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Probabilistic grammars for equation discovery

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Equation discovery

(symbolic regression)

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Data

v_1	v_2	$\ldots$	v_n
$v_{1,1}$	$v_{2,1}$	$\ldots$	$v_{n,1}$
$v_{1,2}$	$v_{2,2}$	$\ldots$	$v_{n,2}$
$\vdots$	$\vdots$	$\ddots$	$\vdots$
$v_{1,m}$	$v_{2,m}$	$\ldots$	$v_{n,m}$

Equation discovery algorithm

Closed-form equations(s)

$$x_i = f(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots x_n)$$

Background knowledge

Two components:

Structure identification
- Background knowledge
- Expression generation
- Search method

Parameter estimation
- Numeric optimization
- Error-of-fit
- Well studied

Equation discovery at JSI

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Grammars



Probabilistic grammars

1990 2000 2020

Process-based models

Autoencoders




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Types of equations

Algebraic equations

$$y = f(x_1, x_2, \dots, x_m)$$

Newton's 2nd law

$$F = m \cdot a$$

Relativistic momentum

$$p = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Gaussian function

$$f = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(\theta - \theta_0)^2}{2\,\sigma^2}}$$

Systems of differential equations

$$\dot{x_1} = f(x_1, x_2, \dots, x_m)$$

…

$$\dot{x_m} = f(x_1, x_2, \dots, x_m)$$

Lorenz system

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z$$

Glider system

$$\dot{x} = -\sin y - Dx^2$$
$$\dot{y} = -\frac{\cos x}{x} + x$$

Van der Pol oscillator

$$\ddot{x} = -x - \mu(x^2 - 1)\dot{x}$$

Integer sequences

$$a_n = f(n, a_{n-1}, \dots, a_{n-m})$$
$$n, a_{n-1}, \dots, a_{n-m} \in \mathbb{Z}$$

Fibonacci sequence:

$$a_n = a_{n-1} + a_{n-2}$$

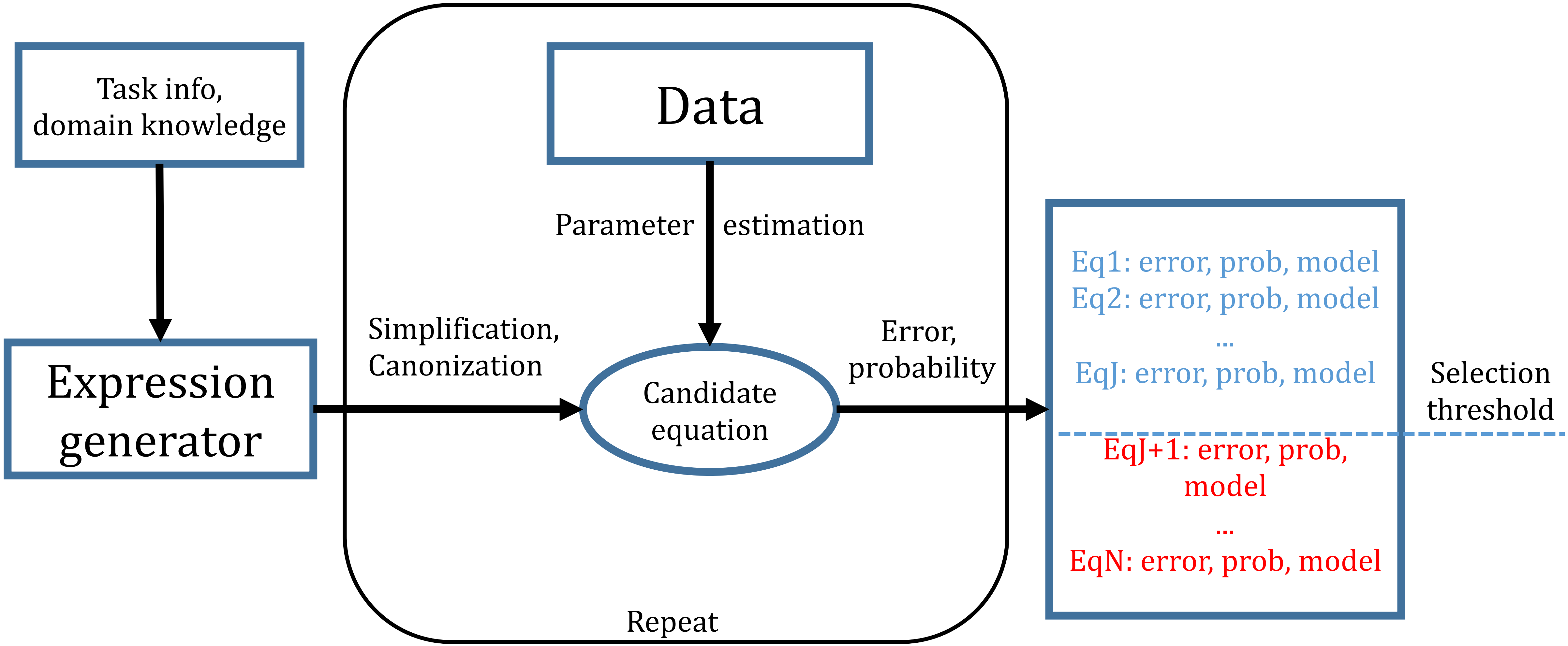
Tetrahedral numbers:

$$a_n = \frac{n(n+1)}{2}$$

Jacobsthal sequence:

$$a_n = 2^n - \mathrm{a}_{n-1}$$

Algorithm: Monte-Carlo sampling



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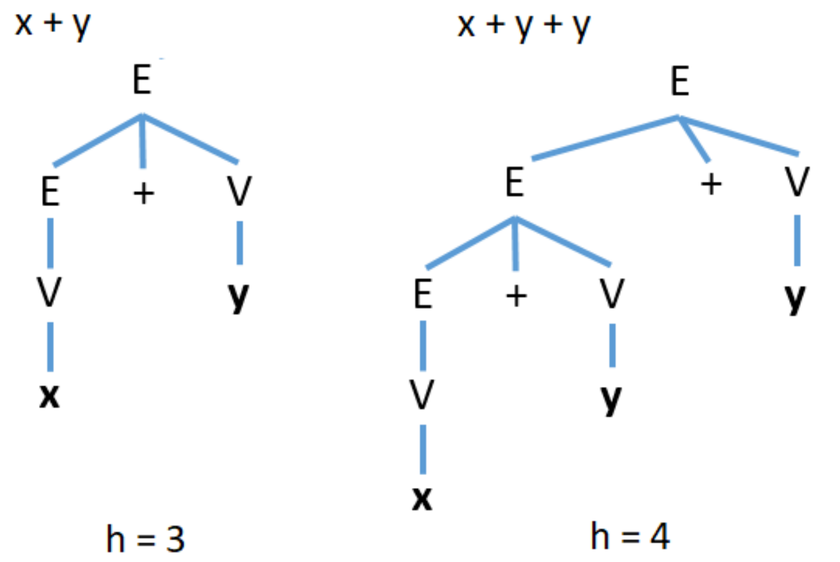
Probabilistic grammars - PCFG

Traditionally: a formal specification of a language

In our case: - the specification of the search space

- the generator of candidate expressions
- defines distribution over equations

$$
\begin{aligned}
E &\rightarrow E + V \; [p] \\
E &\rightarrow V \; [1 - p] \\
V &\rightarrow x \; [q] \\
V &\rightarrow y \; [1 - q]
\end{aligned}
$$



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Parsimony in equation discovery

- Parsimony principle:
  simpler explanations are more likely to be correct.
- Model selection: error vs. complexity
- Common solution: regularization term
- Inherent in PCFGs:

$$P(\psi) = \prod_{(A \to \alpha) \in \mathcal{R}} P(A \to \alpha)^{f(A \to \alpha, \psi)}$$

recursive production

p governs parsimony

$$\boldsymbol{E} \to \boldsymbol{E} + \boldsymbol{V}\ [\boldsymbol{p}]$$
$$E \to V\ [1-p]$$
$$V \to x\ [q]$$
$$V \to y\ [1-q]$$

J. Brence et al. (2021). "Probabilistic grammars for equation discovery". Knowledge-Based Systems 224: 107077.

Results – Feynman database*

- Popular benchmark for equation discovery / symbolic regression
- 100 algebraic equations from physics texbooks by R. Feynman
- Used generator: universal arithmetic grammar

```
exp(-theta**2/2)/sqrt(2*pi)
exp(-(theta/sigma)**2/2)/(sqrt(2*pi)*sigma)
exp(-((theta-theta1)/sigma)**2/2)/(sqrt(2*pi)*sigma)
sqrt((x2-x1)**2+(y2-y1)**2)
G*m1*m2/((x2-x1)**2+(y2-y1)**2+(z2-z1)**2)
m_0/sqrt(1-v**2/c**2)
x1*y1+x2*y2+x3*y3
mu*Nn
q1*q2*r/(4*pi*epsilon*r**3)
q1*r/(4*pi*epsilon*r**3)
```

Successfully reconstructed equations: 36

-> limits of Monte-Carlo

-> unconstrained space, no background knowledge

* Udrescu, S. M., & Tegmark, M. (2020). AI Feynman: A physics-inspired method for symbolic regression. Science Advances, 6(16), eaay2631.

Constraints on the search space

- Search space is generally infinite → need for constraints
- Background knowledge → constraints

$$
\begin{aligned}
E &\rightarrow E + V \ [0.4] \\
E &\rightarrow V \ [0.6] \\
V &\rightarrow x \ [0.75] \\
V &\rightarrow y \ [0.25]
\end{aligned}
$$

Production rules
- **hard** constraints

Rule probabilities
- **soft** constraints

Domain-specific knowledge

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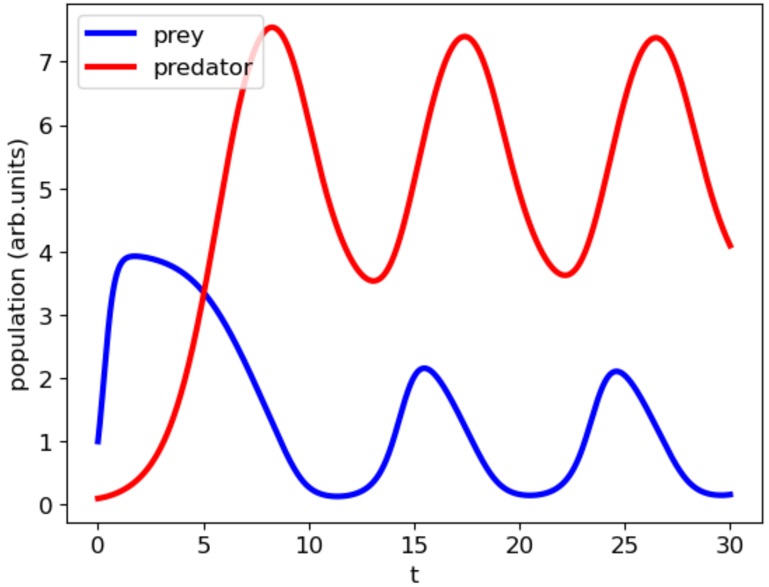
State oscillators

- Polynomials
- Population models: the monod function $\frac{v}{v+c}$

$$E \rightarrow E + T \mid T$$
$$T \rightarrow T * V \mid T * M \mid c$$
$$M \rightarrow \frac{x}{x+c} \mid \frac{y}{y+c}$$
$$V \rightarrow x \mid y$$

Example – predator-prey

$$\dot{x} = x\left(b - x - \frac{y}{y+1}\right)$$
$$\dot{y} = y\left(\frac{x}{x+1} - ay\right)$$



Domain-specific knowledge

Phase oscillators:

- Linear combination of terms
- Terms: sin and cos of variables
- Arguments: linear functions

$$E \rightarrow E + c * T \mid c * T \mid \mathrm{c}$$

$$T \rightarrow \sin(L) \mid \cos(\mathrm{L})$$

$$L \rightarrow L + c * V \mid c$$
$$V \rightarrow x \mid y$$

Example - bar magnets

$$\dot{x} = K\sin(x-y) - \sin(x)$$
$$\dot{y} = K\sin(y-x) - \sin(y)$$

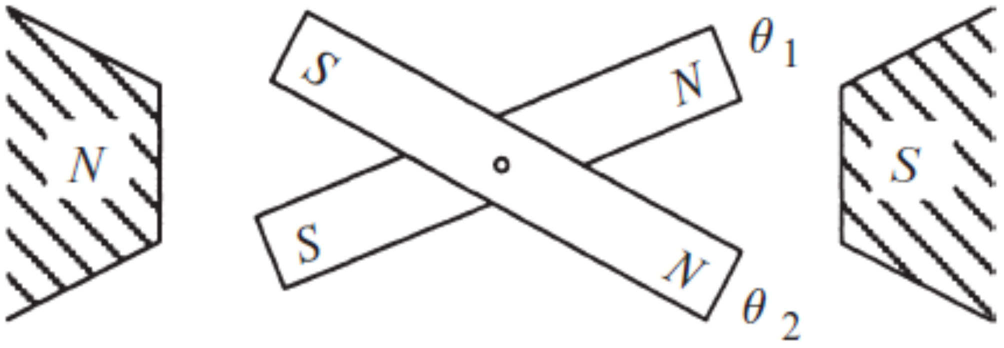


Image from Steven H. Strogatz, "Nonlinear Dynamics and Chaos with Student Solutions Manual", 2015.

Results – dynamical systems

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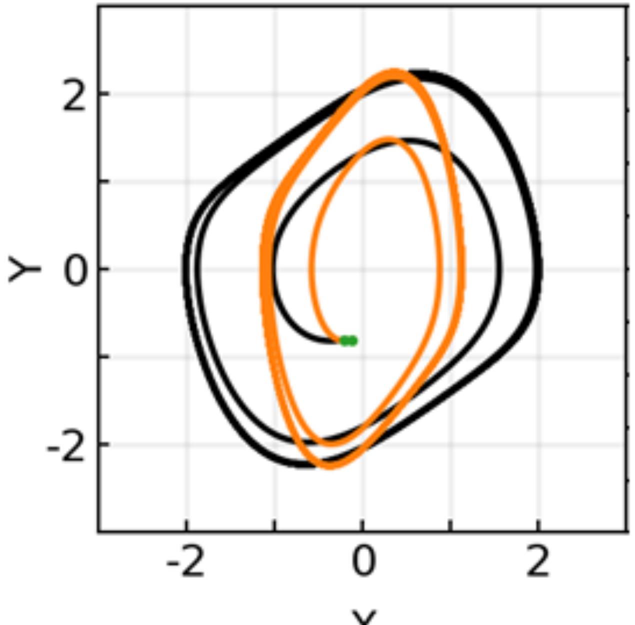
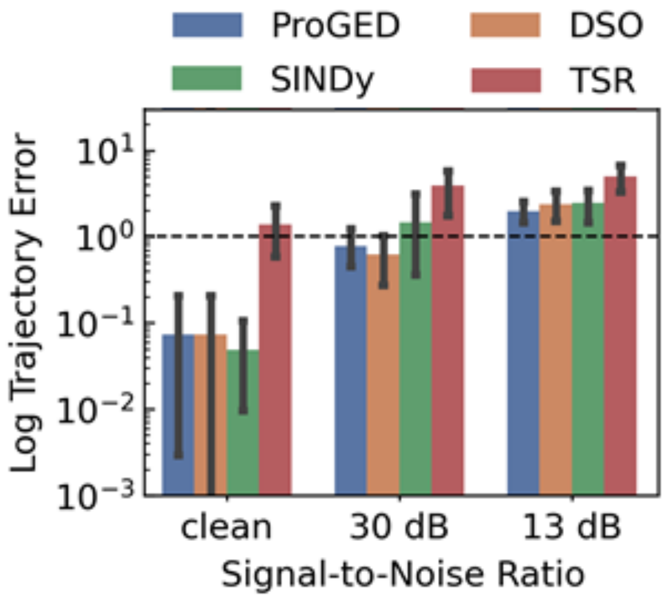
- **Competitive results** for fully-observed systems
- Can handle **partially-observed** systems well



Extended Strogatz benchmark:
10 dynamical systems



N. Omejc, et al. (2023). "Probabilistic grammars for modeling dynamical systems from coarse, noisy, and partial data". In review.

Learning from equation corpora

- Grammar probabilities – “soft” encoding of knowledge

Initial grammar

$E \rightarrow E + F\ [0.2]\ |\ E - F\ [0.2]\ |\ F\ [0.6]$

$F \rightarrow F * T\ [0.2]\ |\ F / T\ [0.2]\ |\ T\ [0.6]$

$T \rightarrow R\ [0.2]\ |\ V\ [0.4]\ |\ c\ [0.4]$

$R \rightarrow (E)\ [0.6]\ |\ \sin(\mathrm{E})\ [0.1]\ |\ \cos(\mathrm{E})\ [0.1]$

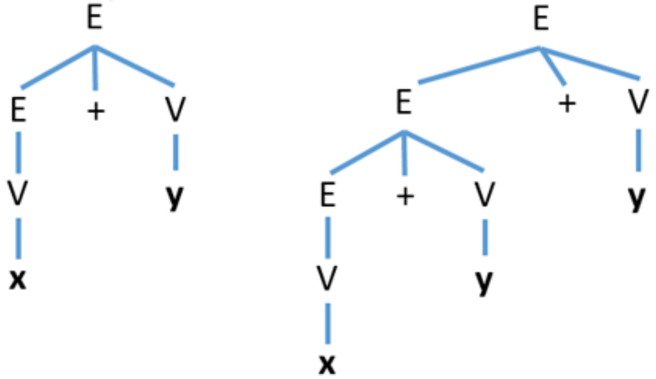
$\rightarrow \sqrt{E}\ [0.1]\ |\ \exp(E)\ [0.1]$

Parse

Corpus of equations

n_rho*mom*tanh(mom*B/(kb*T))
mom*H/(kb*T)+(mom*alpha)/(epsilon*c**2*kb*T)*M
mom*(1+chi)*B
Y*A*x/d
Y/(2*(1+sigma))
1/(exp((h/(2*pi))*omega/(kb*T))-1)
(h/(2*pi))*omega/(exp((h/(2*pi))*omeg

Parse trees



Production frequencies

Updated grammar

$E \rightarrow E + F\ [0.10]\ |\ E - F\ [0.15]\ |\ F\ [0.75]$

$F \rightarrow F * T\ [0.36]\ |\ F / T\ [0.24]\ |\ T\ [0.40]$

$T \rightarrow R\ [0.15]\ |\ V\ [0.72]\ |\ c\ [0.13]$

$R \rightarrow (E)\ [0.56]\ |\ \sin(\mathrm{E})\ [0.12]\ |\ \cos(\mathrm{E})\ [0.09]$

$\rightarrow \sqrt{E}\ [0.14]\ |\ \exp(E)\ [0.09]$

General knowledge: dimensions

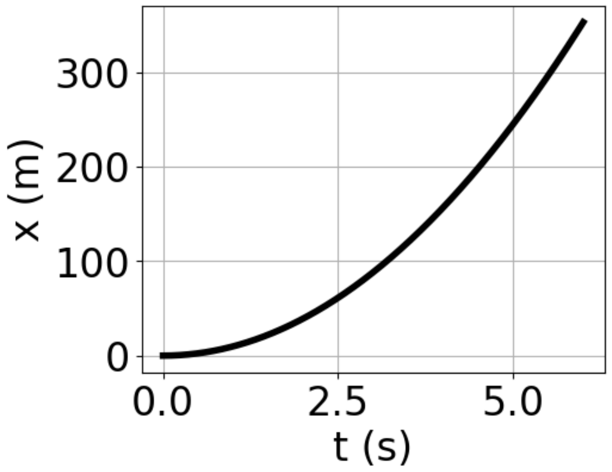
- Units of measurement
- Related: Buckingham PI theorem, dimensional analysis
- Impose constraints on the structure of expressions

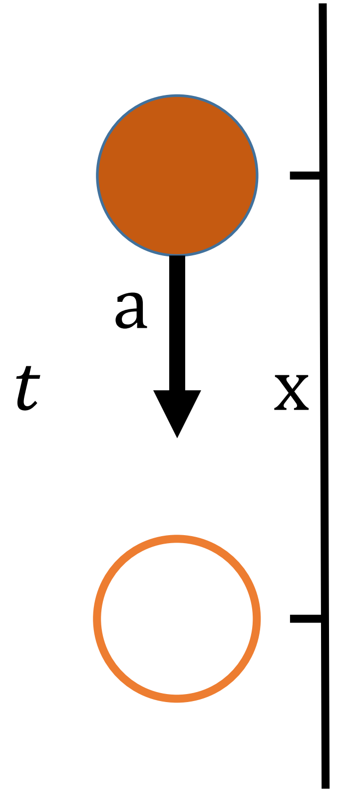
$$u(x) = \boldsymbol{m} = (1,0)$$
$$u(t) = \boldsymbol{s} = (0,1)$$
$$u(a) = \frac{\boldsymbol{m}}{\boldsymbol{s}^2} = (1,-2)$$

$$u(v_1 \pm v_2) = u(v_1) = u(v_2)$$

$$u(v_1 * v_2) = u(v_1) + u(v_2)$$
$$u(v_1 / v_2) = u(v_1) - u(v_2)$$

$$\boldsymbol{x = at^2}$$





General knowledge: dimensions

Attribute grammars

- Nonterminals can have *attributes*
- *Attribute rules* encode knowledge

Dimensional attribute grammar

$$
\begin{array}{lll}
P & \rightarrow P + c * M & \{P1.u = P2.u = M.u\} \\
 & \rightarrow c * M & \{P.u = M.u\} \\
M & \rightarrow M * V & \{M1.u = M2.u + V.u\} \\
 & \rightarrow V & \{M.u = V.u\} \\
V & \rightarrow a & \{V.u = a.u\} \\
 & \rightarrow t & \{V.u = t.u\}
\end{array}
$$

transform ⇒

Dimensionally-consistent context-free grammar

$$
\begin{array}{ll}
P_{(1,0)} & \rightarrow P_{(1,0)} + c * M_{(1,0)} \\
 & \rightarrow c * M_{(1,0)} \\
M_{(1,0)} & \rightarrow M_{(1,-1)} * V_{(0,1)} \\
 & \rightarrow V_{(0,1)} \\
\ldots & \\
V_{(1,0)} & \rightarrow x \\
V_{(0,1)} & \rightarrow t
\end{array}
$$

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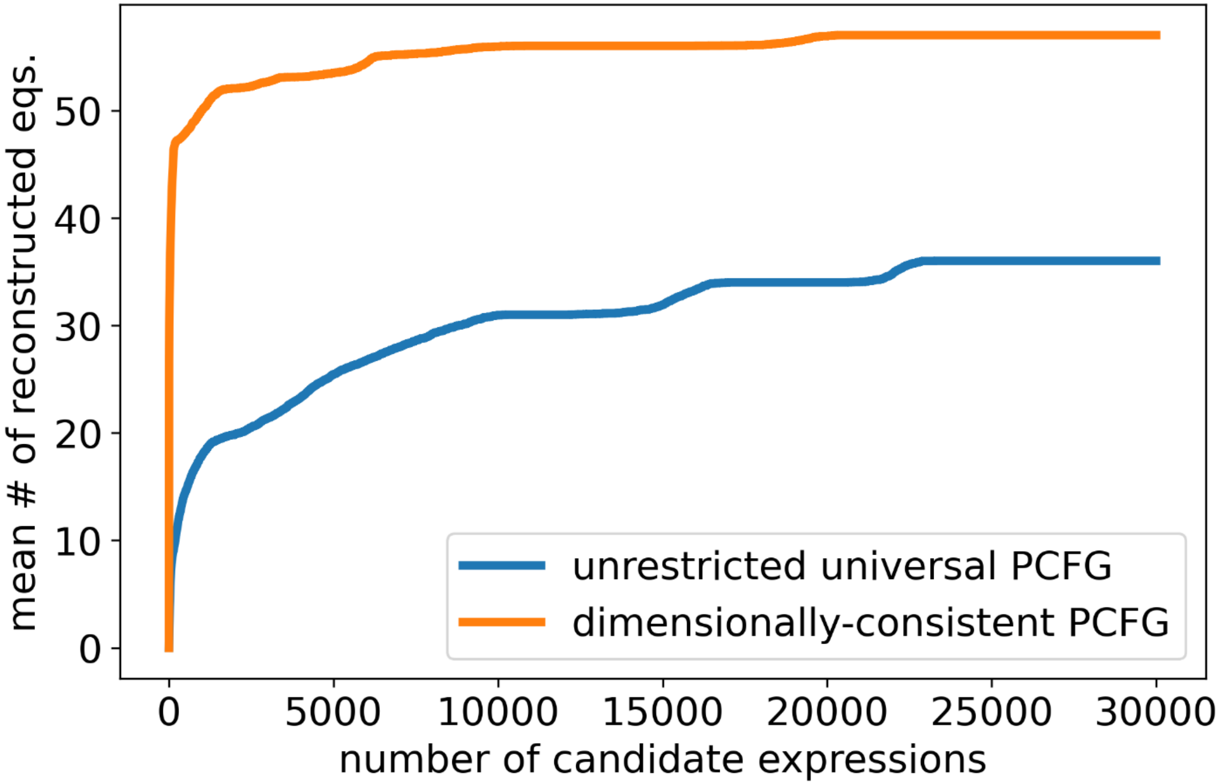
Results – Feynman database, again

- Total equations: **100**
- Universal grammar: **36**
- Dimensionally-consistent universal grammar: **58**



Dimensional consistency enables

-> more successes

-> with fewer candidates

J. Brence, et al. (2023). "Dimensionally consistent equation discovery through probabilistic attribute grammars". Information Sciences.

Summary

Probabilistic grammars enable

- inherent and intuitive control over **parsimony**,
- the encoding of general and domain-specific **background knowledge,**
- both hard and **soft constraints** on the space of equations.

Attribute grammars are a promising framework for more complex types of background knowledge.

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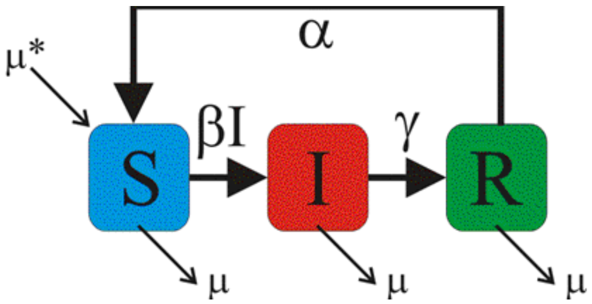
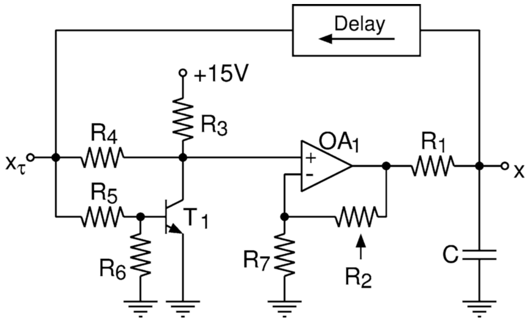
Further work

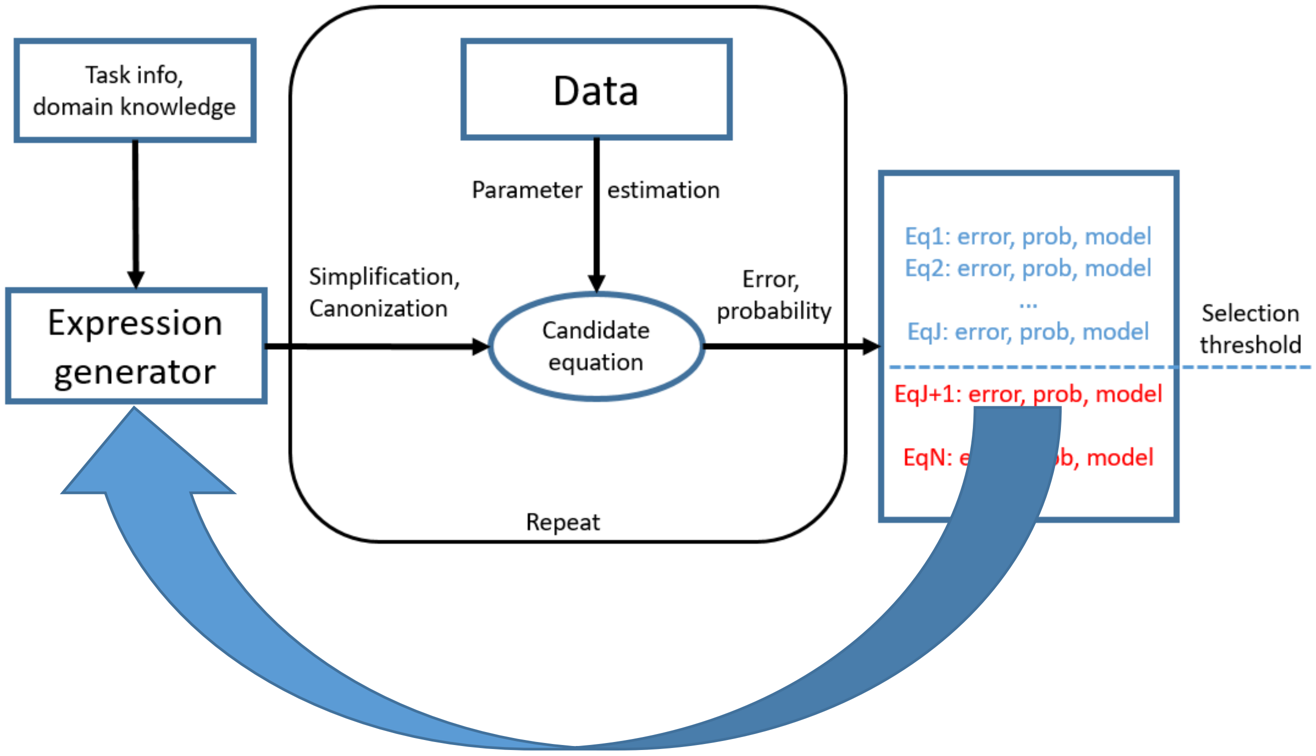
Attribute grammars

- Direct sampling
- Other types of knowledge:
  - Process-based models
  - Compartmental models
  - Electronic circuits
  - ...





Algorithmic improvement



Iterative grammar updating

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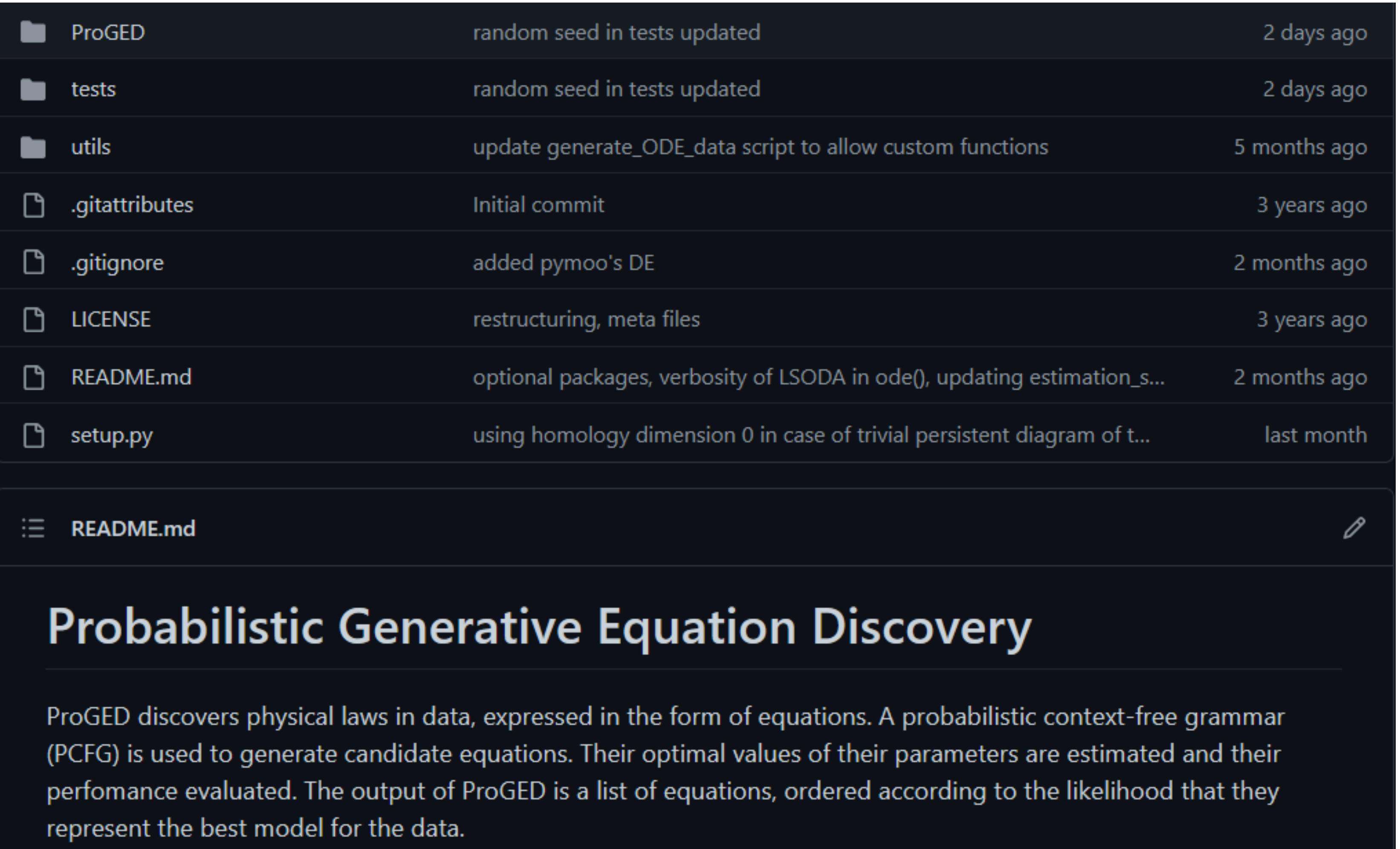
ProGED

https://github.com/brencej/ProGED



ProGED	random seed in tests updated	2 days ago
tests	random seed in tests updated	2 days ago
utils	update generate_ODE_data script to allow custom functions	5 months ago
.gitattributes	Initial commit	3 years ago
.gitignore	added pymoo's DE	2 months ago
LICENSE	restructuring, meta files	3 years ago
README.md	optional packages, verbosity of LSODA in ode(), updating estimation_s...	2 months ago
setup.py	using homology dimension 0 in case of trivial persistent diagram of t...	last month

README.md

Probabilistic Generative Equation Discovery

ProGED discovers physical laws in data, expressed in the form of equations. A probabilistic context-free grammar (PCFG) is used to generate candidate equations. Their optimal values of their parameters are estimated and their perfomance evaluated. The output of ProGED is a list of equations, ordered according to the likelihood that they represent the best model for the data.

- Python package
- Open source
- Active development

Thank you for your attention!

Extras

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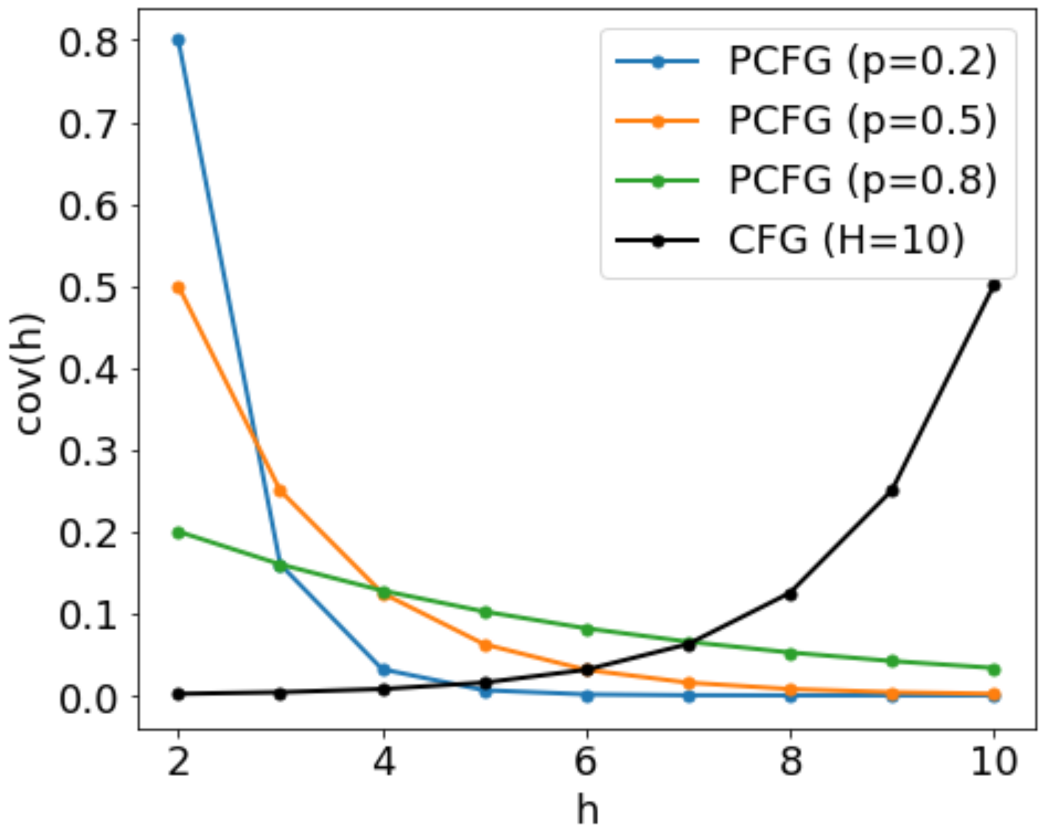
CFG vs PCFG

- **cov** - prob. of all parse trees with height h
- Number of parse trees increases with height.
- In CFGs, all parse trees are equally likely.

- PCFG: cov drops exponentially
- CFG: cov rises exponentially



Domain-specific knowledge

Dynamical systems:
- Systems of ODEs
- Linear combinations of a few terms:
  - Low order monomials
  - Simple rational functions
  - sin or cos functions

Example: glider

$$\dot{x} = -\sin(y) - Dx^2$$

$$\dot{y} = -\frac{\cos(y)}{x} + x$$

$$
\begin{aligned}
E &\rightarrow E + T \ [0.6] \quad | \ T/(D) \ [0.15] \quad | \ T \ [0.25] \\
D &\rightarrow D + T \ [0.5] \quad | \ T \ [0.5] \\
T &\rightarrow T * V \ [0.3] \quad | \ T * R \ [0.1] \quad | \ c \ [0.6] \\
R &\rightarrow \sin(M) \ [0.5] \quad | \ \cos(M) \ [0.5] \\
M &\rightarrow M * V \ [0.5] \quad | \ c \ [0.5] \\
V &\rightarrow x \ [0.5] \quad | \ y \ [0.5]
\end{aligned}
$$