

Određivanje dinamike fizikalnih sustava pomoću strojnog učenja

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Mentor

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1 Uvod

2 Teorijska pozadina

3 Primjeri i rezultati

4 Zaključak

Diferencijalne jednačbe → rješenja

- Newtonova jednačba

$$\mathbf{F} = m\ddot{\mathbf{r}}$$

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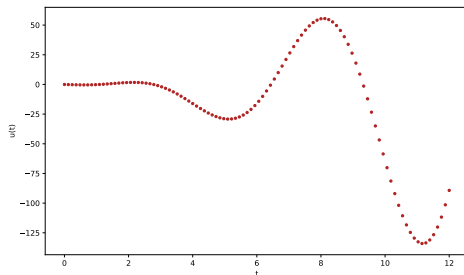
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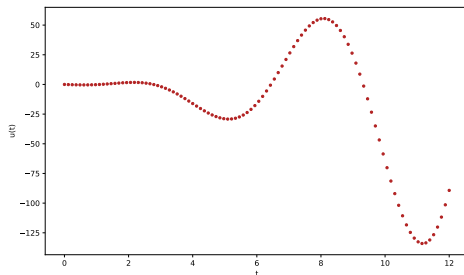
- Schrödingerova jednačba (vremenski neovisna)

$$\frac{-\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) + V(\mathbf{r})\psi(\mathbf{r}, t) = E\psi(\mathbf{r}, t)$$

Podatci → diferencijalna jednadžba

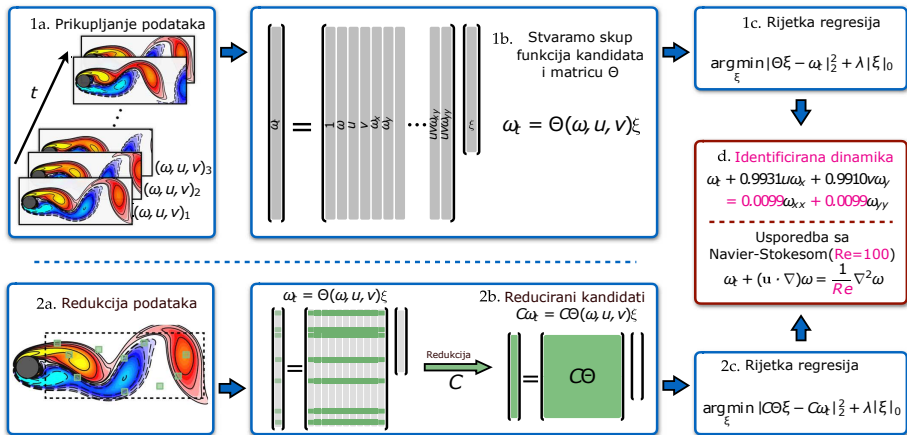


Podatci → diferencijalna jednadžba



$$\ddot{u} = 1.6 \sin(2t) + 2.9u - 3|u|\dot{u} + \dots$$

Ilustracija algoritma



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- Model

$$u_{tt} = F(u, u_x, u_{xy}, \dots, \mathbf{r}, t, \mu)$$

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$$t \rightarrow (t_1, t_2, \dots, t_m)$$

$$x \rightarrow (x_1, x_2, \dots, x_n)$$

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$$x \rightarrow (x_1, x_2, \dots, x_n)$$

- Diskretizacija vektora

$$\mathbf{U} \equiv \begin{bmatrix} u(x_0, t_0) \\ u(x_1, t_0) \\ \vdots \\ u(x_{n-1}, t_m) \\ u(x_n, t_m) \end{bmatrix}$$

- Diskretizacija modela

$$\left[\begin{array}{c} | \\ \mathbf{U}_{tt} \\ | \end{array} \right] = \left[\begin{array}{cccc} | & | & | & | \\ \mathbf{1} & \mathbf{U} & \mathbf{U}^2 & \mathbf{U}\mathbf{U}_t \\ | & | & | & | \end{array} \right] \left[\begin{array}{c} | \\ \xi \\ | \end{array} \right]$$

- Diskretizacija modela

$$\begin{bmatrix} \text{U} \\ \text{t} \\ \text{t} \end{bmatrix} = \begin{bmatrix} \mathbf{1} & \mathbf{U} & \mathbf{U}^2 & \mathbf{U}\mathbf{U}_t \end{bmatrix} \begin{bmatrix} \xi \end{bmatrix}$$

Primjer: harmonijski oscilator ($\omega = 1$)

$$\text{Rješenje: } \xi_0 = \begin{bmatrix} 0 \\ -1 \\ 0 \\ 0 \end{bmatrix} \implies \ddot{u} = -u$$

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- Generalizacija modela

- Linearna regresija

$$\mathbf{U}_{tt} = \Theta(\mathbf{U}, \mathbf{Q})\xi \implies \xi_0 = \underset{\xi}{\operatorname{argmin}} \|\Theta\xi - \mathbf{U}_{tt}\|_2^2$$

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$$\mathbf{U}_{tt} = \Theta(\mathbf{U}, \mathbf{Q})\xi \implies \xi_0 = \underset{\xi}{\operatorname{argmin}} \left\{ \|\Theta\xi - \mathbf{U}_{tt}\|_2^2 + \lambda\|\xi\|_2^2 \right\}$$

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- STRidge algoritam

- Čisti podatci – metoda konačnih razlika

$$f'(x) = \frac{f(x + \Delta) - f(x - \Delta)}{2\Delta} + O(\Delta^2)$$

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$$f'(x) = \frac{f(x + \Delta) - f(x - \Delta)}{2\Delta} + O(\Delta^2)$$

- Podatci sa šumom – interpolacija polinoma
- Konvolucija sa Gaussijanom, metoda konačnih razlika

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- Stvaranje podataka

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```
PDJ dobivena pomoću STRidge:  
u_tt = (-0.051289 +0.000000i)  
      + (1.406844 +0.000000i)u_t  
      + (-0.952997 +0.000000i)u  
      + (0.032605 +0.000000i)u^2  
      + (-1.301716 +0.000000i)u^2u_t
```

```
PDJ dobivena pomoću STRidge:  
u_tt = (1.500808 +0.000000i)u_t  
      + (-0.979745 +0.000000i)u  
      + (-1.461608 +0.000000i)u^2u_t
```

```
PDJ dobivena pomoću STRidge:  
u_tt = (1.454861 +0.000000i)u_t  
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      + (-1.394386 +0.000000i)u^2u_t
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```
PDJ dobivena pomoću STRidge:  
u_tt = (1.440753 +0.000000i)u_t  
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      + (0.041961 +0.000000i)u^2  
      + (-1.370771 +0.000000i)u^2u_t
```

- Stvaranje podataka
- Čisti podatci i podatci sa šumom
- 10 iteracija
- Srednja jednadžba

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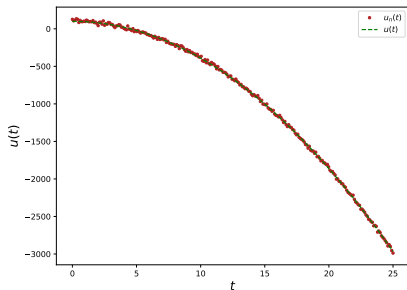
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Diferencijalna jednačba

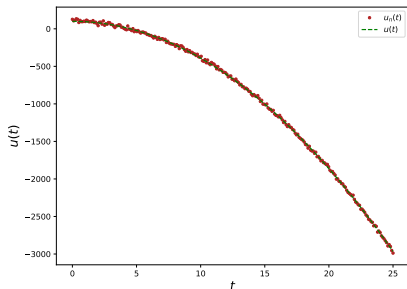
$$\ddot{u} = -g; \quad g = 9.81$$



Diferencijalna jednačina

$$\ddot{u} = -g; \quad g = 9.81$$

- PDE-FIND

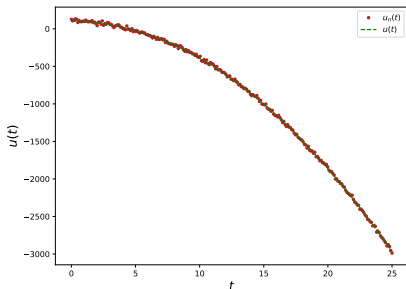


$$\ddot{u} = -9.81$$

$$\Delta\xi = 0\%$$

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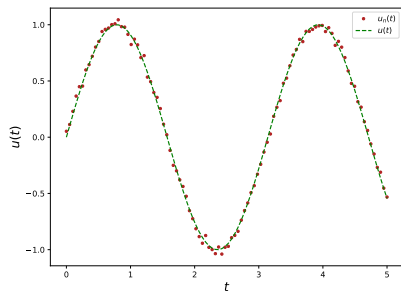
- PDE-FIND sa šumom
($\mu_N = 0, \sigma_N = 15$)

$$\ddot{u} = -9.795279$$

$$\Delta\xi = (1.0 \pm 0.5)\%$$

Diferencijalna jednažba

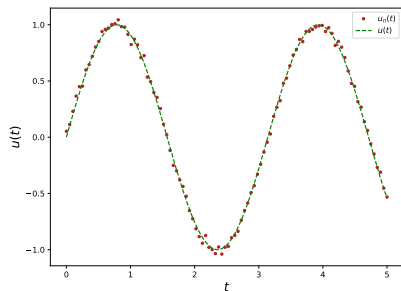
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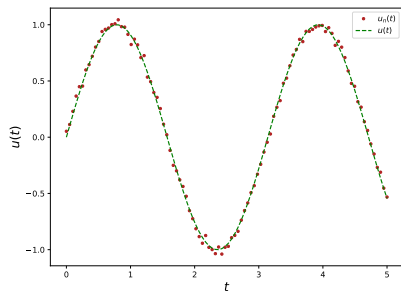


$$\ddot{u} = -3.99687u$$

$$\Delta\xi = 0.08\%$$

Diferencijalna jednačba

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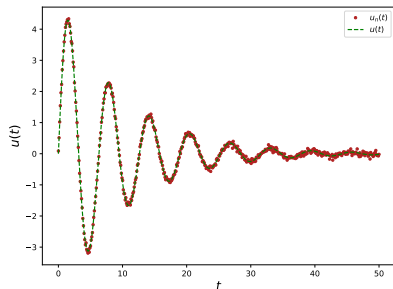
- PDE-FIND sa šumom
($\mu_N = 0, \sigma_N = 0.03$)

$$\ddot{u} = -3.879961u$$

$$\Delta\xi = (3.0 \pm 1.6)\%$$

Diferencijalna jednačba

$$\ddot{u} = -2\zeta\dot{u} - \omega^2 u; \quad \omega = 1, \quad \zeta = 0.1$$



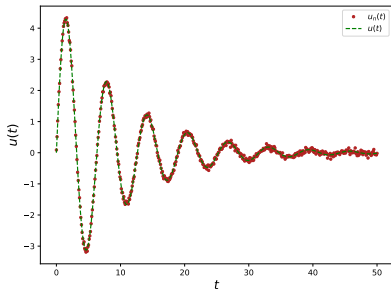
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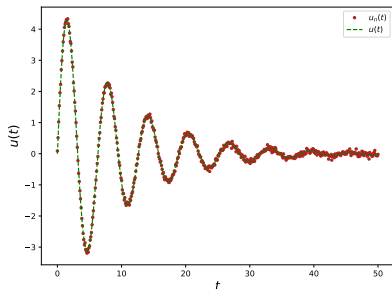
$$\ddot{u} = -0.200179\dot{u} - 0.999128u$$

$$\Delta\xi = 0.09\%$$



Diferencijalna jednačina

$$\ddot{u} = -2\zeta\dot{u} - \omega^2 u; \omega = 1, \zeta = 0.1$$



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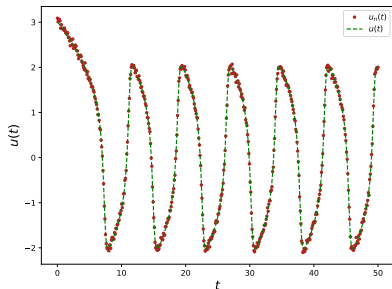
- PDE-FIND sa šumom
($\mu_N = 0, \sigma_N = 0.05$)

$$\ddot{u} = -0.188519\dot{u} - 0.982673u$$

$$\Delta\xi_{max} = (6 \pm 2)\%$$

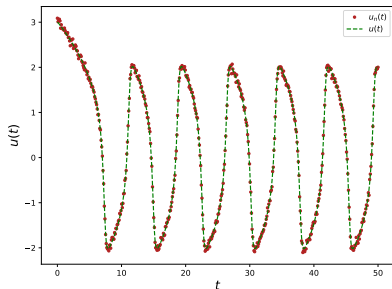
Diferencijalna jednađba

$$\ddot{u} = \mu(1 - u^2)\dot{u} - \omega^2 u; \omega = 1$$



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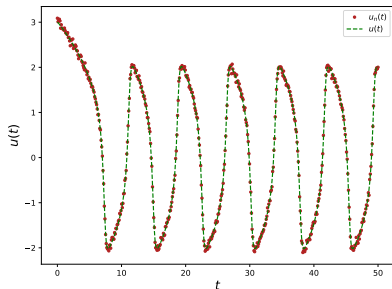


- 3 parametra μ

$$\mu = 0.1, 2 \text{ i } 5$$

Diferencijalna jednažba

$$\ddot{u} = \mu(1 - u^2)\dot{u} - \omega^2 u; \omega = 1$$



- 3 parametra μ

$$\mu = 0.1, 2 \text{ i } 5$$

- 3 početna uvjeta (x_0, \dot{x}_0)

$$(5, 1), (3, 0) \text{ i } (0, -5)$$

Diferencijalna jednačba

$$\ddot{u} = \mu(1 - u^2)\dot{u} - \omega^2 u; \omega = 1$$

Tablica: Van der Polov oscilatora bez šuma

μ	PDE-FIND	Max. greška
0.1	$\ddot{u} = 0.099726\dot{u} - 0.999290u - 0.099848u^2\dot{u}$	0.27%
2	$\ddot{u} = 1.941602\dot{u} - 0.972596u - 1.942509u^2\dot{u}$	2.92%
5	$\ddot{u} = 4.926123\dot{u} - 0.976853u - 4.905555u^2\dot{u}$	2.31%

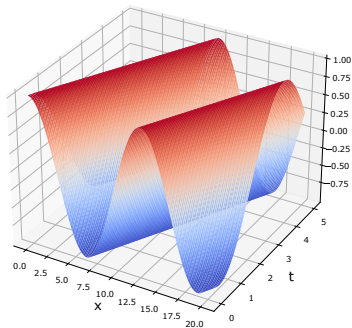
Diferencijalna jednačba

$$\ddot{u} = \mu(1 - u^2)\dot{u} - \omega^2 u; \omega = 1$$

μ	PDE-FIND srednja jednačba	Parametri μ_N i σ_N	Max. greška
0.1	$\ddot{u} = -0.016188 + 0.076330\dot{u} - 0.983806u$ $+ 0.006127u^2 - 0.002214u\dot{u} - 0.088699u^2\dot{u}$	$\mu_N = 0, \sigma_N = 0.05$	$(26 \pm 12)\%$
2	$\ddot{u} = -0.033608 + 1.412393\dot{u} - 0.928338u$ $+ 0.023849u^2 - 0.004304u\dot{u} - 1.357691u^2\dot{u}$	$\mu_N = 0, \sigma_N = 0.05$	$(32 \pm 3)\%$
5	$\ddot{u} = -0.010158 + 3.237894\dot{u} - 1.027299u$ $+ 0.002301u^2 - 0.005109u\dot{u} - 3.034661u^2\dot{u}$	$\mu_N = 0, \sigma_N = 0.05$	$(39 \pm 3)\%$

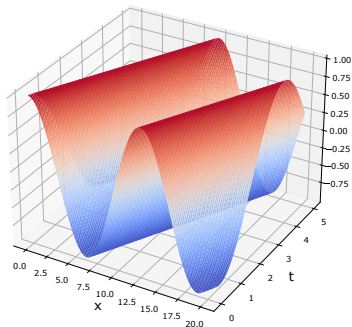
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$$\dot{u} = cu', \quad c = -2$$



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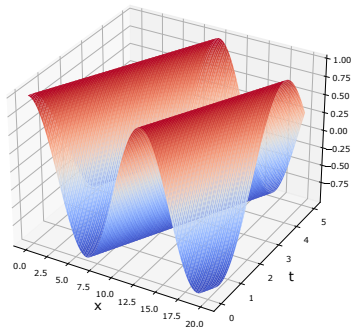
- PDE-FIND

$$\dot{u} = -2.002414u'$$

$$\Delta\xi = 0.1\%$$

Diferencijalna jednažba

$$\dot{u} = cu', \quad c = -2$$



- PDE-FIND

$$\dot{u} = -2.002414u'$$

$$\Delta\xi = 0.1\%$$

- PDE-FIND sa šumom
($\mu_N = 0, \sigma_N = 0.1$)

$$\dot{u} = -1.969783u'$$

$$\Delta\xi = (1.5 \pm 0.3)\%$$

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PDE Functional Identification of Nonlinear Dynamics

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Pozitivno

- Višedimenzionalni podatci i podatci sa šumom
- Brz, efikasan i robustan
- Fizika, kemija, biologija, ekonomija, ...

Identifikacija dinamike

PDE Functional Identification of Nonlinear Dynamics

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- Višedimenzionalni podatci i podatci sa šumom
- Brz, efikasan i robustan
- Fizika, kemija, biologija, ekonomija, ...

Negativno

- Visoka rezolucija
- Puno parametara
- Osjetljivost



Samuel H. Rudy, Steven L. Brunton, Joshua L. Proctor, and J. Nathan Kutz.

Data-driven discovery of partial differential equations.
Science Advances, 3(4):e1602614, 2017.



Steven L. Brunton, Joshua L. Proctor, and J. Nathan Kutz.

Discovering governing equations from data by sparse identification of nonlinear dynamical systems.



Proceedings of the National Academy of Sciences, 113(15):3932–3937, 2016.



R.J. LeVeque.

Finite Difference Methods for Ordinary and Partial Differential Equations: Steady-State and Time-Dependent Problems.

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-  R. González-García, R. Rico-Martínez, and I. G. Kevrekidis.
Identification of distributed parameter systems: A neural net based approach.
Computers and Chemical Engineering, 22(SUPPL.1):S965–S968, 1998.
-  Henning U. Voss, Paul Kolodner, Markus Abel, and Jürgen Kurths.
Amplitude equations from spatiotemporal binary-fluid convection data.
Phys. Rev. Lett., 83:3422–3425, Oct 1999.

Kraj prezentacije

<https://github.com/VinkoGitHub/Samostalni-seminar>