0, 1)$$

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The function \mathbb{HIB}

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$$(v_1, \dots, v_{d+1}) \xrightarrow{\mathbb{HIB}} \{0, 1\}^{d+1^{d+1}}$$

$$\mathbb{HIB}(\mathbf{v})_\alpha = \begin{cases} 1 & \text{if there exists a Hilbert basis element in box } \alpha \\ 0 & \text{otherwise} \end{cases}$$

Why bother?

FACT:

If z in $\Pi \cap \mathbb{Z}^{d+1}$ lies in box with indices $\alpha = (i_1, \dots, i_{d+1})$, then

$$\text{height}(z) = \left\lceil \frac{i_1 + \dots + i_{d+1}}{d+1} \right\rceil$$

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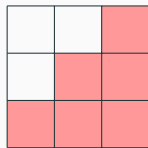
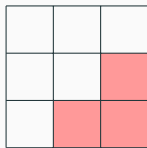
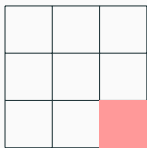
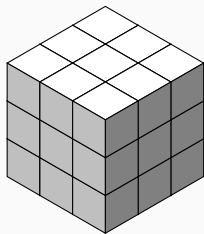
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CONSEQUENCE:

We can detect IDP by looking at support of $\text{IHIB}(\mathbf{v})$.



Defining $\widehat{\text{IDP}}$ via $\widehat{\text{HB}}$

$\widehat{\text{IDP}}$ is the the composite function:

$$\mathbf{v} \xrightarrow{\widehat{\text{HB}}} \{0, 1\}^{d+1^{d+1}} \xrightarrow{\text{supp}} \{0, 1\}$$

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$$\text{cutoff}(x) = \begin{cases} 1 & \text{if } x \geq \eta \\ 0 & \text{if } x < \eta \end{cases}$$

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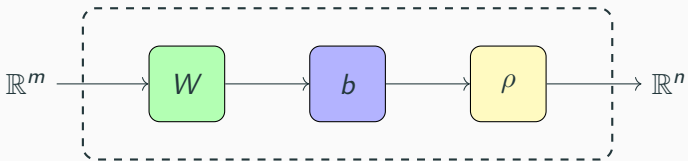
A general method for creating piece-wise linear approximations

The building blocks

matrix: $W \in \mathbb{R}^{n \times m}$ (weights)

vector: $b \in \mathbb{R}^n$ (biases)

function: $\rho(z) = \max(0, z)$ coordinatewise

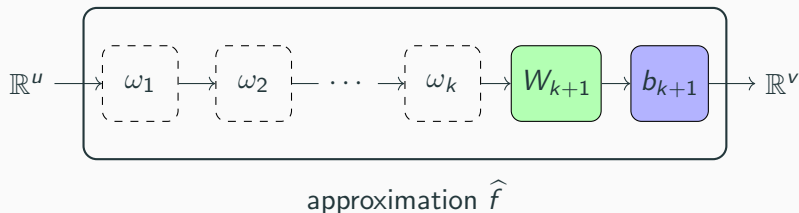


$$\omega(x) = \rho(Wx + b)$$

An initial approximation of $f : \mathbb{R}^u \rightarrow \mathbb{R}^v$

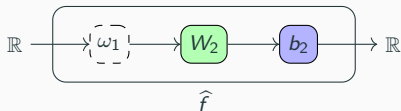
Pick positive integers k and l_1, \dots, l_k ,

Set weights W_i and biases b_i randomly for $\omega_i : \mathbb{R}^{l_i} \rightarrow \mathbb{R}^{l_{i+1}}$



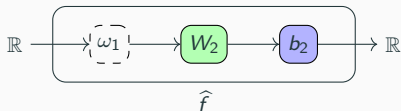
Note: \hat{f} is piece-wise linear

EXAMPLE: $f(x) = \log(x)$ on interval $[1, 3]$



$$W_1 = [0.75, -0.5]^T \quad b_1 = [-0.75, 1] \quad W_2 = [1, 1] \quad b_2 = [-0.5]$$

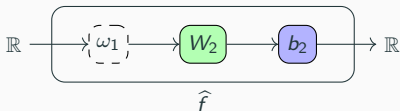
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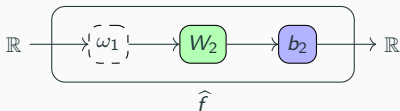


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$$= [1, 1]\rho \left(\begin{bmatrix} 0.75 \\ -0.5 \end{bmatrix} [x] + \begin{bmatrix} -0.75 \\ 1 \end{bmatrix} \right) + [-0.5]$$

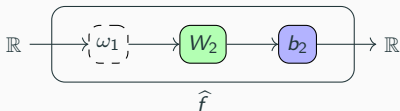
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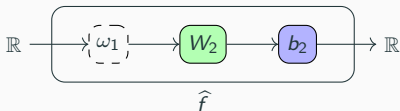
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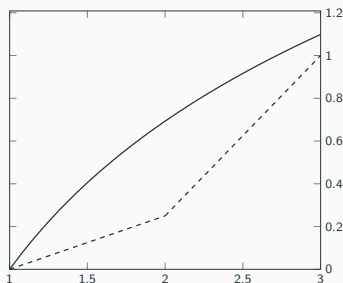
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f and \hat{f} (dashed)

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For sufficiently small ϵ , we expect that $L_{p'}(x) < L_p(x)$

Our new approximation is \hat{f} with the updated parameters p'

$f(x) = \log(x)$ continued

Let $x = 1.5$ and use Euclidean distance loss function

$$L(x) = \left\| \log(x) - \hat{f}(x) \right\|$$

$$\nabla L = \left\langle \frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial b_1}, \frac{\partial L}{\partial W_2}, \frac{\partial L}{\partial b_2} \right\rangle_{x=1.5}$$

$$= \langle -1.5, -1.5, -1, -1, -0.375, -0.25, -1 \rangle.$$

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For $\epsilon = 0.02$, the update $p' = p - \epsilon \nabla L$ is given by

$$W_1 = [0.78, -0.47]^T \quad b_1 = [-0.73, 1.02]$$

$$W_2 = [1.0075, 1.0075] \quad b_2 = [-0.48]$$

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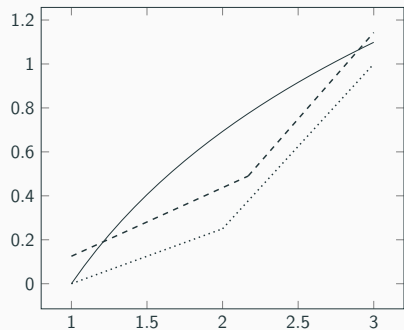
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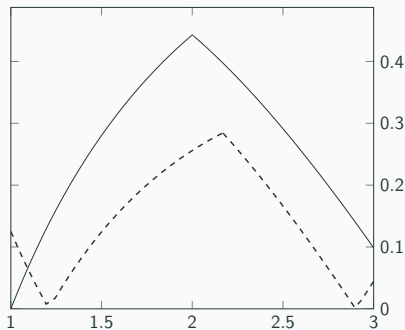
The updated approximation is

$$\hat{f}(x) = \begin{cases} 0.312x - 0.187 & 1 \leq x \leq 2.17 \\ 0.786x - 1.215 & 2.17 < x \leq 3 \end{cases}$$

$f(x) = \log(x)$ continued



$\hat{f}(x; p)$ (dotted) and
 $\hat{f}(x; p')$ (dashed)



Loss for $\hat{f}(x; p)$ and
 $\hat{f}(x; p')$ (dashed)

Implementation

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We restrict to the case that $d = 4$ and \mathbf{v} is of the form:

- $v_i = e_i$ for $1 \leq i \leq d$, and
- $v_{d+1} = (-\lambda_1, -\lambda_2, -\lambda_3, -\lambda_4)$ with $1 \leq \lambda_i \leq 25$

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Using Normaliz, we compute $\mathbb{H}\mathbb{B}(\mathbf{v})$ for 50,000 such examples drawn uniformly at random.

Hyperparameters



Trainable parameters: \approx 12million

Learning rate: $\epsilon = 10^{-4}$

Number of updates: 200,000 batches of size 25

Binary Cross Entropy: For f a 0/1 function, \hat{f} real valued,

$$\text{BCE}(x) = (f - 1) \cdot \log(1 - \sigma \circ \hat{f}) - f \cdot \log(\sigma \circ \hat{f})$$

where σ is the *sigmoid function* $\sigma(z) = (1 + e^{-z})^{-1}$.

Results

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$$\widehat{\text{HTB}}(\mathbf{v}) = (4.4e-23, 1.9e-12, 4.6e-28, 1.3e-13, 1.0e-11, 7.0e-14, 1.0e-01, \dots)$$

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$$\text{with } \eta = 0.1, \quad \text{cutoff}(\widehat{\text{HTB}}(\mathbf{v})) = (0, 0, 0, 0, 0, 0, 1, \dots)$$

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$$\widehat{f}(\mathbf{v}) = (-51.4, -26.9, -62.9, -29.6, -25.2, -30.2, -2.1, \dots)$$

$$\widehat{\text{HTB}}(\mathbf{v}) = (4.4e-23, 1.9e-12, 4.6e-28, 1.3e-13, 1.0e-11, 7.0e-14, 1.0e-01, \dots)$$

with $\eta = 0.1$, $\text{cutoff}(\widehat{\text{HTB}}(\mathbf{v})) = (0, 0, 0, 0, 0, 0, 1, \dots)$

$\eta = 0.1$	PREDICTED 0	PREDICTED 1
ACTUAL 0	2,705	160
ACTUAL 1	1	11

$$\lambda = (5, 11, 11, 20)$$

$$\hat{f}(\mathbf{v}) = (-51.4, -26.9, -62.9, -29.6, -25.2, -30.2, -2.1, \dots)$$

$$\widehat{\text{HTB}}(\mathbf{v}) = (4.4e-23, 1.9e-12, 4.6e-28, 1.3e-13, 1.0e-11, 7.0e-14, 1.0e-01, \dots)$$

$$\text{with } \eta = 0.1, \quad \text{cutoff}(\widehat{\text{HTB}}(\mathbf{v})) = (0, 0, 0, 0, 0, 0, 1, \dots)$$

$\eta = 0.1$	PREDICTED 0	PREDICTED 1
ACTUAL 0	2,705	160
ACTUAL 1	1	11

$$\text{specificity (top row)} = \frac{\text{true negatives}}{\text{true negatives} + \text{false positives}} = 94\%$$

$$\text{sensitivity (bottom row)} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}} = 92\%$$

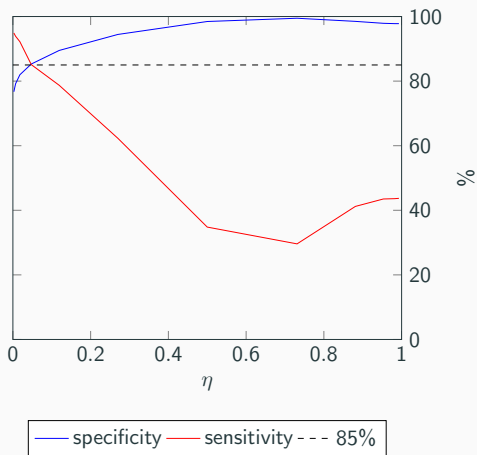
5,000 random samples aggregated

$\eta = 0.01$	PREDICTED 0	PREDICTED 1
ACTUAL 0	11,448,675	2,845,413
ACTUAL 1	6,572	92,971

specificity = 80%

sensitivity = 93%

Effect on \widehat{HIB} of varying η



In the sample of 5,000 simplices, there were 112 IDP examples
($\approx 2.4\%$)

The resulting approximation $\widehat{\text{IDP}}$

In the sample of 5,000 simplices, there were 112 IDP examples ($\approx 2.4\%$)

Result of applying $\widehat{\text{IDP}}$ to the sample:

$\tau \backslash \eta$	0.5	0.25	0.12	0.05
0	3/7 (42.9%)	3/4 (75.0%)	3/3 (100.0%)	3/3 (100.0%)
10	21/320 (6.6%)	11/38 (29.0%)	8/21 (38.1%)	6/12 (50.0%)
20	46/1026 (4.5%)	21/102 (20.6%)	11/45 (24.4%)	8/27 (29.6%)
30	65/1770 (3.7%)	35/196 (17.9%)	23/103 (22.3%)	16/64 (25.0%)

The IDP examples predicted by $\widehat{\text{IDP}}$ ($\eta = 0.1, \tau = 65$)

1,1,1,1	1,1,3,9	1,1,21,24	1,2,14,10	1,2,14,10	24,2,1,16
1,3,16,3	1,3,24,1	1,4,2,16	1,4,20,20	1,8,1,1	24,4,2,4
1,10,10,8	1,10,24,24	1,12,4,12	1,15,3,1	1,18,1,6	24,24,23,12
1,21,1,4	1,24,1,9	1,24,14,2	1,24,17,1	1,24,18,1	24,24,6,24
1,24,18,4	1,24,24,20	2,2,2,7	2,3,12,18	2,8,8,4	23,24,24,12
2,10,1,16	2,20,10,5	3,1,1,9	3,6,12,1	3,12,2,24	23,18,3,24
3,14,21,3	3,19,3,1	3,23,15,3	4,1,1,4	4,8,2,16	23,2,2,6
4,20,1,14	4,20,10,20	4,23,4,12	4,24,1,16	6,1,2,12	22,22,20,1
6,2,6,3	6,2,18,9	6,6,6,3	6,14,6,15	6,17,9,18	22,16,22,1
7,3,21,7	7,7,1,7	7,7,16,16	8,1,8,2	8,2,12,24	22,16,4,1
8,16,4,2	9,1,1,9	9,6,18,2	9,9,4,4	9,18,4,4	22,2,2,22
9,18,18,6	9,22,1,11	10,1,5,22	10,5,10,9	10,24,4,1	21,21,16,4
11,22,5,5	12,1,2,6	12,1,24,19	12,2,3,12	12,2,18,3	20,22,1,22
12,3,2,6	12,3,11,6	12,6,1,1	12,6,1,3	12,12,4,12	20,20,4,20
12,16,1,16	12,24,2,24	12,24,6,1	13,2,2,20	14,6,14,7	20,20,4,1
14,7,2,24	14,7,12,1	15,1,13,15	15,15,1,1	16,1,6,6	20,20,1,20
16,4,2,16	16,7,16,16	16,8,4,2	16,16,12,3	16,24,1,22	20,14,24,1
17,1,7,1	17,17,8,4	17,17,17,1	18,1,1,15	18,2,6,6	
18,2,22,1	18,10,1,15	19,19,1,16	20,2,1,12	20,8,19,8	

The big search

We computed the value of $\widehat{\text{IDP}}$ for all 390,625 $\Delta_{(1,q)}$ simplices with q -vector in $[1, 25]^4$ using $\eta = 0.007$ and $\tau = 50$.

The computation produced 3,773 predicted positives.

We then computed IDP for these examples and found that 856 were IDP.

This corresponds to a specificity of about 23%.

1. If we train our approximation $\widehat{\text{HIB}}$ to have high sensitivity, then we can recover a set of lattice points containing the Hilbert basis. If the specificity is high, then reducing this set will require fewer steps than reducing the entire fundamental parallelepiped.
2. If we record the number of FPP points in each bin instead of the presence of Hilbert basis elements, then we have a model for predicting **unimodality** of the h^* -vector.