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Discrete Control + Continuous Dynamics

Discrete Control + Continuous Dynamics



Parameters

 $flow_3$:

- ε : external stimulus current to cell

 $+\frac{w}{2\cdot(1+e^{-2k_{so}(u-u_{so})})\cdot\tau}, \qquad u \ge \theta_{v} \qquad -\frac{1}{\tau_{so1} + \frac{\tau_{so2} - \tau_{so1}}{1+e^{-2k_{so}(u-u_{so})}}}$

З

Cardiac Cell Action Potential Model (BCF Model[Bueno2008])

State Variables

- u: cell's transmembrane potential -flowcurrent at fast channeflogate $\frac{du}{dt} = \varepsilon - \frac{1}{\tau_{so1} + \frac{\tau_{so2} - \tau_{so1}}{1 + e^{-2k_{so}(u-u_{so})}}} \qquad \qquad \frac{du}{dt} = \varepsilon + \frac{v(u - \theta_v)(u_u - u)}{\tau_{fi}}$ - $\frac{du}{dt}$, s: $\frac{du}{\tau_{a1}}$ rents at two slow $\frac{du}{dt} \in \operatorname{ham}_{\tau_{a2}}^{u}$ gate $u \ge \theta_o$ $\frac{dv}{dt} = -\frac{v}{\tau_{v^2}}$ $\frac{dv}{dt} = \frac{1-v}{\tau_{v1}}$ $u \ge \theta_w$

Discrete Control + Continuous Dynamics

Prostate Cancer Treatment Model [Bing2015]



Control (cancer therapy)

x: Population of HSCs (Hormone Sensitive Cells) y: Population of CRCs (Cancer Resistant Cells) Plant (cancer progression)

z: Androgen concentration

v: PSV level, biomarker for the total population of cancer cells





Power Train Control (Toyota Research)



Autonomous Vehicle (CMU ECE)



Microfluidic Chip Design (Univ. of Waterloo)

Improper functioning of cardiac cell ionic channels can cause the cells to lose excitability, which disorders electric wave propagation and leads to cardiac abnormalities such as ventricular tachycardia or fibrillation.





Normal Condition

Atrial Fibrillation



Cardiac Cell Action Potential

Can we find a set of initial values/parameters for which a cardiac cell loses excitability? (= can it reach mode 4?)



- CAS(Continuous Androgen Suppression) is known to fail.
- IAS(Intermittent Androgen Suppression) works better



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- However, we need to identify patient-specific schedules.



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- IAS(Intermittent Androgen Suppression) works better
- However, we need to identify patient-specific schedules.



Can we find a personalized treatment schedule which prevents the cancer recurrence in N days?



Control (cancer therapy)

x: Population of HSCs (Hormone Sensitive Cells) y: Population of CRCs (Cancer Resistant Cells) Plant (cancer progression)

z: Androgen concentration

v: PSV level, biomarker for the total population of cancer cells



y Analysis of Hybrid Systems

nalized treatment schedule which prevents :e in N days?



Figure 7: Model prediction vs. experimental data.

Can we automate a non-trivial parking?



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"Tesla Motors will be rolling out an automated car passing feature, but which is initiated by the human driver as a way to make the latter ultimately responsible for the outcomes."

Matthew O'Kelly, Houssam Abbas, Sicun Gao, Shin'ichi Shiraishi, Shinpei Kato, and Rahul Mangharam ,

"Tesla Motors will be rolling out an automated car passing feature, but which is initiated by the human driver as a way to make the latter ultimately responsible for the outcomes."

"Randomized testing, where the configurations are sampled from hypercubes of parameters, is not a scalable solution: suppose we decide to sample only 10 points in the range of every state variable. For our 7D model, and with 2 cars, this yields a total of 10^{14} simulations. Say we wish to simulate 10 seconds. Even if a simulation runs in realtime, this still requires $10*10^{14}$ seconds = 30 million years to complete."

Matthew O'Kelly, Houssam Abbas, Sicun Gao, Shin'ichi Shiraishi, Shinpei Kato, and Rahul Mangharam,

Can we do validated planning?



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Can we do validated planning?



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Can a hybrid system reach a goal region of its state space?

Can a hybrid system reach a goal region of its state space?



Can a hybrid system reach a goal region of its state space?



The standard bounded reachability problems for simple hybrid systems are **undecidable**[Alur et al, 1992].

The standard bounded reachability problems for simple hybrid systems are **undecidable**.

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I. Give up



"I can't find an algorithm, but neither can all these famous people."

The standard bounded reachability problems for simple hybrid systems are **undecidable**.

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2. Don't give Up

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A. Find a decidable fragment and solve it

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Given $\delta \in \mathbb{Q}^+$, $\llbracket H^{\delta} \rrbracket$ and $\llbracket goal^{\delta} \rrbracket$ over-approximate $\llbracket H \rrbracket$ and $\llbracket goal \rrbracket$

 δ -reachability problem asks for one of the following answers:



Unreachable

δ-reachable

δ [[H]] [goal]^δ

Given $\delta \in \mathbb{Q}^+$, $\llbracket H^{\delta} \rrbracket$ and $\llbracket goal^{\delta} \rrbracket$ over-approximate $\llbracket H \rrbracket$ and $\llbracket goal \rrbracket$

 δ -reachability problem asks for one of the following answers:



- Decidable for a wide range of nonlinear hybrid systems
 - polynomials, log, exp, trigonometric functions, ...

Given $\delta \in \mathbb{Q}^+$, $\llbracket H^{\delta} \rrbracket$ and $\llbracket goal^{\delta} \rrbracket$ over-approximate $\llbracket H \rrbracket$ and $\llbracket goal \rrbracket$

 δ -reachability problem asks for one of the following answers:



- Decidable for a wide range of nonlinear hybrid systems
- Reasonable complexity bound (PSPACE-complete)



Unreachable

I. "Unreachable" answer is sound.



2. Analysis is parameterized by δ

If using a delta (δ) leads to an **infeasible** counterexample, you may try a **smaller delta** (δ ') and possibly get rid of it.



3. Robustness (in verification context)



3. Robustness (in verification context) If your safe system is δ -unsafe under a reasonably small δ , then it indicates that your system is not robust.
δ-Reachability Analysis of Hybrid Systems

"δ-reachability analysis checks robustness which implies safety."

δ-Reachability Analysis of Hybrid Systems



dReach: Bounded delta-reachability analysis tool for Hybrid Systems

Encode reachability problems of hybrid systems to first-order formulas over real numbers, which are solved by a delta-decision procedure, dReal.

Input Format (drh) for Hybrid System

```
#define D 0.45
#define K 0.9
[0, 15] x;
                                                              12
[9.8] g;
[-18, 18] v;
                                                                      21
[0, 3] time;
{
   mode 1;
    invt: (v <= 0);
          (x >= 0);
    flow: d/dt[x] = v;
                                                                         25 31
                                                                   17
          d/dt[v] = -q - (D * v ^ 2);
    jump: (x = 0) = 0 (and (x' = x) (v' = -K * v)); }
{
    mode 2;
    invt: (v >= 0);
          (x >= 0);
    flow: d/dt[x] = v;
          d/dt[v] = -q + (D * v ^ 2);
    jump: (v = 0) = 0 (and (x' = x) (v' = v)); }
init: (1 (and (x \ge 5) (v = 0)));
goal: (and (x \ge 0.45));
```

Inelastic bouncing ball with air resistance

Can a system run into an **unsafe** region after making k steps?



Can a system run into an **unsafe** region after making k steps?



$$Init(\vec{x}_{0}) \wedge flow_{q_{0}}(\vec{x}_{0}, \vec{x}_{0}^{t}, t_{0}) \wedge jump_{q_{0} \to q_{1}}(\vec{x}_{0}^{t}, \vec{x}_{1})$$

$$x_{0}^{t} = x_{0} + \int_{0}^{t_{0}} v \, dt$$

$$v_{0}^{t} = v_{0} + \int_{0}^{t_{0}} -9.8 - 0.45v^{2} \, dt$$

Can a system run into an unsafe region after making k steps?



Can a system run into an **unsafe** region after making k steps?



 $Init(\vec{x}_{0}) \wedge flow_{q_{0}}(\vec{x}_{0}, \vec{x}_{0}^{t}, t_{0}) \wedge jump_{q_{0} \to q_{1}}(\vec{x}_{0}^{t}, \vec{x}_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge jump_{q_{1} \to q_{2}}(\vec{x}_{1}^{t}, \vec{x}_{2})$

Can a system run into an unsafe region after making k steps?



 $Init(\vec{x}_{0}) \wedge flow_{q_{0}}(\vec{x}_{0}, \vec{x}_{0}^{t}, t_{0}) \wedge jump_{q_{0} \to q_{1}}(\vec{x}_{0}^{t}, \vec{x}_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge jump_{q_{1} \to q_{2}}(\vec{x}_{1}^{t}, \vec{x}_{2}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge jump_{q_{1} \to q_{2}}(\vec{x}_{1}^{t}, \vec{x}_{2}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{2}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, t_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, t_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, t_{1}^{t}$

 $flow_{q_k}(\vec{x}_k, \vec{x}_k^t, t_k)$

Can a system run into an unsafe region after making k steps?



$$Init(\vec{x}_{0}) \wedge flow_{q_{0}}(\vec{x}_{0}, \vec{x}_{0}^{t}, t_{0}) \wedge jump_{q_{0} \to q_{1}}(\vec{x}_{0}^{t}, \vec{x}_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge jump_{q_{1} \to q_{2}}(\vec{x}_{1}^{t}, \vec{x}_{2}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge jump_{q_{1} \to q_{2}}(\vec{x}_{1}^{t}, \vec{x}_{2}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{2}^{t}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{2}^{t}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{2}^{t}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{1}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{2}^{t}) \wedge flow_{q_{1}}(\vec{x}_{1}, \vec{x}_{2}^{t}, t_{1}) \wedge flow_{q_{1}}(\vec{x}_{1}, t_$$

 $flow_{q_k}(\vec{x}_k, \vec{x}_k^t, t_k) \wedge Unsafe(\vec{x}_k^t)$

Can a system run into an unsafe region after making k steps?



$$\exists \vec{x}_0, \vec{x}_1, \dots, \vec{x}_k \exists \vec{x}_0^t, \vec{x}_1^t, \dots, \vec{x}_k^t \exists t_0, t_1, \dots, t_k \\ Init(\vec{x}_0) \land flow_{q_0}(\vec{x}_0, \vec{x}_0^t, t_0) \land jump_{q_0 \to q_1}(\vec{x}_0^t, \vec{x}_1) \land \\ flow_{q_1}(\vec{x}_1, \vec{x}_1^t, t_1) \land jump_{q_1 \to q_2}(\vec{x}_1^t, \vec{x}_2) \land$$

 $flow_{q_k}(\vec{x}_k, \vec{x}_k^t, t_k) \wedge Unsafe(\vec{x}_k^t)$

Decision Problem



Standard Form

$$\phi := \exists^{\mathbf{I}} \mathbf{x} \bigvee_{i} \bigwedge_{j} f_{i,j}(\mathbf{x}) = 0$$

δ-Decision Problem



 $\delta \text{-Weakening of } \varphi$ $\phi^{\delta} := \exists^{\mathbf{I}} \mathbf{x} \bigvee_{i} \bigwedge_{j} |f_{i,j}(\mathbf{x})| \leq \delta$



- SAT solver finds a satisfying Boolean assignment
- Theory solver checks whether the assignment is feasible under the first order theory of Real



- SAT solver finds a satisfying Boolean assignment
- Theory solver checks whether the assignment is feasible under the first order theory of Real



$$\exists x. \ (l_1 \land l_2) \implies (l_3 \lor l_4 \lor l_5)$$
$$l_1 := x > 4$$
$$l_2 := x < 10$$
$$l_3 := x^2 < 10$$
$$l_4 := x^2 - 6x + 9 = 0$$
$$l_5 := \cos(x) < 0.5$$

- SAT solver finds a satisfying Boolean assignment
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Main Algorithm of Theory Solver



Main Algorithm of Theory Solver: ICP(Interval Constraint Propagation)



Main Algorithm of Theory Solver: ICP(Interval Constraint Propagation)



Contracting interval domains associated to variables of Real without removing any value that is consistent with a set of constraints

Main Algorithm of Theory Solver: ICP(Interval Constraint Propagation)



Two Termination Conditions of ICP



 $\exists x, y \in [0.5, 1.0] : y = sin(x) \land y = atan(x)$



ANSWER: UNSAT



 $\exists x, y \in [0.5, 1.0] : y = \sin(x) \land y = \operatorname{atan}(x)$







 $\exists x, y \in [0.5, 1.0] : y = \sin(x) \land y = atan(x)$



x : [0.524, 1.0], *y* : [0.5, 0.841]





- $y' = y \cap \operatorname{atan}(x)$
 - $= [0.5, 0.841] \cap atan([0.546, 1.0])$
 - $= [0.5, 0.841] \cap [0.5, 1.0]$
 - = [0.5, 0.785]

 $\exists x, y \in [0.5, 1.0] : y = sin(x) \land y = atan(x)$



x : [0.524, 1.0], *y* : [0.5, 0.785]


















Unsat



ANSWER: SAT

 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$



 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$

Begin 🛛 🗴 dim : 🛛 x 😒 y dim : 🛛 y 😂 Next



Pruning Applied

 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$

Begin 🗴 dim : 🗙 📀 y dim : y 📀 Next



After steps, pruning reaches a fixed point.

 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$

Begin X dim : 🗴 😒 Y dim : 🗴 🗘 Next



Branching on X

 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$

Begin 🛛 🗴 dim : 🛛 x 😒 y dim : 🛛 y 😂 🛛 Next



Apply Pruning on the Left-hand Box

 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$

Begin 🗴 dim : 🗙 📀 y dim : y 📀 Next



After pruning steps, it shows that left-hand box contains NO solution.

 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$

Begin 🗴 dim : 🗴 📀 y dim : 🗴 y 😂 Next



Apply Pruning on the Right-hand Box

 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$

Begin 🛛 🗴 dim : 🛛 x 😒 y dim : 🛛 y 😒 🛛 Next



Apply Pruning on the Right-hand Box

 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$

Begin 🗴 dim : 🗙 📀 y dim : y 📀 Next



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Apply Pruning on the Right-hand Box

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Begin 🗴 dim : 🗙 😒 y dim : y 😂 Next



 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$



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 $\exists x \in [0.5, 2.0], y \in [0.0, 2.0] : y = sin(x) \land y = atan(x)$

Begin 🛛 🗴 dim : 🛛 x 😒 y dim : 🛛 y 😒 🛛 Next



Found a small enough Box (width <= 0.001) Answer: delta-SAT

Main Algorithm of ICP

```
Algorithm 1: Theory Solving in DPLL(ICP)
    input : A conjunction of theory atoms, seen as constraints,
              c_1(x_1,...,x_n),...,c_m(x_1,...,x_n), the initial interval bounds on all
              variables B^0 = I_1^0 \times \cdots \times I_n^0, box stack S = \emptyset, and precision \delta \in \mathbb{Q}^+.
    output: \delta-sat, or unsat with learned conflict clauses.
 1 S.\operatorname{push}(B_0);
 2 while S \neq \emptyset do
        B \leftarrow S.pop();
 3
        while \exists 1 \leq i \leq m, B \neq \text{Prune}(B, c_i) do
 4
             //Pruning without branching, used as the assert() function.
 5
                                                                                                        Pruning
             B \leftarrow \operatorname{Prune}(B, c_i);
        \mathbf{end}
 6
         //The \varepsilon below is computed from \delta and the Lipschitz constants of
 7
         functions beforehand.
        if B \neq \emptyset then
 8
             if \exists 1 \leq i \leq n, |I_i| \geq \varepsilon then
 9
                  \{B_1, B_2\} \leftarrow \text{Branch}(B, i); //\text{Splitting on the intervals}
10
                  S.push(\{B_1, B_2\});
                                                                                                      Branching
             else
11
                 return \delta-sat; //Complete check() is successful.
12
             end
13
       \mathbf{end}
14
15 end
16 return unsat;
```

Pruning using ODEs

$$X_t = X_0 + \int_0^T flow(x(s)) \mathrm{d}s$$



pruning on Xt

How can we prune X_t ?



(numerically) Compute the enclosures of the solutions of ODE



(numerically) Compute the enclosures of the solutions of ODE



Take the intersection between the Enclosure and Xt

Pruning using ODEs (Backward)



Pruning on X₀

Pruning using ODEs (on Time)



Pruning using ODEs (on Time)



Pruning using ODEs (on Time)



Pruning using ODEs (using Invariant)



dReach: δ-Reachability Analysis of Hybrid Systems



- Open Source, available at <u>https://dreal.github.io</u>
- Support polynomials, transcendental functions and nonlinear ODEs
- Formulas with 100+ ODEs have been solved.

Visualization of Counterexample


Visualization of Counterexample

3-mode Oscillator Model

Mode1 Mode2 Mode3 Mode1 Mode2 Mode3 -1 --2 --3 --4 --5 -Ζ 0.0 --0.5 --1.0 --1.5 --2.0 -Λ -0.5 -1.0 Х -1.5 6 4 2 0 tau 2.5 2.0 1.5 1.0 0.5 0.0 omega2 2.0 1.5 1.0 0.5 omega1

Applications

- * Cardiac Cells, Prostate Cancer (CMU, GIT, TU Vienna)
- * Prostate Cancer (CMU, UPITT)
- * Power-train Control, Validated Planning (Toyota Research Labs)
- * Microfluidic Chip Designs (Univ. of Waterloo)
- * Analog Circuits (City University London)
- * Quadcopter Control, Autonomous Driving (CMU)
- * FDA-accepted non-linear hybrid physiological model for diabetes, (UPENN)

Tools based on dReal/dReach

- * APEX: A Tool for Autonomous Vehicle Plan Verification and Execution (Toyota)
- * ProbReach: Probabilistic reachability analysis of hybrid systems (Univ. of Newcastle)
- * BioPSy: Parameter set synthesis on biological models (Univ. of Newcastle)
- * SReach: Bounded model checker for stochastic hybrid systems (CMU)
- * Osmosis: Semantic importance sampling for statistical model checking (CMU SEI)
- * Sigma: Probabilistic programming language (MIT)

Conclusion

- * δ-reachability analysis checks robustness of hybrid systems which implies safety.
- * **Decidable** (PSPACE-Complete)
- * Use dReal, δ -SMT solver supporting nonlinear functions/ODEs
- * Based on DPLL (ICP) framework
- * Open-source: available at <u>http://dreal.github.io</u>

Future Work

- * Scalability
 - * Learning & Non-chronological Backtracking in ICP
 - * Parallelization
- * Expressiveness
 - * Support Exist-Forall formulas (for optimization problems)
 - * Support PDEs (Partial Differential Equations)
- * Generating Certificate for UNSAT cases
 - * Already have a prototype independent type-checker
 - * Plan to generate Lean/Coq proofs

147. Table 3 / Carrom Table Function [58] (Continuous, Differentiable, Non-Separable, Non-Scalable, Multimodal)

$$f_{147}(\mathbf{x}) = -[(\cos(x_1)\cos(x_2)) \\ \exp|1 - [(x_1^2 + x_2^2)^{0.5}]/\pi|)^2]/30$$

subject to $-10 \le x_i \le 10$. x2 -10 -10 x1 -5 -5 0 5 0 10 5 0 10 -5 -10 -15 -20 f(-9.6709, -9.6584) = -24.3100 -25

Momin Jamil and Xin-She Yang, A literature survey of benchmark functions for global optimization problems, Int. Journal of Mathematical Modelling and Numerical Optimisation Whitley Function [86] (Continuous, Differentiable, Non-Separable, Scalable, Multimodal)



Momin Jamil and Xin-She Yang, A literature survey of benchmark functions for global optimization problems, Int. Journal of Mathematical Modelling and Numerical Optimisation

Any Questions?

FAQs

Q1. How to pick ϵ from a given $\delta \in Q^+$ in ICP Algorithm? A1:

- For all $f_i,$ find ϵ_i such that

$$\forall \vec{x}, \vec{y} \in B, ||x - y|| < \epsilon_i \implies |f_i(\vec{x}) - f_i(\vec{y})| < \delta$$

- Fix ϵ be the minimum of $\epsilon_i s$

$$\epsilon = \min(\epsilon_1, \ldots, \epsilon_n)$$

FAQs

Q2. Lipschitz continuity?

A2: A Lipschitz continuous function is limited in how fast it can change: there exists a definite real number K such that, for every pair of points on the graph of this function, the absolute value of the slope of the line connecting them is not greater than this real number; this bound is called a "Lipschitz constant" of the function (or "modulus of uniform continuity").

$$\frac{d_Y(f(x_1), f(x_2))}{d_X(x_1, x_2)} \le K.$$