Quasi-Newton methods for solving nonsmooth optimization problems in learning and control

Adeyemi Damilare Adeoye

Supervisor: Prof. Alberto Bemporad

PhD Thesis Defence
IMT School for Advanced Studies Lucca, Italy

Jury: Prof. Mikael Johansson (KTH Royal Institute of Technology, Stockholm, Sweden), Prof. Panagiotis Patrinos (KU Leuven, Leuven, Belgium), Dr. Puya Latafat (IMT School for Advanced Studies Lucca, Italy)

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Outline

Introduction: Neural networks for function approximation

RNN for Markovian state-space dynamics

DCRNN: An RNN for Markovian state-space approximation

iSQPRL: An inexact SQP approach for recurrent learning

Recurrent-Control Neural Network

Generalized Gauss-Newton with self-concordant regularization

Conclusions and future directions

Some challenges in modeling, optimizing, and controlling the physical entities of a nonlinear dynamical system from first principles

As an example, some questions that concern arterial blood flow with no known straightforward answers:

- is a Newtonian or non-Newtonian model more appropriate?
- is there any universally accepted model for blood flow?
- how to choose parameters for any given model?
- efficient numerical methods for solving the governing equations under any given circumstance?
- are there efficient (numerical) methods to handle the high-complexity of realistic geometries?

Some challenges in modeling, optimizing, and controlling the physical entities of a nonlinear dynamical system from first principles

Notable remarks:

- **known fact:** blood is a non-Newtonian fluid
  (its viscosity changes with the wall shear rate)
- no known non-Newtonian model accurately describes the rheological behaviour of blood [1]
- governing equations computationally intensive to solve
  (a new problem needs to be solved for each new configuration)
- studies suggest that a Newtonian model can be a good approximation (especially for large arteries) [2][1]

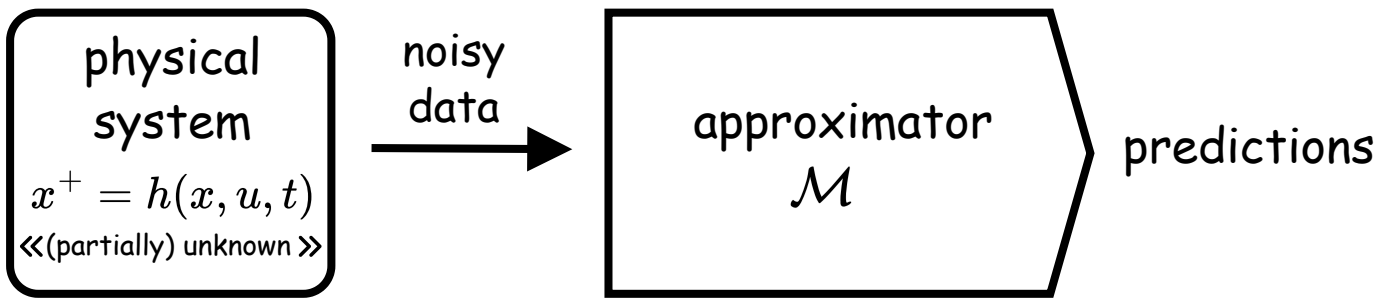
...still... there is no universally accepted model for blood flow!

[1] Johnston et al. 2006
[2] Johnston et al. 2004

A search for fast and accurate approximations of complex dynamical models

now, on the modeling aspect:

from (noisy) experimental data, can we "learn" models that provide real-time approximations to explicit (constitutive) models while accurately capturing the high-complexities in them?

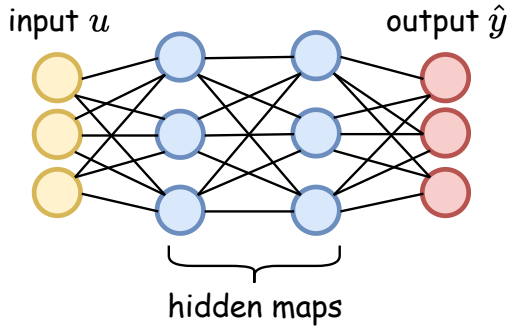


Neural networks for function approximation

Neural network:

$$\mathcal{M}(u;\theta) = \sigma_L(W_L\sigma_{L-1}(W_{L-1}\cdots\sigma_1(W_1u+b_1)\cdots+b_{L-1})+b_L)$$

- powerful tool for approximating complex functions from data



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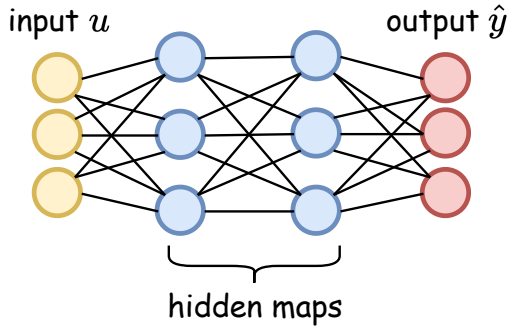
- data $\{(u_i, y_i)\}_{i=1}^m$
  model $\mathcal{M}(u;\theta)$, $u = [u_1, \ldots, u_m]^\top$
  predictions $\hat{y}_i = \mathcal{M}(u_i;\theta)$



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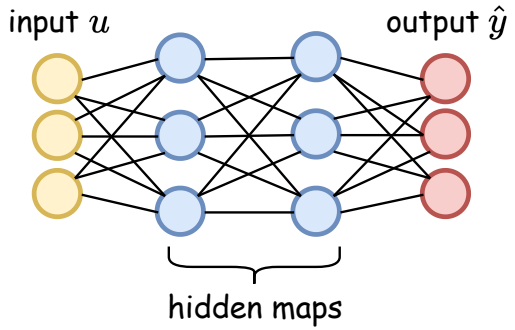
- $\theta \triangleq \{(W_l, b_l)\}_{l=1}^{L}$ is learned by empirical risk minimization:

$$\min_{\theta\in\mathcal{C}\subseteq\mathbb{R}^n} f(\theta) \triangleq \frac{1}{m}\sum_{i=1}^{m}\ell\left(y_i,\hat{y}_i\right)$$



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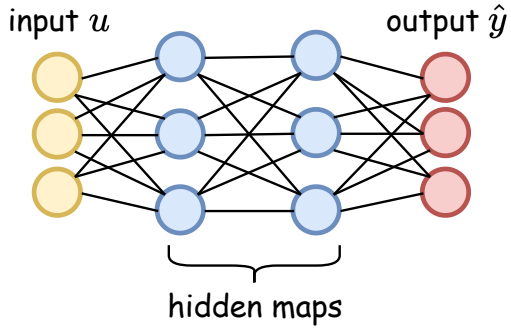

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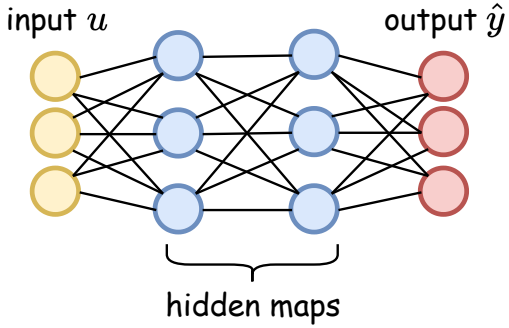
- breaks the classical *curse of dimensionality* [3]



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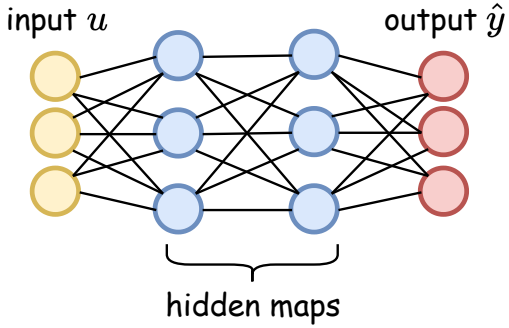

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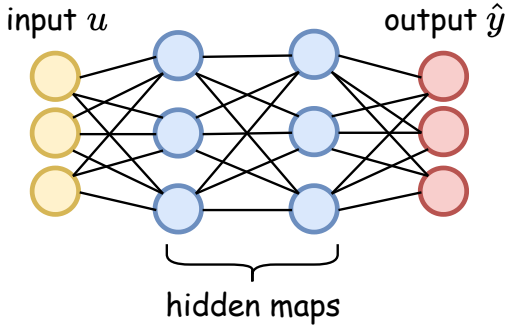

MNIST [4] (28×28 pixels per image), CIFAR-10/100 [5] (32×32 pixels per image), ImageNet [6] (224×224 pixels per image), ...

As per classical theory for 1-Lipschitz functions [7], we would need $\mathcal{O}(1/\varepsilon^{784})$ parameters to achieve a uniform ε-error for MNIST.

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Neural networks for function approximation

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- yet, deep neural networks perform astonishingly well in this *high-dimensional* regime!
- **why?**

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- yet, deep neural networks perform astonishingly well in this *high-dimensional* regime!
- **why?** ...some explanations exist[9], e.g., manifold assumption, random sampling, PDE assumptions,...

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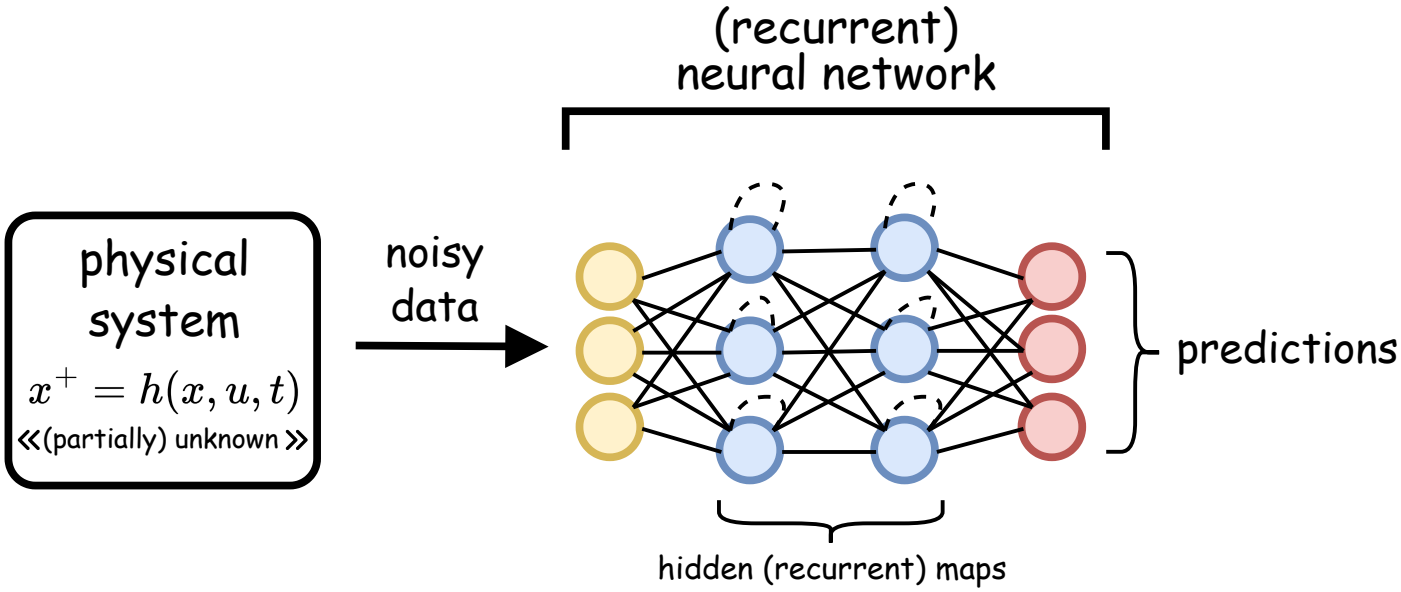
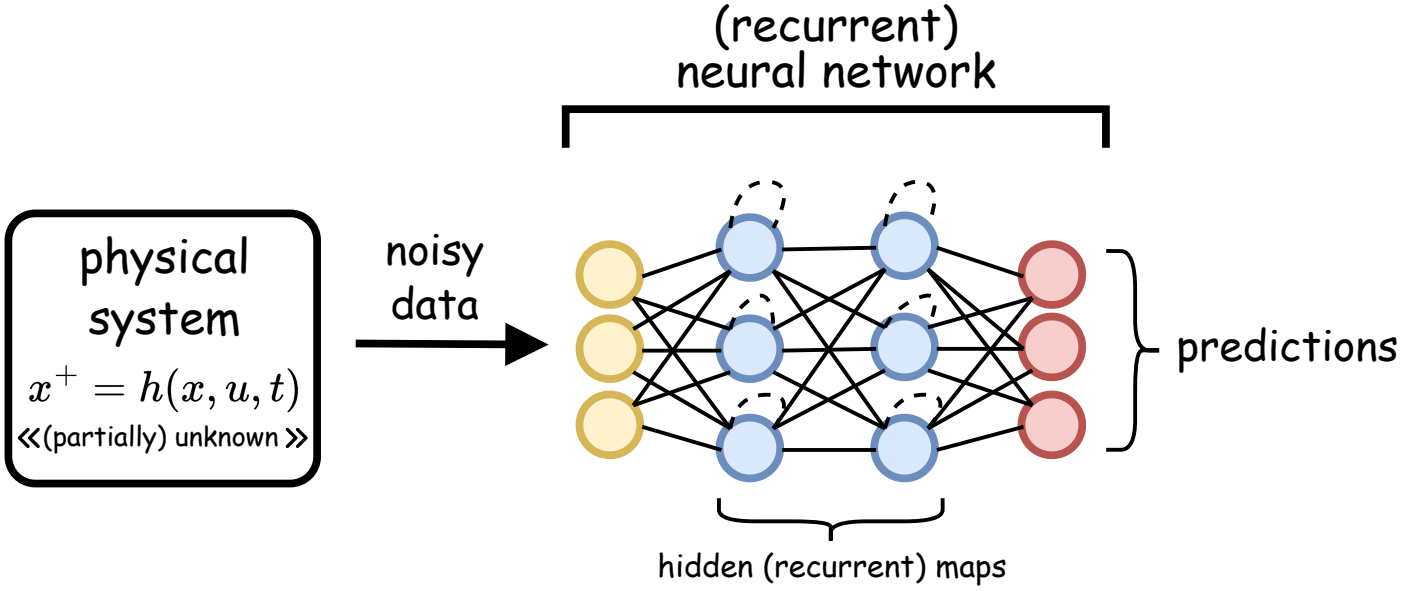
Neural networks for dynamical systems

- compared to FNNs, RNNs can capture temporal dependencies in data via feedback loops [10]



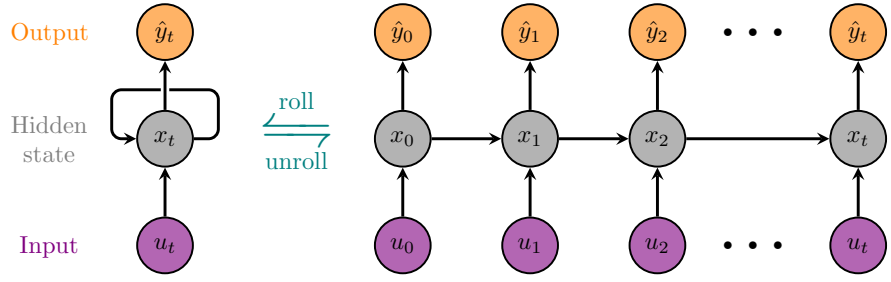
[10] Rumelhart, Hinton, and Williams 1986

Neural networks for dynamical systems



The vanilla RNN in state-space form:

$$x_{t+1} = \sigma_x(W_{xu}u_t + W_{xx}x_t + b_x)$$
$$\hat{y}_t = \sigma_y(W_{yx}x_t + b_y)$$



The approach (Motivation)

Architecture: a structured RNN for two-stage POMDP

- system identification: train the RNN to approximate the environment's Markovian state-space dynamics;
- optimal control policy selection by a FNN

The two stages combined constitutes the "agent's model".

[10] Bengio, Simard, and Frasconi 1994; Hochreiter 1998.
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Learning issues with BPTT algorithms:

- vanishing- and exploding-gradients[10]
- slow convergence of common BPTT algorithms[11]

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Two common remedies: (see Ref.[12])

- (approximate) second-order algorithms, e.g., generalized Gauss-Newton (GGN), Levenberg-Marquardt (LM), CG, etc....
- nonlinear sequential state-estimation techniques, e.g., EKF

[10] Bengio, Simard, and Frasconi 1994; Hochreiter 1998.
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RNN for Markovian state-space dynamics

Consider an RNN model of the form:

$$x_{t+1} = \sigma_x(W_{xu}u_t + W_{xy}y_t + W_{xx}x_t + b_x)$$
$$\hat{y}_t = \sigma_y(W_{yx}x_t + b_y)$$

σ_x: a nonlinear function (element-wise)
$u_t \in \mathbb{R}^{n_u}$: input at time t to the RNN
$y_t \in \mathbb{R}^{n_y}$: "observable" output at time t
$x_t \in \mathbb{R}^{n_x}$: RNN hidden state at time t
$\hat{y}_t \in \mathbb{R}^{n_y}$: RNN prediction at time t
$\theta_x \triangleq vec([W_{xu}\ W_{xy}\ W_{xx}\ b_x]) \in \mathbb{R}^{n_{\theta_x}}$
$\theta_y \triangleq vec([W_{yx}\ b_y]) \in \mathbb{R}^{n_{\theta_y}}$

e.g., an agent uses what it perceives of y_t for future predictions/actions

---

[13] McCloud 1993; Tumblr 2012
[14] Ha and Schmidhuber 2018.

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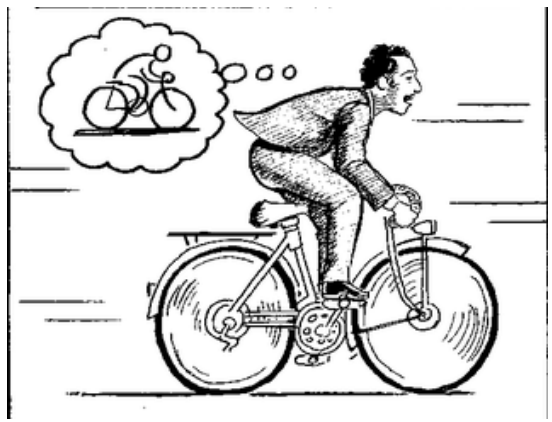
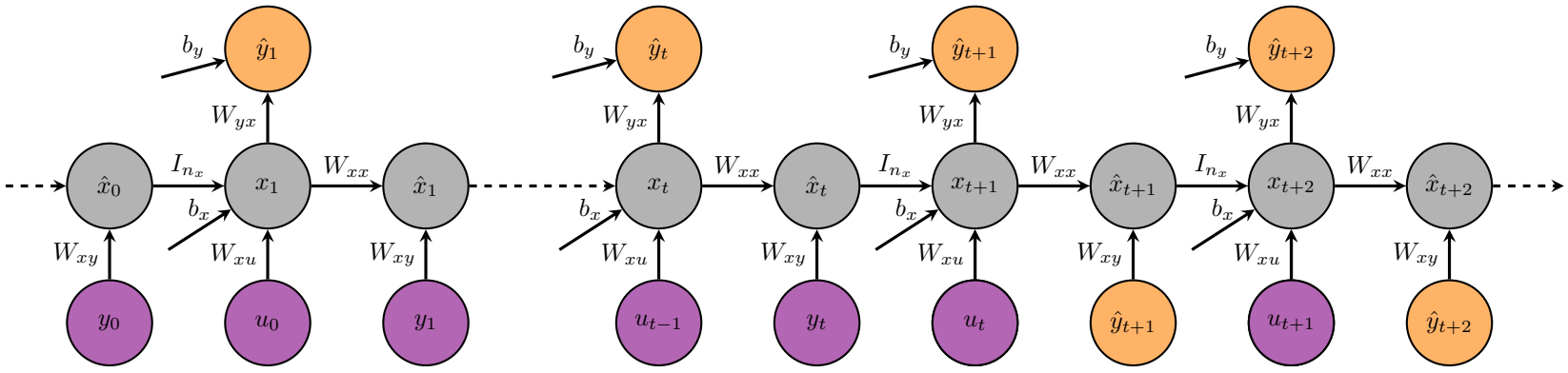


A World Model.[13]

Humans develop a mental model of the world based on what they are able to perceive with their limited senses.[14]

[13] McCloud 1993; Tumblr 2012
[14] Ha and Schmidhuber 2018.

DCRNN: An RNN for system identification



Unrolled RNN with dynamically consistent overshooting (DCRNN).

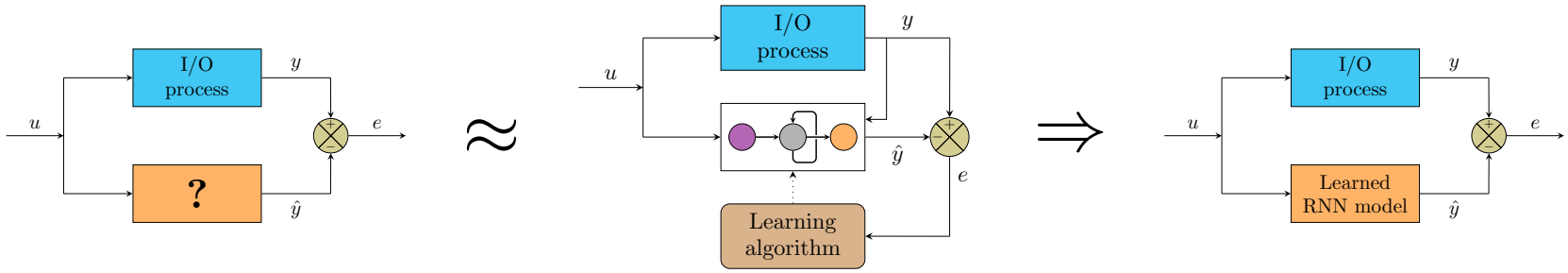
State-space equations of DCRNN[15]:

$$x_{t+1} = \sigma_x(\mathrm{I}\hat{x}_t + W_{xu}u_t + b_x), \qquad \hat{x}_t = \begin{cases} W_{xx}x_t + W_{xy}y_t, & \forall 0 \leq t \leq m_-, \\ W_{xx}x_t + W_{xy}\hat{y}_t, & \forall m_- < t \leq N, \end{cases}$$
$$\hat{y}_t = W_{yx}x_t + b_y$$

$N = m_- + m_+$, m_- is the finite truncation time of the RNN unrolling and $m_+ > 1$ is the number of overshooting time steps into the future.

[15] Zimmermann et al. 2006.

Learning the DCRNN – Optimization problem



Learn x_t, θ_y, θ_x in parallel by solving equality-constrained optimization problem[16]: (RNN training problem = optimal control problem)[17]

$$\min_z \quad f(z) \triangleq \sum_{t=0}^{N-1} (y_t - \hat{y}_t)^2 + \mathcal{R}(x_0, \theta_x, \theta_y)$$

$$\text{s.t.} \quad c_t(z) = 0, \quad \forall t = 0, \dots, N,$$

$$\text{with} \quad c_t(z) \triangleq x_{t+1} - \sigma_x(\mathrm{I}\hat{x}_t + W_{xu} u_t + b_x), \quad z \triangleq [x_1^\top \cdots x_{N-1}^\top \, x_0^\top \, \theta_y^\top \, \theta_x^\top]^\top$$

$$\hat{x}_t = \begin{cases} W_{xx} x_t + W_{xy} y_t, & \forall 0 \le t \le m_-, \\ W_{xx} x_t + W_{xy} \hat{y}_t, & \forall m_- < t \le N-1 \end{cases}$$

---

[16] Adeoye and Bemporad 2025.

[17] Bemporad 2022; Bemporad 2023.

SQP approach

1. Define the Lagrangian:

$$\mathcal{L}(z, \lambda) \triangleq f(z) - \lambda^\top c(z), \qquad \lambda \in \mathbb{R}^m$$

2. Iteratively model the QP subproblem (iSQPRL):

$$\begin{aligned} \min_{d_z} \quad & \frac{1}{2} d_z^\top H_k d_z + \nabla f(z_k)^\top d_z \\ \text{s.t.} \quad & J_k d_z + c(z_k) = 0, \end{aligned}$$

with $J_k \equiv \nabla c(z_k) = [\nabla c_0(z_k) \cdots \nabla c_{N-1}(z_k)]^\top \in \mathbb{R}^{m \times n}$,
$H_k \equiv \nabla^2 \mathcal{L}(z_k, \lambda_k)$.

Newton-KKT solution

1. Define necessary (KKT) optimality conditions:

$$\tilde{\mathcal{F}}(z_k, \lambda_k) \triangleq \begin{bmatrix} \nabla \mathcal{L}(z_k, \lambda_k) \\ c(z_k) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

[18] Saad and Schultz 1986.

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2. Derive the *Newton-KKT* system: For an optimal multiplier $\tilde{\lambda}$, we have

$$\underbrace{\begin{bmatrix} H_k & J_k^\top \\ J_k & 0 \end{bmatrix}}_{A_k} \underbrace{\begin{bmatrix} d_z \\ -\tilde{\lambda} \end{bmatrix}}_{d_k} = \underbrace{\begin{bmatrix} -g_k \\ -c_k \end{bmatrix}}_{b_k}$$

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3. Solve the system for d_k:
   - use a (modified) BFGS update of H_k
   - solve the resulting system using the *restarted GMRES*[18]

[18] Saad and Schultz 1986.

Local convergence

A local two-step superlinear convergence with $H_k \succ 0$:

Lemma (Powell 1978b, Theorem 1)

Under twice-differentiability, compactness and convexity assumptions, we have

$$\lim_{k\to\infty} \frac{\|(P_k(H_k - \nabla^2\mathcal{L}^*)P_k)d_z\|}{\|d_z\|} = 0 \quad \textit{implies} \quad \lim_{l\to\infty} \frac{\|z_{l+1} - z^*\|}{\|z_{l-1} - z^*\|} = 0,$$

where P_k is the projection matrix $P_k = I - J_k(J_k^\top J_k)^{-1}J_k^\top$.

Requires only that a projection of each H_k is close to a projection of $\nabla^2\mathcal{L}^*$.

Globalization (line-search)

For globalization, we define a merit function such as

$$\mathcal{M}_1(z_k;\rho_k) = f_k + \frac{\rho_k}{\omega}\|c_k\|_1, \qquad \frac{\rho_k}{\omega} > 0$$

with the heuristic choice $\omega \geq 2$.
Ideally, we want some $\alpha_k > 0$ such that d_k satisfies

$$\mathcal{M}_1(z_k + \alpha_k d_z;\rho_k) \leq \mathcal{M}_1(z_k;\rho_k) + \nu\alpha_k \nabla_{d_z}\mathcal{M}_1(z_k;\rho_k)$$

$0 < \nu \leq 0.5$ is a small value and $\nabla_{d_z}\mathcal{M}_1(z_k;\rho_k)$ is the directional derivative of $\mathcal{M}_1$ along d_z.
Finally, we update (z, λ) using

$$z_{k+1} = z_k + \alpha_k d_z, \quad \lambda_{k+1} = \lambda_k + \alpha_k(\tilde{\lambda} - \lambda_k). \tag{3}$$

Globalization conditions for inexact SQP

- **key requirement:** account for the error r_k due to inexactness: $A_k d_k = b_k + r_k$
- thanks to the restarted GMRES, we have $\|r_k\| \leq \sigma_4 \|b_k\|, 0 < \sigma_4 < 1$

Proposition (Partial)

If we choose $\rho_k > \omega \|\tilde{\lambda}\|_\infty$, then d_z is guaranteed to be a descent direction for $\mathcal{M}_1$, and $\nabla_{d_z} \mathcal{M}_1(z_k; \rho_k) < 0$ at nonstationary points of iSQPRL problem.

Globalization conditions for inexact SQP

Corollary

The following property holds:

$$\rho_k \geq \frac{\omega}{2}\left[\frac{g_k^\top d_z + d_z^\top H_k d_z - d_z^\top r_z}{\|c_k\|_1 - \|r_\lambda\|_1} + \|\tilde{\lambda}\|_\infty\right]. \tag{4}$$

choose $\omega \geq 2$.

Our *safeguarding* rule, slightly modifying Powell 1978a, is (for $\bar{\rho} > 0$)

$$\rho_k = \begin{cases} \max\{\omega\|\tilde{\lambda}\|_\infty + \bar{\rho},\ \frac{1}{\omega}(\rho_{k-1} + \omega\|\tilde{\lambda}\|_\infty + \bar{\rho})\}, \forall k \neq 1 \\ \omega\|\tilde{\lambda}\|_\infty + \bar{\rho}, \quad \text{if } k = 1. \end{cases} \tag{5}$$

Convergence to a stationary point

Theorem

Let $\rho_k > \omega\|\tilde{\lambda}\|_\infty$ hold according to the safeguarding rule. Let $\{\lambda_k\}$ be bounded and $\{\alpha_k\}$ be bounded below by some positive constant. Then the sequence of iterates $\{z_k\}$, starting from an arbitary point, converges to a stationary point of $\mathcal{M}_1$.

A direct consequence of the descent property of $\mathcal{M}_1$ at d_k such that the line-search succeeds for all k. (Practical refinements are needed!)

[19] Panier and Tits 1991

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A direct consequence of the descent property of $\mathcal{M}_1$ at d_k such that the line-search succeeds for all k. (Practical refinements are needed!)

- To avoid so-called "Maratos effect", incorporate, e.g., a nonmonotone line-search procedure.

Q-superlinear convergence preserved! [19] (Even though now $\mathcal{M}_1$ is not forced to reduce at initial steps.)

[19] Panier and Tits 1991

Numerical illustration

RL problem (mountain-car env): The car's motion is described by

$$\bar{y}_{t+1} = \bar{y}_t + \dot{\bar{y}}_t, \quad \dot{\bar{y}}_{t+1} = \dot{\bar{y}}_t + 0.001 u_t - 0.0025 \cos(3\bar{y}_t),$$

$y_t = [\bar{y}_t, \dot{\bar{y}}_t]$, $-1.2 \leq \bar{y}_t \leq 0.5$, $-0.07 \leq \dot{\bar{y}}_t \leq 0.07$, $\bar{y}_t$: car's position at time t, $\dot{\bar{y}}_t$: car's velocity at time t, $u_t \in \{-1, 0, 1\}$: control action (applied force), $\sigma_x = \tanh$, $\sigma_y =$ identity; bounds on y_t enforced through $t_{a_i, b_i}(\hat{y}_i) = \frac{b_i + a_i}{2} + \frac{b_i - a_i}{2} \left(\frac{2\hat{y}_i}{1 + \hat{y}_i} \right)$.

Numerical illustration

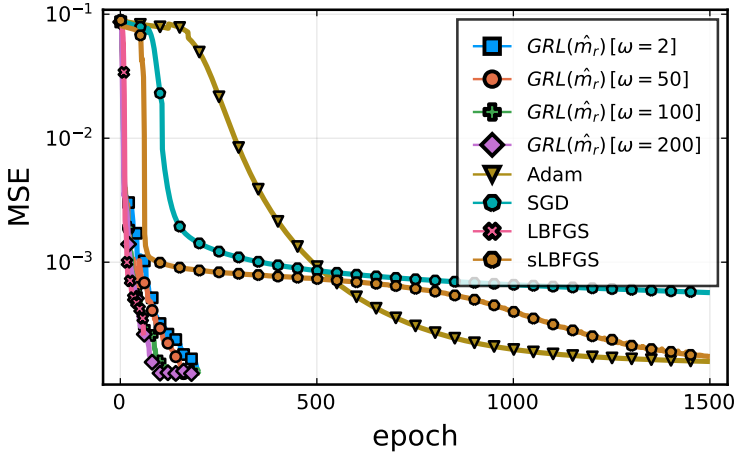
CSTR problem (ethylene oxidation): The reactor's dynamics are described by

$$
\begin{aligned}
\dot{\bar{y}}_1 &= u_1(1-\bar{y}_1\bar{y}_4)\\
\dot{\bar{y}}_2 &= u_1(u_2-\bar{y}_2\bar{y}_4) - A_1\, e^{\gamma_1/\bar{y}_4}(\bar{y}_2\bar{y}_4)^{0.5} - A_2\, e^{\gamma_2/\bar{y}_4}(\bar{y}_2\bar{y}_4)^{0.25}\\
\dot{\bar{y}}_3 &= -u_1\bar{y}_3\bar{y}_4 + A_1\, e^{\gamma_1/\bar{y}_4}(\bar{y}_2\bar{y}_4)^{0.5} - A_3\, e^{\gamma_3/\bar{y}_4}(\bar{y}_3\bar{y}_4)^{0.5}\\
\dot{\bar{y}}_4 &= \frac{u_1}{\bar{y}_1}(1-\bar{y}_4) + \frac{B_1}{\bar{y}_1}\, e^{\gamma_1/\bar{y}_4}(\bar{y}_2\bar{y}_4)^{0.5} + \frac{B_2}{\bar{y}_1}\, e^{\gamma_2/\bar{y}_4}(\bar{y}_2\bar{y}_4)^{0.25}\\
&\quad + \frac{B_3}{\bar{y}_1}\, e^{\gamma_3/\bar{y}_4}(\bar{y}_3\bar{y}_4)^{0.5} - \frac{B_4}{\bar{y}_1}(\bar{y}_4 - T_c)
\end{aligned}
$$

$y_t = [\bar{y}_1, \bar{y}_2, \bar{y}_3, \bar{y}_4]$ represent the gas density, ethylene concentration, ethylene oxide concentration, and temperature in the reactor; $u_t = [u_1, u_2]$, where u_1 is the feed volumetric flow rate and u_2 is the concentration of ethylene in the feed; $0.0704 \le u_1 \le 0.7042$, $0.2465 \le u_2 \le 2.4648$.

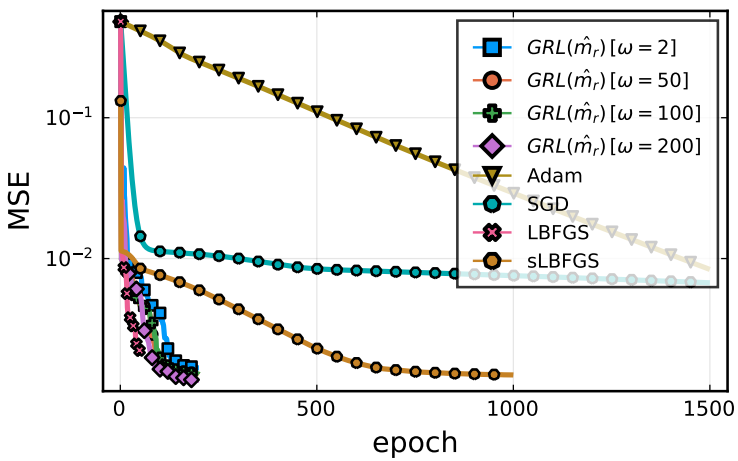
Numerical illustration

- mountain-car environment:



BPTT algorithm	Approximation error (MSE)	Iter	CPU time [s]
SGD	5.6828×10^{-4}	1500	5.6584×10
Adam	1.5821×10^{-4}	1500	4.9532×10
LBFGS	7.1389×10^{-4}	30	2.8670×10^{0}
sLBFGS	3.9884×10^{-4}	1000	2.8071×10
GRL($\hat{m}_r$), $\omega = 2$	1.3451×10^{-4}	200	6.4956×10
GRL($\hat{m}_r$), $\omega = 50$	$\mathbf{1.2702 \times 10^{-4}}$	200	1.0091×10^{2}
GRL($\hat{m}_r$), $\omega = 100$	1.3164×10^{-4}	200	5.6220×10
GRL($\hat{m}_r$), $\omega = 200$	1.2707×10^{-4}	200	1.1914×10^{2}

- ethylene oxidation:



BPTT algorithm	Approximation error (MSE)	Iter	CPU time [s]
SGD	6.7298×10^{-3}	1500	5.3596×10
Adam	8.3706×10^{-3}	1500	4.4071×10
LBFGS	1.5866×10^{-3}	46	1.6200×10^{0}
sLBFGS	1.4902×10^{-3}	1000	1.9693×10
GRL($\hat{m}_r$), $\omega = 2$	1.6720×10^{-3}	200	4.3819×10
GRL($\hat{m}_r$), $\omega = 50$	1.4948×10^{-3}	200	4.2956×10
GRL($\hat{m}_r$), $\omega = 100$	1.5043×10^{-3}	200	4.4190×10
GRL($\hat{m}_r$), $\omega = 200$	$\mathbf{1.3642 \times 10^{-3}}$	200	4.5000×10

Recurrent-Control Neural Network

- fix the DCRNN weights and train an FNN model on top of it to select future optimal control inputs $\hat{u}_t$:

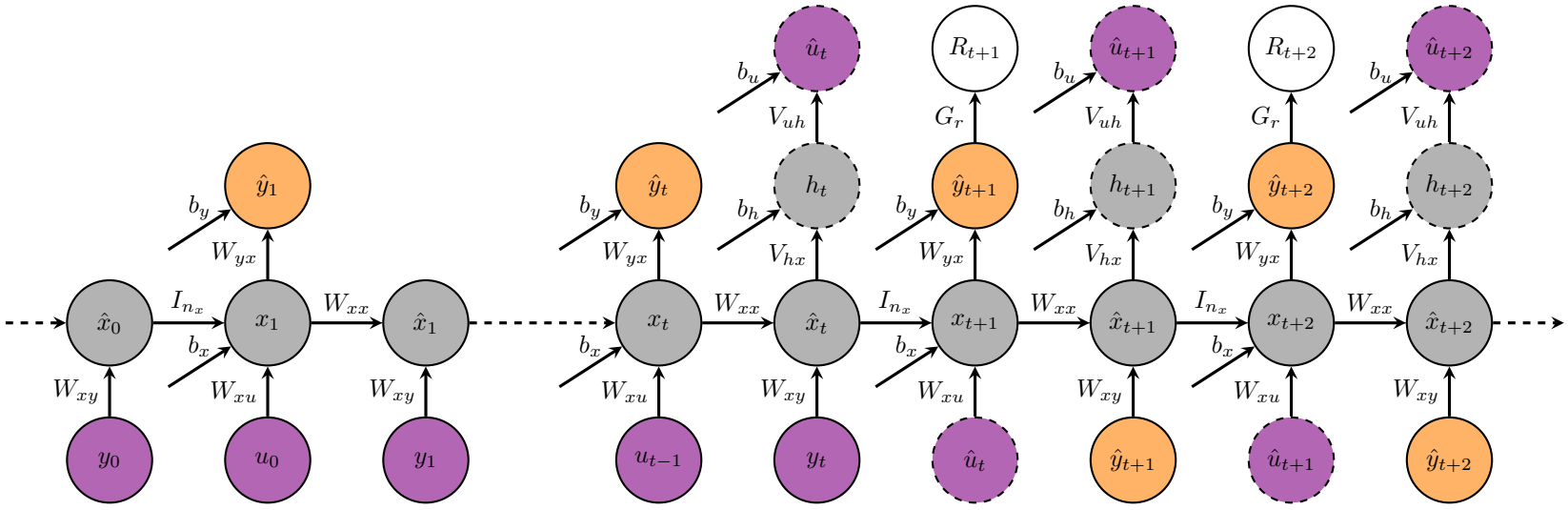
$$\hat{u}_t = \sigma_u(V_{uh}\sigma_h(V_{hx}\hat{x}_t + b_h) + b_u), \quad \forall m_- \leq t \leq N$$

$$x_{t+1} = \begin{cases} \sigma_x(\mathrm{I}\hat{x}_t + W_{xu}u_t + b_x), & \forall 0 \leq t < m_- \\ \sigma_x(\mathrm{I}\hat{x}_t + W_{xu}\hat{u}_t + b_x), & \forall m_- < t \leq N \end{cases}$$

$$R_t = G_r\sigma_r(W_{yx}x_t + b_y), \quad \forall m_- < t \leq N$$

$$\text{with} \quad \hat{x}_t = \begin{cases} W_{xx}x_t + W_{xy}y_t, & 0 \leq t \leq m_- \\ W_{xx}x_t + W_{xy}\hat{y}_t, & m_- < t \leq N \end{cases}$$

- $V_{uh} \in \mathbb{R}^{n_u \times n_h}$, $V_{hx} \in \mathbb{R}^{n_h \times n_x}$, $b_h \in \mathbb{R}^{n_h}$, $b_u \in \mathbb{R}^{n_u}$ are FNN parameters
- σ_u, σ_h are activation functions
- G_r, σ_r model problem's reward/cost function $R_t \equiv R(x_t, \hat{y}_t; \hat{u}_t)$



Architecture of recurrent control neural network (RCNN).

Learning the FNN — Optimization problem

Define the finite-sum

$$\bar{f}(\theta_u) \triangleq \sum_{t=m_-}^{N-1} R_t,$$

and consider the *regularized* optimization problem:

$$\min_{\theta_u} \quad \bar{f}(\theta_u) + \lambda_{\bar{r}} \bar{r}(\theta_u),$$

where $\theta_u \triangleq vec([\,V_{uh}\ V_{hx}\ b_h\ b_u]) \in \mathbb{R}^{n_{\theta_u}}$, $\lambda_{\bar{r}} > 0$.

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- specifically, solve using a *pseudo*-online generalized Gauss-Newton (GGN) algorithm for problems of the form

$$\min_{x \in \mathbb{R}^n} f(x) \triangleq \bar{f}(x) + g(x)$$

Newton's algorithm ($g = 0$)

Newton's update: $x_{k+1} = x_k - \nabla^2 f(x)^{-1} \nabla f(x)$

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- inverting $\nabla^2 f(x) \in \mathbb{R}^{n \times n}$ often highly expensive
- approximation: replace $\nabla^2 f(x)$ with $H_f \approx \nabla^2 f(x)$
- e.g., GGN approximation: $H_f = J_f^\top Q_f J_f$
  - let $m = N - m_-$
  - $J_f \in \mathbb{R}^{m \times n}$: Jacobian of $\hat{u}$ wrt x_k
  - $Q_f \in \mathbb{R}^{m \times m}$: Hessian of f wrt $\hat{u}$ at x_k

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- GGN iteration:
  $x_{k+1} = x_k - (J_f^\top Q_f J_f)^{-1} \nabla f(x)$
- or,
  $x_{k+1} = x_k - (J_f^\top Q_f J_f)^{-1} J_f^\top e_f$

- $\nabla f(x_k) \equiv J_f^\top e_f$
- e_f: gradient of f wrt $\hat{u}$ at x_k

GGN algorithm (g smooth)

Consider $g(x)$ smooth, e.g., $g(x) = \lambda \|x\|_2^2$

- GGN algorithm:
  $$x_{k+1} = x_k - (J_f^\top Q_f J_f + \nabla^2 g(x_k))^{-1}(J_f^\top e_f + \nabla g(x_k))$$

[20] Adeoye and Bemporad 2023a.

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- rewrite via our stylized augmentation:
- consider $y_i \in \mathbb{R}$, and define

$$J = \left[\begin{array}{c} J_f \\ \hdashline \nabla g(x_k)^\top \end{array}\right], Q = \left[\begin{array}{c:c} Q_f & 0 \\ \hdashline 0 & 0 \end{array}\right], e = \left[\begin{array}{c} e_f \\ \hdashline 1 \end{array}\right]$$

[20] Adeoye and Bemporad 2023a.

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then[20]

$$x_{k+1} = x_k - (J_f^\top Q_f J_f + \nabla^2 g(x_k))^{-1}(J_f^\top e_f + \nabla g(x_k))$$

$$\Leftrightarrow$$

$$x_{k+1} = x_k - (J^\top Q J + \nabla^2 g(x_k))^{-1} J^\top e$$

[20] Adeoye and Bemporad 2023a.

GGN algorithm (g smooth)

GGN algorithm: $x_{k+1} = x_k - (J^\top Q J + \nabla^2 g(x_k))^{-1} J^\top e$

an interesting matrix identity[21]:
$(D - VA^{-1}B)^{-1} VA^{-1} = D^{-1}V(A - BD^{-1}V)^{-1}$

[21] Duncan 1944; Guttman 1946.

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so then (if $m < n$), cheaper updates for GGN:

$$x_{k+1} = x_k - \nabla^2 g(x_k)^{-1} J^\top (\underbrace{I_m + QJ \nabla^2 g(x_k)^{-1} J^\top}_{m \times m})^{-1} e$$

[21] Duncan 1944; Guttman 1946.

Self-concordant optimization ($g = 0$)

Both *pure* Newton and GGN algorithms may fail globally

- global properties of Newton's method are well-established for (generalized) self-concordant functions
- a *convex* function f is (M_f, ν)-generalized self-concordant (SC) if $\left|\left\langle \nabla^3 f(x)[v_1]v_2, v_2 \right\rangle\right| \leq M_f \|v_2\|_x^2 \|v_1\|_x^{\nu-2} \|v_1\|^{3-\nu}, \forall v_1, v_2 \in \mathbb{R}^n, M_f \geq 0, \nu > 0;$ local norm: $\|d\|_x \triangleq \langle \nabla^2 f(x) d, d \rangle^{1/2}$

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- standard SC if $\nu = 3, v_1 = v_2$

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- standard SC if $\nu = 3, v_1 = v_2$

globalization of Newton's method $\Leftrightarrow$ step-size *damping*:
$x_{k+1} = x_k - \bar{\alpha}_k \nabla^2 f(x)^{-1} \nabla f(x), \qquad 0 < \bar{\alpha}_k \leq 1$ (damping parameter)

Self-concordant optimization ($g = 0$)

damped Newton: $x_{k+1} = x_k - \bar{\alpha}_k \nabla^2 f(x)^{-1} \nabla f(x)$

- affine-invariant *local quadratic convergence* guarantee
- *global convergence* guarantee for an appropriately-chosen $\bar{\alpha}_k$

[22] Nemirovski 2004; Nesterov and Nemirovskii 1994.
[23] Sun and Tran-Dinh 2019.

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- for standard SC f[22]: $\bar{\alpha}_k = \frac{1}{1+M_f \underbrace{\|\nabla f\|^*_{x_k}}_{\text{Newton decrement}}}$

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- for standard SC f[22]: $\bar{\alpha}_k = \dfrac{1}{1+M_f \underbrace{\|\nabla f\|^*_{x_k}}_{\text{Newton decrement}}}$
- convergence theory extends for generalized SC functions[23]
- several customized algorithms and robust loss functions arising from this notion, e.g., in nonsmooth composite optimization, regression problems and robust statistics, etc....

---

[22] Nemirovski 2004; Nesterov and Nemirovskii 1994.

[23] Sun and Tran-Dinh 2019.

Self-concordant regularization

assume $g \neq 0$ is (M_g, ν)-generalized SC

- choose $\bar{\alpha}_k = \frac{\alpha_k}{1 + M_g \|\nabla g\|^*_{x_k}}, \qquad 0 < \alpha_k \leq 1$
- GGN-SCORE algorithm: $x_{k+1} = x_k - \bar{\alpha}_k (J^\top Q J + \nabla^2 g(x_k))^{-1} J^\top e$
- if $m < n$,
  $x_{k+1} = x_k - \bar{\alpha}_k \nabla^2 g(x_k)^{-1} J^\top (\underbrace{I_m + Q J \nabla^2 g(x_k)^{-1} J^\top}_{m \times m})^{-1} e$

Self-concordant regularization: what we get...

local linear-quadratic convergence guarantee for (strongly) convex problems[24]

Assume:

- f, g are γ_l, γ_a-strongly convex
- f, g have γ_u, γ_b-Lipschitz continuous first derivatives
- f, g have γ_f, γ_g-Lipschitz continuous second derivatives H_f, H_g
- g is $(M_g, 3)$-generalized SC (and scaled by $\lambda \geq 0$)

Key Remark

There exist $\beta, \tilde{\beta}, K_1 > 0$, with $Q \leq K_1 I$, such that $\|e\| \leq \beta, \|J\| \leq \tilde{\beta}$, and hence

$$\|\lambda I + QJH_g^{-1}J^T\| \leq \lambda + (K/\gamma_a), \qquad \boxed{K = K_1\tilde{\beta}^2, H_g = \nabla^2 g}$$

[24] Adeoye and Bemporad 2023a.

Self-concordant regularization: what we get...

Theorem (local loss behaviour and suboptimality)

If $\alpha_k = \alpha = \frac{\sqrt{\gamma_a}}{\beta_1}(K + \lambda\gamma_a)$, *and under given regularity and unbiasedness conditions on the GGN matrices and gradients,*

$$\mathbb{E}[\mathcal{L}(x_{k+1})] \leq \mathcal{L}(x_k) - \left(\frac{\lambda\omega(\zeta_k)}{M_g^2} + \frac{\gamma_l \omega''(\tilde{\zeta}_k)}{2\gamma_a} - \xi \right)$$

$$\mathbb{E}\|x_{k+1} - x^*\|_{x_{k+1}} \leq \vartheta \|x_k - x^*\|_{x_k} + \frac{\gamma_u}{\beta_1}\|x_k - x^*\| + \frac{\gamma_g}{2}\|x_k - x^*\|^2$$

$$\omega(t) \triangleq t - \ln(1+t), \quad \zeta_k \triangleq \frac{M_g}{1+\tilde{\zeta}_k},$$

$$\tilde{\zeta}_k \triangleq M_g \|\nabla g\|^*_{x_k}, \quad \xi \triangleq \frac{2(\gamma_u + \lambda\gamma_b)}{\sqrt{\gamma_a}}, \beta_1 \triangleq \beta\tilde{\beta}$$

$$\vartheta \triangleq 1 + \frac{\lambda}{\sqrt{\gamma_a}\beta_1(1 - M_g\|x_k - x^*\|_{x_k})}.$$

Self-concordant regularization: what we get...

non-asymptotic guarantee for the last-iterate convergence of neural network predictions to the outputs of a given target function[25]
Consider a two-layer neural network:

$$u \mapsto \mathcal{M}(u; x) \triangleq \kappa(p) \sum_{i=1}^{p} v_i \sigma(w_i u), \tag{7}$$

where $\kappa(p)$ is some scaling that depends on n, e.g., $\kappa(p) = 1/\sqrt{p}$.

[25] Adeoye, Petersen, and Bemporad 2024.

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where $\kappa(p)$ is some scaling that depends on n, e.g., $\kappa(p) = 1/\sqrt{p}$.
learning problem (ERM):

$$\min_{x \in \mathbb{R}^n} \mathcal{L}(x) \triangleq \hat{R}_s(\mathcal{M}) + g(x), \tag{8}$$

where $\hat{R}_s(\mathcal{M}) \triangleq \frac{1}{m} \sum_{i=1}^{m} \ell(\mathcal{M}(u_i;x), y_i)$ (assumed strongly convex wrt $\mathcal{M}$), $\ell \colon \mathbb{R}^{n_L} \times \mathbb{R}^{n_L} \to \mathbb{R}$ is loss function.

---

[25] Adeoye, Petersen, and Bemporad 2024.

Self-concordant regularization: what we get...

Assume standard regularity assumptions on the GGN matrices and the gradient terms.

Theorem (nonasymptotic convergence)

After $K \triangleq \frac{1}{\bar{\alpha}} \log((1 + \|\mathcal{M}_0 - \mathcal{M}^*\|^2)/\epsilon)$ *iterations, for any* $\epsilon, \bar{\alpha} \in (0, 1)$,

$$\|\mathcal{M}_K - \mathcal{M}^*\|^2 \leq \epsilon$$

where $\mathcal{M}^*$ *is a target function (e.g., a teacher network).*

Theorem (regularized loss evolution)

The "unaugmented" J_k *is* $mC\kappa(p)$*-Lipschitz,* C *constant, and for all* k,

$$\mathcal{L}(x_{k+1}) \leq \mathcal{L}(x_k) - \xi_k$$

where $\xi_k = \mathcal{O}\left(\hat{\beta}_1^2 \bar{c}_k / \hat{\beta}_m^4\right)$ *is positive,* $\hat{\beta}_1 \triangleq \sigma_{\max}(J_k)$, $\hat{\beta}_m \triangleq \sigma_{\min}(J_k)$ *(augmented).*

Self-concordant smoothing

constructing an SC g:

- **approach**: epi-smoothing by infimal convolution[26]: $g_s(x;\mu) = g \square h_\mu \triangleq \inf_{w \in \mathbb{R}^n} \left\{ g(w) + h_\mu(x-w) \right\}, \quad h_\mu(\cdot) \triangleq \mu h\left(\frac{\cdot}{\mu}\right), \quad \mu \in \mathbb{P}$
- consider a parameterized family of regularization kernels $\mathcal{H} \triangleq \left\{ (x,w) \mapsto h_\mu(x-w) \mid x, w \in \mathbb{R}^n, \mu \in \mathbb{P} \right\}$

  $h_\mu \in \mathcal{H}$ with $h(x) \triangleq \sum_{i=1}^{n} \phi(x_i)$, $\liminf_{\|x\| \to \infty} \frac{\phi(x)}{\|x\|} = +\infty$ and $\phi \in \mathcal{F}_{M_\phi, \nu}$

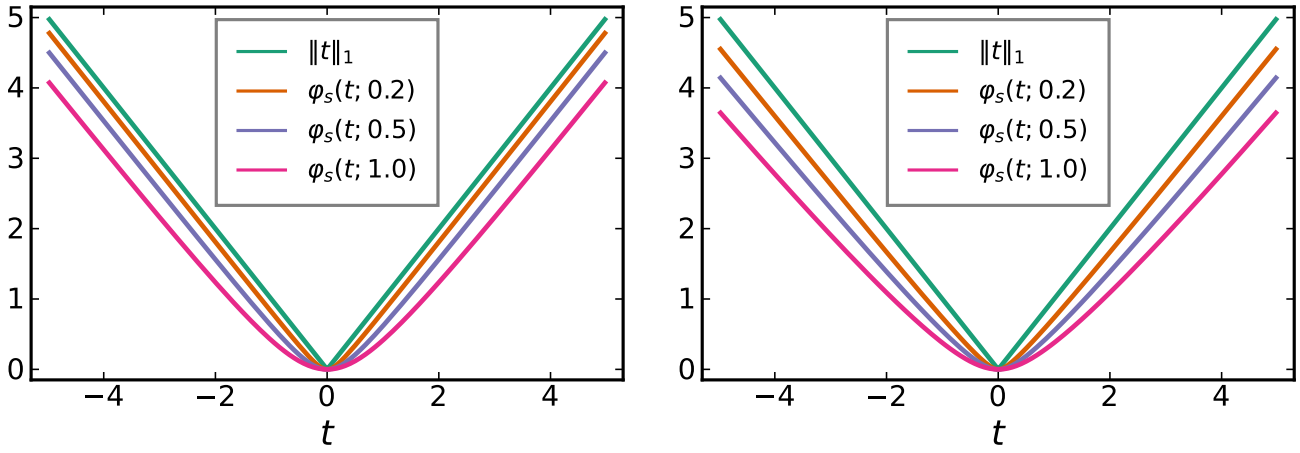
Let $\varphi_s(t;\mu) \triangleq (\varphi \square \phi_\mu)(t)$; then $g_s \triangleq g \square h_\mu \equiv \sum_{i=1}^{n} \varphi_s(x_i;\mu)$ is (M_g, ν)-generalized SC![27]

---

[26] Burke and Hoheisel 2017.

[27] Adeoye and Bemporad 2023b

Self-concordant smoothing



Generalized self-concordant smoothing of $\|\cdot\|_1$ with $\phi(t) = \sqrt{1+|t|^2} - 1$ (left) and $\phi(t) = \frac{1}{2}\left[\sqrt{1+4t^2} - 1 + \log\left(\frac{\sqrt{1+4t^2}-1}{2t^2}\right)\right]$ (right). The smooth approximation is shown for $\mu = 0.2, 0.5, 1.0$.

Julia package

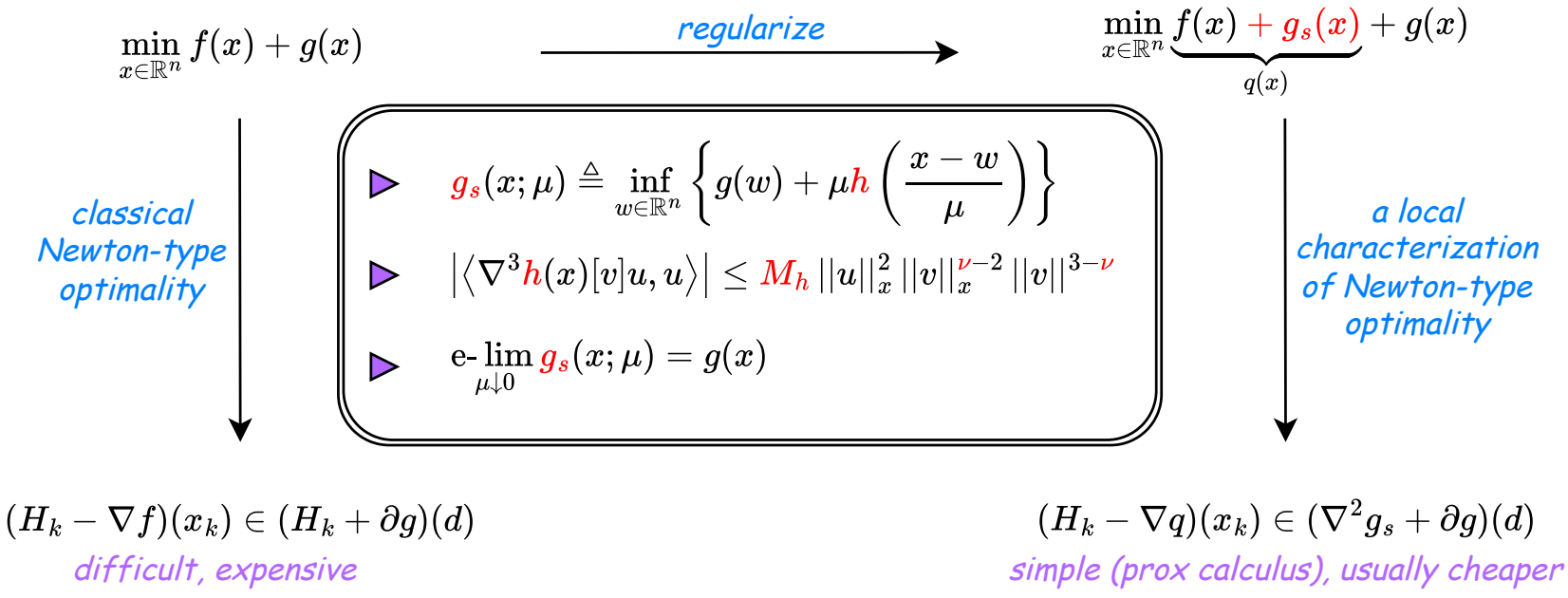
All implemented in a Julia package,

`SelfConcordantSmoothOptimization.jl`

A Python port is available:

`https://github.com/adeyemiadeoye/pySCSOpt`

Self-concordant smoothing in proximal quasi-Newton methods



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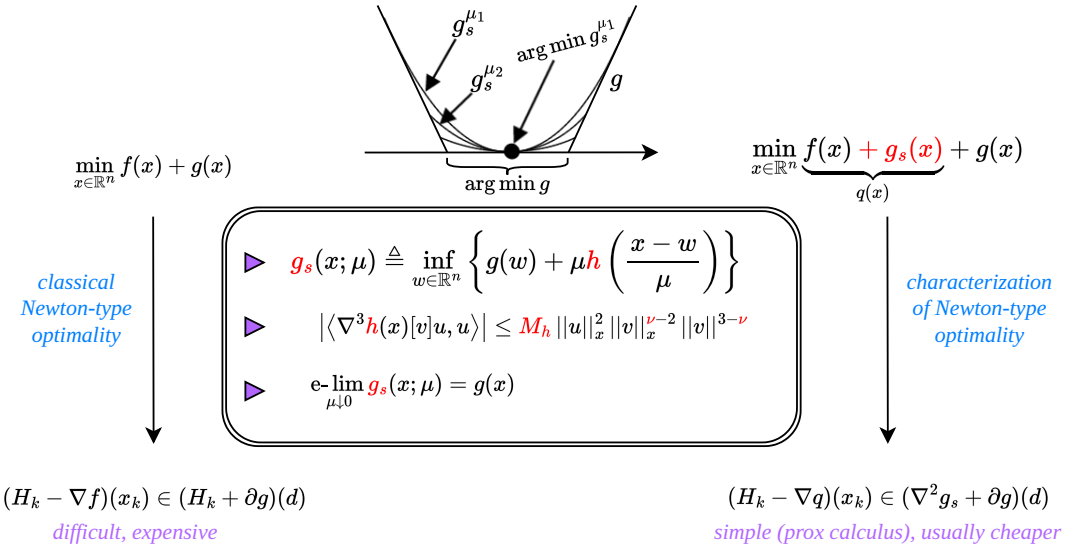


each g_s^μ is ε^μ-optimal for g (ε-$\operatorname{argmin} g \triangleq \{x \mid g(x) \le \inf g + \varepsilon\}$)

ideally, one wants g_s with parametrization set $\{g_s^\mu\}_{\mu>0}$ satisfying

$$\limsup_{\mu} (\operatorname{argmin} g_s^\mu) \subset \operatorname{argmin} g$$

"every cluster point of the minimizers of $\{g_s^\mu\}_{\mu>0}$ is a minimizer of g"[a]

[a] Rockafellar and Wets 2009.

A proximal GGN algorithm

Algorithm `Prox-GGN-SCORE`

Require: $x_0 \in \mathbb{R}^n$, f, g, $g_s \in \mathcal{S}^{\mu}_{M_g,\nu}$, $\mathcal{M}$, $\{u_i, y_i\}_{i=1}^m$ with $y_i \in \mathbb{R}^{n_y}$, $\alpha \in (0, 1]$

for $k = 0, \dots$ **do**
  $H_g \leftarrow \nabla^2 g_s(x_k)$; $\eta_k \leftarrow \left\| \nabla g_s(x_k) \right\|_{H_g}^*$ ▷ NOTE: H_g is diagonal
  $\bar{\alpha}_k \leftarrow \frac{\alpha}{1 + M_g \eta_k}$
  if $m + n_y \leq n$ **then**
    $\delta_k^{\mathrm{ggn}} = -H_g^{-1} J_k^\top (I_m + Q_k J_k H_g^{-1} J_k^\top)^{-1} u_k$
  else
    $\delta_k^{\mathrm{ggn}} = -(J_k^\top Q_k J_k + H_g)^{-1} J_k^\top u_k$
  end if
  $x_{k+1} \leftarrow \mathrm{prox}_{\alpha g}^{H_g}(x_k + \bar{\alpha}_k \delta_k^{\mathrm{ggn}})$ ▷ simplified by prox-calculus[28]
end for

[28] Becker, Fadili, and Ochs 2019.

Convergence properties

assumptions:

- f is convex and $f \in \mathcal{C}^{2,2}_{L_f}(\mathbb{R}^n)$
- $\rho_0 I_n \leq \nabla^2 f(x^*) \leq L I_n$, $\rho I_n \leq \nabla^2 g_s(x^*) \leq L_0 I_n$ locally with $L \geq \rho_0 > 0$ and $L_0 \geq \rho > 0$
- $g \in \Gamma_0(\mathbb{R}^n)$
- $g_s \in \mathcal{S}^{\mu}_{M_g,\nu}$

Convergence properties

Theorem

Starting from an arbitrary point, `Prox-GGN-SCORE` *converges to a solution, with* $\mathcal{L}$ *evolving as*

$$\mathcal{L}(x_{k+1}) \leq \mathcal{L}(x_k) - (L_f/6)\|x_{k+1} - x_k\|^3$$

Convergence properties

$$d_\nu(x,y) \triangleq \begin{cases} M_g\|y-x\| & \text{if } \nu = 2, \\ \left(\frac{\nu}{2}-1\right) M_g \|y-x\|_2^{3-\nu} \|y-x\|_x^{\nu-2} & \text{if } \nu > 2 \end{cases}$$

$$\omega_\nu(\tau) \triangleq \begin{cases} \frac{\exp(\tau)-\tau-1}{\tau^2} & \text{if } \nu = 2, \\ \frac{-\tau-\ln(1-\tau)}{\tau^2} & \text{if } \nu = 3, \\ \frac{(1-\tau)\ln(1-\tau)+\tau}{\tau^2} & \text{if } \nu = 4, \\ \left(\frac{\nu-2}{4-\nu}\right)\frac{1}{\tau}\left[\frac{\nu-2}{2(3-\nu)\tau}\left((1-\tau)^{\frac{2(3-\nu)}{2-\nu}}-1\right)-1\right] & \text{otherwise} \end{cases}$$

$$R_\nu(\tau) \triangleq \begin{cases} \left(\frac{3}{2}+\frac{\tau}{3}\right)\exp(\tau) & \text{if } \nu = 2, \\ \frac{1-(1-\tau)^{\frac{4-\nu}{\nu-2}}-\left(\frac{4-\nu}{\nu-2}\right)\tau(1-\tau)^{\frac{4-\nu}{\nu-2}}}{\left(\frac{4-\nu}{\nu-2}\right)\tau^2(1-\tau)^{\frac{4-\nu}{\nu-2}}} & \text{if } \nu \in (2,3] \end{cases}$$

$$\bar{\omega}_\nu(\tau) \triangleq \begin{cases} \frac{2\exp\left(\frac{\tau}{2}\right)-2}{\tau} & \text{if } \nu = 2, \\ -\frac{\ln(1-\tau)}{\tau} & \text{if } \nu = 3, \\ \left(\frac{\nu-2}{\nu-3}\right)\frac{1-(1-\tau)^{\frac{\nu-3}{\nu-2}}}{\tau} & \text{otherwise} \end{cases}$$

Convergence properties

local assumptions:

- $\|J_k v\| \geq \beta_1 \|v\|$, $\beta_1 > 0$, for any $v \in \mathbb{R}^n$
- $\left\|e_f(x_k)\right\| \leq \beta_2$, $\|Q_f(x_k)\| \leq \beta_3$ for some $\beta_2, \beta_3 > 0$

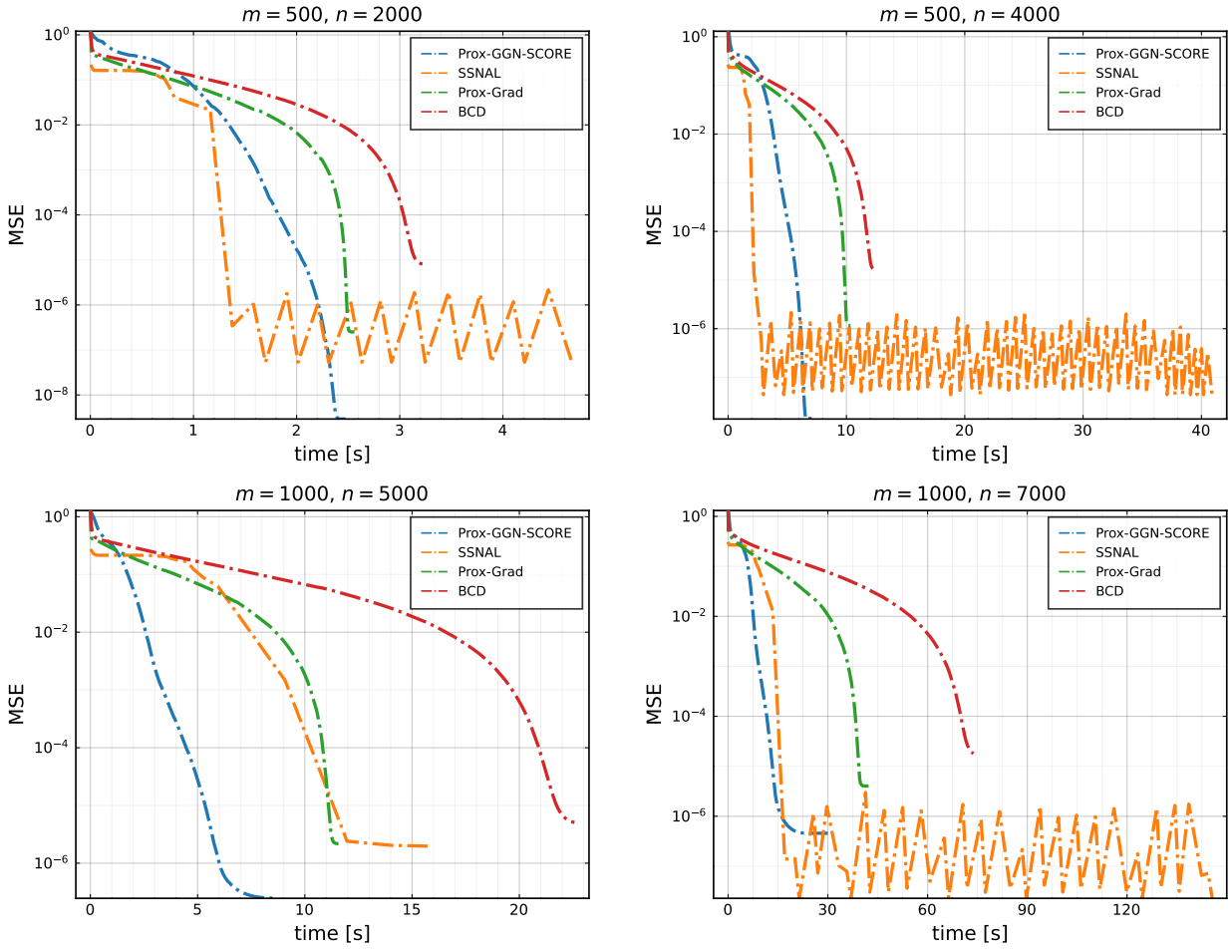
let $\tilde{\beta} \triangleq \beta_2 \beta_3$, $\alpha_k \equiv \alpha \in (0, 1]$, $\lambda_k \triangleq 1 + M_g \omega_\nu(-d_\nu(x^*, x_k)) \|x_k - x^*\|_{x_k}$,
$\vartheta_k \triangleq \left(\frac{\lambda_k - \alpha_k}{\lambda_k}\right) \bar{\omega}_\nu(d_\nu(x^*, x_k)) + \frac{L_f}{2\sqrt{\rho}}$, $R_k \triangleq R_\nu(d_\nu(x^*, x_k)) d_\nu(x^*, x_k)$

Theorem (local suboptimality of `Prox-GGN-SCORE` iterates)

Starting from $x_0 \in \mathcal{E}_r(x^*)$, if $d_\nu(x^*, x_k) < 1$, then

$$\|x_{k+1} - x^*\|_{x^*} \leq \frac{L(\lambda_k - \alpha_k)}{\lambda_k \sqrt{\rho}} + \frac{\tilde{\beta}\left\|x_k - x^*\right\|}{\sqrt{\rho}} + R_k \|x_k - x^*\|_{x^*} + \vartheta_k \|x_k - x^*\|^2$$

Sparse group lasso test



$$\min_{x \in \mathbb{R}^n} \underbrace{\frac{1}{2}\|Ax - y\|^2}_{=:f(x)} + \underbrace{\beta\|x\|_1 + \beta_{\mathcal{G}} \sum_{j \in \mathcal{G}} \omega_j \|x_j\|}_{=:g(x)}$$

Learning the FNN with GGN-SCORE

$$\min_{\theta_u \equiv \bar{z}} \quad \bar{f}(\theta_u) + \lambda_{\bar{r}} \bar{r}(\theta_u), ;\ n_d = n_y \cdot n_b;\ n_b = \text{mini-batch size}$$

$$\bar{z}_{k+1} = \bar{z}_k - \frac{\sigma}{1 + M_{\bar{r}} \bar{\eta}_k} \bar{H}_k^{-1} \bar{J}_k \bar{B}_k^{-1} \bar{e}_k, \quad \bar{B}_k \triangleq \lambda_{\bar{r}} \mathrm{I} + \bar{Q}_k \bar{J}_k \bar{H}_k^{-1} \bar{J}_k^\top,$$

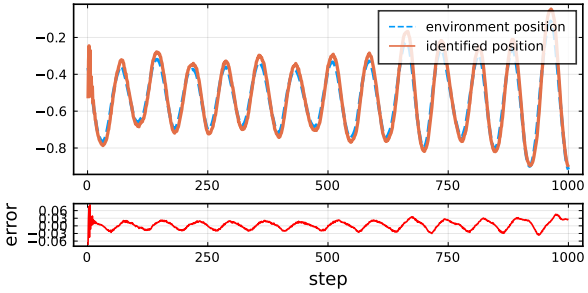
$$\bar{J}_k^\top = \left[\begin{array}{c:c} J_{\hat{y}}^\top & \lambda_{\bar{r}} \bar{g}_k \end{array} \right], \bar{Q}_k = \left[\begin{array}{c:c} Q_{\bar{f}} & 0 \\ \hdashline 0 & 0 \end{array} \right], \bar{e}_k = \left[\begin{array}{c} g_{\bar{f}} \\ \hdashline 1 \end{array} \right],$$

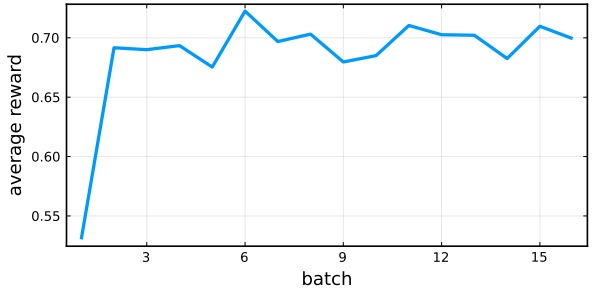
$\bar{H}_k \in \mathbb{R}^{n_{\theta_u} \times n_{\theta_u}}$: Hessian of $\bar{r}$ with respect to θ_u, $J_{\hat{y}} \in \mathbb{R}^{n_d \times n_{\theta_u}}$: Jacobian of $\hat{y}_k$ with respect to θ_u, $\bar{g}_k$: gradient of $\bar{r}$ with respect to θ_u, $g_{\bar{f}} \in \mathbb{R}^{n_d}$: residual vector defined as the gradient of $\bar{f}$ with respect to $\hat{y}_k$, $Q_{\bar{f}} \in \mathbb{R}^{n_d \times n_d}$: Hessian of $\bar{f}$ with respect to $\hat{y}_k$.

choose: $0 < \sigma \leq 1$, $\bar{\eta}_k = \left\langle \bar{g}_k, \bar{H}_k^{-1} \bar{g}_k \right\rangle^{1/2}$, and $M_{\bar{r}} \geq 0$ is associated with $\bar{r}$.

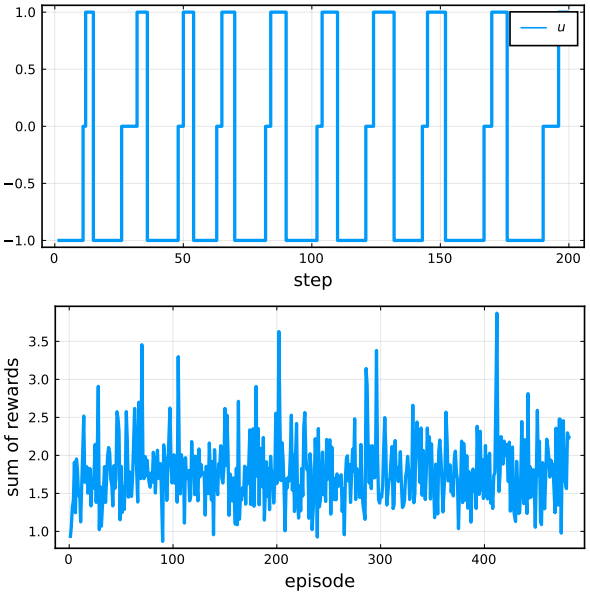
use: $\bar{B}_k^{-1} \approx \underline{\mathrm{B}}_k$ with $\underline{\mathrm{B}}_k \in \mathbb{R}^{n_{\theta_u} \times n_{\theta_u}}$ with entries $\underline{\mathrm{b}}_{i,j} = \bar{\delta}_{i,j} / \bar{b}_{i,i}$, where $\bar{\delta}_{i,j}$ is the Kronecker delta function and $\bar{b}_{i,i}$ are the diagonal entries of $\bar{B}_k$.

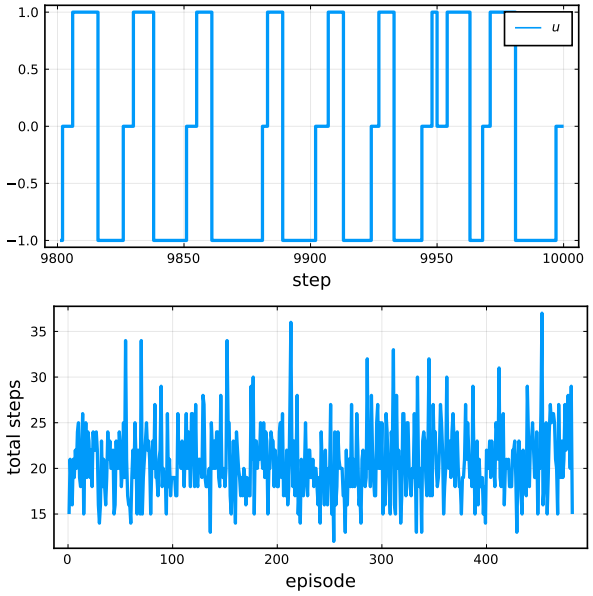
Full RCNN simulation results (mountain car)





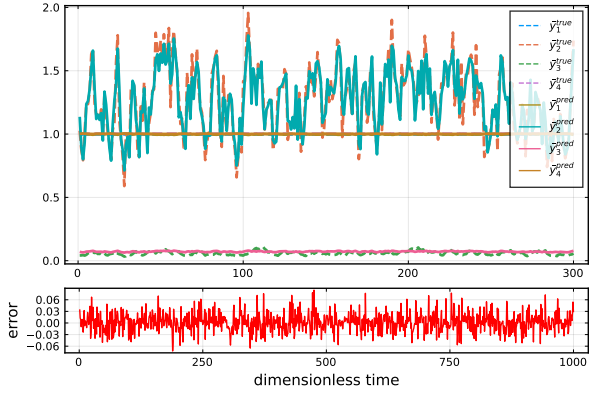
Left: DCRNN identified model in stage I. **Right**: Stage II FNN training.

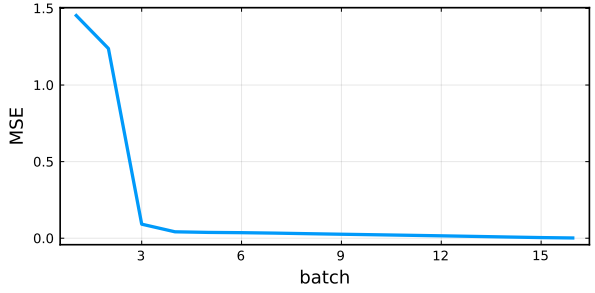




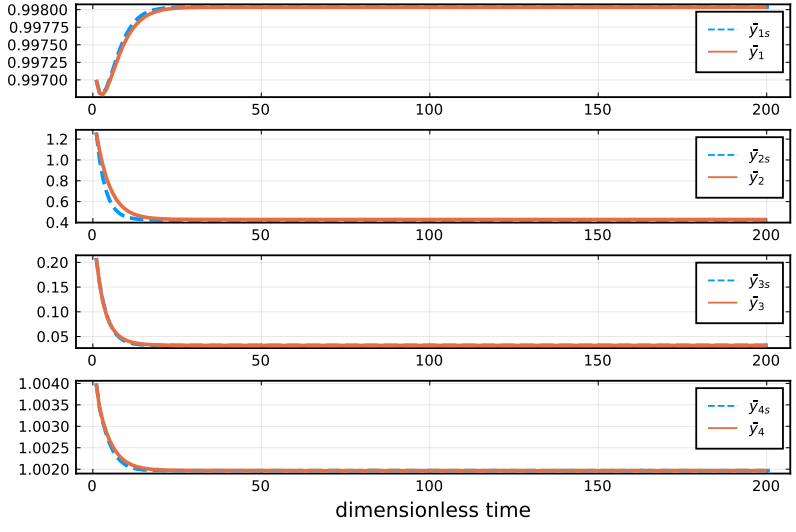
Real-time control performance. $G_r = [1, 0]$, $R_t = \text{logistic}_{10}(\hat{y}_t - 0.5)$, $\text{logistic}_{10}(x) \triangleq \frac{1}{1+e^{-10x}}$, $\sigma_u = \tanh$ (+ *bucketing* for inference), $\sigma_h =$ relu.

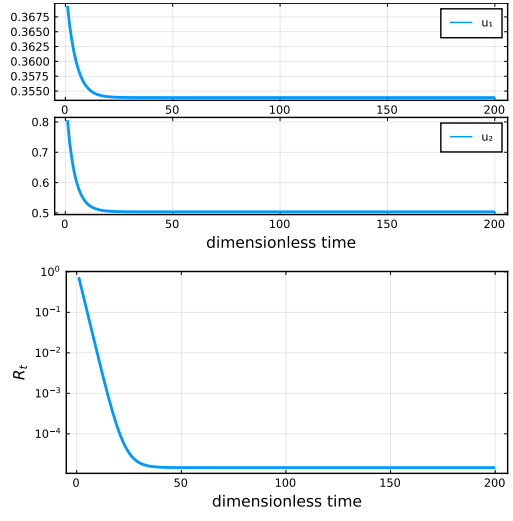
Full RCNN simulation results (ethylene oxidation)





Left: DCRNN identified model in stage I. **Right**: Stage II FNN training.





Real-time control performance. ; $G_r = [1, 1, 1, 1]$, $R_t = (\hat{y}_t - y^{ref})$, $\sigma_u = \tanh$, $\sigma_h =$ relu.

Conclusions

- designed and analyzed quasi-Newton optimization algorithms within a learning and control context
- addressed structural issues with RNNs
- proposed "self-concordant regularization" for quasi-Newton methods
- featured an approximation technique in GGN-SCORE that's useful for overparameterized models and mini-batch updates
- achieved faster convergence and better prediction quality than first-order methods
- proved the first (nonasymptotic, last-iterate) convergence result for GGN in optimizing neural networks with explicit regularization

Conclusions

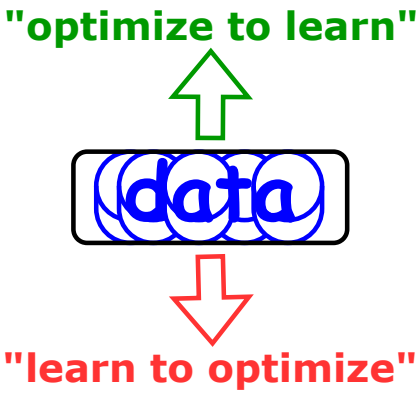
Future directions:

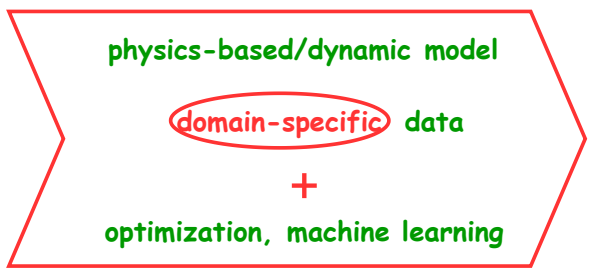
- extensions to explicitly handle more general constraints
- automatic or adaptive selection of optimal smoothing parameters in the proximal SCORE framework
- application and/or analysis of online/stochastic versions of the proximal SCORE framework
- explore parallel and distributed versions of quasi-Newton methods
- improve/solidify theoretical guarantees on the newly proposed techniques

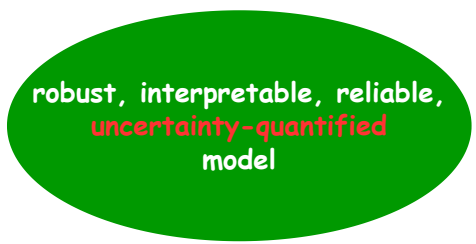
Conclusions

Future directions:

- uncertainty quantification in neural network predictions, e.g., (probabilistic) Bayesian neural networks, for reliability and robustness
- hybrid models (data + physics) for improved interpretability and robustness







- **applications**: large-scale industrial and engineering problems, e.g., computational fluid dynamics, optimal experimental design, optimal power flow, . . .

Thank you!

References

 Adeoye, Adeyemi D and Alberto Bemporad (2023a). "SCORE: approximating curvature information under self-concordant regularization". In: *Computational Optimization and Applications* 86.2, pp. 599–626.

 — (2023b). "Self-concordant Smoothing for Convex Composite Optimization". In: *arXiv preprint arXiv:2309.01781*.

 Adeoye, Adeyemi D. and Alberto Bemporad (2025). "An Inexact Sequential Quadratic Programming Method for Learning and Control of Recurrent Neural Networks". In: *IEEE Transactions on Neural Networks and Learning Systems* 36.2, pp. 2762–2776. DOI: 10.1109/TNNLS.2024.3354855.

 Adeoye, Adeyemi D, Philipp Christian Petersen, and Alberto Bemporad (2024). "Regularized Gauss-Newton for Optimizing Overparameterized Neural Networks". In: *arXiv preprint arXiv:2404.14875*.

References


Atiya, Amir F and Alexander G Parlos (2000). "New results on recurrent network training: unifying the algorithms and accelerating convergence". In: *IEEE transactions on neural networks* 11.3, pp. 697–709.


Becker, Stephen, Jalal Fadili, and Peter Ochs (2019). "On quasi-Newton forward-backward splitting: proximal calculus and convergence". In: *SIAM Journal on Optimization* 29.4, pp. 2445–2481.


Bellman, Richard (1952). "On the theory of dynamic programming". In: *Proceedings of the national Academy of Sciences* 38.8, pp. 716–719.


Bemporad, Alberto (2022). "Recurrent neural network training with convex loss and regularization functions by extended Kalman filtering". In: *IEEE Transactions on Automatic Control* 68.9, pp. 5661–5668.

References

- Bemporad, Alberto (2023). "Training recurrent neural networks by sequential least squares and the alternating direction method of multipliers". In: *Automatica* 156, p. 111183.
- Bengio, Yoshua, Patrice Simard, and Paolo Frasconi (1994). "Learning long-term dependencies with gradient descent is difficult". In: *IEEE transactions on neural networks* 5.2, pp. 157–166.
- Berner, Julius et al. (2021). "The modern mathematics of deep learning". In: *arXiv preprint arXiv:2105.04026* 78.
- Burke, James V and Tim Hoheisel (2017). "Epi-convergence properties of smoothing by infimal convolution". In: *Set-Valued and Variational Analysis* 25, pp. 1–23.
- Deng, Jia et al. (2009). "Imagenet: A large-scale hierarchical image database". In: *2009 IEEE conference on computer vision and pattern recognition*. Ieee, pp. 248–255.
- DeVore, Ronald A (1998). "Nonlinear approximation". In: *Acta numerica* 7, pp. 51–150.

References

- Duncan, William Jolly (1944). "LXXVIII. Some devices for the solution of large sets of simultaneous linear equations: With an appendix on the reciprocation of partitioned matrices". In: *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* 35.249, pp. 660–670.
- Guttman, Louis (1946). "Enlargement methods for computing the inverse matrix". In: *The annals of mathematical statistics*, pp. 336–343.
- Ha, David and Jürgen Schmidhuber (2018). "Recurrent world models facilitate policy evolution". In: *Advances in neural information processing systems* 31.
- Hochreiter, Sepp (1998). "Recurrent neural net learning and vanishing gradient". In: *International Journal Of Uncertainity, Fuzziness and Knowledge-Based Systems* 6.2, pp. 107–116.

References

- Johnston, Barbara M et al. (2004). "Non-Newtonian blood flow in human right coronary arteries: steady state simulations". In: *Journal of biomechanics* 37.5, pp. 709–720.
- — (2006). "Non-Newtonian blood flow in human right coronary arteries: transient simulations". In: *Journal of biomechanics* 39.6, pp. 1116–1128.
- Krizhevsky, Alex, Geoffrey Hinton, et al. (2009). "Learning multiple layers of features from tiny images". In.
- LeCun, Yann et al. (1998). "Gradient-based learning applied to document recognition". In: *Proceedings of the IEEE* 86.11, pp. 2278–2324.
- McCloud, Scott (1993). *Understanding Comics: The Invisible Art*. Tundra Publishing.
- Nemirovski, Arkadi (2004). "Interior point polynomial time methods in convex programming". In: *Lecture notes* 42.16, pp. 3215–3224.

References

- Nesterov, Yurii and Arkadii Nemirovskii (1994). *Interior-point polynomial algorithms in convex programming*. SIAM.
- Novak, Erich and Henryk Woźniakowski (2009). "Approximation of infinitely differentiable multivariate functions is intractable". In: *Journal of Complexity* 25.4, pp. 398–404.
- Panier, Eliane R and André L Tits (1991). "Avoiding the Maratos effect by means of a nonmonotone line search I. General constrained problems". In: *SIAM Journal on Numerical Analysis* 28.4, pp. 1183–1195.
- Powell, Michael JD (1978a). "A fast algorithm for nonlinearly constrained optimization calculations". In: *Numerical analysis*. Springer, pp. 144–157.
- — (1978b). "The convergence of variable metric methods for nonlinearly constrained optimization calculations". In: *Nonlinear programming 3*. Elsevier, pp. 27–63.

References


Rockafellar, R Tyrrell and Roger J-B Wets (2009). *Variational analysis*. Vol. 317. Springer Science & Business Media.


Rumelhart, David E, Geoffrey E Hinton, and Ronald J Williams (1986). "Learning representations by back-propagating errors". In: *nature* 323.6088, pp. 533–536.


Saad, Youcef and Martin H Schultz (1986). "GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems". In: *SIAM Journal on scientific and statistical computing* 7.3, pp. 856–869.


Sun, Tianxiao and Quoc Tran-Dinh (2019). "Generalized self-concordant functions: a recipe for Newton-type methods". In: *Mathematical Programming* 178.1-2, pp. 145–213.


Tumblr, Meme Engine (2012). *More thoughts from Understanding Comics by Scott McCloud*. Retrieved from Meme Engine Tumblr.

References

 Zimmermann, Hans-Georg et al. (2006). "Identification and forecasting of large dynamical systems by dynamical consistent neural networks". In: *New Directions in Statistical Signal Processing: From Systems to Brain*, pp. 203–242.