

Can we extrapolate?

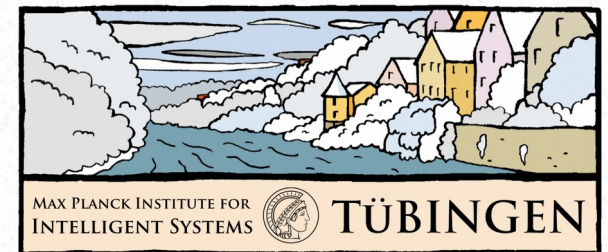
Equation identification for Extrapolation and Control

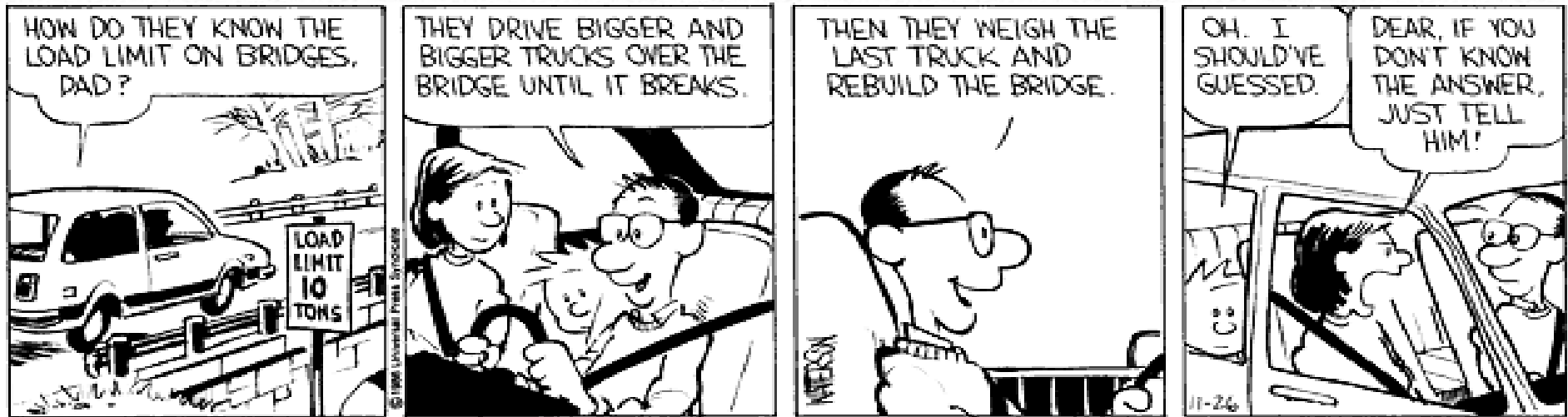
by Georg Martius

MPI for Intelligent Systems, Tübingen
Autonomous Learning Group



MAX-PLANCK-GESELLSCHAFT



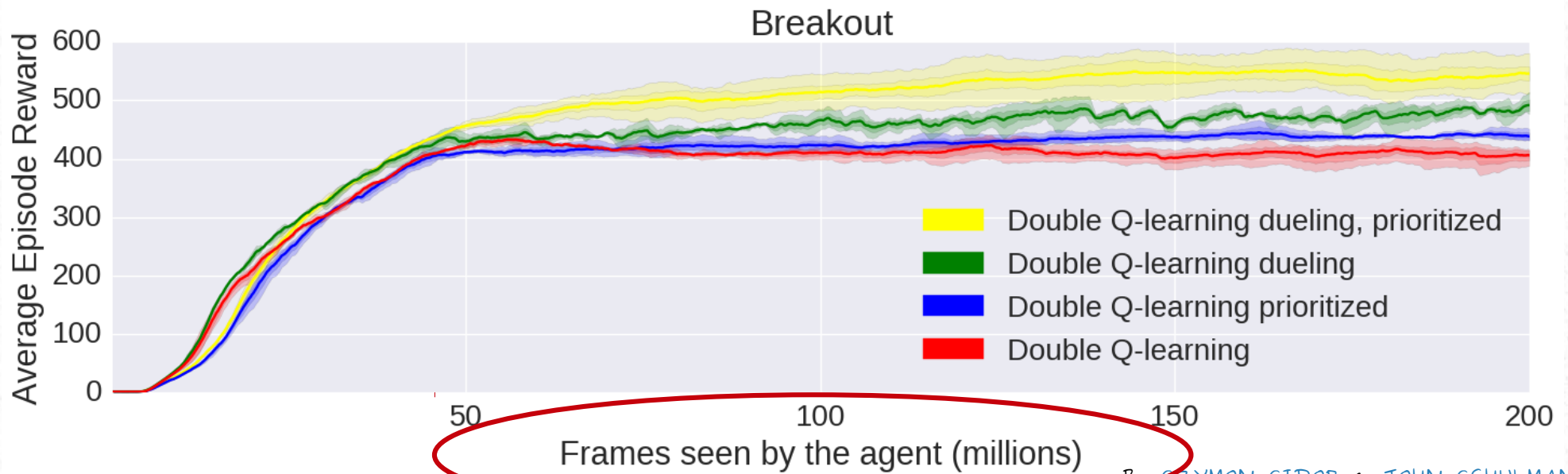


Watterson, B.: [Calvin and Hobbes](#)

Want:

- › extrapolate to unseen domains
- › by identify underlying equations (from observed data)
- › use it to efficiently control a robot
- › get interpretable models

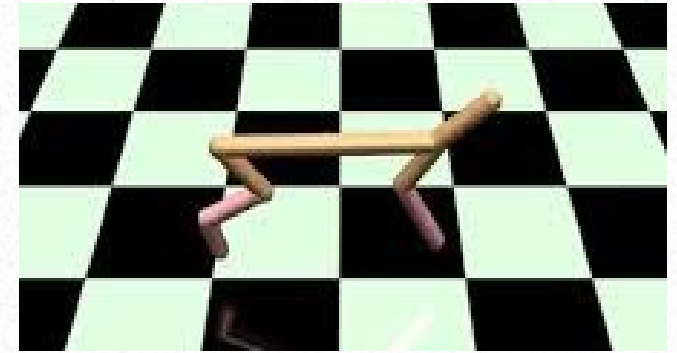
Reinforcement Learning today



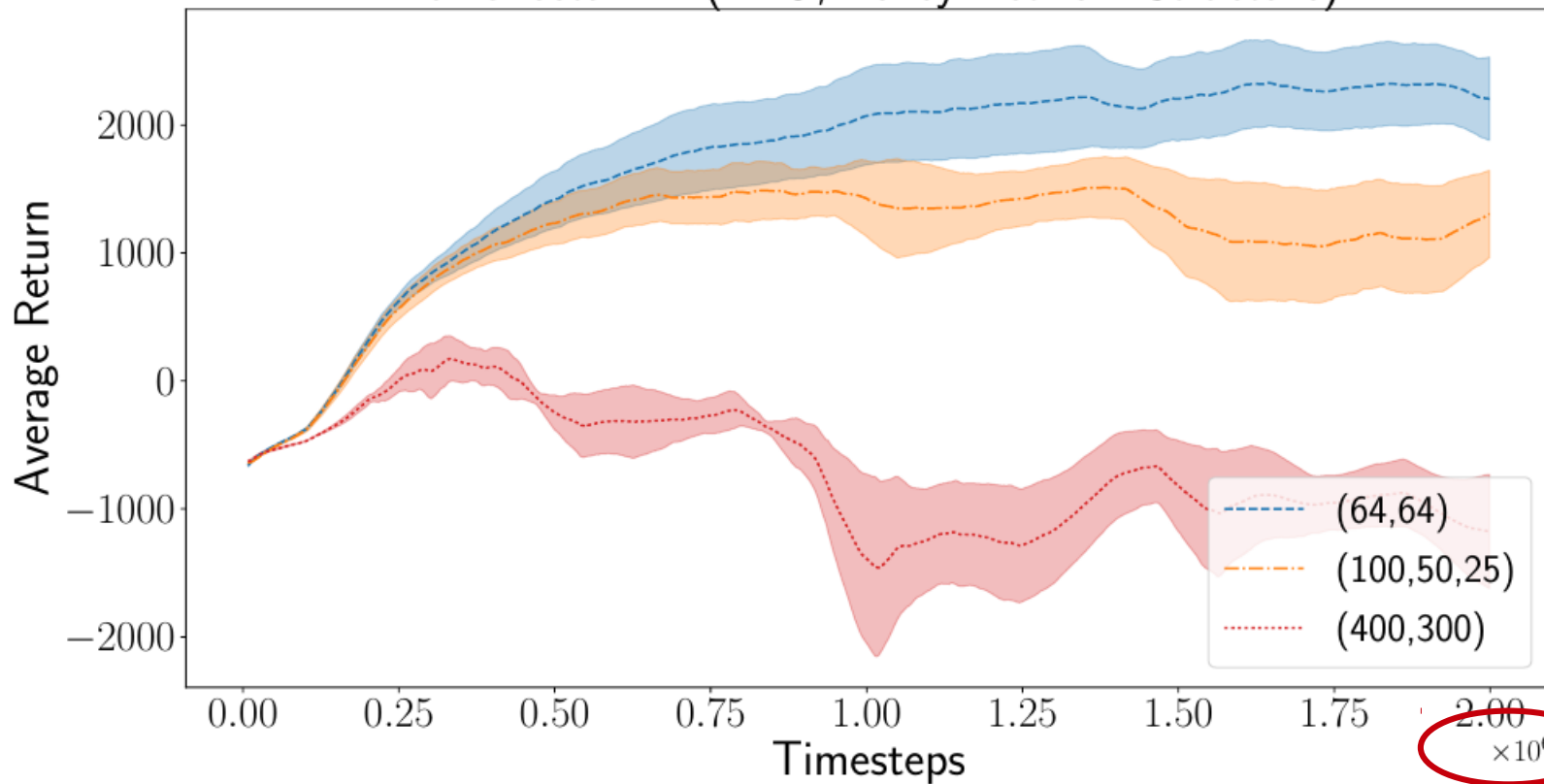
By SZYMON SIDOR & JOHN SCHULMAN
(openai.com)

Reinforcement Learning today

OpenAi Gym Half Cheetah environment



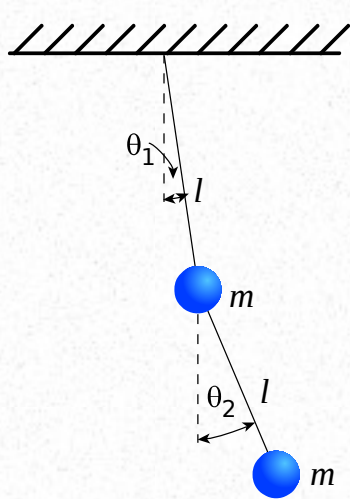
HalfCheetah-v1 (PPO, Policy Network Structure)



Henderson et al 2017

Learning the physics of the world

Example: Learn equation of double pendulum from interaction



$$\dot{\omega}_1 = \frac{g \sin(\theta_1 - 2\theta_2) + 3g \sin(\theta_1) + l\omega_1^2 \sin(2\theta_1 - 2\theta_2) + \dots}{2l(\cos(\theta_1 - \theta_2)^2 - 2)}$$
$$\dot{\omega}_2 = \frac{(-g \sin(2\theta_1 - \theta_2) + g \sin(\theta_2) - 2l\omega_1^2 \sin(\theta_1 - \theta_2) - \dots}{l(\cos(\theta_1 - \theta_2)^2 - 2)}$$

Want:

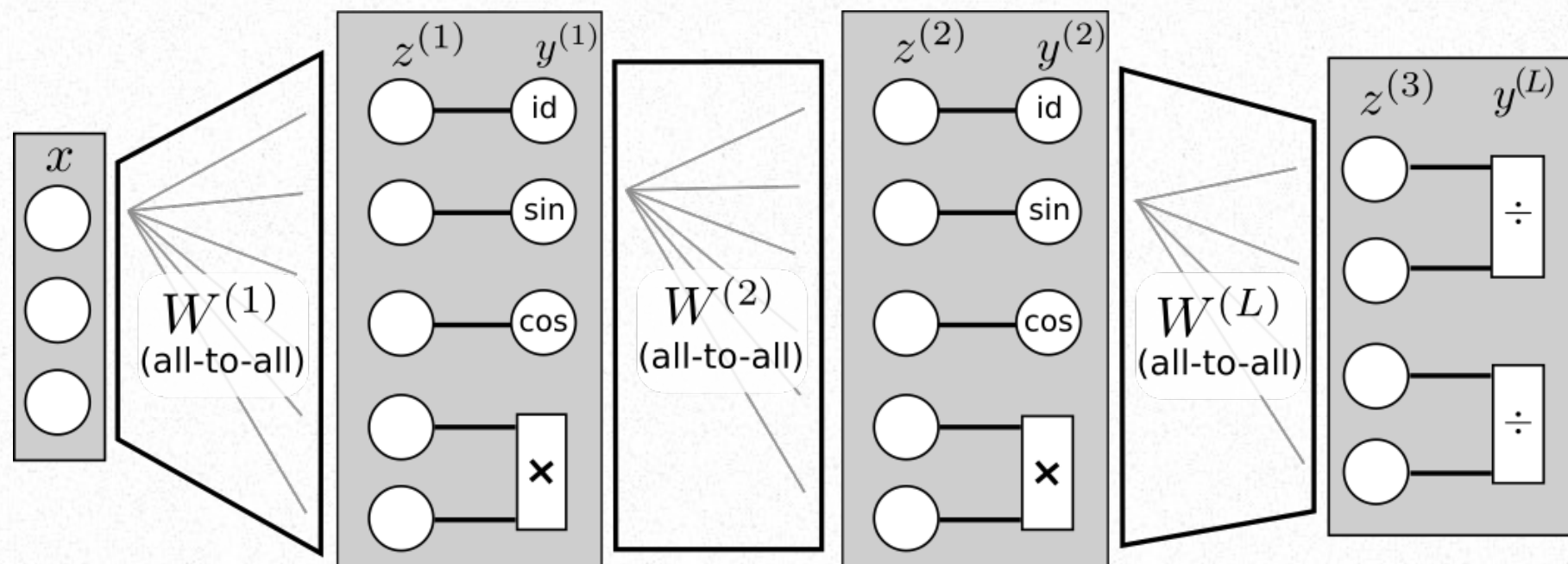
- > identify underlying equations
- > extrapolate to unseen domains

Differentiable Architecture for Equation Learning

Data: $\{(x_1, y_1), (x_2, y_2), \dots\}$

Assumption: $y = f(x) + \text{noise}$

f is in the model class



Replace standard units of NN

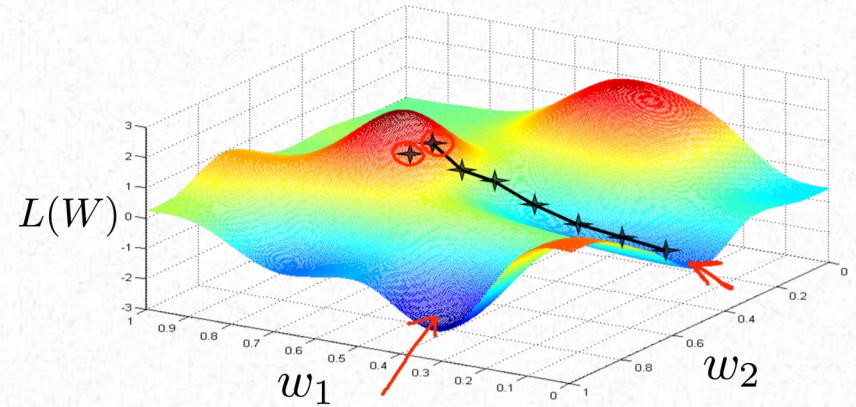
by id , sin , cos , multiplication and division.

Regression with sparsity regularization

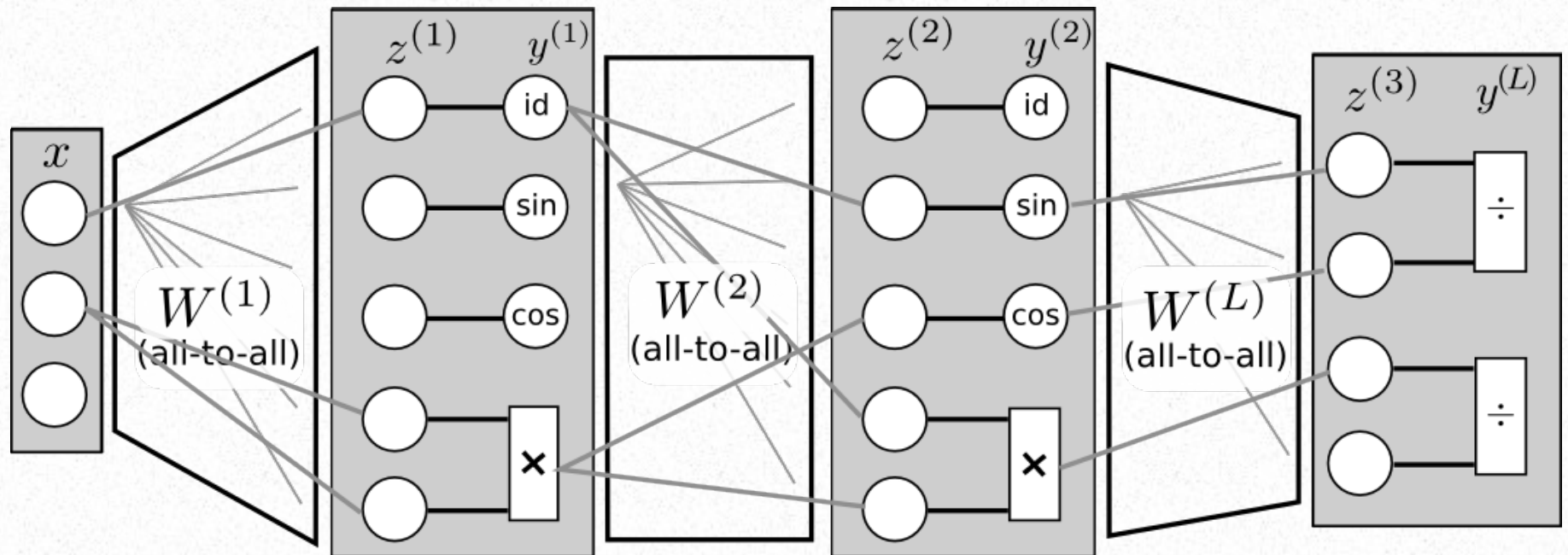
$$E = \sum_{i=1}^n |f(x_i, W) - y_i|^2 + \lambda |W|^1$$

Training by gradient descent

$$\Delta W \propto -\frac{\partial E}{\partial W}$$



if right formula is learned \rightarrow
great extrapolation

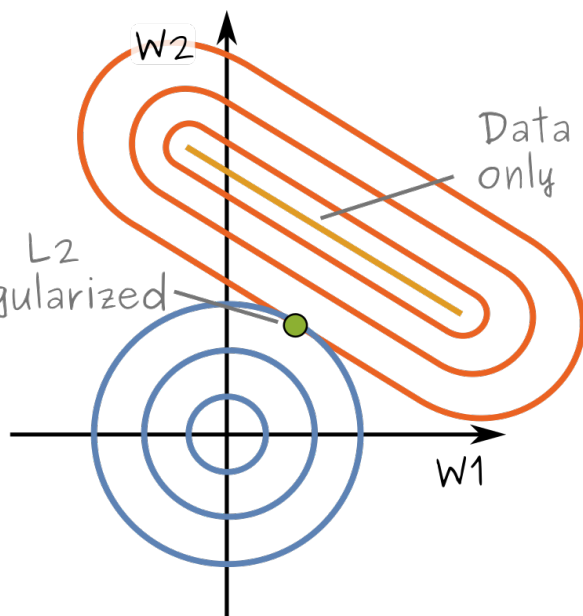


Regularization Phases

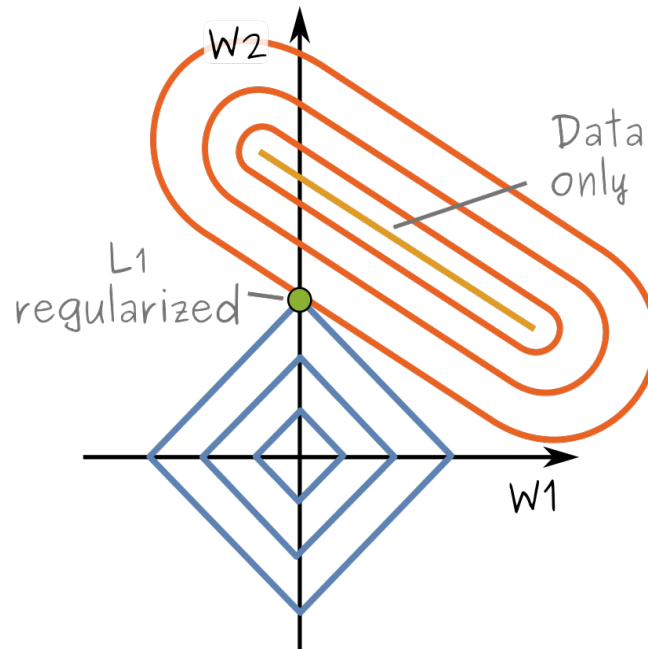
> Want: sparse solution



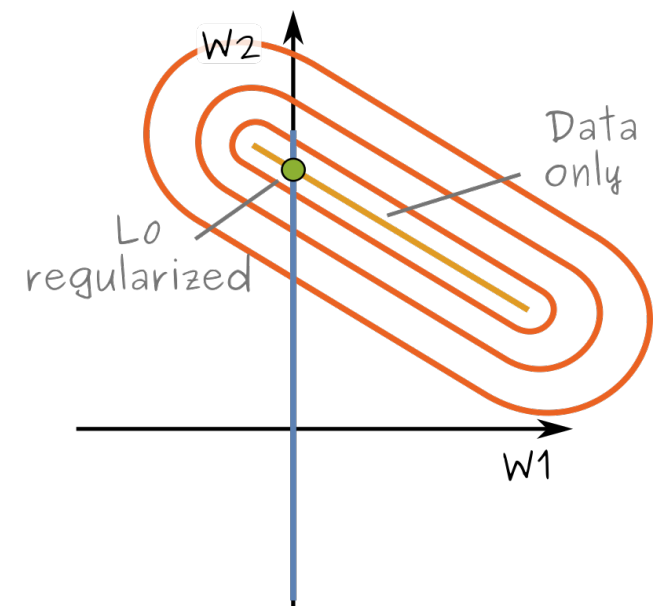
$$L2 - |W|_2^2$$



$$L1 - |W|_1$$



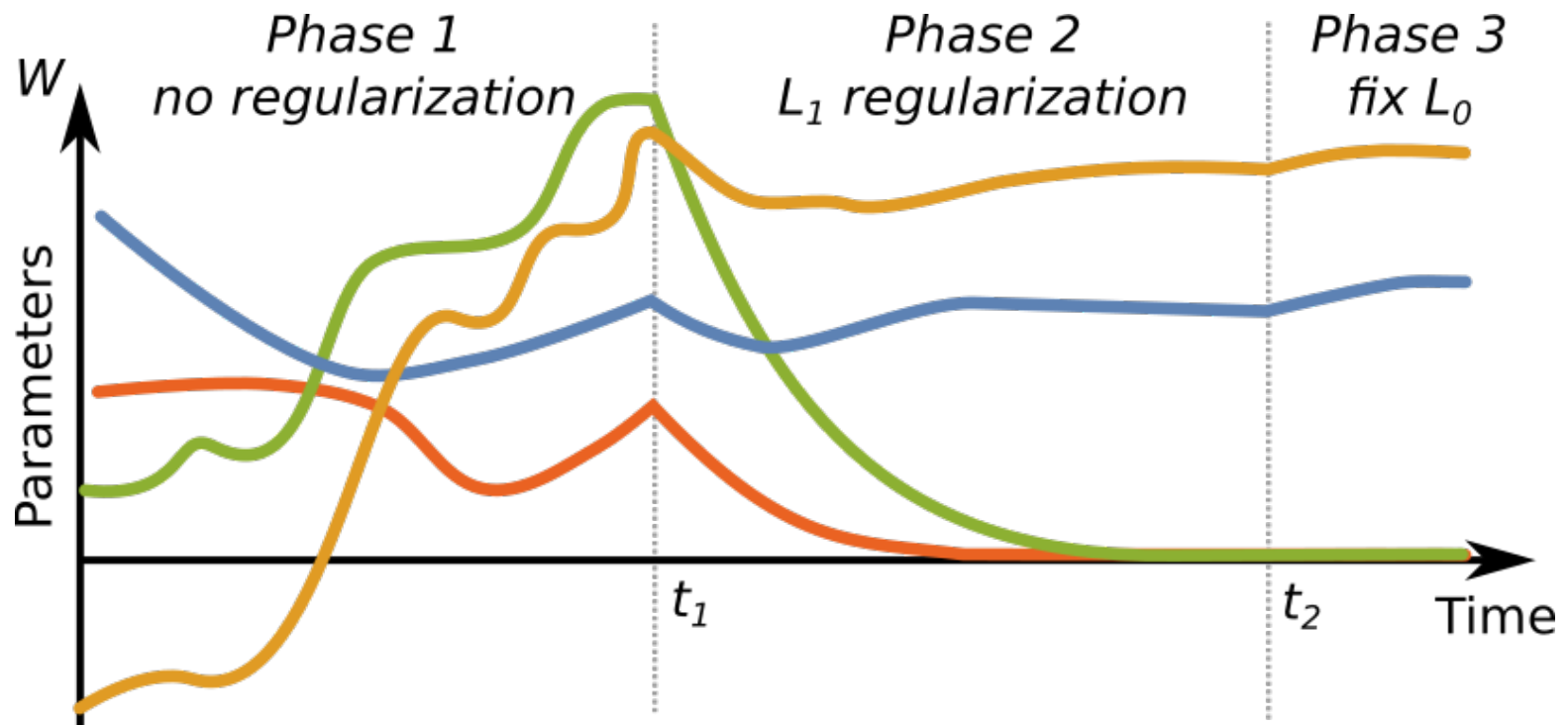
fix $L0$



> (keep tiny weights at 0)

> sparse solution without tradeoff

Regularization Phases



New ways to achieve sparsity: Bayesian compression/learned dropout
ICLR 2018, ArXiv: 1712.01312 by
Christos Louizos, Max Welling, Diederik P. Kingma

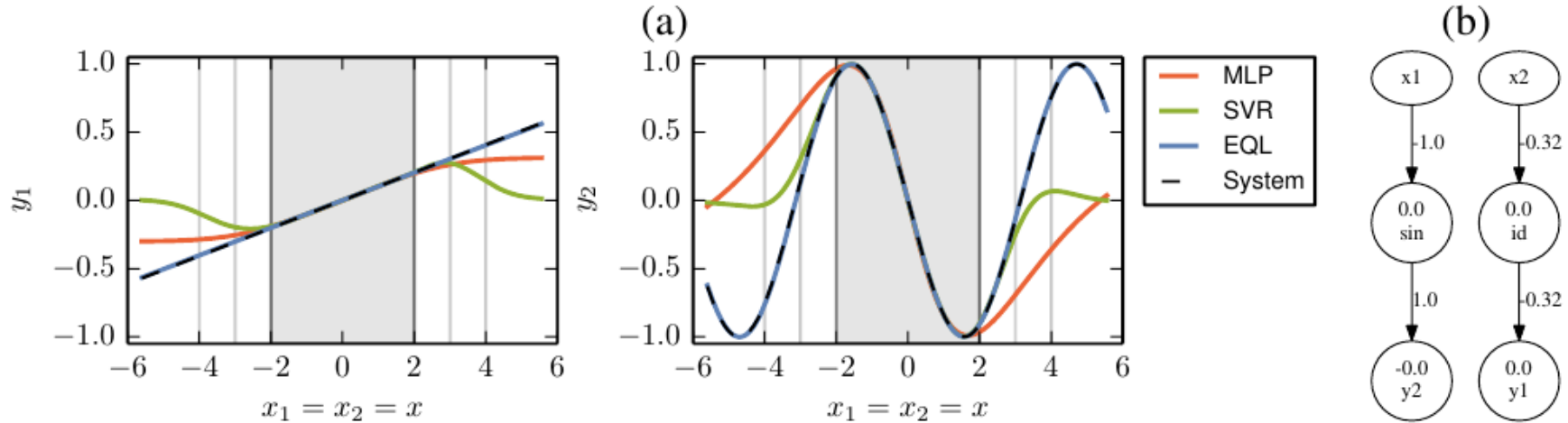
Martius, Lampert arXiv 2016

Pendulum Dynamics

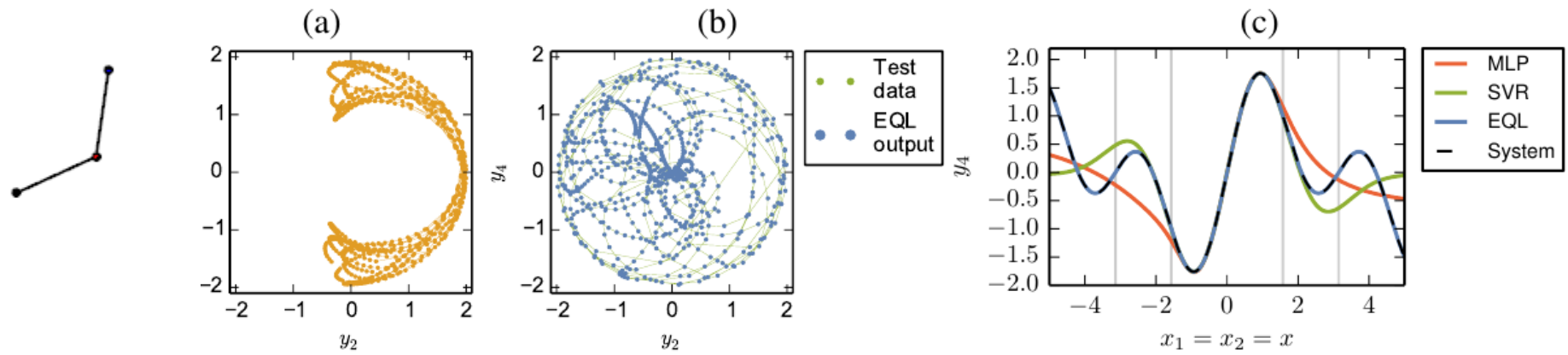
$$\dot{x}_1 = x_2$$

and

$$\dot{x}_2 = -g \sin(x_1),$$



Double Pendulum Kinematics



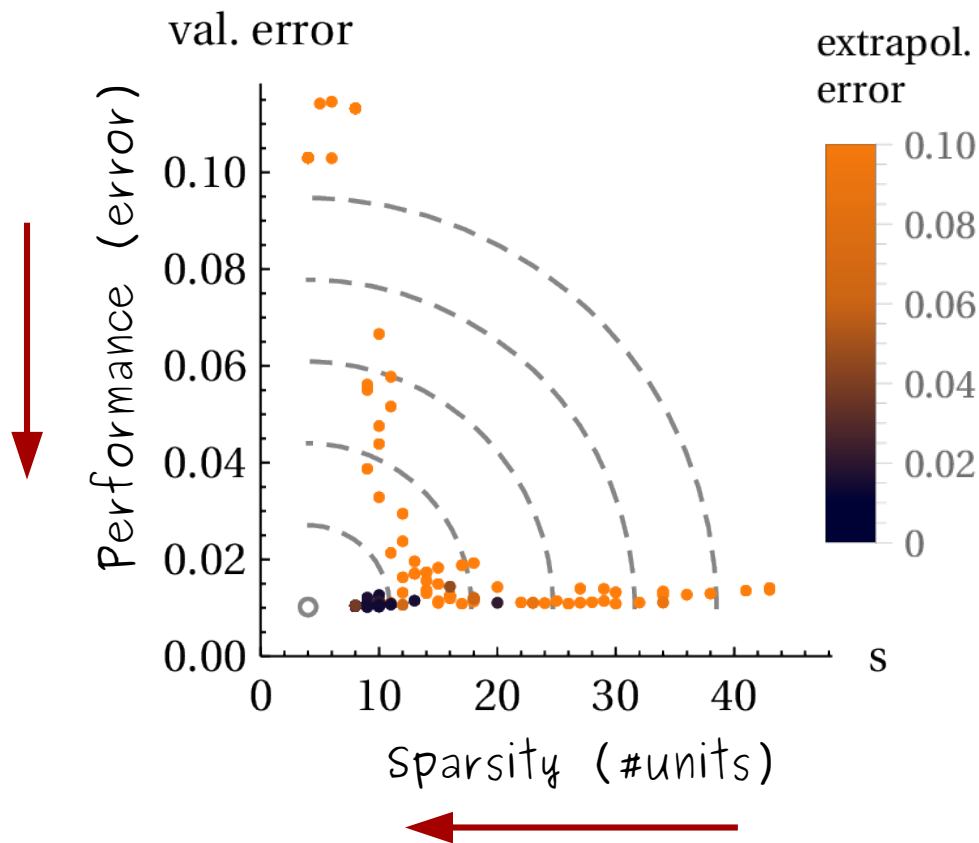
	EQL	MLP	SVR
(d) extrapolation error	0.0003 ± 0.00003	0.58 ± 0.03	0.25

Model Selection

Occams Razor: Most simple formula is most likely the right one.

But too simple can also be wrong!

Multiobjective: simple and good performance

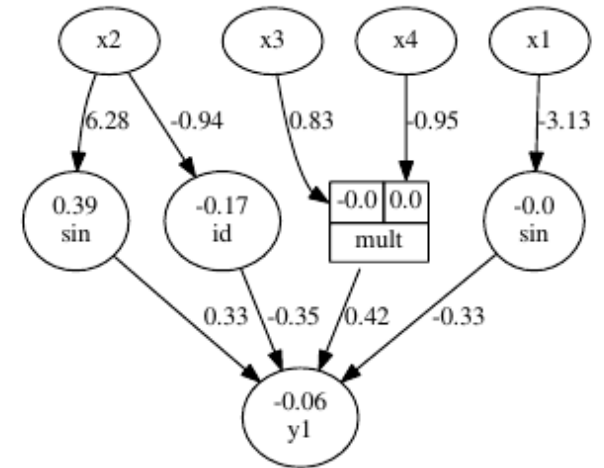
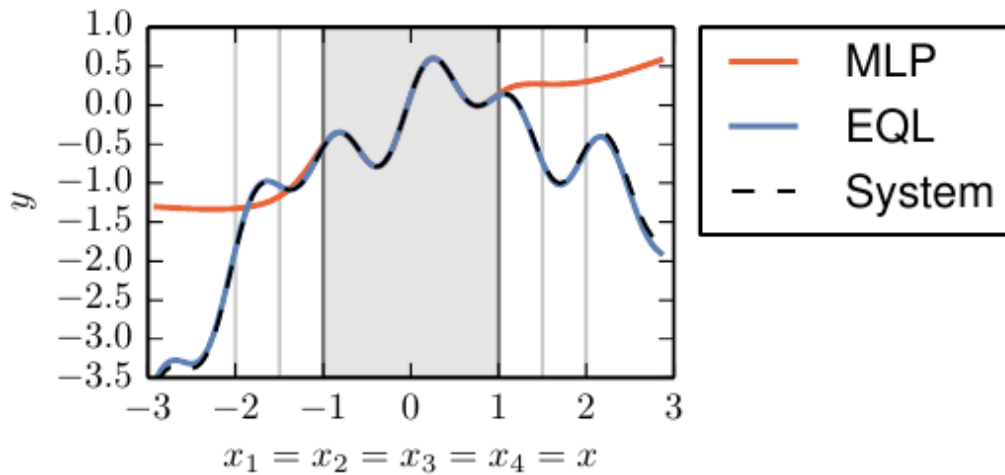


$$\arg \min_{\phi} [\tilde{v}(\phi)^2 + \tilde{s}(\phi)^2]$$

normalized values

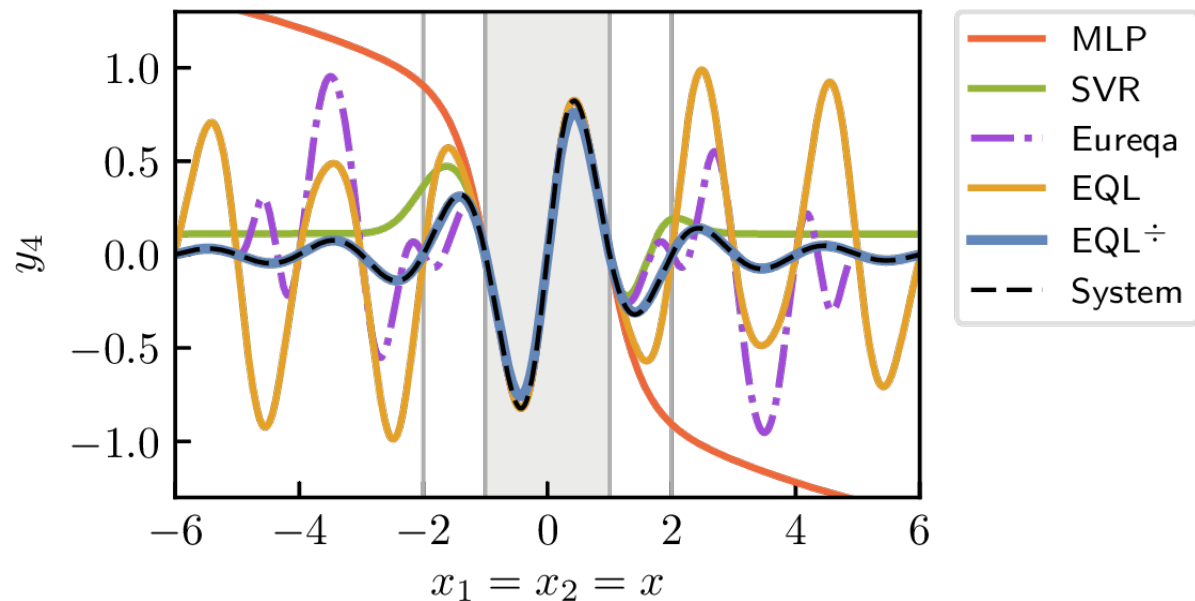
some formulas

$$y = 1/3 (\sin(\pi x_1) + \sin(2\pi x_2 + \pi/8) + x_2 - x_3 x_4)$$



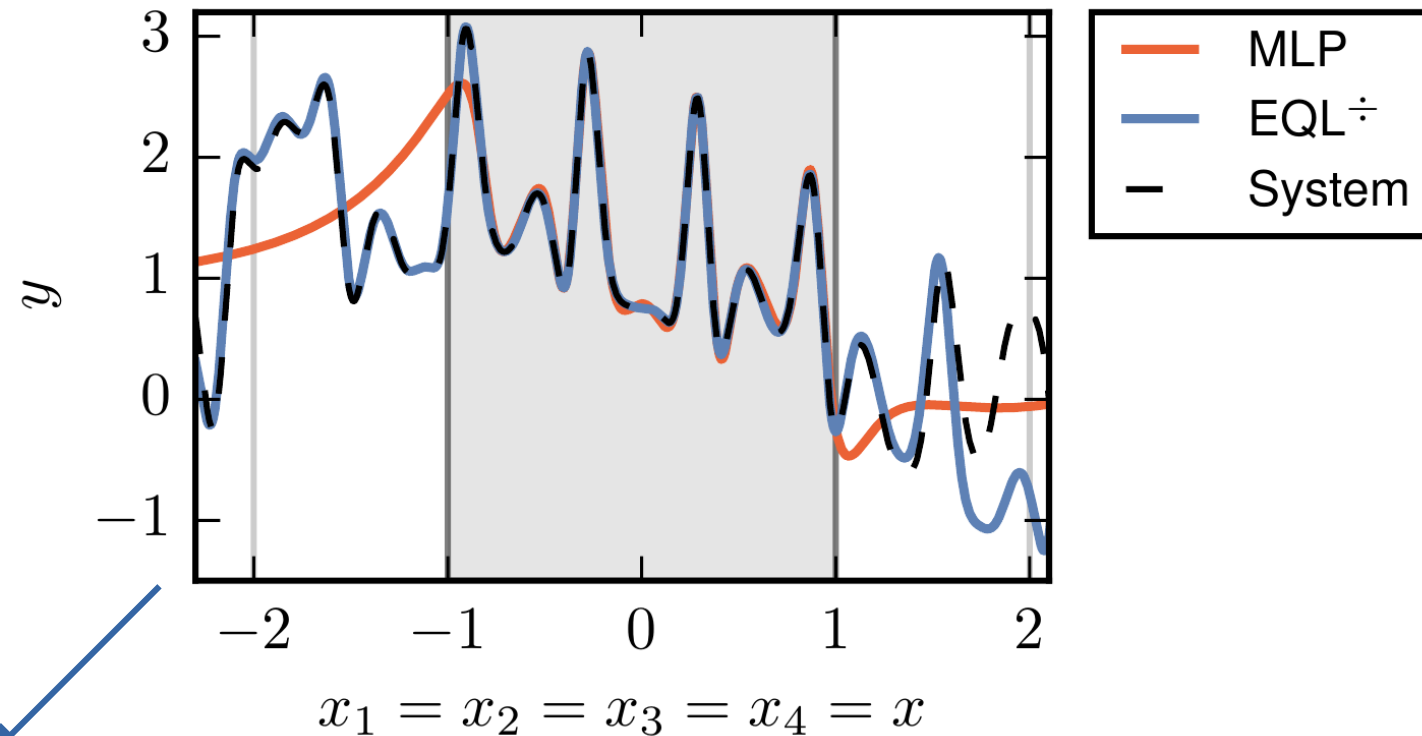
learned formula: $-0.33 \sin(-3.13x_1) + 0.33 \sin(6.28x_2 + 0.39) + 0.33x_2 - 0.056 - 0.33x_3x_4$

$$y = \frac{\sin(\pi x_1)}{(x_2^2 + 1)}$$



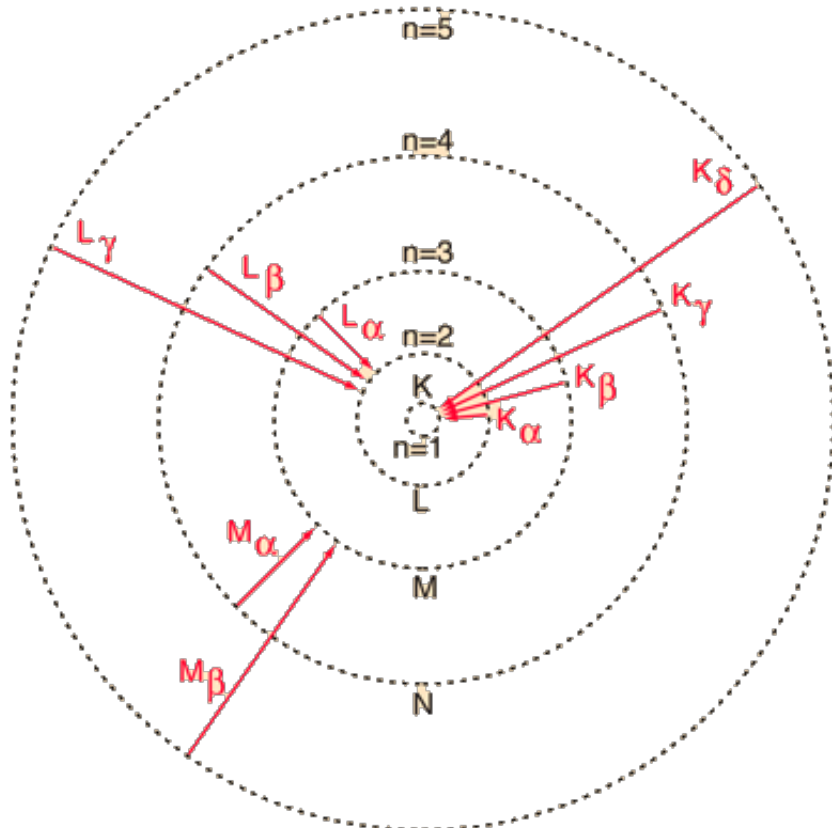
Random formulas

random formula
(RE2-2)



	RE2-1	RE2-2	RE2-3 ✗	RE2-4	RE3-1 ✗	RE3-2	RE3-3	RE3-4
EQL \div V ^{ex} -S	0.05±0.05	0.07±0.02	0.70±0.12	0.01±0.00	0.89±0.56	0.47±0.45	0.10±0.12	0.53±0.32
EQL \div V ^{int} -S	0.17±0.14	0.27±0.11	3.21±5.02	0.01±0.00	4.66±11.50	1.62±1.67	0.35±0.43	1.41±2.42
MLP V ^{ex}	1.55±0.07	1.04±0.04	1.03±0.25	0.97±0.10	1.11±0.20	1.89±0.20	0.70±0.42	1.77±0.25
MLP V ^{int}	1.57±0.07	1.05±0.03	1.45±0.15	1.00±0.09	1.32±0.17	2.03±0.16	1.30±0.47	1.86±0.17
SVR V ^{ex}	1.15	1.06	0.59	1.51	0.75	1.81	0.37	1.23
SVR V ^{int}	1.20	2.12	17.72	13.89	11.79	11.28	0.37	17.67
Const 0	6.73	2.57	0.50	5.36	1.65	72.26	17.67	3.15

X-Ray transition energies



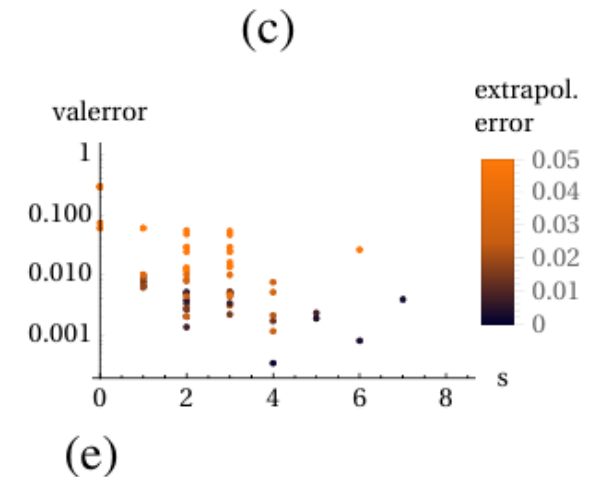
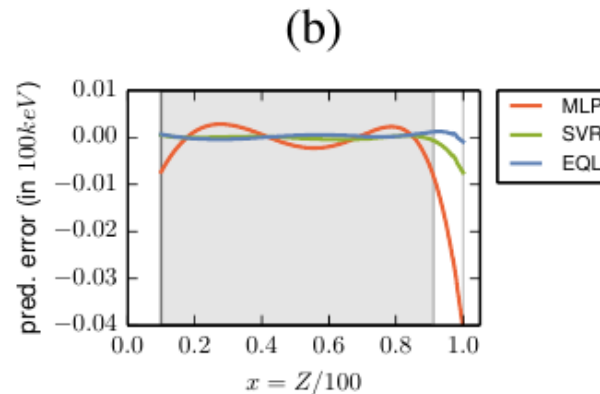
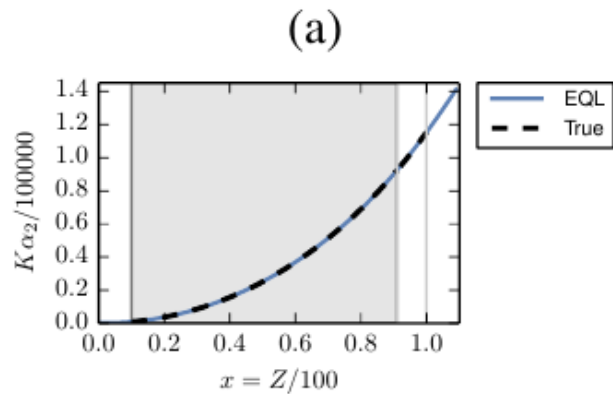
1 1,008* H hydrogen	2 4,003 He helium																
3 6,94* Li litium	4 9,012 Be beryllium																
11 22,99 Na natrium	12 24,31* Mg magnesium																
19 39,10 K kalium	20 40,08 Ca kalsium	21 44,96 Sc scandium	22 47,87 Ti titan	23 50,94 V vanadium	24 52,00 Cr krom	25 54,94 Mn mangan	26 55,85 Fe jern	27 58,93 Co kobolt	28 58,69 Ni nikkel	29 63,55 Cu kobber	30 65,38* Zn sink	31 69,72 Ga gallium	32 72,63 Ge germanium	33 74,92 As arsen	34 78,96* Se selen	35 79,90* Br brom	36 83,80 Kr krypton
37 85,47 Rb rubidium	38 87,62 Sr strontium	39 88,91 Y yttrium	40 91,22 Zr zirkonium	41 92,91 Nb niob	42 95,96* Mo molybden	43 [98] Tc technetium	44 101,1 Ru ruthenium	45 102,9 Rh rhodium	46 106,4 Pd palladium	47 107,9 Ag sølv	48 112,4 Cd kadmium	49 114,8 In indium	50 118,7 Sn tinn	51 121,8 Sb antimon	52 127,6 Te tellur	53 126,9* I jod	54 131,3 Xe xenon
55 132,9 Cs cesium	56 137,3 Ba barium	57-71 Fr francium	72 178,5 Hf hafnium	73 180,9 Ta tantal	74 183,8 W wolfram	75 186,2 Re rhenium	76 190,2 Os osmium	77 192,2 Ir iridium	78 195,1 Pt platina	79 197,0 Au gull	80 200,6 Hg kvikksølv	81 204,4* Tl thallium	82 207,2 Pb bly	83 209,0 Bi vismut	84 [209] Po polonium	85 [210] At astat	86 [222] Rn radon
			104 [267] Rf rutherfordium	105 [268] Db dubnium	106 [269] Sg seaborgium	107 [270] Bh bohrium	108 [269] Hs hassium	109 [278] Mt meitnerium	110 [281] Ds darmstadtium	111 [281] Rg roentgenium	112 [285] Cn copernicium	113 [286] Uut ununtrium	114 [289] Ff flerovium	115 [288] Uup ununpentium	116 [293] Lv livermorium	117 [294] Uus ununseptium	118 [294] Uuo ununoctium
			57 138,9 La lantan	58 140,1 Ce cerium	59 140,9 Pr praseodym	60 144,2 Nd neodym	61 [145] Pm promethium	62 150,4 Sm samarium	63 152,0 Eu europium	64 157,3 Gd gadolinium	65 158,9 Tb terbium	66 162,5 Dy dysprosium	67 164,9 Ho holmium	68 167,3 Er erbitium	69 168,9 Tm thulium	70 173,1 Yb ytterbium	71 175,0 Lu lutetium
			89 [227] Ac actinium	90 232,0 Th thorium	91 231,0 Pa protactinium	92 238,0 U uran	93 [237] Np neptunium	94 [244] Pu plutonium	95 [243] Am americium	96 [247] Cm curium	97 [247] Bk berkelium	98 [251] Cf californium	99 [252] Es einsteinium	100 [257] Fm fermium	101 [258] Md mendelevium	102 [259] No nobelium	103 [262] Lr lawrencium

*H: 1,00784, 1,00811
 Li: 6,938, 6,997
 B: 10,806, 10,821
 C: 12,0096, 12,0116
 N: 14,00643, 14,00728
 O: 15,99903, 15,99977
 Mg: [24,304, 24,307]
 Si: [26,084, 26,086]
 S: [32,059, 32,076]
 Cl: [35,446, 35,453]
 Br: [79,901, 79,907]
 Ti: [204,382, 204,385]
 Zn: 65,38(2)
 Se: 78,96(3)
 Mo: 95,96(2)

wikimedia

<http://hyperphysics.phy-astr.gsu.edu>

X-Ray transition energies



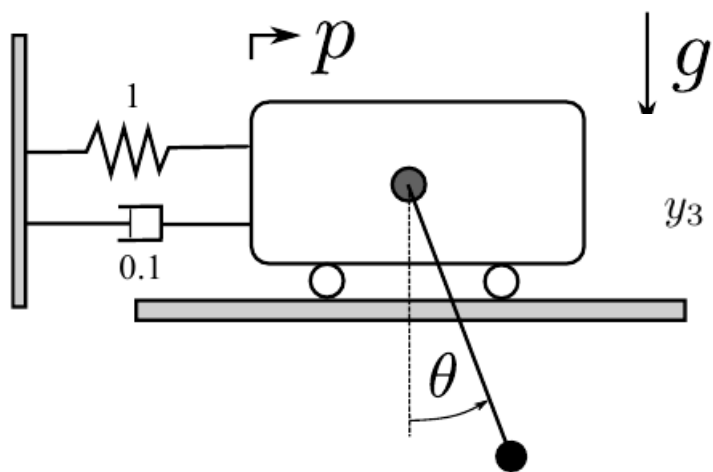
(d)

	interpolation	extrapolation
EQL	0.00042	0.0061 ± 0.0038
MLP	0.002	0.0180 ± 0.0024
SVR	0.00067	0.0057 ± 0.0014

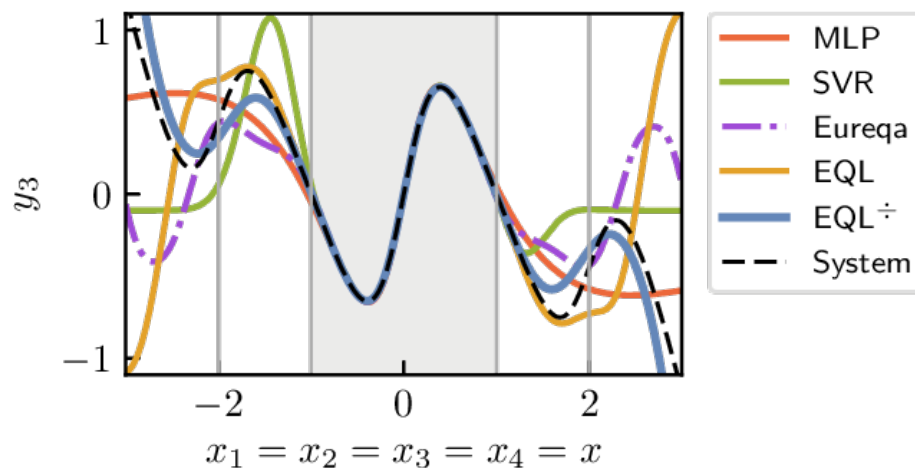
(e)

s	formula
1	$y = 1.28x^2 - 0.183x + 0.026$
2	$y = 1.98x^2 - 1.42x + 0.618 - 1.45\text{sigm}(-3.65x - 0.3)$
3	$y = -0.38z + 2.47\text{sigm}(-2.25z - 2.77) + 0.38$ with $z = \cos(2.32x - 0.08)$
4	$y = 0.221z + 0.42\text{sigm}(0.75z - 3.73)$ with $z = 4.65x^2 - 0.229x$

Cart-Pendulum dynamics



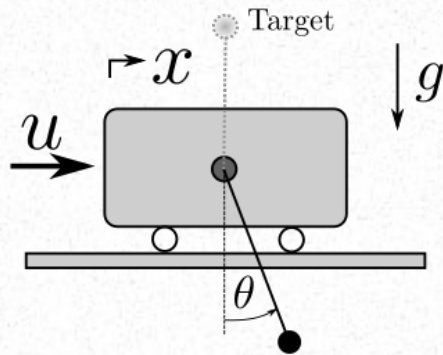
$$y_3 = \frac{-x_1 - 0.01x_3 + x_4^2 \sin(x_2) + 0.1x_4 \cos(x_2) + 9.81 \sin(x_2) \cos(x_2)}{\sin^2(x_2) + 1},$$



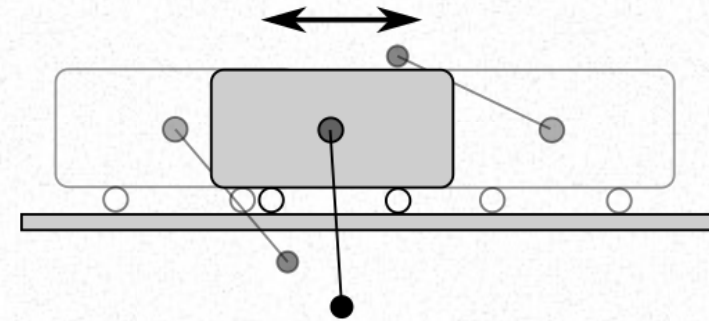
Able to learn dynamics equations

Learning Cart-Pole swingup

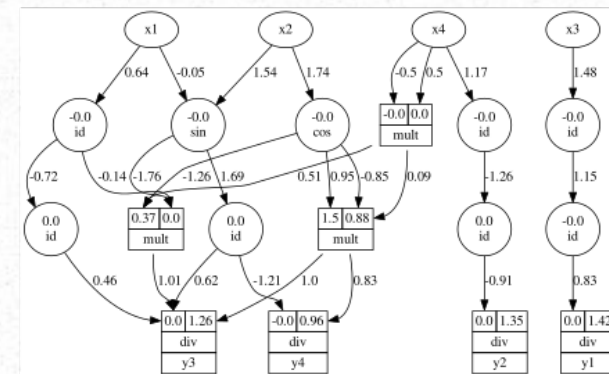
Robot



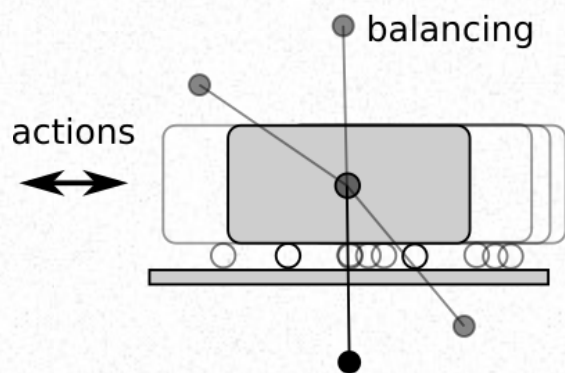
random movements



Learning Equation



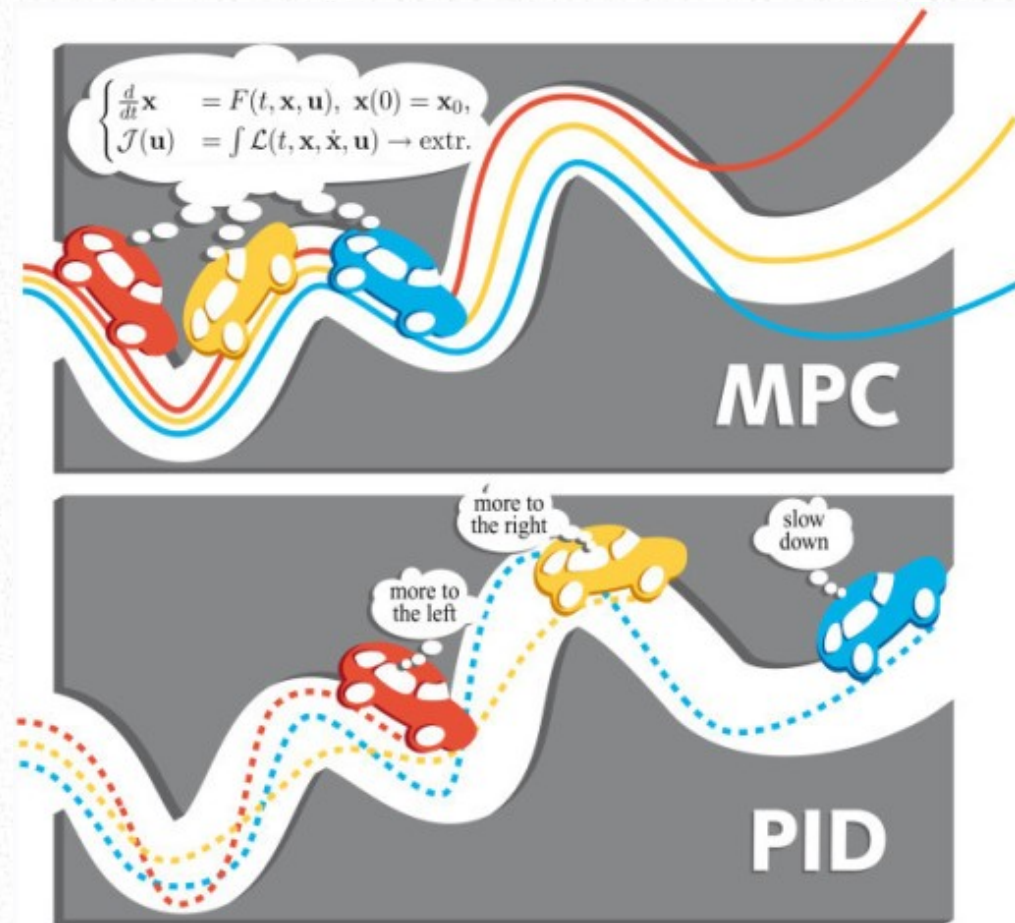
Control



Model predictive Control,
random shooting method

Model Predictive Control

- plan ahead with model
- take best action
- replan



(openi.nlm.nih.gov)

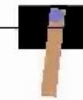
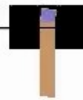
here: planning = many random rollouts

Learning Equations for Extrapolation and Control

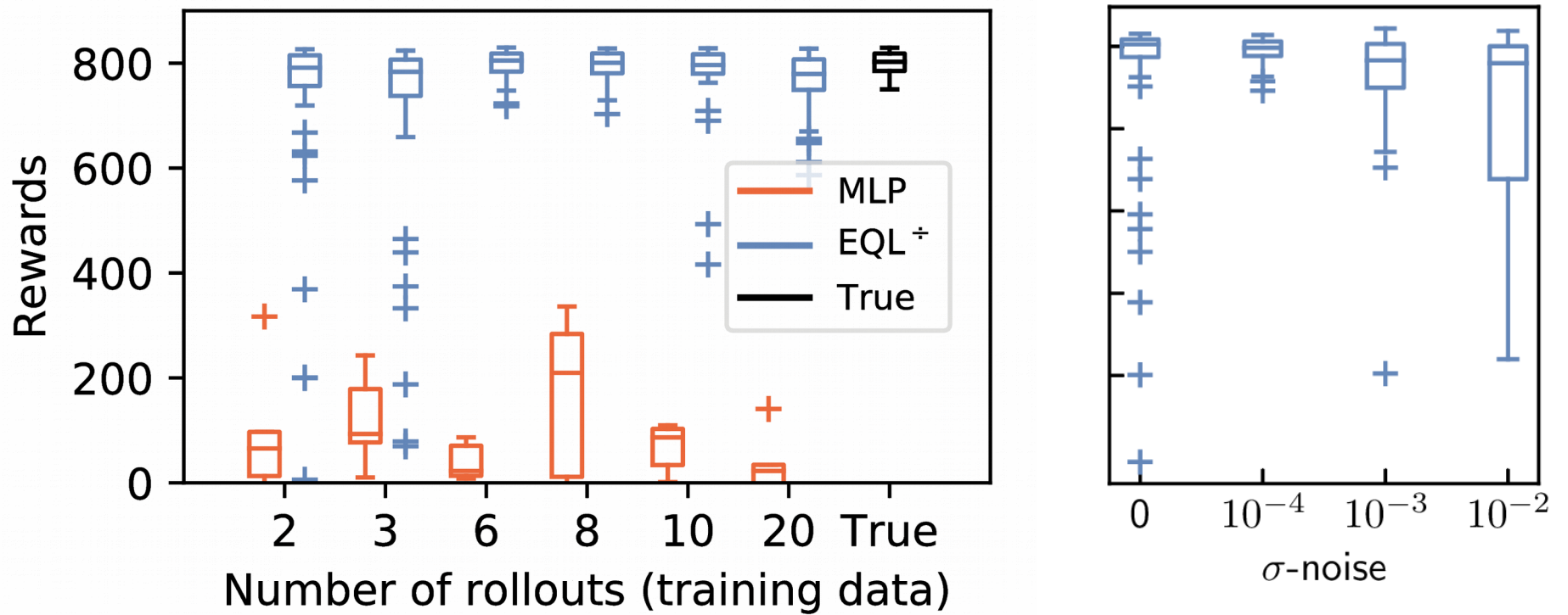
by S.S.Sahoo, C.H.Lampert and G.Martius, ICML 2018

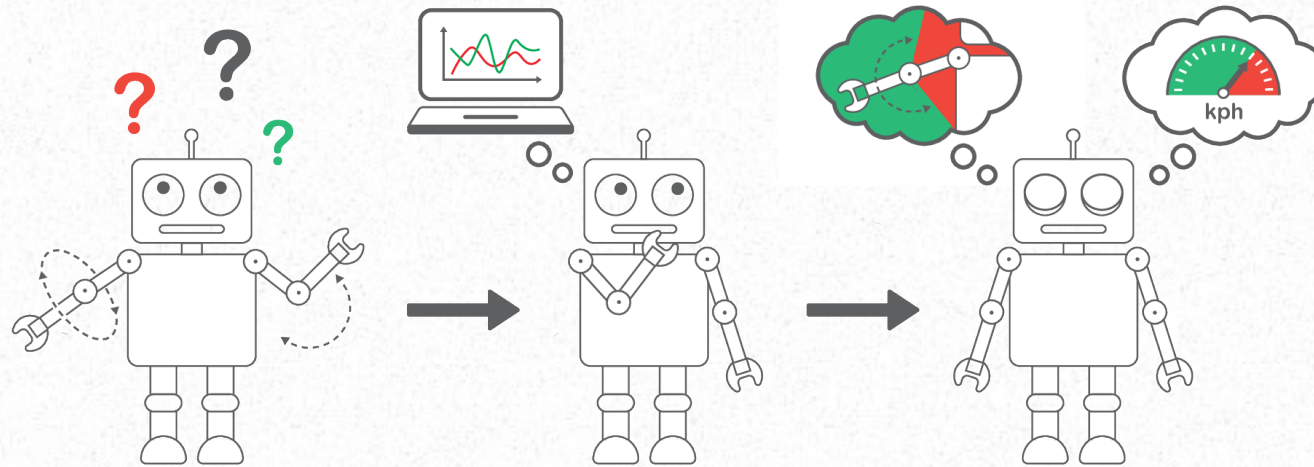
Training
1 Random rollout

Validation
1 Random rollout
(stronger actions)



Cart-pole Swingup





- › Robots need good learned models to become efficient
- › Learning Equation from data
 - exquisite extrapolation capabilities

Code on github.com/martius-lab

With



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