The Deep Mathematics Behind A.I. and Deep Learning

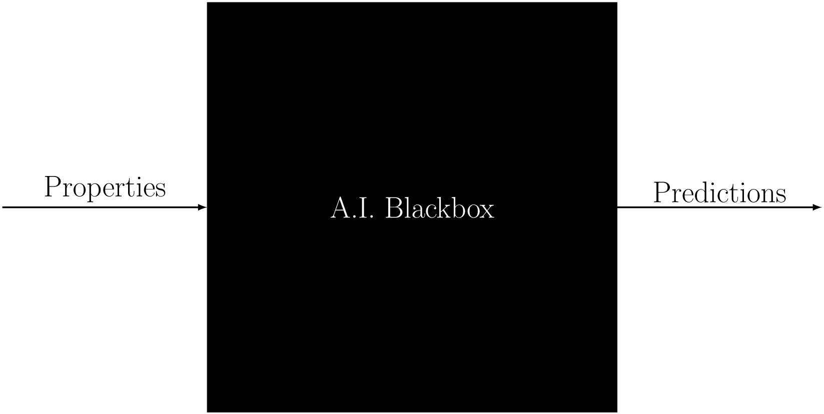
A mathematical generalisation and important theorems in contemporary A.I. and deep learning problems.

Sepehr Saryazdi

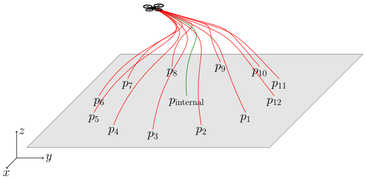
University of Sydney

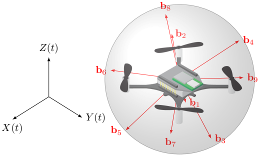
March 8, 2023

Why learn the math behind AI?



Who am I?


p_8
p_9
p_{10}
p_{11}
p_7
p_6
p_{internal}
p_{12}
p_5
p_1
p_4
p_3
p_2
z
y
x


$Z(t)$
$Y(t)$
$X(t)$
$\mathbf{b}_8$
$\mathbf{b}_2$
$\mathbf{b}_4$
$\mathbf{b}_6$
$\mathbf{b}_9$
$\mathbf{b}_1$
$\mathbf{b}_5$
$\mathbf{b}_7$
$\mathbf{b}_3$


aws
certified
Machine Learning
SPECIALTY

Overview

The Face-Space Problem

Some Subset of the Face-Space

Logical Boundaries (Logic Values = $\{0, 1\}$)

Some Subset of the Face-Space

Logical Boundaries (Logic Values = $\{0, 1\}$)

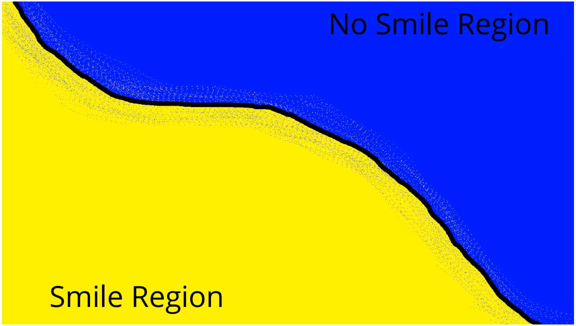
Some Subset of the Face-Space

Fuzzy Logic (Logic Values = $[0, 1] \subseteq \mathbb{R}$)

Some Subset of the Face-Space

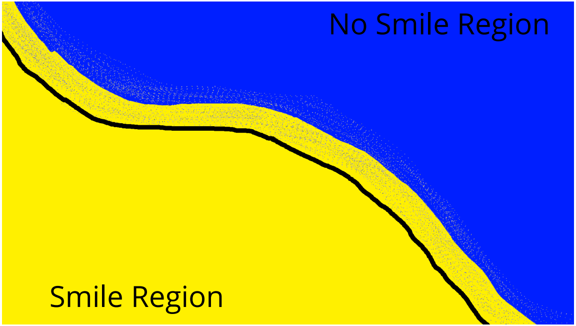
ROC/Confusion Matrix Adjustment

- ROC (Receiver Operating Characteristic Curve) / Confusion Matrices quantify where things are going wrong for each boundary function choice.



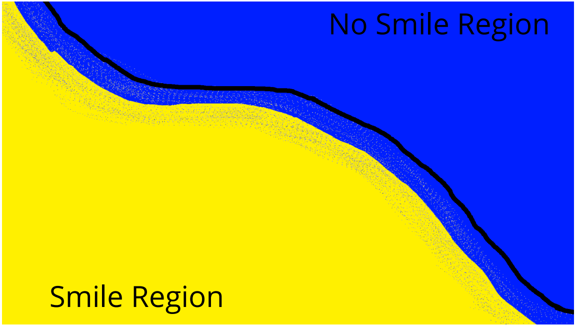
ROC/Confusion Matrix Adjustment

- ROC (Receiver Operating Characteristic Curve) / Confusion Matrices quantify where things are going right/wrong for each boundary function choice.



ROC/Confusion Matrix Adjustment

- ROC (Receiver Operating Characteristic Curve) / Confusion Matrices quantify where things are going right/wrong for each boundary function choice.



A.I. Model Representations

- Let P be a topological space, representing the model's parameters (i.e. $P = \mathbb{R}^n$).
- Let X, Y be topological spaces, and let $C(X, Y)$ be the space of continuous functions from X to Y.
- Let a map that takes a parameter to A.I. models for $X \to Y$ be denoted by $\mathcal{M}$.

A.I. Model Representations

Every A.I. model may be viewed as a function $\mathcal{M}$ that maps parameters to continuous functions from $X \to Y$.

$$\mathcal{M} : P \to C(X, Y)$$

A.I. Model Representations

A.I. Model Representations

Every A.I. model may be viewed as a function $\mathcal{M}$ that maps parameters to continuous functions from $X \to Y$.

$$\mathcal{M} : P \to C(X, Y)$$

Example 1: $\mathbb{R} \to \mathbb{R}$ Linear Model

$$P = \mathbb{R}^2, (a, b) \in P, X = Y = \mathbb{R}$$

$$(\mathcal{M}(a, b))(x) := a + bx$$

A.I. Model Representations: $\mathbb{R} \to \mathbb{R}$ Linear Model

$$(\mathcal{M}(a, b))(x) := a + bx$$

A.I. Model Representations: $\mathbb{R} \to \mathbb{R}$ Quadratic Model $(\mathcal{M}(a,b,c))(x) := a + bx + cx^2$

A.I. Model Representations: $\mathbb{R} \to \mathbb{R}^2 \to \mathbb{R}$ Neural Network Model

Example 3: $\mathbb{R} \to \mathbb{R}^2 \to \mathbb{R}$ Neural Network Model

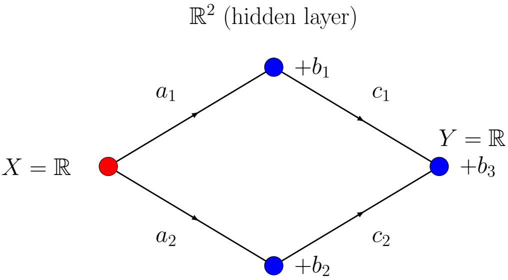
$$P = \mathbb{R}^7, (a_1, a_1, b_1, b_2, b_3, c_1, c_2) \in P, X = Y = \mathbb{R}$$

$$(\mathcal{M}(a_1, a_1, b_1, b_2, b_3, c_1, c_2))(x)$$

$$:= \left(\mathrm{ReLU}\left(\begin{pmatrix} a_1 & a_2 \end{pmatrix} x + \begin{pmatrix} b_1 & b_2 \end{pmatrix}\right)\right) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} + b_3$$

$$\mathrm{ReLU}(x_1, x_2) := \begin{pmatrix} \max(x_1, 0) & \max(x_2, 0) \end{pmatrix}$$

A.I. Model Representations: $\mathbb{R} \to \mathbb{R}^2 \to \mathbb{R}$ Neural Network Model



Generalised Loss Functions

- Let P, X, Y be topological spaces and $\mathcal{M} : P \to C(X, Y)$ a function.
- Let $d : C(X, Y) \times C(X, Y) \to \mathbb{R}_{\geq 0}$ be a metric.
- Let L_f for some $f \in C(X, Y)$ be named a “loss function”.

Generalised Loss Functions

Define the loss function $L_f : P \to \mathbb{R}_{\geq 0}$ to satisfy

$$L_f(p) := d(f, \mathcal{M}(p))$$

Generalised Loss Functions

Example: $L^2(X, \mathbb{R}_{\geq 0})$ Loss Function

$$L_f(p) = \int_X ||f(x) - (\mathcal{M}(p))(x)||^2 \mathrm{d}x$$

Loss Surfaces: $f(x) := \sin x$, $(M(a,b))(x) := a + bx$, L^2-Loss Function

Loss Surfaces: Optimal Parameter Search

- Let $(p_n)_{n\in\mathbb{N}} \subseteq P$ be a sequence of parameters.

Optimal Parameter Search

An optimal parameter search is an algorithm where for any $p_0 \in P$, it returns a sequence $(p_n)_{n\in\mathbb{N}} \subseteq P$ such that

$$L_f(p_n) \xrightarrow[n\to\infty]{} \inf_{p\in P} L_f(p)$$

- Note: Such a sequence need not have a unique limit, as P and $\mathcal{M}$ may over-cover the goal function f.

Loss Surfaces: Gradient Descent

Loss Surfaces: Gradient Descent

- Let $\gamma \in \mathbb{R}_{>0}$ be named the "learning rate".
- Let ∇L_f denote the gradient function of L_f.

Gradient Descent Optimal Parameter Search Algorithm

Assuming $p_0 \in P$ is given, construct the sequence $(p_n)_{n\in\mathbb{N}} \subseteq P$ with recursion given by

$$p_{n+1} = p_n - \gamma(\nabla L_f)(p)$$

- In practice, a fixed γ causes either zero movement or large oscillations near local minima of L_f, so a strictly decreasing sequence $(\gamma_n)_{n\in\mathbb{N}} \subseteq \mathbb{R}_{>0}$ is often used, or similar ideas like "momentum".

Loss Surfaces: Gradient Descent

Loss Functions: Finite Sampling of $f : X \to Y$

- In practice, we can only sample $N \in \mathbb{N}$ finitely many points $(x_i, y_i) \in X \times Y$ with $f(x_i) = y_i$.
- This collapses the L^2 loss function to a finite sum.

Finite Sampling of $L^2(X, \mathbb{R}_{\geq 0})$ Loss Function (MSE)

$$L_f(p) \approx \frac{1}{N} \sum_{i=1}^{N} ||f(x_i) - (\mathcal{M}(p))(x_i)||^2$$

- As $N \to \infty$ and assuming the sampling is distributed uniformly over X, then this will approach the true L^2 loss function.

Kolmogorov–Arnold Representation Theorem

- This is a solution to the famous 13th Hilbert Problem.
- Colloquially, this theorem says that the "only true continuous multivariable function is the sum".

KA Representation Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}^m$ with $f(\mathbf{x}) := f(x_1, \ldots, x_n)$ be a continuous function. Then there exists univariate functions $\Phi_q : \mathbb{R} \to \mathbb{R}^m, \phi_{q,p} : \mathbb{R} \to \mathbb{R}$ such that:

$$f(\mathbf{x}) = \sum_{q=0}^{2n} \Phi_q \left(\sum_{p=1}^{n} \phi_{q,p}(x_p) \right)$$

Consequences of KA Representation Theorem

- From this theorem, feature engineering was born.
- This theorem allows us to transform each data column independently before combining them with sums in an A.I. algorithm.

x_1	x_2	x_3
10	99	85
67	13	8
82	48	89
$\vdots$	$\vdots$	$\vdots$
7	76	25

$\longrightarrow$

$0.5x_1 + 2x_2 - x_3$
118
51.5
48
$\vdots$
130.5

Universal Approximation Theorem

- This says that neural networks can be used to approximate any continuous function if X is closed and bounded.

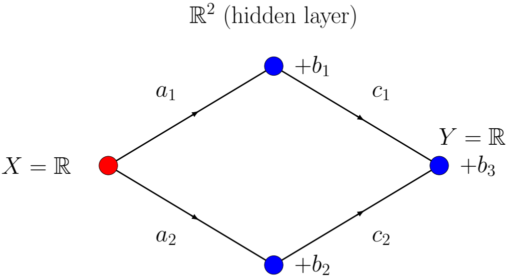
Universal Approximation Theorem

If given $f : X \subseteq \mathbb{R}^n \to \mathbb{R}^m$ and a valid non-polynomial function $\sigma : \mathbb{R} \to \mathbb{R}$, then $L_f(p) := ||f - \mathcal{M}(p)||_\infty$ can be made arbitrarily small where

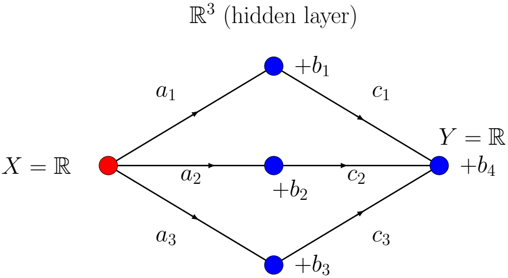
$$(\mathcal{M}(p))(x) := C_p\left(\sigma \circ (A_p(x) + b)\right)$$

$$p \in P := \mathbb{R}^{k(1+m+n)}, A_p \in \mathbb{R}^{k\times n}, C_p \in \mathbb{R}^{m\times k}, b \in \mathbb{R}^k$$

Universal Approximation Theorem

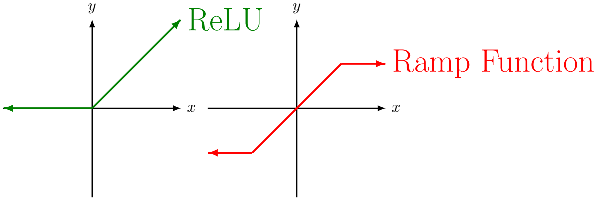


Universal Approximation Theorem



Universal Approximation Theorem: How It Works

- The choice of $\sigma : \mathbb{R} \to \mathbb{R}$ was really the crucial part of the entire theorem.
- This is because σ acts as a tool for approximating the 'ramp' function and this can then approximate any continuous function.



Spin Hamiltonian-Loss Correspondence

The Fundamental Issue of Machine Learning

How do we know we have found the global minima of $L_f : P \to \mathbb{R}_{\geq 0}$?

- Fear not! It turns out for large neural networks, any local minima is good enough under reasonable sampling!
- This is thanks to the Spin-Glass Hamiltonian and Neural Network Loss Function Correspondence.

Spin Hamiltonian-Loss Correspondence: Hamiltonians

- Hamiltonians are a concept from Physics; they quantify how much energy a system is capable of moving around.

Example: Particle in Gravity Hamiltonian

$$\mathcal{H}(x, v) = \frac{1}{2}mv^2 - \frac{GMm}{|x|}$$

Spin Hamiltonian-Loss Correspondence: Hamiltonians

Example: Particle in Gravity Hamiltonian

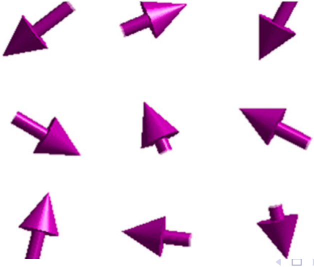
$$\mathcal{H}(x, v) = \frac{1}{2}mv^2 - \frac{GMm}{|x|}$$

- The natural state of the system (when energy moves around the least) occurs whenever $(x_n, v_n)_{n\in\mathbb{N}} \subseteq \mathbb{R}^2$ is a sequence such that

$$\mathcal{H}(x_n, v_n) \xrightarrow[n\to\infty]{} \inf_{(x,v)\in\mathbb{R}^2} \mathcal{H}(x, v)$$

Spin Hamiltonian-Loss Correspondence: Spin-Glass

- Physicists have been interested in how magnets work for a long time.
- They modelled a block magnet as being made up of locally frozen magnets on the unit sphere $S^2 \subset \mathbb{R}^3$ that align/repel neighbouring magnets.



Spin Hamiltonian-Loss Correspondence: Spin-Glass

- Bumping up to N-dimensional magnets and only considering interactions between $p \geq 2$ closest neighbouring magnets, we get the p-Spin Glass Model.

The Spin-Glass Hamiltonian

$$\mathcal{H}_{N,p}(\sigma) = \frac{1}{N^{(p-1)/2}} \sum_{i_1,\cdots,i_p=1}^{N} J_{i_1,\cdots,i_p} \sigma_{i_1} \cdots \sigma_{i_p}$$

$$\sigma = (\sigma_1, \cdots, \sigma_N) \in S^{(N-1)/\sqrt{N}}, \sum_{i=1}^{N} \sigma_i^2 = N$$

Spin Hamiltonian-Loss Correspondence: Hamiltonian Local Minima

- With reasonable (but technical) distribution assumptions, one can show that any local minima of $\mathcal{H}_{N,p}$ is good enough (Auffinger A. et. al., 2011).

The Spin-Glass Global-Local Minima Proximity

If $\sigma_{\min} \in S^{(N-1)/\sqrt{N}}$ is a local minima of $\mathcal{H}_{N,p}$, then we expect its Hamiltonian value $\mathcal{H}_{N,p}(\sigma_{\min})$ to be close to the globally smallest value $\inf_{\sigma \in S^{(N-1)/\sqrt{N}}} \mathcal{H}_{N,p}(\sigma)$.

$$\mathcal{H}_{N,p}(\sigma_{\min}) \approx \inf_{\sigma \in S^{(N-1)/\sqrt{N}}} \mathcal{H}_{N,p}(\sigma)$$

Spin Hamiltonian-Loss Correspondence

- It turns out that the loss function L_f of a neural network (under certain assumptions) can be bijectively mapped to $\mathcal{H}_{N,p}$ (Choromanska A. et. al, 2015).

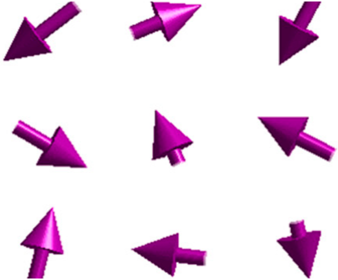
Spin Hamiltonian-Loss Correspondence

$$\sigma_{\min} \in S^{(N-1)/\sqrt{N}} \Leftrightarrow p_{\min} \in P$$

$$\mathcal{H}_{N,p}(\sigma_{\min}) \approx \inf_{\sigma \in S^{(N-1)/\sqrt{N}}} \mathcal{H}_{N,p} \Leftrightarrow L_f(p_{\min}) \approx \inf_{p \in P} L_f(p)$$

Spin Hamiltonian-Loss Correspondence

- This theorem explains why A.I. works reasonably well even when only approaching one local minima (assuming certain distributional assumptions hold).



Representer Theorem: Regularisation

- A technical issue that arises, when sampling finitely many points of an infinite space, is the bias-variance tradeoff.
- If you want your model to generalise faster (less variance in predictions), it needs to be more biased!

L^2 Regularisation Bias (Hyper-Parameter $\lambda > 0$)

$$L_{f,\lambda}(p) := \int_X ||f(x) - (M(p))(x)||^2 dx + \lambda ||M(p)||_2^2$$

$$||M(p)||_2^2 = \int_X ||(M(p))(x)||^2 dx$$

Representer Theorem: Hilbert Spaces

- Due to some nice mathematics, L^2 is what's called a *Hilbert Space* $\mathcal{H}$, i.e. it has a notion of 'angles' which allows for a faster way of measuring how similar two functions are.

Hilbert Space Inner Product

$$\langle f, g \rangle_{\mathcal{H}} = \int_X f(x)g(x)dx = ||f||_{\mathcal{H}}||g||_{\mathcal{H}} \cos\theta$$

Representer Theorem: Kernels

- Kernels show up everywhere in machine learning due to something called the *Kernel Trick*.
- The idea is to lift our sample points $(x_i, y_i) \in X \times Y := X \times \mathbb{R}$ into a higher dimensional Hilbert Space, then use the inner product as a 'similarity' measure for any two data points.
- Let $\kappa : X \times X \to \mathbb{R}$ be the Kernel which lifts the data via a transformation $g : X \to \mathcal{H}$ and evaluates the inner product, defined as

Kernel Function

$$\kappa(x, y) := \langle g(x), g(y) \rangle_{\mathcal{H}}$$

Representer Theorem: Reproducing Kernel Hilbert Space

Representer Theorem: Minimiser A.I. Model

L^2 Regularisation Bias (Hyper-Parameter $\lambda > 0$)

$$L_{f,\lambda}(p) \approx \frac{1}{N}\sum_{i=1}^{N} ||f(x_i) - (M(p))(x_i)||^2 + \lambda ||M(p)||_2^2$$

- The Representer Theorem beautifully constructs an A.I. model function M^* which becomes linear in the coefficients and directly keeps track of all the sampled data points, enabling data efficiency.

Representer Theorem: Minimiser A.I. Model

Representer Theorem

There exists $p = (p_1, \cdots, p_N) \in P := \mathbb{R}^N$ and $M^* : \mathbb{R}^N \to C(X, \mathbb{R})$ which minimises the loss function $L_{f,\lambda}$ given as

$$(M^*(p))(x) = \sum_{i=1}^{N} p_i \kappa(x, x_i) \in \text{span}_{\mathbb{R}}\{\kappa(x, x_i) \mid i \in \{1, \cdots, N\}\}$$

Representer Theorem: Applications

- This shows up in reinforcement learning, where the goal function $f : \mathcal{S} \to \mathcal{A}$ is a decision process function with state-space $\mathcal{S}$ and action-space $\mathcal{A}$.
- Since $\mathcal{S} \subseteq \mathbb{R}^n$ for continuously moving objects, then this is an infinite-dimensional space so making f linearly represented by a finite function basis generated by the Kernel $\kappa : \mathcal{S} \times \mathcal{S} \to \mathbb{R}$ is very data-efficient.

Conclusions

- Overall, A.I. is secretly the study of functions.
- The KA Representation Theorem justifies the univariate transformation of features in feature engineering.
- The Universal Approximation Theorem explains why neural networks are so successful at approximating continuous functions.
- The Spin Hamiltonian-Loss Correspondence explains why local minima of loss in neural networks are close to the global minima.
- The Representer Theorem allows for a linear representation of the A.I. model that utilises the "similarity" measure (the Kernel) about all the data points, so it's data-efficient.