## Input Attribution for Statistical Model Checking using Logistic Regression

Jeff Hansen

September 23, 2016

Software Engineering Institute Carnegie Mellon University Pittsburgh, PA 15213



This material is based upon work funded and supported by the Department of Defense under Contract No. FA8721-05-C-0003 with Carnegie Mellon University for the operation of the Software Engineering Institute, a federally funded research and development center.

NO WARRANTY. THIS CARNEGIE MELLON UNIVERSITY AND SOFTWARE ENGINEERING INSTITUTE MATERIAL IS FURNISHED ON AN "AS-IS" BASIS. CARNEGIE MELLON UNIVERSITY MAKES NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED, AS TO ANY MATTER INCLUDING, BUT NOT LIMITED TO, WARRANTY OF FITNESS FOR PURPOSE OR MERCHANTABILITY, EXCLUSIVITY, OR RESULTS OBTAINED FROM USE OF THE MATERIAL. CARNEGIE MELLON UNIVERSITY DOES NOT MAKE ANY WARRANTY OF ANY KIND WITH RESPECT TO FREEDOM FROM PATENT, TRADEMARK, OR COPYRIGHT INFRINGEMENT.

[Distribution Statement A] This material has been approved for public release and unlimited distribution. Please see Copyright notice for non-US Government use and distribution.

This material may be reproduced in its entirety, without modification, and freely distributed in written or electronic form without requesting formal permission. Permission is required for any other use. Requests for permission should be directed to the Software Engineering Institute at permission@sei.cmu.edu.

DM-0004023



Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Carnegie Mellon University

## **Motivating Example**

### Pursuer/Evader Example

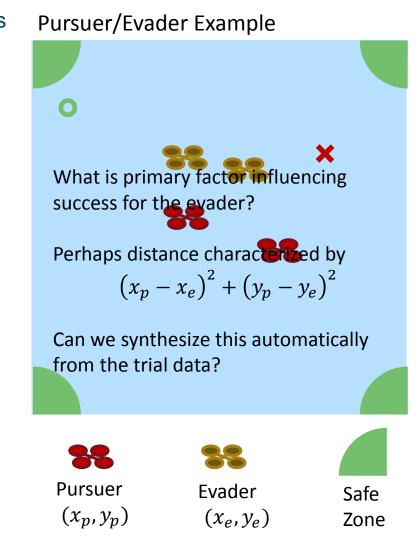
- Pursuer and Evader given random initial positions  $(x_p, y_p)$  and  $(x_e, y_e)$  near center of region.
- Evader attempts to reach safe zone in corner.
- Faster moving pursuer attempts to catch evader before it reaches safe zone.

### Statistical Model Checking (SMC)

- Let  $\mathcal{M}$  be the model for the pursuer/evader scenario and  $\Phi$  be the property "the evader reaches safe zone".
- SMC attempts to answer the question, "What is the probability that *M* ⊨ Φ? "

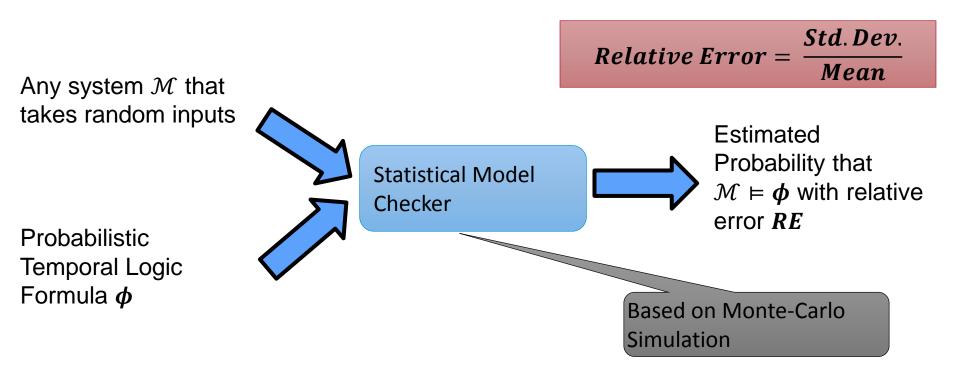
### Input Attribution (IA)

- Asks the question "Why do I get a particular probability estimate?"
- Analog to counter-example in model checking.
- Expressed in terms of the inputs as approximation for the model?



Distribution Statement A Approved for Public Release; Distribution is Unlimited

## **Statistical Model Checking (SMC)**



- System properties described in formal language (UTSL, BLTL, etc.)
- Property is tested on "sample trajectories" (sequence of states)
- Each outcome can be treated as a Bernoulli random variable (i.e., coin flip)

### **Statistical Model Checking with Crude Monte-Carlo**

The probability that condition  $\Phi$  holds in model  $\mathcal{M}$  when the input  $\vec{x}$  is distributed according to joint pdf  $f(\vec{x})$  is the expected value of that indictor function and can be calculated as:

$$p = E[I_{\mathcal{M} \models \Phi}(\vec{x})] = \int I_{\mathcal{M} \models \Phi}(\vec{x}) f(\vec{x}) d\vec{x}$$

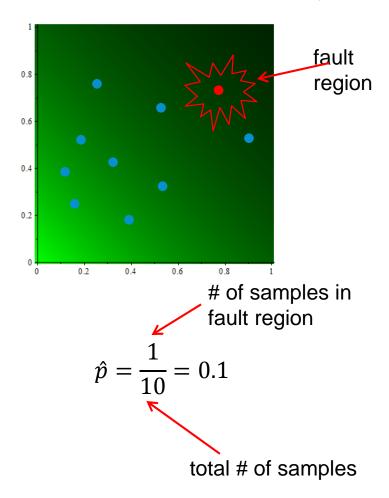
where  $I_{\mathcal{M}\models\Phi}(\vec{x})$  is an indicator function for the model. This can be estimated with Crude Monte-Carlo simulation as:

$$\hat{p} = \frac{1}{N} \sum_{i=1}^{N} I_{\mathcal{M} \models \Phi}(\vec{x}_i)$$

where each  $\vec{x}_i$  is a sample vector drawn from  $f(\vec{x})$ . As *N* gets large,  $\hat{p}$  will converge to *p*.

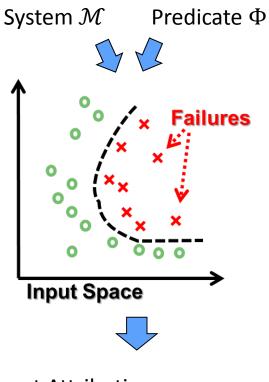
For low probabilities, approximate number of samples required to evaluate to a relative error of RE is:  $N \approx \frac{1}{p(RE)^2}$ 

#### **Estimated Failure Probability**



Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Carnegie Mellon University

## Input Attribution – The "Why" of SMC



#### **Input Attribution**

Expression	p-Value
$0.62(a - 1.01d)^2$	0.0013
4.3 <i>b</i>	0.0042
$1.3(2.3-c)^{2}$	0.0172

Problem – Standard SMC provides an estimate on probability that a predicate is satisfied, but does not address why a particular result was obtained.

Goal – Provide investigator with informative nonredundant representation of how system inputs relate to the property being tested:

- 1. Describes relationship that actually exists in data
- 2. Is presented in a way that is quantitative and understandable
- 3. Gives investigator new insights
- 4. Is resilient to randomness in the system

Approach – Apply machine learning and feature extraction techniques.

- Use *Logistic Regression* to identify "predictors" that affect the probability that a predicate is satisfied.
- Calculate p-values for predictors to indicate significance.
- Look for sets of predictors that can be factored into larger expressions.

## **Odds vs Probability**

Logistic Regression reasons about "odds"

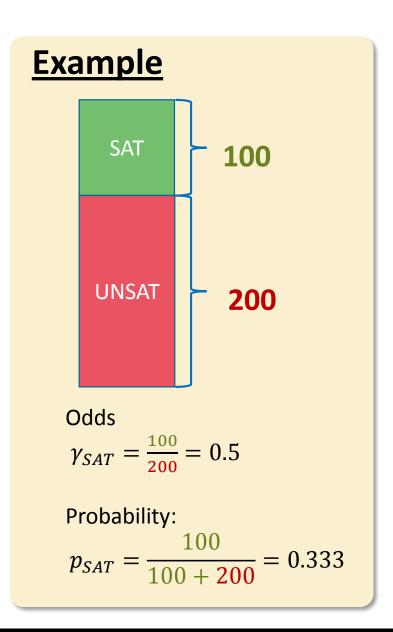
- Alternate representation of probability
- Think of horse racing odds like "7:1".
- The odds γ of event is related to the probability p as:

$$p = \frac{\gamma}{\gamma + 1} = \frac{1}{1 + 1/\gamma}$$

Odds fall in interval:

 $0 < \gamma < \infty$ 

- Log of odds fall in interval:  $-\infty < \log(\gamma) < \infty$
- Unbounded nature of "log odds" makes it suitable for linear regression analysis.



Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Carnegie Mellon University

## Logistic Regression (LR)

Logistic Regression

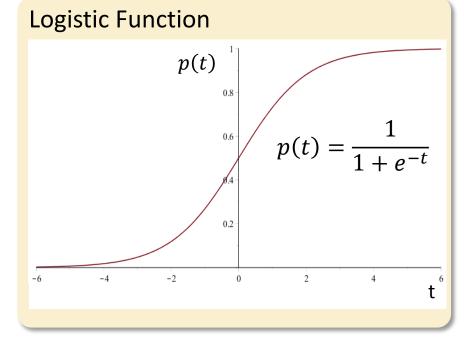
- Regression model useful when dependent variable is Boolean.
- Based on the logistic function.
- Linear fit of the log of the "odds".
- Estimates probability that for a particular input the result variable will be true.

Input

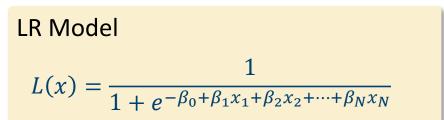
 Set of "trials" consisting of vectors of "predictors" (e.g., input variables) and a dependent Boolean random variable.

### Output

- Set of coefficients for each predictor that fit a linear expression.
- Standard error for each predictor from which a p-Value can be computed.



Log Odds or "Logit"  $t = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_N x_N$ 



Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Carnegie Mellon University 10

## **Evaluating LR Results (Linear Case)**

The factor by which the log odds of a predicate will increase per unit increase of input. Positive values represent increase and negative values represent decrease.

	Name	ß	Std.Err.	p-Value		
Constant Term	_	-4.28	0.874	0.0000		
ſ	а	0.154	0.0138	0.0000		
Predictors	b	-1.91	0.3551	0.0000		
Predictors	С	0.0635	0.0277	0.0219		
l	d	5.05	2.77	0.0685	}	
Error in estimation of $\beta$ .						

- Calculated by applying inverse normal distribution to ratio of standard error and β.
- Represents probability that  $\beta = 0$  can explain the data.
- Values above a threshold (e.g., 0.05) indicate relation between input and predicate is not statistically significant.

This predictor is not statistically significant since its p-value is greater than 0.05.

## **Polynomial Input Attribution**

### **Non-Linear Predictors**

- By including non-linear predictors, it may be possible to find a statistically significant solution when linear only terms fail.
- In our work to date, we have focused on quadratic terms (e.g., x<sup>2</sup>, y<sup>2</sup>, xy)
- Higher order or non-polynomial terms could be useful for some systems.

### Factoring

- Factored polynomials are easier for humans to understand.
- Since coefficients are approximated, perfect factorings may not be possible.
- Look for approximate factorings which do not adversely affect original coefficients.

# Find variable pairs with squares and cross terms

squares and cross terms					
Name	β	Std.Err.	p-Value		
:	÷	:	:		
a <sup>2</sup>	1.01	0.0148	0.0000		
ab	-2.04	0.0362	0.0000		
$b^2$	1.02	0.0193	0.0219		
:	:	:	:		

 $1.01(a - 1.01b)^2$ 

Complete square to create candidate factoring

$$1.01a^2 - 2.04ab + 1.03b^2$$

Re-expand and accept approximation if error is within set factor of std. error.

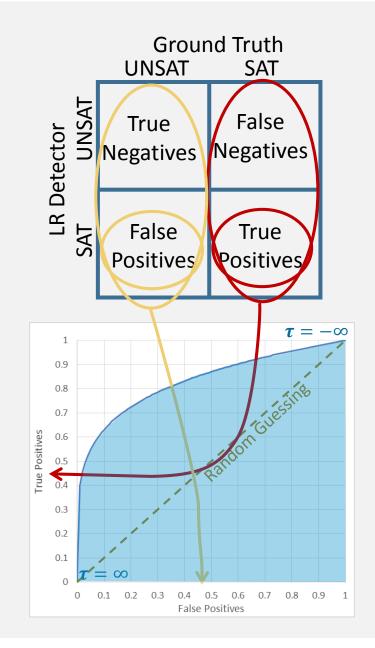
## **Evaluating LR Fit**

Model Verification

- Results of LR only meaningful if overall model fits data.
- LR model *L*(*x*) predicts probability that input *x* will satisfy predicate.

**ROC** Analysis

- ROC curve is plot of
  - true positives  $P[L(x_i) > \tau | \phi_i]$  vs
  - false positives  $P[L(x_i) > \tau | \overline{\phi_i}]$
  - for  $-\infty < \tau < \infty$
- Area Under Curve (AUC)
  - Represents  $P[L(x_{SAT}) > L(x_{UNSAT})]$  where  $x_{SAT}$  and  $x_{UNSAT}$  are arbitrary inputs resulting in SAT and UNSAT of  $\Phi$ .
  - Values range between 0.5 (model is no better than chance) to 1.0 (perfect fit).



Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Carnegie Mellon University 13

## **Evaluating LR Fit**

### Model Verification

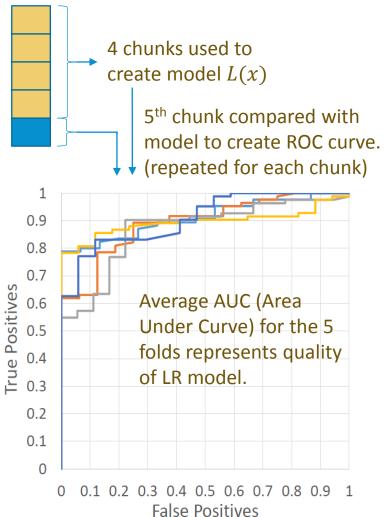
- Results of LR only meaningful if overall model fits data.
- LR model *L*(*x*) predicts probability that input *x* will satisfy predicate.

### **ROC** Analysis

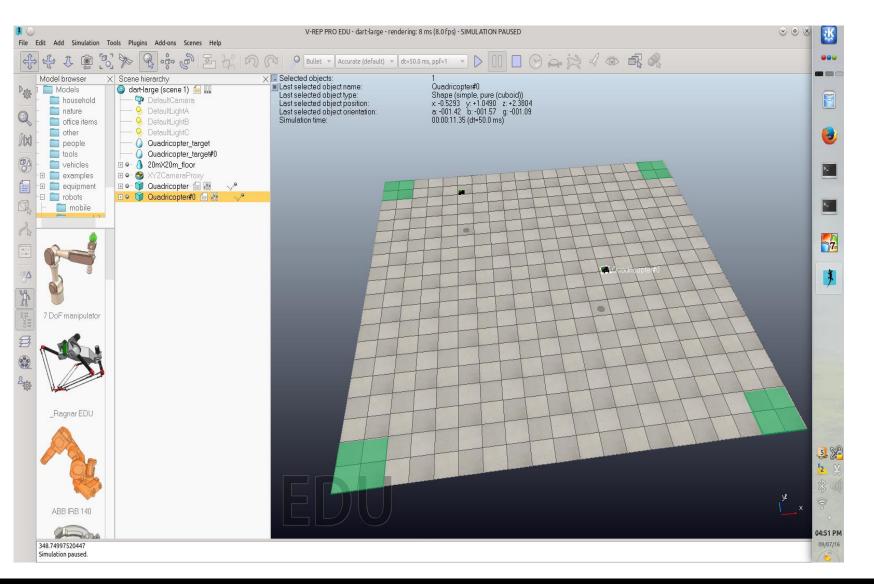
- ROC curve is plot of
  - true positives  $P[L(x_i) > \tau | \phi_i]$  vs
  - false positives  $P[L(x_i) > \tau | \overline{\phi_i}]$
  - for  $-\infty < \tau < \infty$
- Area Under Curve (AUC)
  - Represents  $P[L(x_{SAT}) > L(x_{UNSAT})]$  where  $x_{SAT}$  and  $x_{UNSAT}$  are arbitrary inputs resulting in SAT and UNSAT of  $\Phi$ .
  - Values range between 0.5 (model is no better than chance) to 1.0 (perfect fit).
  - Use average of 5-fold cross validation to avoid bias.

#### 5-Fold Cross Validation

Simulation data with input and predicate results  $x_i$ ,  $\phi_i$  partitioned into 5 chunks



### **V-REP Simulator**





Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Carnegie Mellon University

Distribution Statement A Approved for Public Release; Distribution is Unlimited

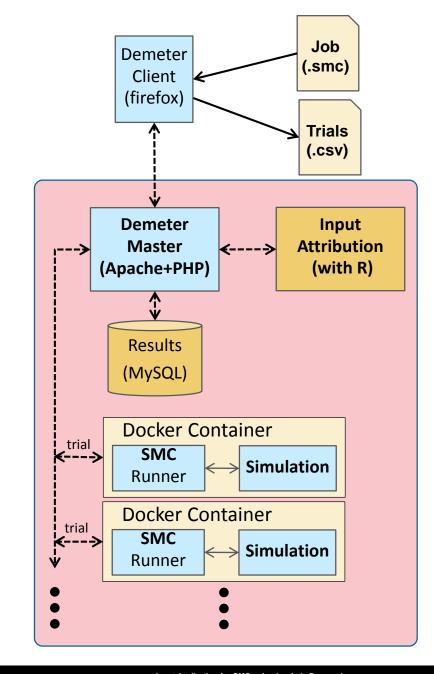
### Demeter

Goal: Develop parallel infrastructure for SMC of systems with probabilistic behaviors.

Primary target is autonomous systems.

Demeter components

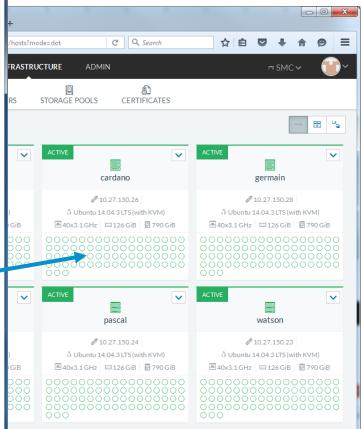
- Client runs in web browser (e.g. firefox)
- Master runs in Apache server with PHP
- Data stored in MySQL database
- Input Attribution uses R statistical system
- Individual simulations conducted in Docker containers. Managed by "Runner".



Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Camegie Mellon University 16

Demeter ← → C'	× watson.ssdla	ab.sei.cmu.edu/smc/						2 ×
E.		Software Engineering Institute     DEMETEI     (Distributed Execution or and Transfer of Empiric	R of Multiple Experiments					
Jobs Trials Runners Machines Log Help		SMC Runners						
Bugs	prev 1 2	3 4 5 6 9 next				Total	of 216 records.	
Č.	Id 🔝	URL	Host	Registered	Status	Job #	Trial #	
	1	http://10.42.185.160:5649	cardano:5:25b03941a080	2016-06-06 14:08:07	Online	169	3206076	
	2	http://10.42.58.227:5649	pascal:2:6b31603b164c	2016-06-06 14:08:07	Online	169	3206077	
	3	http://10.42.174.124:5649	bose:4:f20141699640	2016-06-06 14:08:07	Online	169	3206078	
	4	http://10.42.254.239:5649	germain:6:095c8ec71a29	2016-06-06 14:08:07	Online	169	3206079	
	5	http://10.42.46.139:5649	pascal:8:bf86002bb5d4	2016-06-06 14:08:07	Online	169	3206080	
	6	http://10.42.76.10:5649	cardano:11:57cd640be75c	2016-06-06 14:08:07	Online	169	3206081	
	7	http://10.42.32.223:5649	watson:9:c3770ba616cf	2016-06-06 14:08:07	Online	169	3206082	
	8	http://10.42.73.243:5649	hubble:7:d61840ef695b	2016-06-06 14:08:07	Online	169	3206083	
	9	http://10.42.71.249:5649	hubble:13:caaf57937ffe	2016-06-06 14:08:07	Online	169	3206084	
	10	http://10.42.85.55:5649	hubble:1:b3e12b602606	2016-06-06 14:08:07	Online	169	2205000	
	11	http://10.42.158.117:5649	watson:3:8f918537ad67	2016-06-06 14:08:07	Online	109	3206086	
	12	http://10.42.188.80:5649	watson:15:563d4fc83c75	2016-06-06 14-09 37	Online	169	3206087	
	13	http://10.42.62.115:5649	cardano:17:c5a3091f8fb9 🗖	2016-06-06 14:08:07	Online	169	3206088	
	14	http://10.42.147.142:5649	germain:19:c020f78e4d18	2016-06-06 14:08:07	Online	169	3206089	
	15	http://10.42.187.174:5649	germain:12:8289d11871ef	2016-06-06 14:08:07	Online	169	3206090	
	16	http://10.42.123.138:5649	bose:10:1baf30ac2fae	2016-06-06 14:08:07	Online	169	3206091	
	17	http://10.42.205.24:5649	bose:16:c05500c2e80f	2016-06-06 14:08:07	Online	169	3206092	
	18	http://10.42.201.6:5649	watson:21:f905e333e15e	2016-06-06 14:08:07	Online	169	3206093	
	19	http://10.42.153.133:5649	pascal:14:080c0b5ffdf1	2016-06-06 14:08:07	Online	169	3206094	
	20	http://10.42.194.97:5649	pascal:20:6950d188cc0a	2016-06-06 14:08:07	Online	169	3206095	
	21	http://10.42.223.166:5649	hubble:18:a143bd1136c3	2016-06-06 14:08:07	Online	169	3206096	
	22	http://10.42.54.162:5649	cardano:23:68ff0f727849	2016-06-06 14:08:07	Online	169	3206097	
	23	http://10.42.212.143:5649	bose:22:3c8e474a355e	2016-06-06 14:08:07	Online	169	3206098	
	24			2016-06-06 14:08:07	Online	1(0	3206099	
	24	http://10.42.250.15:5649	pascal:26:b457408b7978	2010-00-00 14:08:07	Onnne	169	5200099	

SMC-Runner operate as a Docker container. Each Docker container is managed by Rancher



Active Job: 169 (batch 111), Runners: 216 (216 busy)



Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Carnegie Mellon University

### **Target/Threat Experiment**

#### Scenario

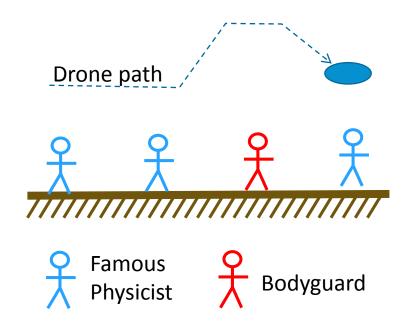
- Drone flies pre-programmed path over area.
- Along path are "targets" to be photographed.
  - Close to ground  $\rightarrow$  Better chance of good photo.
- Path also includes "threats" to be avoided.
  - Close to ground  $\rightarrow$  More likely to be destroyed.
- Adaptive algorithm with imperfect sensors, sense threats ahead and controls altitude.

#### Inputs

- Number of targets/threats
- Target detector range (down)
- Target/Threat detector range/accuracy (forward)
- Threat range

#### Predicate

• Drone photographs at least 50% of targets while avoiding being destroyed by threats.



Distribution Statement A Approved for Public Release; Distribution is Unlimited

## Target/Threat Experiment

#### **Key Observations**

- False positives on threats reduce the probability of detecting targets.
  - Reacting to threats that are not there results in drone flying at higher altitude when not necessary and missing some targets.
- Increasing number of targets reduces probability of survival.
  - Drone takes more risks by flying lower to photograph targets.
- False negatives on threat and target detection do not have statistically significant effect on mission, detection or survival probabilities.
  - Verified with additional simulations varying false negative rate. Could indicate problem with adaptation algorithm controlling drone.

#### **Simulation Results**

#Trials:	22,560
P[SAT-mission]:	0.308
P[SAT-survive]:	0.618
P[SAT-detect]:	0.361
<b>Relative Error:</b>	0.05
Batch Size:	120
Run Time:	10 hours, 6 min

#### Input Attribution (AUC=0.926)

•	Name	β mission	β detect	β survive
	Target Detector Range	1.33	1.46	
	Threat Range	-1.57	-1.189	-2.37
	Threat Lookahead	0.233	0.194	0.377
	Number of Threats	-0.0892	-0.0943	-0.0792
	Number of Targets			-0.0296
	Target False Positives			-17.81
	Threat False Positives	-3.26	-10.04	32.74

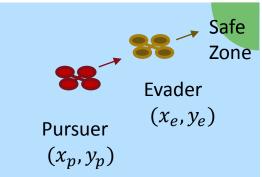
Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Carnegie Mellon University

#### Software Engineering Institute Carnegie Mellon University

Distribution Statement A Approved for Public Release; Distribution is Unlimited

## **Motivating Example - Revisited**

Pursuer/Evader Example



Initial hypothesis was that initial distance between pursuer and evader was deciding factor for survival of evader.

Factoring the IA predictors gives us:  $0.0602(x_e - 1.03x_p)^2 + 0.0561(y_e - 1.09y_p)^2$ 

With error less than  $4se(\beta)$  on each coefficient.

Resulting IA expression very close to square of Euclidean distance. Constant factor represents relation between distance and log odds of survival.

Simulation Results				
#Trials:	36,960			
# SAT:	7,900			
P[SAT]:	0.214			
<b>Relative Error:</b>	0.01			
Batch Size:	120			
Run Time:	5 hours, 20 min			

#### Input Attribution (AUC=0.77)

β	se(β)	p-value			
-0.124	0.0027	$< 10^{-4}$			
-0.122	0.0027	$< 10^{-4}$			
0.06	0.0031	$< 10^{-4}$			
0.056	0.0031	$< 10^{-4}$			
0.056	0.0031	$< 10^{-4}$			
0.056	0.0031	$< 10^{-4}$			
	-0.124 -0.122 0.06 0.056 0.056	-0.124       0.0027         -0.122       0.0027         0.06       0.0031         0.056       0.0031         0.0056       0.0031			

Input Attribution for SMC using Logistic Regression September 29, 2016 © 2016 Carnegie Mellon University 222

### Summary

### Addresses the "Why" of SMC

- Concise human understandable justification for SMC probability estimate
- Modeled as expression correlated with the predicate
- Shows which variables are most important

### **Uses Logistic Regression**

- Regression model useful when dependent variable is Boolean.
- Not dependent on input distribution.
- Commonly used in machine learning applications.

### Extended to Non-Linear Attribution

- Adds non-linear functions of inputs as predictors to model.
- Can find attributions where linear attribution fails.