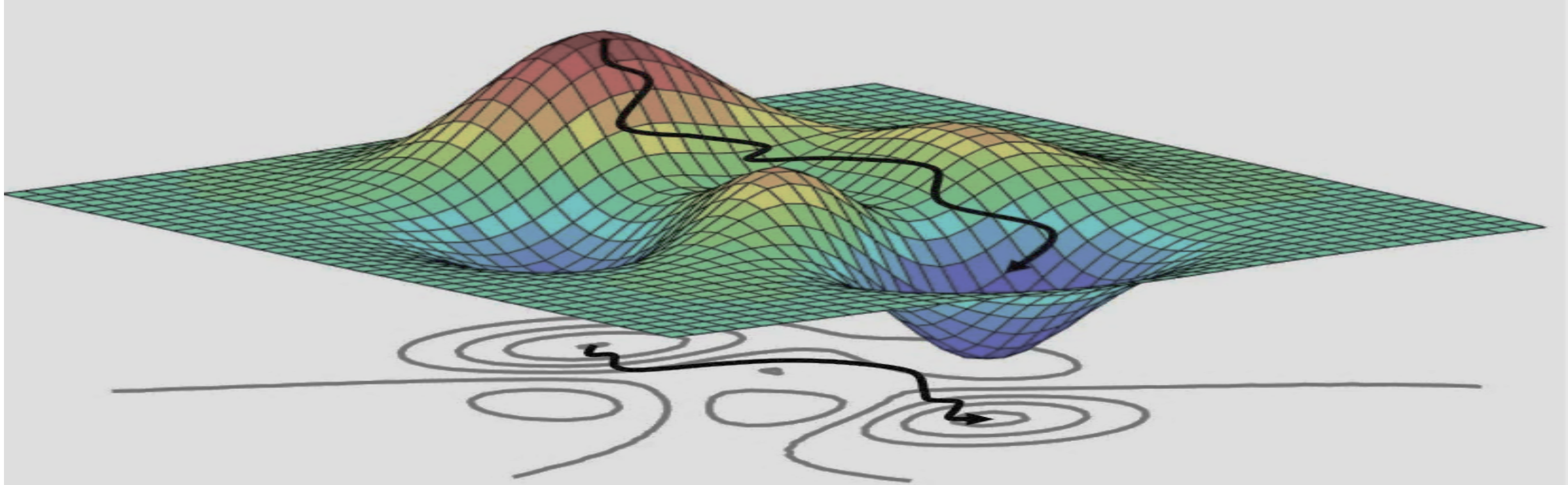


Learning to Optimize with Convergence Guarantees

using nonlinear system theory[1]

Luca Furieri

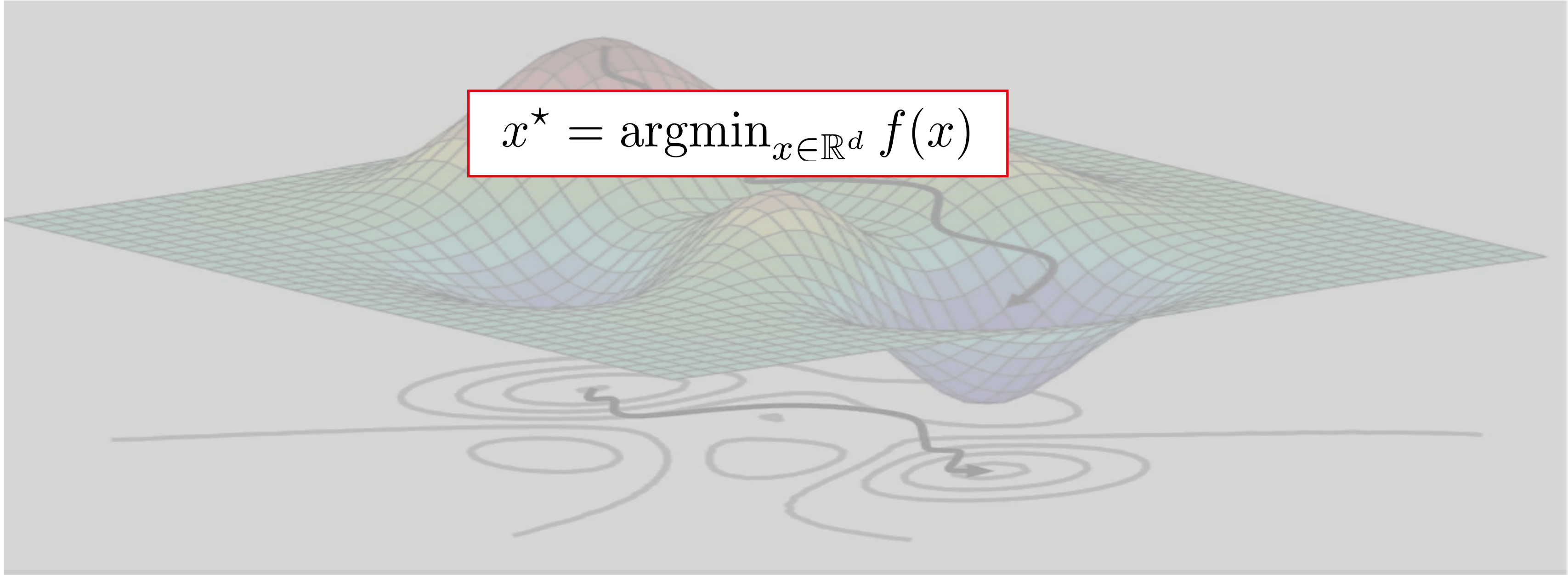
[1] Andrea Martin and Luca Furieri, “Learning to optimize with convergence guarantees using nonlinear system theory”, IEEE Control System Letters, 2024

École polytechnique fédérale de Lausanne

Swiss National Science Foundation

NCCR Automation

Optimization across disciplines



$$x^\star = \text{argmin}_{x \in \mathbb{R}^d} f(x)$$

Optimization across disciplines

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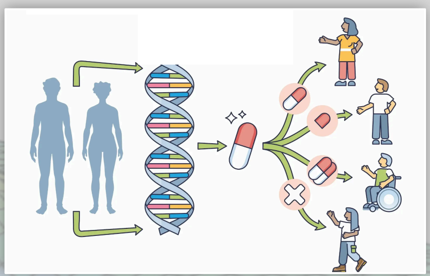

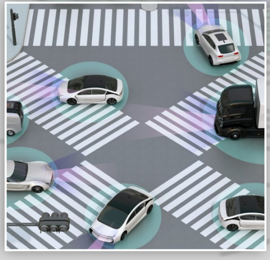

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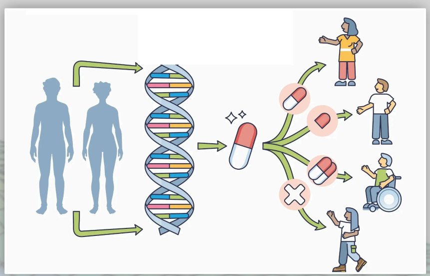

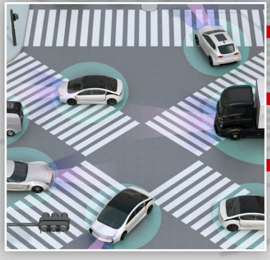

Nonconvex

Large scale

No analytical solution

Iterative optimization algorithms

$$x_{t+1} = x_t + \mathrm{update}_t(f, x_t)$$ *…until convergence*

(Hard) questions for the algorithm designer

1. ***Convergence*** as $t \to \infty$? From which initial guesses x_0?
2. ***How many interations*** for the algorithm to converge?
3. **Does the algorithm find a *«good» solution***?

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Examples

- Steepest descent algorithm: $x_{t+1} = x_t - \eta \nabla f(x_t)$

1. **Any x0** 2. **Linear rate.** 3. **Closest stationary point**

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Examples

- Steepest descent algorithm: $x_{t+1} = x_t - \eta \nabla f(x_t)$

  1. Any x0 2. Linear rate. 3. Closest stationary point

- Newton-Raphson algorithm: $x_{t+1} = x_t - \left(\nabla^2 f(x_t)\right)^{-1} \nabla f(x_t)$

  1. (x0 close to x*, global variants) 2. Quadratic rate 3. Stationary point

(Hard) questions for the algorithm designer

1. ***Convergence*** as $t \to \infty$? From which initial gue... $_0$?
2. ***How m...***
3. **Does th...**

Hyper-parameter tuning

- Step-size, 1° and 2° momentum…
- Lack of a general theory beyond convex
  - In ML, best practices and know-how

→ **Design of new algorithms**

- Steepest de...

1. **Any x0** 2...

- Newton-Raph...

1. **(x0 close to** ... **tationary point**

- Adam algorithm *(Kingma et al., 2014)*

1. **May diverge on convex** 2. **Empirical** 3. **Deep learning, empirical**

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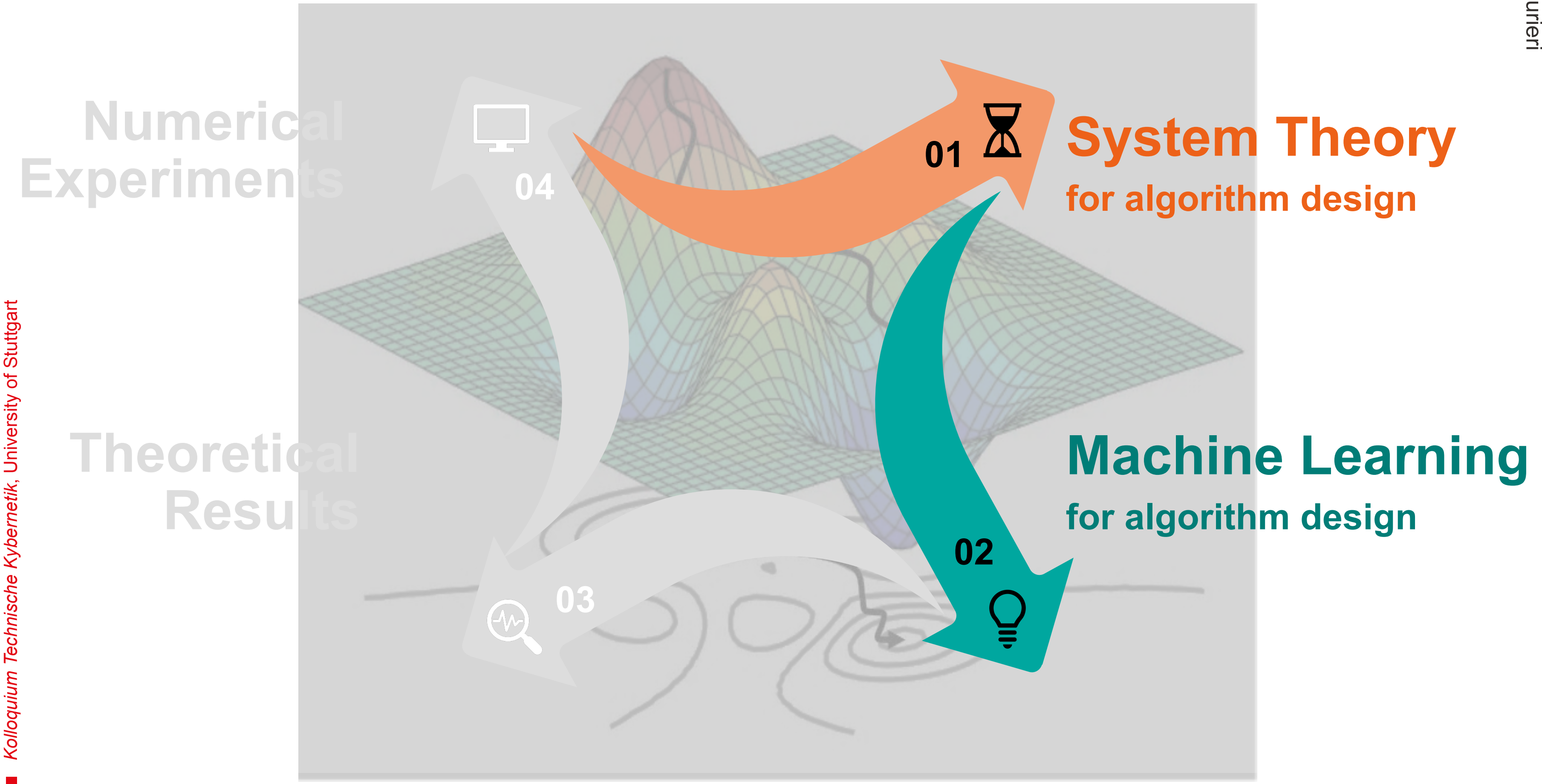
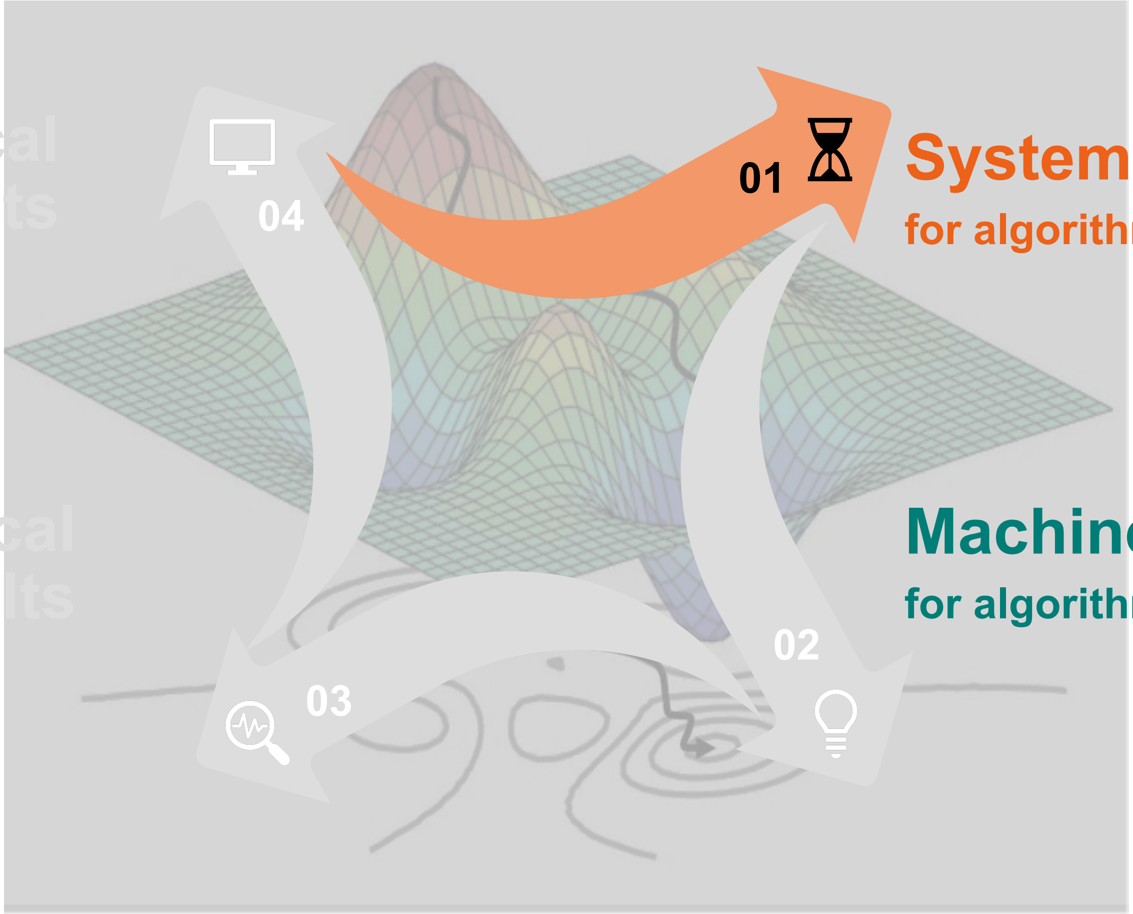


Design of new optimization algorithms



Numerical Experiments

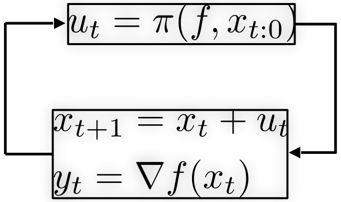
Theoretical Results

System Theory
for algorithm design

Machine Learning
for algorithm design

Success stories from system theory

Classical Algorithms $\equiv$ Control policies[1],[2]



$$
u_t = \begin{cases} -\eta \nabla f(x_t) & \text{(gradient descent)} \\ -\eta \nabla f(x_t) + \beta(x_t - x_{t-1}) & \text{(heavy ball)}^{[1]} \\ -\left(\nabla^2 f(x_t)\right)^{-1} \nabla f(x_t) & \text{(Newton-Raphson)} \\ \dots \end{cases}
$$

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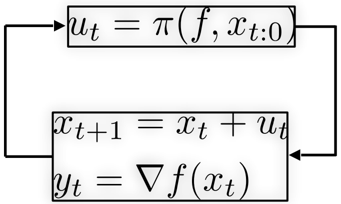

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Algorithm design $\equiv$ *Robust* control problem

For every cost function f in a class $\mathcal{F}$, designed algo must achieve:

1. ***Convergence:*** regulate $y_t = \nabla f(x_t)$ to zero
2. ***Speed:*** $\mathcal{H}_2/\mathcal{H}_\infty$ guarantees, exponential stability…
3. ***Solution quality:*** e.g., performance of equilibria

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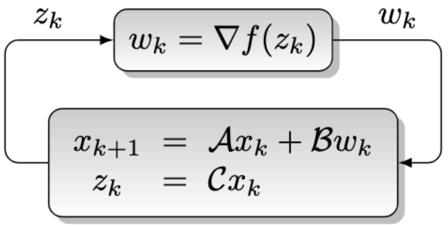
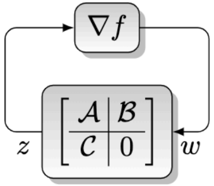
Success stories from system theory

- Classical algorithms equivalent to uncertain LTIs



$$\left(\begin{array}{c|c} \mathcal{A} & \mathcal{B} \\ \hline \mathcal{C} & 0 \end{array}\right) = \left(\begin{array}{cc|c} (1+\beta)I_d & -\beta I_d & -\alpha I_d \\ I_d & 0 & 0 \\ \hline (1+\gamma)I_d & -\gamma I_d & 0 \end{array}\right)$$

- ball algorithm by Polyak:



- … **is a Lure's system**[1,2]! We know a lot about them…

[1] Lessard, L., Recht, B., & Packard, A. (2016). Analysis and design of optimization algorithms via integral quadratic constraints. *SIAM Journal on Optimization*, *26*(1), 57-95.

[2] Scherer, C., & Ebenbauer, C. (2021). Convex synthesis of accelerated gradient algorithms. *SIAM Journal on Control and Optimization*, *59*(6), 4615-4645.

Success stories from system theory

- **Breakthrough[1,2]:** convex design of algorithm $\mathcal{A}, \mathcal{B}, \mathcal{C}$ such that

$$||x_k - x^\star|| \leq K\rho^k ||x_0 - x^\star|| \qquad K > 0,\ \ \rho \in (0,1)$$

for all cost functions that are **(strongly)-convex and smooth**

- Integral Quadratic Constraints (IQCs) for optimal worst-case convergence rates[1,2]
- Extrememum–seeking control, algorithms with delayed info…[2]

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A main take-away

Crucial role of nonlinear, robust system theory

for the next generation of optimization algorithms

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EPFL

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  $\in (0, 1)$

  for all cost functio

- Integral Quadratic … gence rates[1,2]
- Extrememum–seek…

Open challenges

- Algorithms for **non-convex** cost functions
- Scaling to very large problems
- Beyond worst-case rates? (e.g. solution quality)

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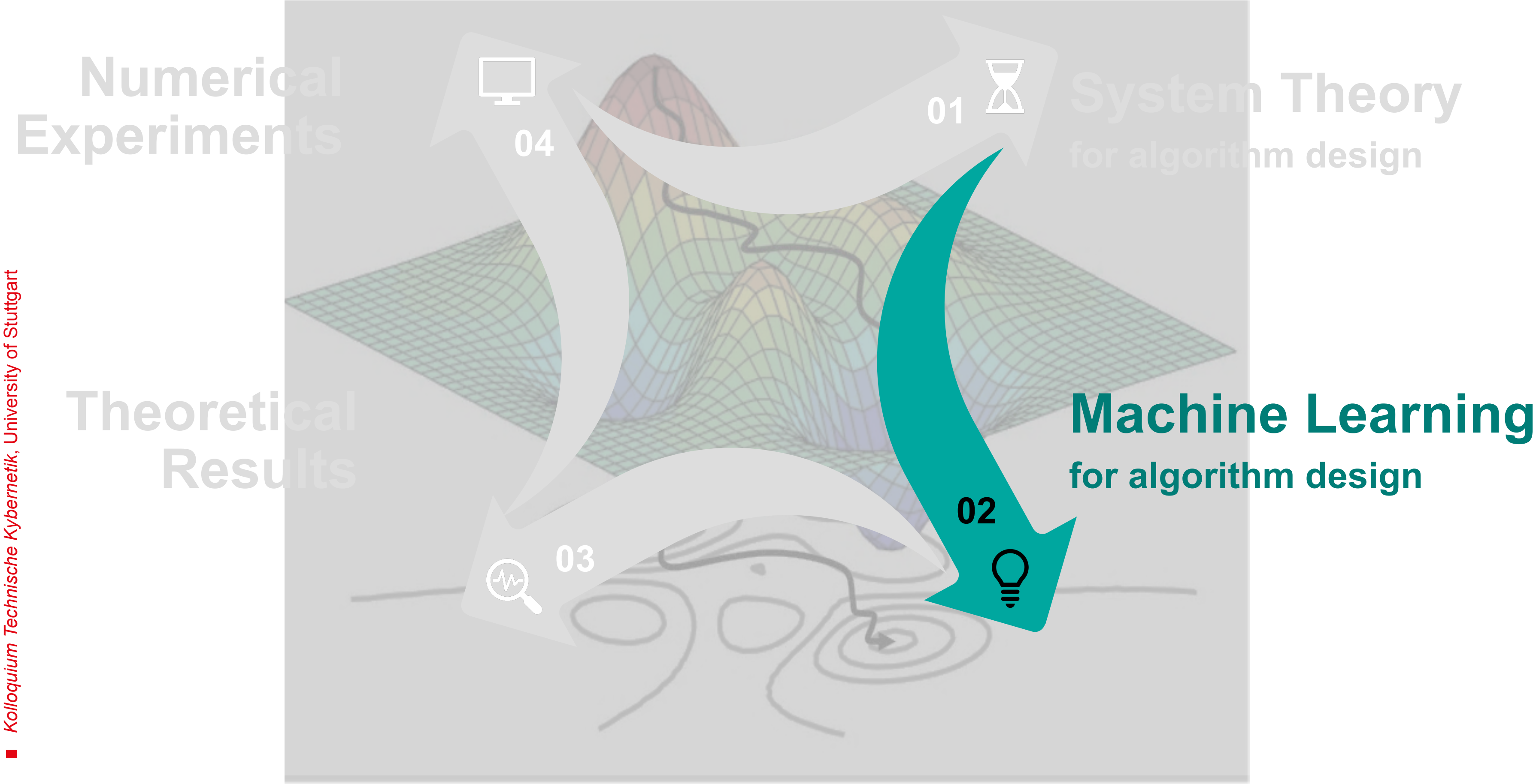
Design of new optimization algorithms



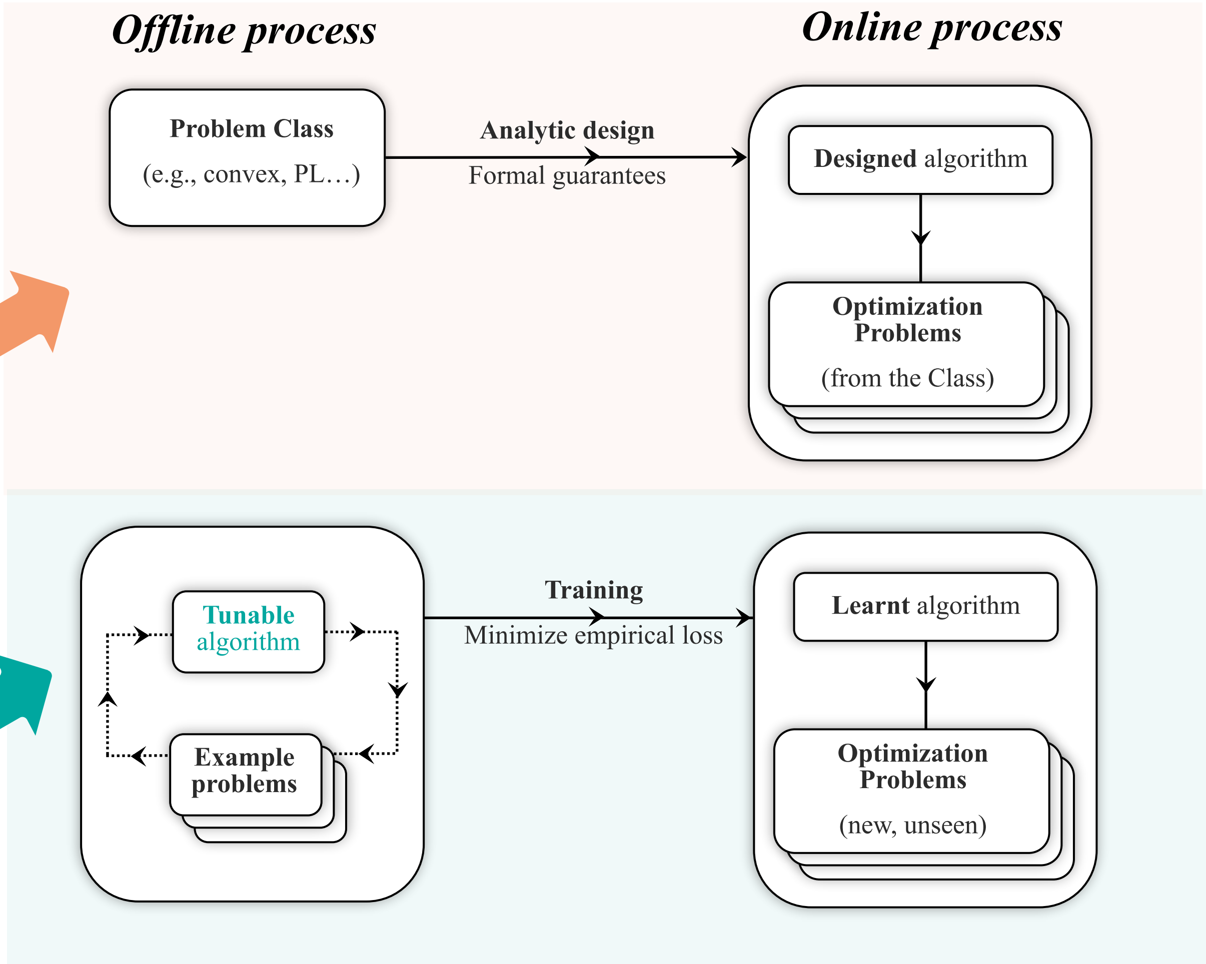
Different philosophies for algorithm design

	Offline process	*Online process*
System theory point-of-view		
Machine learning point-of-view		

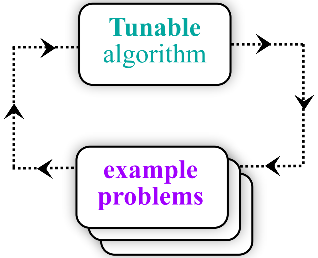
Different philosophies for algorithm design

System theory point-of-view

Machine learning point-of-view

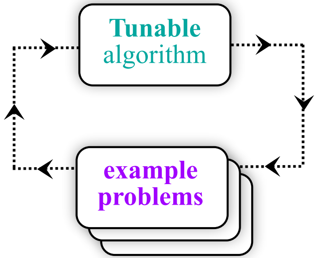


«Learning To Optimize» (L2O) for optimal control



«Learning To Optimize» (L2O) for optimal control

L. Furieri



- **Crucial**: «distribution» of **example problems**
  - *generalizability* VS *performance*
- Rule of thumb
  - *effective when* ***example problems*** *are representative of future instances*

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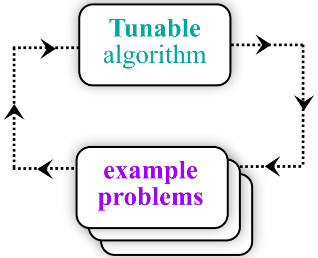

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  - *effective when **example problems** are representative of future instances*

Prime example: Nonlinear Model Predictive Control (NMPC)

Repeatedly solve…

$$u^\star(x(t)) = \arg\min_{\{u_k\}_{k=0}^{N-1}} \sum_{k=0}^{N-1} l(x_k, u_k) + l_f(x_N)$$

$$\text{subject to} \quad x_0 = x(t), \quad x_{k+1} = f(x_k, u_k)$$

$$x_k \in \mathcal{X}, \; u_k \in \mathcal{U}, \; x_N \in \mathcal{X}_f$$

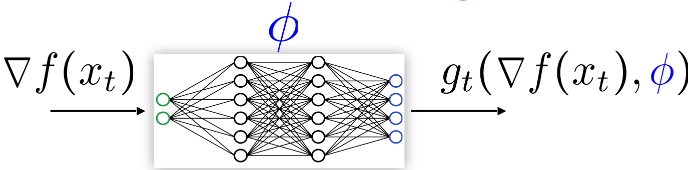
"examples"

A learnt algorithm can discover shortcuts unknown to standard interior-point solvers

Success of L2O in machine learning[1,2,3]

- **Parametrize** algorithms as follows:

$$x_{t+1} = x_t + g_t(\nabla f(x_t), \phi)$$



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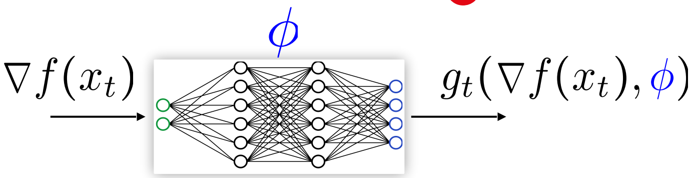

- **Measure performance** of an algorithm over T steps:

$$L(\phi) = \mathbb{E}_{f \sim \mathcal{F}, x_0 \sim X_0} \sum_{t=0}^{T} f(x_t)$$

where $\mathcal{F}$ is the set of «*example problems*»

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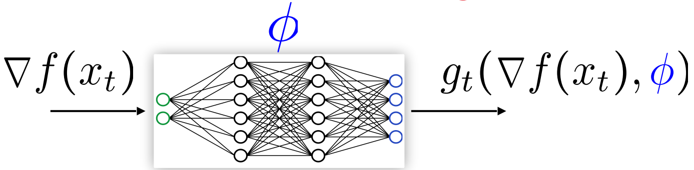

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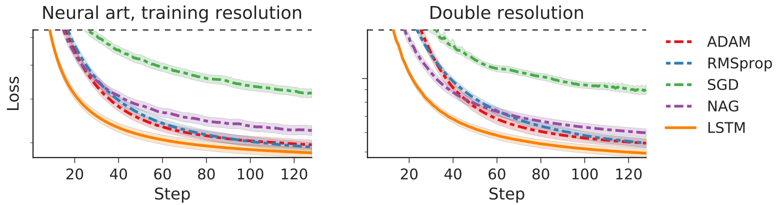

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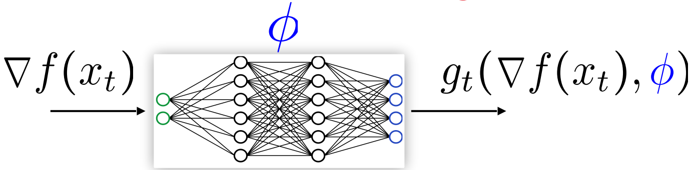

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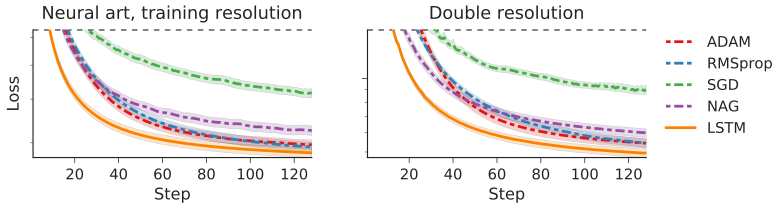

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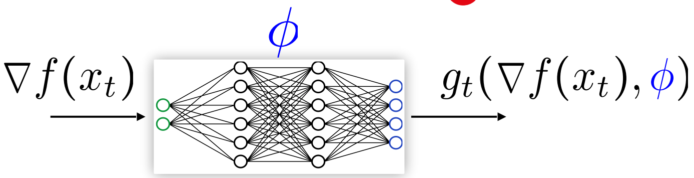

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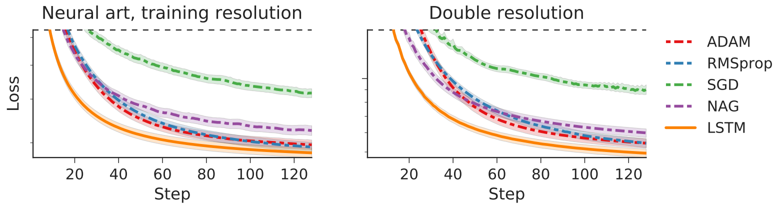

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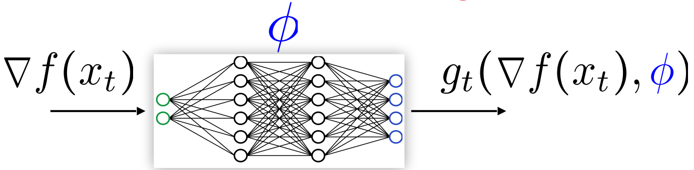

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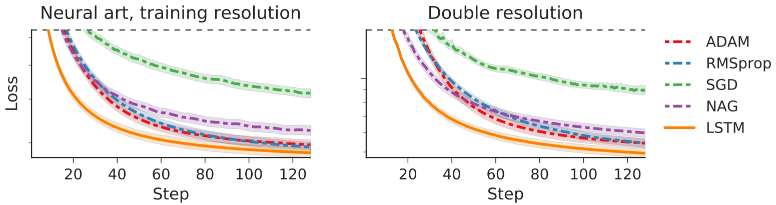

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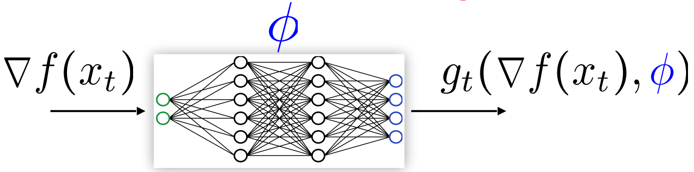

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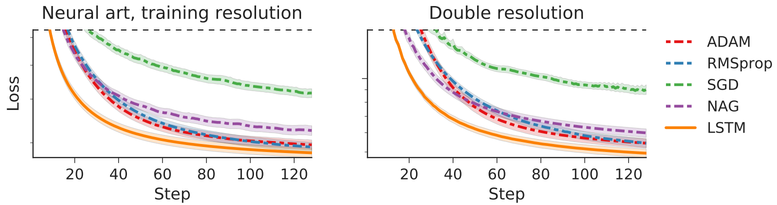

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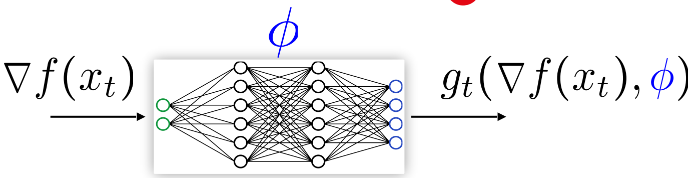

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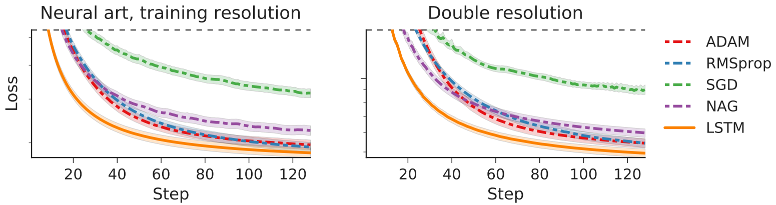

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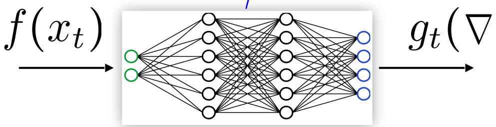

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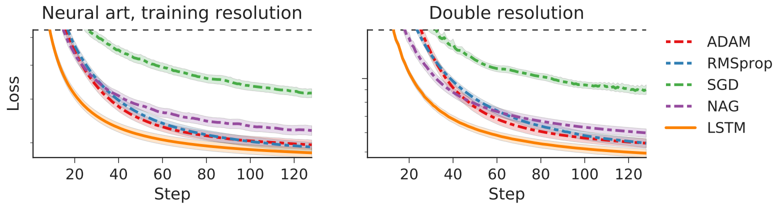

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Success of L2O in machine learning[1,2,3]

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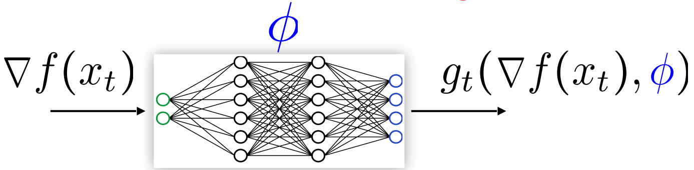

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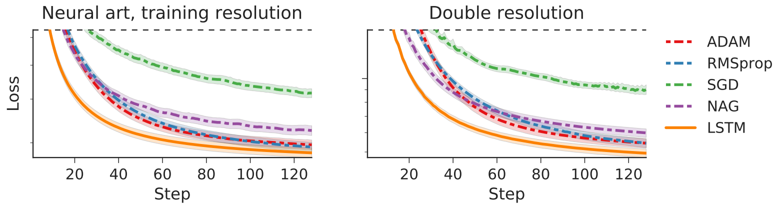

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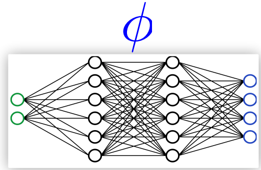
$\nabla f(x_t) \rightarrow$  $\rightarrow g_t(\nabla f(x_t), \phi)$

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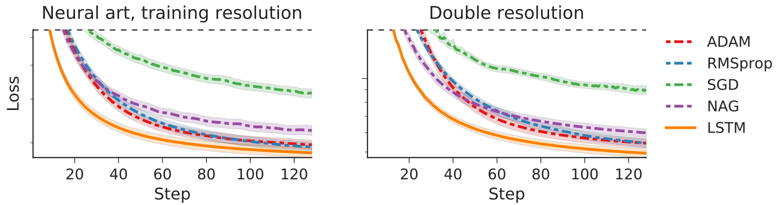

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Convergence: no guarantees![1]

- Requires conservative **fallback mechanisms**… …even for the convex case[2]

[1] Harrison, James, Luke Metz, and Jascha Sohl-Dickstein. "*A closer look at learned optimization: Stability, robustness, and inductive biases*." NeurIPS, 2022

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Focus of this work

- **Learn convergent algorithms** for smooth non-convex functions
  - …beyond conservative heuristics[1,2]

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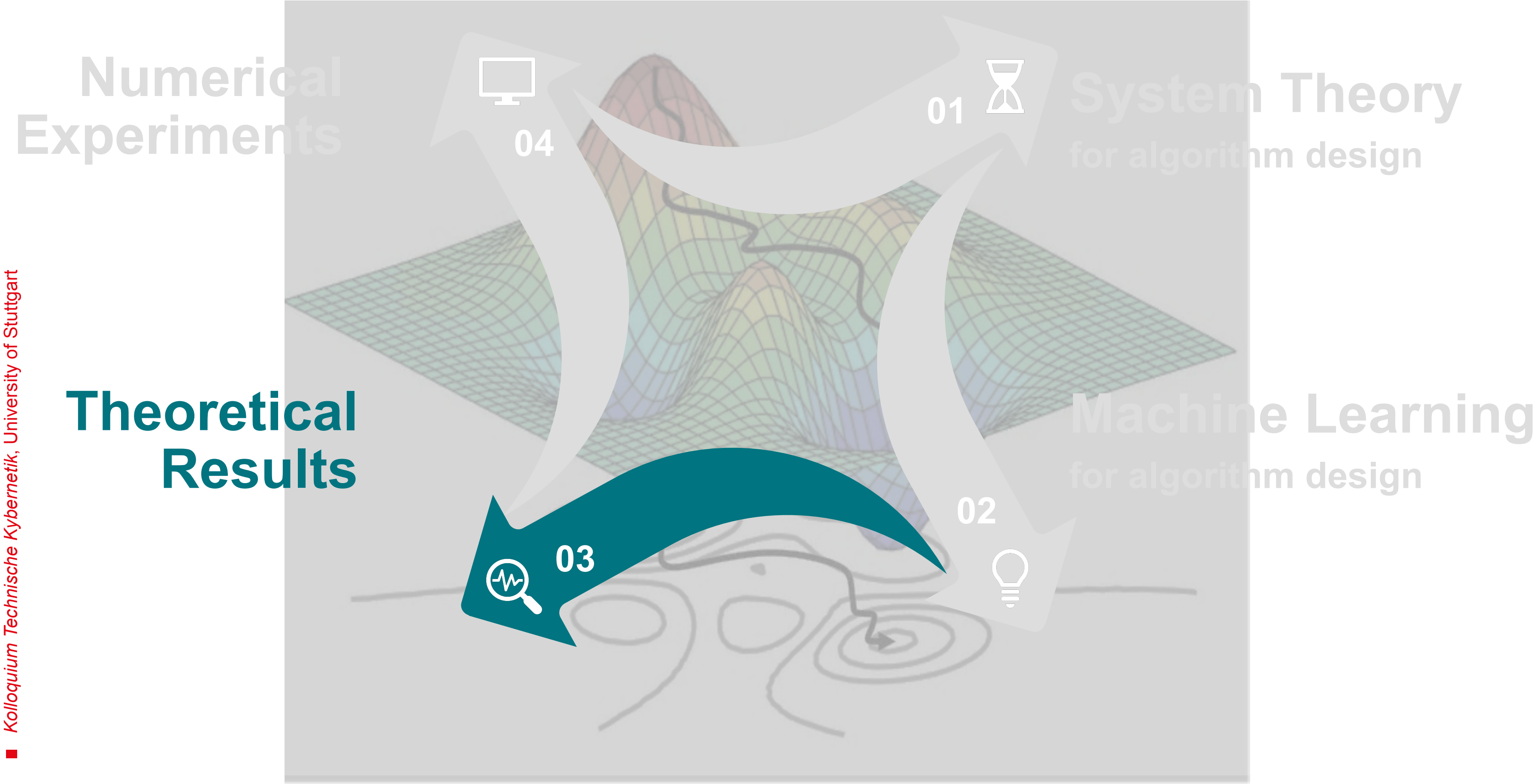
Design of new optimization algorithms



Problem Formulation (1)

- Denote as $\mathcal{S}_\beta$ the set of **non-convex** cost functions with β- Lipschitz gradients:

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$$\begin{cases} x_{t+1} = x_t + \pi_t(f, x_t) \\ x_0 = x_0 \end{cases} \iff z\mathbf{x} = \mathbf{x} + \boldsymbol{\pi}(f, \mathbf{x}) + z\boldsymbol{\delta}_0$$

$z \equiv$ one-time-step shift

$\mathbf{x} = (x_0, x_1, x_2, \ldots)$

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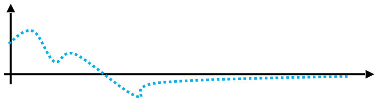

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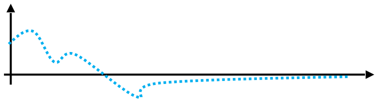

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- **Algorithms that convergence for a function** $f \in \mathcal{S}_\beta$

> "$\boldsymbol{\pi}$ *is **sum-square convergent** for f*" $\iff$ $\|\nabla f(\boldsymbol{x})\|^2 < \infty \quad \|\boldsymbol{\pi}(f, \boldsymbol{x})\|^2 < \infty,$
> "$\boldsymbol{\pi} \in \Sigma(f)$" $\left(= \sqrt{\sum_{t=0}^{\infty} |\nabla f(x_t)|^2}\right)$

Problem Formulation (2)

- **Problem**: *design an optimal robustly convergent algorithm*

$$\begin{aligned} \min_{\boldsymbol{\pi}} \quad & \mathbb{E}_{f\sim\text{Examples}, x_0 \sim \mathcal{X}_0} \left[\texttt{AlgoPerf}(f, \mathbf{x})\right] \\ \text{s.t.} \quad & x_{t+1} = x_t + \pi_t(f, x_{t:0}), \\ & \boldsymbol{\pi}(f, \mathbf{x}) \in \Sigma(f), \ \forall f \in \mathcal{S}_\beta \,, \end{aligned}$$

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  - E.g.: $\pi(f, x_t) = -\eta \nabla f(x_t)$ belongs to $\Sigma(f)$ for every $f \in \mathcal{S}_\beta$, if $\eta < \beta^{-1}$[1]
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- **Performance metric**:

$$\texttt{AlgoPerf}(f,\mathbf{x}) = \sum_{t=0}^{T} \alpha_t |\nabla f(x_t)|^2 + \gamma_t f(x_t)\,,$$

to balance fast convergence and solution quality

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Main result 1: a separation principle

- Consider the following algorithm:

$$\boldsymbol{\pi}(f, \mathbf{x}) = -\eta \nabla f(\mathbf{x}) + \mathbf{v}$$

- **Key idea:** separate algorithms into two addends

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Result: The algorithm above is sum-square convergent for all $f \in \mathcal{S}_\beta$ if:

- $\eta < \beta^{-1}$
- $\mathbf{v}$ is a bounded-energy ℓ_2 signal, that is, $\sum_{t=0}^{\infty} ||v_t||^2 \leq \infty$

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$$\boxed{\implies ||\nabla f(\mathbf{x})||_2^2 \leq K_1 + K_2||\mathbf{v}||_2^2 \leq \infty}$$

[1] Khalil, Hassan K. *Control of nonlinear systems*. Prentice Hall, New York, NY, 2002.
[2] Andrea Martin and Luca Furieri, *Learning to optimize with convergence guarantees using nonlinear system theory,* IEEE Control System Letters, 2024

Main result 2: completeness

(Crucial) question: can *any* algorithm that robustly converges on $\mathcal{S}_\beta$ be expressed as

$$\boldsymbol{\pi}(f, \mathbf{x}) = -\eta \nabla f(\mathbf{x}) + \mathbf{v} \quad ?$$

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$$\boldsymbol{\pi}(f, \mathbf{x}) \in \Sigma(f), \ \forall f \in \mathcal{S}_\beta \, .$$

Then, there exists an $\mathcal{L}_2$ operator $\mathbf{V}$ such that the algorithm

$$\boldsymbol{\pi}'(f, \mathbf{x}) = -\eta \nabla f(\mathbf{x}) + \mathbf{V}(x_0)$$

yields the same trajectories as $\boldsymbol{\pi}$, for every x_0 and every $f \in \mathcal{S}_\beta$.

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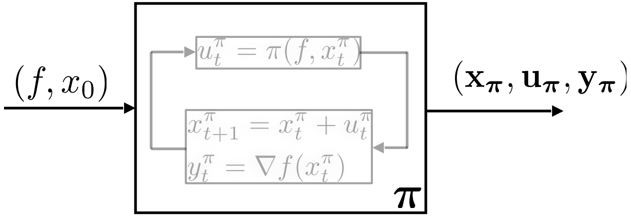
Proof sketch:



is an $\mathcal{L}_2$ operator.

Then $\mathbf{V}(x_0) = \eta\nabla f(\mathbf{x}_{\boldsymbol{\pi}}(x_0)) + \mathbf{u}_{\boldsymbol{\pi}}(x_0)$ achieves desired behavior, and also lies in $\mathcal{L}_2$

[1] Andrea Martin and Luca Furieri, *Learning to optimize with convergence guarantees using nonlinear system theory,* IEEE Control System Letters, 2024

Importance of main results 1 and 2

One-to-one parametrization

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EPFL

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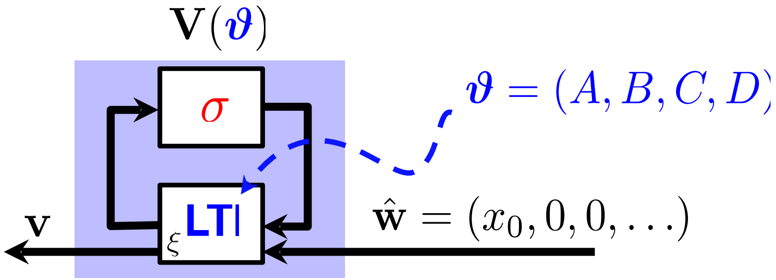
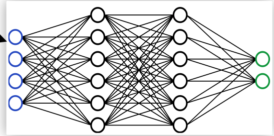
How do we search over these operators?

Unconstrained parametrizations of $\mathbf{V} \in \mathcal{L}_2$



- Expressive models including

$$\xi_t = \hat{A}\xi_{t-1} + \hat{B}\,\mathrm{NN}(\xi_{t-1}, \hat{\mathbf{w}}_t)$$
$$u_t = \hat{C}\xi_t + \hat{D}\,\mathrm{NN}(\xi_t, \hat{\mathbf{w}}_t)$$



- $\mathbf{V}(\vartheta) \in \mathcal{L}_2$ if there is a storage function $S(\xi) = \xi^\mathsf{T} P \xi$ verifying

$$S(\xi_{t+1}) - S(\xi_t) \leq \gamma^2 |x_0| - |u_t|$$

[1] Kim, K. K., E. Ríos Patrón, and R. D. Braatz. *Standard representation and unified stability analysis for dynamic artificial neural network models,* Transactions on Neural Networks, 2018
[2] Revay, M, R. Wang, and I.R. Manchester. *Recurrent equilibrium networks: Flexible dynamic models with guaranteed stability and robustness*. IEEE TAC 2023

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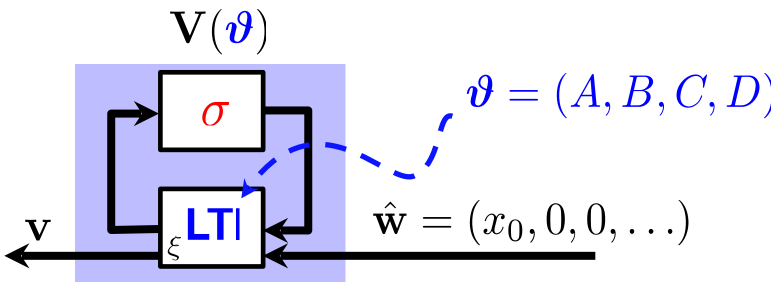

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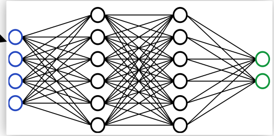

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⇩

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Challenges for effective L2O

1. **Insufficient features**
   - Learning to map $x_0 \in \mathbb{R}^d \rightarrow \mathbf{v}^\star \in \mathbb{R}^\infty$ is hard
2. **Full gradient measurements** for convergence

[1] Kim, K. K., E. Ríos Patrón, and R. D. Braatz. S… *network models,* Transactions on Neural Networks…
[2] Revay, M, R. Wang, and I.R. Manchester. *Recu… …dynamic models with guaranteed stability and robustness*. IEEE TAC 2023

1) Enriching the input features with $[I, f, \nabla f](x_t)$

- Parametrize additional signal with rich input features (**not in** ℓ_2):

$$\boldsymbol{\omega}(\boldsymbol{\varphi}) = \boldsymbol{\Omega}(\mathbf{x}, f(\mathbf{x}), \nabla f(\mathbf{x}), \boldsymbol{\varphi})$$

- Construct a combined signal $\mathbf{z}(\boldsymbol{\varphi}, \boldsymbol{\Theta})$ <u>which is ℓ_2 by construction</u>:

$$z_t(f, \nabla f, x_{t:0}, \boldsymbol{\varphi}, \boldsymbol{\Theta}) = \frac{\omega_t(f, \nabla f, x_{t:0}, \boldsymbol{\varphi})}{|\omega_t(f, \nabla f, x_{t:0}, \boldsymbol{\varphi})|} |v_t(x_0, \boldsymbol{\Theta})|$$

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Preserves one-to-one parametrization!

$$-\eta \nabla f(\mathbf{x}) + \frac{\boldsymbol{\Omega}(f, \nabla f, \mathbf{x})}{|\boldsymbol{\Omega}(f, \nabla f, \mathbf{x})|} |\mathbf{V}(x_0)| \equiv \boldsymbol{\pi}(f, \mathbf{x}) \in \Sigma(f), \ \forall f \in \mathcal{S}_\beta \,.$$

Proof of sufficiency: by construction

Proof of necessity: reduces to previous case by choosing $\boldsymbol{\Omega}(f, \nabla f, \mathbf{x}) = \mathbf{V}(x_0)$

2) Convergence with incomplete gradients

- Typical scenario in machine learning

$$f(x) = \sum_{i \in \text{batches}} f_i(x) \quad \Rightarrow \quad \underline{\text{access to } \nabla f_i(x) \text{ only}}$$

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Result: Convergence (*asymptotic*) is preserved using the update rule

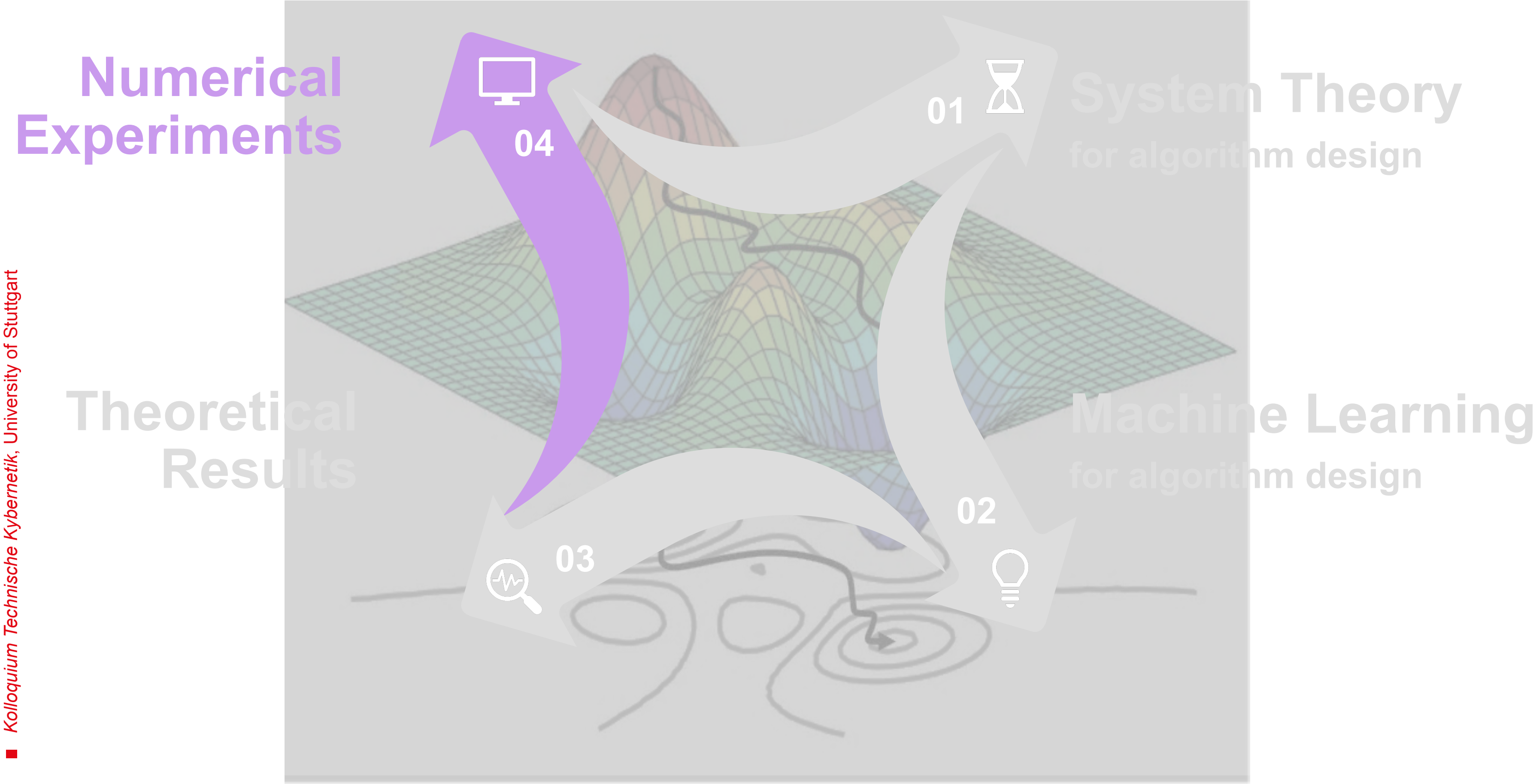
$$\boldsymbol{\pi}_t(x_t) = -\eta_t \nabla f_t(x_t) + v_t$$

as long as $\boldsymbol{\eta} \in \ell_2$ and $|v_t| \leq C\eta_t |\nabla f(x_t)|$.

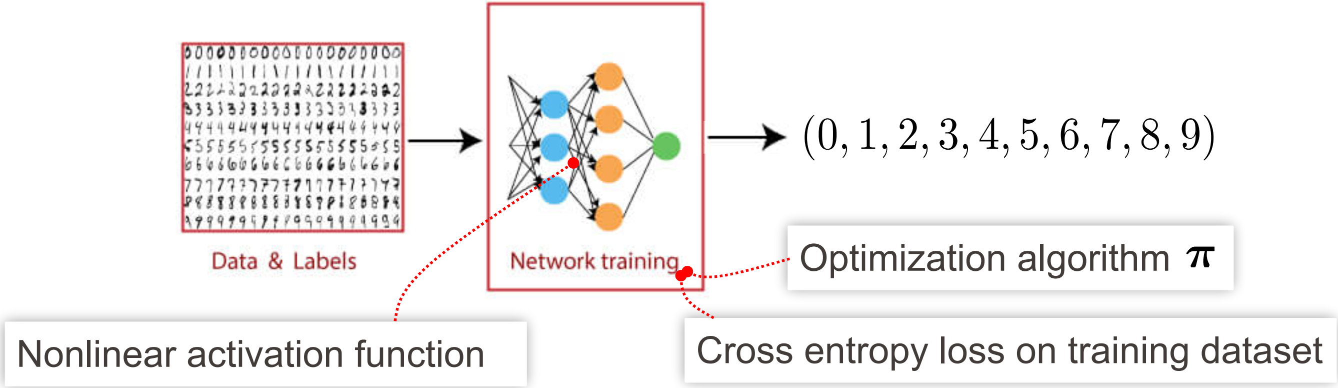
- **Convergence** guarantees of L2O algorithms **compatible with ML tasks**!
- **Only sufficient, only asymptotic convergence**
  - *necessity* relies on full gradient information
  - *asymptotic convergence*: consistent with stochastic gradient descent results

[1] Andrea Martin and Luca Furieri, *Learning to optimize with convergence guarantees using nonlinear system theory*, IEEE Control System Letters, 2024

Design of new optimization algorithms



Numerical experiments: image classification[1]



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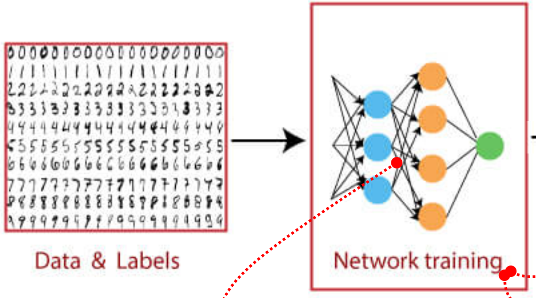

$\longrightarrow (0, 1, 2, 3, 4, 5, 6, 7, 8, 9)$

Optimization algorithm π

Nonlinear activation function

Cross entropy loss on training dataset

- **Algorithm training**: repeatedly optimize from uniformly distributed initial weights
  - $\mathrm{AlgoPerf}$: average algorithm performance (speed and solution quality)
  - We fix $\tanh$ activation function on

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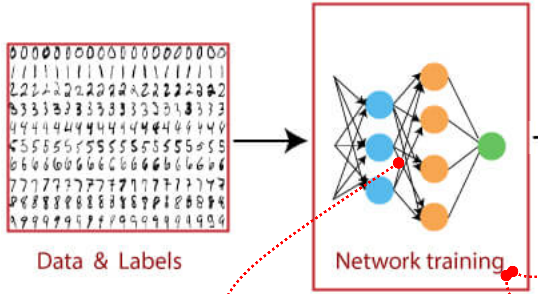

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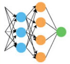
  - We fix $\tanh$ activation function on 
- **Algorithm testing**: compare with classical fine-tuned optimizers
  - Generalization to different activation functions on 
  - Convergence guaranteed by design

[1] LeCun, Y., Cortes, C. and Burges, C.J.C. (1998) The MNIST Database of Handwritten Digits. New York, USA. http://yann.lecun.com/exdb/mnist/

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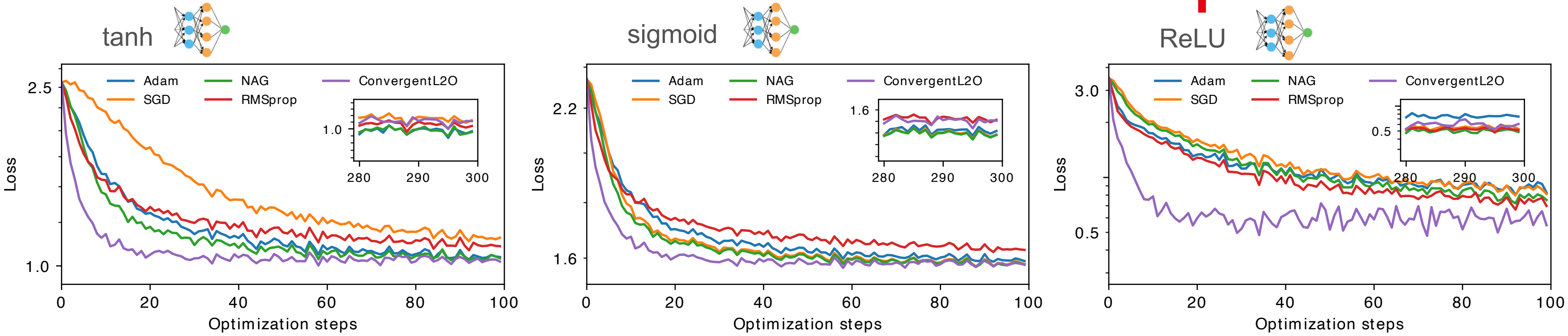

[1] Andrychowicz, Marcin, et al. "Learning to learn by gradient descent by gradient descent." NIPS 2016

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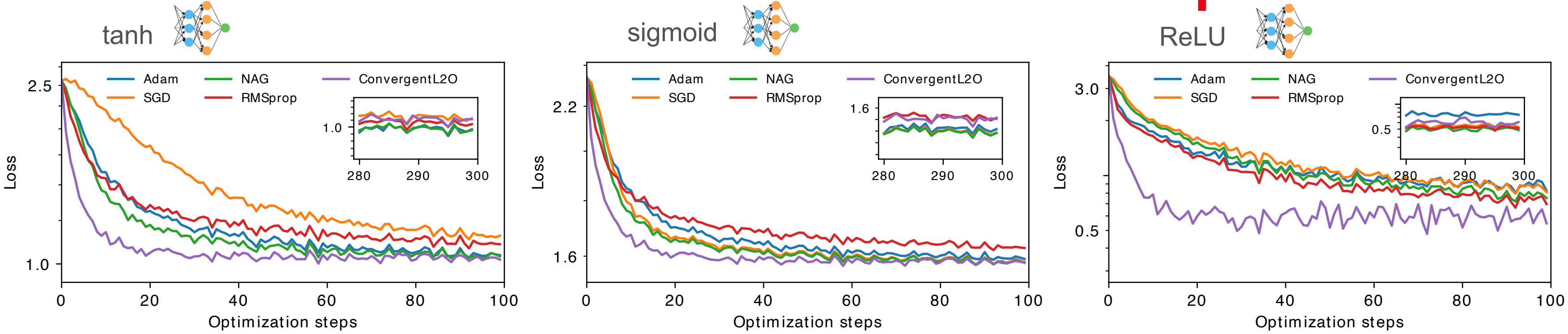

Classification accuracy on test data

Step $t = 20$	tanh	sigmoid	ReLU
Adam	$71.7 \pm 5.1\%$	$76.1 \pm 3.1\%$	$52.7 \pm 11.1\%$
SGD	$44.9 \pm 4.2\%$	$79.7 \pm 1.9\%$	$49.8 \pm 9.3\%$
NAG	$79.7 \pm 1.4\%$	$81.1 \pm 1.5\%$	$52.7 \pm 10.2\%$
RMSprop	$69.4 \pm 2.9\%$	$72.8 \pm 2.3\%$	$61.1 \pm 8.9\%$
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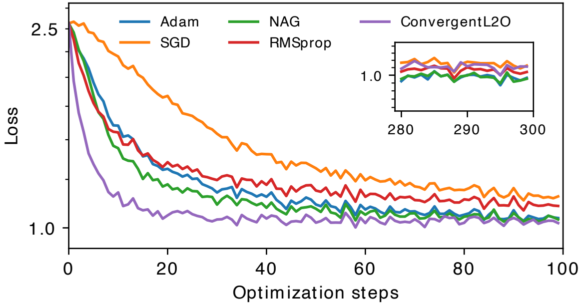
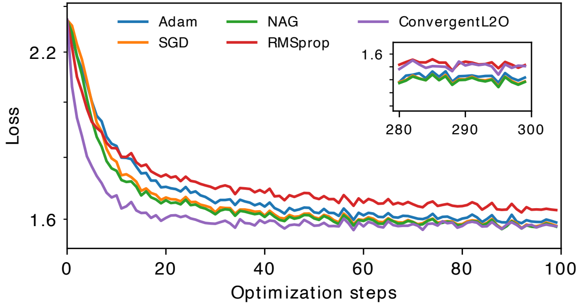
Numerical Experiments

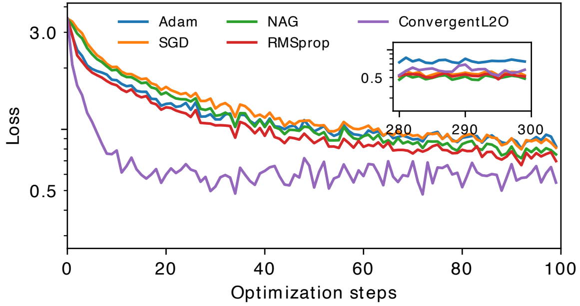
tanh



sigmoid



ReLU



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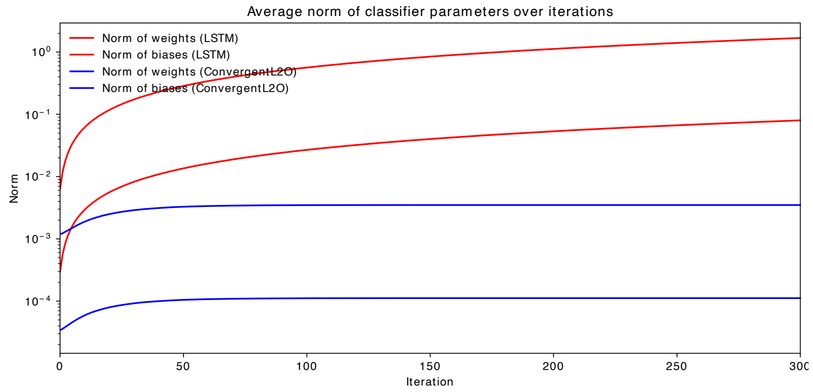
LSTM from [1] diverges!



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Conclusions

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  - With theoretical guarantees by design
  - For non-convex functions

Nonlinear system theory

L2O

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Check out the paper:

Thank you! Questions?

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