MODEL PREDICTIVE CONTROL

LEARNING-BASED MPC

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COURSE STRUCTURE

- Basic concepts of model predictive control (MPC) and linear MPC
- ✓ Linear time-varying and nonlinear MPC
- ✓ Quadratic programming (QP) and explicit MPC
- ✓ Hybrid MPC
- ✓ Stochastic MPC
- Learning-based MPC (or data-driven MPC)

MACHINE LEARNING AND CONTROL ENGINEERING



MPC AND ML

• MPC and ML = main R&D trends in industry for control!

model predictive control



machine learning















(source: https://books.google.com/ngrams)

MACHINE LEARNING (ML)

• Massive set of techniques to extract mathematical models from data



• Good mathematical foundations from artificial intelligence, statistics, optimization

• Works very well in practice (despite training is most often a nonconvex optimization problem ...)

• Used in myriads of very diverse application domains

Availability of excellent open-source software tools also explains success
 scikit-learn, TensorFlow/Keras, PyTorch, JAX, Flux.jl,...
 python julia

MPC DESIGN FROM DATA

- 1. Use machine learning to get a prediction model from data (system identification)
 - Autoencoders, recurrent neural networks (nonlinear models)
 - Online learning of feedforward/recurrent neural networks by EKF
 - Piecewise affine regression to learn hybrid models
- 2. Use reinforcement learning to learn the MPC law from data
 - Q-learning: learn Q-function defining the MPC law from data
 - Policy gradient methods: learn optimal policy coefficients directly from data using stochastic gradient descent
 - Global optimization methods: learn MPC parameters (weights, models, horizon, solver tolerances, ...) by optimizing observed closed-loop performance

LEARNING PREDICTION MODELS FOR MPC



"All models are wrong, but some are useful."

(George E. P. Box)

CONTROL-ORIENTED NONLINEAR MODELS

• Black-box models: purely data-driven. Use training data to fit a prediction model that can explain them (need good data to get a good model)



• Physics-based models: use physical principles to create a prediction model (fewer parameters to learn, better generalizes on unseen data)



$$\begin{array}{c} \begin{array}{c} p_{1} = k_{1}(W_{c} + W_{cpr} - k_{c}p_{1}) + \frac{\hat{T}_{1}}{T_{1}}p_{1} \\ p_{2} = k_{2}(k_{p1} - W_{cpr} - W_{t} + W_{f}) + \frac{\hat{T}_{2}}{T_{2}}p_{2} \end{array} \xrightarrow{ \qquad } \begin{array}{c} \mathcal{X} \end{array} \xrightarrow{ \qquad } \begin{array}{c} prediction \\ model \end{array} \xrightarrow{ } \end{array}$$

• Gray-box (or physics-informed) models: mix of the two, can be quite effective

CONTROL-ORIENTED MODELS

- Complex model = complex controller (controller design and evaluation) Example: Model Predictive Control (MPC)
- Typically look for small-scale models (e.g., ≤ 10 states/inputs/outputs) with a limited number of coefficients (vs. Large Language Models: 2-300 B params)
- Limit nonlinearities as much as possible (e.g., avoid very deep neural networks)
- Need to get the best model within a poor model class from a rich dataset (= limited risk of overfit)
- Computation constraints: solve the learning problem using limited resources (=our laptop, no supercomputing infrastructures)

Solving system identification problems requires different algorithms compared to typical machine learning tasks

NONLINEAR SYS-ID BASED ON NEURAL NETWORKS

• Neural networks proposed for nonlinear system identification since the '90s

(Narendra, Parthasarathy, 1990) (Hunt et al., 1992) (Suykens, Vandewalle, De Moor, 1996)

- NNARX models: use a feedforward neural network to approximate the nonlinear difference equation $y_t \approx \mathcal{N}(y_{t-1}, \dots, y_{t-n_a}, u_{t-1}, \dots, u_{t-n_b})$
- Neural state-space models:
 - w/ state data: fit a neural network model $x_{t+1} \approx \mathcal{N}_x(x_t, u_t), \ y_t pprox \mathcal{N}_y(x_t)$
 - I/O data only: set x_t = value of an inner layer of the network (Prasad, Bequette, 2003) such as an autoencoder (Masti, Bemporad, 2021)
- Alternative for MPC: learn entire prediction (Masti, Smarra, D'Innocenzo, Bemporad, 2020)

$$y_{t+k} = h_k(x_t, u_t, \dots, u_{t+k-1}), k = 1, \dots, N$$



• **Recurrent neural networks** are more appropriate for accurate open-loop predictions, but more difficult to train (see later ...)

NLMPC BASED ON NEURAL NETWORKS

• Approach: use a neural network model for prediction



• MPC design workflow:



LEARNING NONLINEAR STATE-SPACE MODELS FOR MPC

(Masti, Bemporad, 2021)

• Idea: use autoencoders and artificial neural networks to learn a nonlinear state-space model of desired order from input/output data



ANN with hourglass structure

(Hinton, Salakhutdinov, 2006)

LEARNING NONLINEAR STATE-SPACE MODELS FOR MPC

• Training problem: choose n_a, n_b, n_x and solve

$$\min_{f,d,e} \sum_{k=k_0}^{N-1} \alpha \left(\ell_1(\hat{O}_k, O_k) + \ell_1(\hat{O}_{k+1}, O_{k+1}) \right) \\ + \beta \ell_2(x_{k+1}^*, x_{k+1}) + \gamma \ell_3(O_{k+1}, O_{k+1}^*)$$
s.t. $x_k = e(I_{k-1}), k = k_0, \dots, N$
 $x_{k+1}^* = f(x_k, u_k), k = k_0, \dots, N-1$
 $\hat{O}_k = d(x_k), O_k^* = d(x_k^*), k = k_0, \dots, N$



- Model complexity can be reduced by adding group-LASSO penalties
- Quasi-LPV structure for MPC: set $f(x_k, u_k) = A(x_k, u_k) \begin{bmatrix} x_k \\ 1 \end{bmatrix} + B(x_k, u_k)u_k$ (A_{ij}, B_{ij}, C_{ij} = feedforward NNs) $y_k = C(x_k, u_k) \begin{bmatrix} x_k \\ 1 \end{bmatrix}$
- Different options for the state-observer:
 - use encoder e to map past I/O into x_k (deadbeat observer)
 - design extended Kalman filter based on obtained model f, d
 - simultaneously fit state observer $\hat{x}_{k+1} = s(x_k, u_k, y_k)$ with loss $\ell_4(\hat{x}_{k+1}, x_{k+1})$

LEARNING NONLINEAR NEURAL STATE-SPACE MODELS FOR MPC

• Example: nonlinear two-tank benchmark problem



 $\begin{cases} x_1(t+1) = x_1(t) - k_1\sqrt{x_1(t)} + k_2u(t) \\ x_2(t+1) = x_2(t) + k_3\sqrt{x_1(t)} - k_4\sqrt{x_2(t)} \\ y(t) = x_2(t) + u(t) \end{cases}$

Model is totally unknown to learning algorithm

- Artificial neural network (ANN): 3 hidden layers 60 exponential linear unit (ELU) neurons
- For given number of model parameters, autoencoder approach is superior to NNARX
- Jacobians directly obtained from ANN structure for Kalman filtering & MPC problem construction



LEARNING AFFINE NEURAL PREDICTORS FOR MPC

(Masti, Smarra, D'Innocenzo, Bemporad, 2020)

• Alternative: learn the entire prediction

$$y_k = h_k(x_0, u_0, \dots, u_{k-1}), \ k = 1, \dots, N$$



• LTV-MPC formulation: linearize h_k around nominal inputs \bar{u}_j

$$y_k = h_k(x_0, \bar{u}_0, \dots, \bar{u}_{k-1}) + \sum_{j=0}^{k-1} \frac{\partial h_k}{\partial u_j}(x_0, \bar{u}_0, \dots, \bar{u}_{k-1})(\mathbf{u}_j - \bar{u}_j)$$

Example: \bar{u}_k = MPC sequence optimized @k-1

• Avoid computing Jacobians by fitting h_k in the affine form

$$y_k = f_k(x_0, \bar{u}_0, \dots, \bar{u}_{k-1}) + g_k(x_0, \bar{u}_0, \dots, \bar{u}_{k-1}) \begin{bmatrix} u_0 - \bar{u}_0 \\ \vdots \\ u_{k-1} - \bar{u}_{k-1} \end{bmatrix}$$

cf. (Liu, Kadirkamanathan, 1998)

LEARNING AFFINE NEURAL PREDICTORS FOR MPC

Example: apply affine neural predictor to nonlinear	Prediction step	BFR
two-tank benchmark problem	1	0.959
10000 to initiate second as ANNU ith 2 laws of 20 Pall I second	2	0.958
10000 training samples, ANN with 2 layers of 20 ReLU heurons	4	0.948
$\begin{pmatrix} \ \hat{u} - u\ _{2} \end{pmatrix}$	7	0.915
Best fit rate $ ext{BFR} = ext{max} \left\{ 0, 1 - \frac{\ y - y\ _2}{\ y - \overline{y}\ _2} ight\}$	10	0.858

2.0

• Closed-loop LTV-MPC results:

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- Model complexity reduction: add group-LASSO term with penalty λ

λ	BFR (average on all prediction steps)	# nonzero weights	
.01	0.853	328	
0.005	0.868	363	
0.001	0.901	556	
0.0005	0.911	888	
0	0.917	9000	



ON THE USE OF NEURAL NETWORKS FOR MPC

- Neural prediction models can speed up the MPC design a lot
- Experimental data need to well cover the operating range (as in linear system identification)
- No need to define linear operating ranges with NN's, it is a one-shot model-learning step
- Physical models may better predict unseen situations than black box models
- Physical modeling can help driving the choice of the nonlinear model structure to use (gray-box models)
- NN model can be updated online for adaptive nonlinear MPC



0.4075	0.7305	0.2140	0.5296	6.003
1,2334	0.2810	0.1670	0.6116	0.510
5353	0,5882	0.6461	0.8432	0.14
3116	0.5032	0.1803	0.4570	0.5
086	0.5316	0.1165	0.8828	0.
71	0.6063	0.3653	0,4936	0







LEARNING NEURAL NETWORK MODELS FOR CONTROL

TRAINING FEEDFORWARD NEURAL NETWORKS

• Feedforward neural network model:

$$y_{k} = f_{y}(x_{k}, \theta) = \begin{cases} v_{1k} = A_{1}x_{k} + b_{1} \\ v_{2k} = A_{2}f_{1}(v_{1k}) + b_{2} \\ \vdots & \vdots \\ v_{Lk} = A_{Ly}f_{L-1}(v_{(L-1)k}) + b_{L} \\ \hat{y}_{k} = f_{L}(v_{Lk}) \end{cases}$$



$$\theta = (A_1, b_1, \dots, A_L, b_L)$$

E.g.: x_k = current state & input, or $x_k = (y_{k-1}, \dots, y_{k-n_a}, u_{k-1}, \dots, u_{k-n_b})$

• Training problem: given a dataset $\{x_0, y_0, \dots, x_{N-1}, y_{N-1}\}$ solve

$$\min_{\theta} r(\theta) + \sum_{k=0}^{N-1} \ell(y_k, f(x_k, \theta))$$



• It is a nonconvex, unconstrained, nonlinear programming problem that can be solved by stochastic gradient descent, quasi-Newton methods, ... and EKF !

TRAINING FEEDFORWARD NEURAL NETWORKS VIA EKF

(Singhal, Wu, 1989) (Puskorius, Feldkamp, 1994)

• Key idea: treat parameter vector *θ* of the feedforward neural network as a constant state

$$\begin{cases} \theta_{k+1} &= \theta_k + \eta_k \\ y_k &= f(x_k, \theta_k) + \zeta_k \end{cases}$$

and use EKF to estimate θ_k on line from a streaming dataset $\{x_k, y_k\}$

• Ratio $\operatorname{Var}[\eta_k] / \operatorname{Var}[\zeta_k]$ is related to the learning-rate

• Initial matrix $(P_{0|-1})^{-1}$ is related to quadratic regularization on θ

RECURRENT NEURAL NETWORKS

• Recurrent Neural Network (RNN) model:

$$egin{array}{rcl} x_{k+1} &=& f_x(x_k,u_k, heta_x) \ y_k &=& f_y(x_k, heta_y) \ f_x,f_y &=& {
m feedforward neural network} \end{array}$$



(e.g.: general RNNs, LSTMs, RESNETS, physics-informed NNs, ...)

• Training problem: given an I/O dataset $\{u_0, y_0, \ldots, u_{N-1}, y_{N-1}\}$ solve

$$\min_{\substack{\theta_x, \theta_y \\ x_0, x_1, \dots, x_{N-1}}} r(x_0, \theta_x, \theta_y) + \frac{1}{N} \sum_{k=0}^{N-1} \ell(y_k, f_y(x_k, \theta_y))$$

s.t. $x_{k+1} = f_x(x_k, u_k, \theta_x)$

• Main issue: xk are hidden states and hence also unknowns of the problem

GRADIENT DESCENT METHODS FOR TRAINING RNNS

• Problem condensing: substitute $x_{k+1} = f_x(x_k, u_k, \theta_x)$ recursively and solve

$$\min_{\theta_x,\theta_y,x_0} r(x_0,\theta_x,\theta_y) + \frac{1}{N} \sum_{k=0}^{N-1} \ell(y_k, f_y(x_k,\theta_y)) = \lim_{\theta_x,\theta_y,x_0} V(\theta_x,\theta_y,x_0)$$

• Gradient descent (GD) methods: update θ_x, θ_y, x_0 by setting

$$\begin{bmatrix} \theta_x^{t+1} \\ \theta_y^{t+1} \\ x_0^{t+1} \end{bmatrix} = \begin{bmatrix} \theta_x^{t} \\ \theta_y^{t} \\ x_0^{t} \end{bmatrix} - \alpha_t \nabla V(\theta_x^{t}, \theta_y^{t}, x_0^{t})$$

Example: Adam uses adaptive moment estimation to set the learning rate α_t

(Kingma, Ba, 2015)

GRADIENT DESCENT METHODS FOR TRAINING RNNS

- Main issue with GD methods: slow convergence (in theory and in practice)
- Stochastic gradient descent (SGD) can be even less efficient with RNNs:
 - collect a high number of short independent experiments (often impossible)
 - create mini-batches by using multiple-shooting ideas (Forgione, Piga, 2020) (Bemporad, 2023)
- Newton's method: very fast (2nd-order) local convergence but difficult to implement, as we need the Hessian $\nabla^2 V(\theta_x^{\ t}, \theta_y^{\ t}, x_0^t)$
- Quasi-Newton methods: good tradeoff between convergence speed / solution quality and numerical complexity. Only requires the gradient $\nabla V(\theta_x^{\ t}, \theta_y^{\ t}, x_0^t)$

TRAINING RNNS VIA EXTENDED KALMAN FILTERING

TRAINING RNNS BY EKF

• Iterating Extended Kalman Filter (EKF) based on the following model

$$\begin{cases} x_{k+1} = f_x(x_k, u_k, \theta_{xk}) + \xi_k \\ \begin{bmatrix} \theta_{x(k+1)} \\ \theta_{y(k+1)} \end{bmatrix} = \begin{bmatrix} \theta_{xk} \\ \theta_{yk} \end{bmatrix} + \eta_k \\ y_k = f_y(x_k, \theta_{yk}) + \zeta_k \end{cases} \qquad \qquad Q = \operatorname{Var}\left[\begin{bmatrix} \xi_k \\ \eta_k \end{bmatrix}\right] \\ R = \operatorname{Var}[\zeta_k] \\ P_0 = \operatorname{Var}\left[\begin{bmatrix} \theta_x \\ \theta_y \\ x_0 \end{bmatrix}\right]$$

= applying Newton's method incrementally to solve the relaxed problem

$$\min_{\substack{\theta_x, \theta_y \\ 0, x_1, \dots, x_{N-1}}} \left\| \left[\frac{\theta_x}{\theta_y} \right] \right\|_{P_0^{-1}}^2 + \sum_{k=0}^{N-1} \|y_k - f_y(x_k, \theta_y)\|_{R^{-1}}^2 + \sum_{k=0}^{N-2} \left\| \left[\frac{x_{k+1} - f_x(x_k, u_k, \theta_x)}{\theta_{k+1} - \theta_k} \right] \right\|_{Q^{-1}}^2 \right\|_{Q^{-1}}$$
(Humpherys, Redd, West, 2012)

- The ratio Q/R determines the learning-rate of the training algorithm
- The inverse of the initial matrix P_0 is related to ℓ_2 -penalty on θ_x, θ_y , and x_0

• Generalization: train via Moving Horizon Estimation (MHE)

(Løwenstein, Bernardini, Bemporad, Fagiano, 2023)

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TRAINING RNNS BY EKF

• EKF can be generalized to handle general strongly convex and smooth losses $\ell(y_k, \hat{y}_k)$ by taking a local quadratic approximation of the loss around \hat{y}_k :

$$\begin{split} \ell(y_k, \hat{y}) &\approx \quad \frac{1}{2} \Delta y' H(k) \Delta y + \phi'_k \Delta y + \text{const} \\ &= \quad \frac{1}{2} \left\| y_k - H^{-1}(k) \phi_k - \hat{y} \right\|_{H(k)}^2 + \text{const} \quad \begin{aligned} \Delta y &= \hat{y} - \hat{y}_k, \ \phi_k = \frac{\partial \ell(y_k, \hat{y}_k)}{\partial \hat{y}} \\ H(k) &= \frac{\partial^2 \ell(y_k, \hat{y}_k)}{\partial \hat{y}_k^2} \end{aligned}$$

- Strongly convex smooth regularization $r(x_0, \theta_x, \theta_y)$ can be handled similarly
- Can handle ℓ_1 -penalties $\lambda \left\| \begin{bmatrix} \theta_x \\ \theta_y \end{bmatrix} \right\|_1$, useful to sparsify θ_x, θ_y by changing the EKF update into

$$\begin{bmatrix} \hat{x}(k|k)\\ \theta_x(k|k)\\ \theta_y(k|k) \end{bmatrix} = \begin{bmatrix} \hat{x}(k|k-1)\\ \theta_x(k|k-1)\\ \theta_y(k|k-1) \end{bmatrix} + M(k)e(k) - \lambda P(k|k-1) \begin{bmatrix} 0\\ \operatorname{sign}(\theta_x(k|k-1))\\ \operatorname{sign}(\theta_y(k|k-1)) \end{bmatrix}$$

The model $\overline{\theta_x}$, θ_y can be learned offline by processing a given dataset multiple times, and also **adapted on line** from streaming data (u_k, y_k)

TRAINING RNNS BY EKF - EXAMPLES

- Dataset: magneto-rheological fluid damper 3499 I/O data (Wang, Sano, Chen, Huang, 2009)
- N=2000 data used for training, 1499 for testing the model
- Same data used in NNARX modeling demo of SYS-ID Toolbox for MATLAB
- RNN model: 4 hidden states, shallow state-update and output functions
 6 neurons, atan activation, I/O feedthrough
- Compare with gradient descent (Adam)

MATLAB+CasADi implementation (Apple M1 Max CPU)





TRAINING RNNS BY EKF - EXAMPLES

- RNN model: 4 states, shallow NNs with 6 neurons each, atan activation, I/O feedthrough
- Compare BFR wrt NNARX model (SYS-ID TBX):

EKF = **92.82**, Adam = **89.12**, NNARX(6,2) = **88.18** (training) EKF = **89.78**, Adam = **85.51**, NNARX(6,2) = **85.15** (test)

• Repeat training with ℓ_1 -penalty $\tau \left\| \begin{bmatrix} \theta_x \\ \theta_y \end{bmatrix} \right\|_1$





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TRAINING LSTMS BY EKF - EXAMPLES

Use EKF to train Long Short-Term Memory (LSTM) model

(Hochreiter, Schmidhuber, 1997) (Bonassi et al., 2020)

$$\begin{array}{lll} x_a(k+1) &=& \sigma_G(W_F u(k) + U_f x_b(k) + b_f) \odot x_a(k) \\ &+ \sigma_G(W_I u(k) + U_I x_b(k) + b_I) \odot \sigma_C(W_C u(k) + U_C x_b(k) + b_C) \\ x_b(k+1) &=& \sigma_G(W_O u(k) + U_O x_b(k) + b_O) \odot \sigma_C(x_a(k+1)) \\ y(k) &=& f_y(x_b(k), u(k), \theta_y) \end{array}$$

gate activation for $\sigma_G(\alpha) = \frac{1}{1+e^{-\alpha}}$, cell activation for $\sigma_C(\alpha) = \tanh(\alpha)$

• Training results (mean and std over 20 runs):

	BFR	Adam	EKF
RNN	training	89.12 (1.83)	92.82 (0.33)
$n_{\theta} = 107$	test	85.51 (2.89)	89.78 (0.58)
LSTM	training	89.60 (1.34)	92.63 (0.43)
$n_{\theta} = 139$	test	85.56 (2.68)	88.97 (1.31)

• EKF training applicable to arbitrary classes of black/gray box recurrent models!

TRAINING RNNS BY EKF - EXAMPLES

• Dataset: 2000 I/O data of linear system with binary outputs

- N=1000 data used for training, 1000 for testing the model
- Train linear state-space model with 3 states and sigmoidal output function

$$f_1^y(y) = 1/(1 + e^{-A_1^y[x'(k) \ u(k)]' - b_1^y})$$

	EKF accuracy [%]		
σ	test	training	
0.000	98.02	97.91	
0.001	95.33	98.66	
0.010	97.99	98.52	
0.100	94.56	95.44	
0.200	93.71	92.22	

• Training loss: (modified) cross-entropy loss

$$\ell_{CE\epsilon}(y(k), \hat{y}) = \sum_{i=1}^{n_y} -y_i(k) \log(\epsilon + \hat{y}_i) - (1 - y_i(k)) \log(1 + \epsilon - \hat{y}_i)$$

EXAMPLE: MPC OF ETHYLENE OXIDATION PLANT

 Chemical process = oxidation of ethylene to ethylene oxide in a nonisothermal continuously stirred tank reactor (CSTR)

$$\begin{array}{l} C_2H_4 + \frac{1}{2}O_2 \to C_2H_4O \\ C_2H_4 + 3O_2 \to 2CO_2 + 2H_2O \\ C_2H_4O + \frac{5}{2}O_2 \to 2CO_2 + 2H_2O \end{array}$$

• Nonlinear model (dimensionless variables): (Durand, Ellis, Christofides, 2016)

$$\begin{array}{rcl} \dot{x}_1 & = & u_1(1-x_1x_4) & \underbrace{\Upsilon_1}_{x_2} & \underbrace{\Upsilon_2}_{x_4} & \underbrace{\Upsilon_2}_{x_4}(x_2x_4)^{\frac{1}{2}} - A_2e^{\frac{\Upsilon_2}{x_4}}(x_2x_4)^{\frac{1}{4}} \\ \dot{x}_2 & = & u_1(u_2-x_2x_4) - A_1e^{\frac{\Upsilon_1}{x_4}}(x_2x_4)^{\frac{1}{2}} - A_2e^{\frac{\Upsilon_2}{x_4}}(x_2x_4)^{\frac{1}{4}} \\ \dot{x}_3 & = & -u_1x_3x_4 + A_1e^{\frac{\Upsilon_1}{x_4}}(x_2x_4)^{\frac{1}{2}} - A_3e^{\frac{\Lambda_1}{x_4}}(x_3x_4)^{\frac{1}{2}} \\ \dot{x}_4 & = & \underbrace{\frac{\Upsilon_1(1-x_4) + B_1e^{\frac{\Lambda_2}{x_4}}(x_2x_4)^{\frac{1}{2}} + B_2e^{\frac{\Lambda_2}{x_4}}(x_2x_4)^{\frac{1}{4}}}{x_1} \\ & + \frac{B_3e^{\frac{\Upsilon_3}{x_4}}(x_3x_4)^{\frac{1}{2}} - B_4(x_4 - T_C)}{x_1} \\ y & = & x_3 \end{array}$$

 x_1 = gas density x_2 = ethylene concentration x_3 = ethylene oxide concentration x_4 = temperature in reactor

 $u_1 =$ feed volumetric flow rate $u_2 =$ ethylene concentration in feed

• u_1 = manipulated variables, x_3 = controlled output, u_2 = measured disturbance

RNN MODEL OF ETHYLENE OXIDATION PLANT

Train a black-box recurrent neural-network model

$$x_{k+1} = \mathcal{N}_x(x_k, u_k)$$
$$y_k = \mathcal{N}_y(x_k)$$

1,000 training samples $\{u_k, y_k\}$, sample time $T_s = 5$ s 2 layers (6 neurons, 4 neurons), sigmoid activation

ightarrow 95 coefficients

- NN model trained in MATLAB by EKF (Bemporad, 2023) CPU time ≈ 12.58 s [Apple M1 Max]
- Model validated on 1000 samples

BFR (Best Fit Rate)	training	test
	95.1611	84.3623





MPC OF ETHYLENE OXIDATION PLANT

- Nonlinear MPC: $\min \sum_{k=0}^{9} 10(y_{k+1} r_{k+1})^2 + \frac{1}{10}(u_{1,k} u_{1,k-1})^2$ subject to RNN model and input constraints $0.0704 \le u_k \le 0.7042$
- **EKF** used to estimate the hidden state x_k and, possibly, the disturbance d_k



• Model mismatch compensated by output integrator in steady-state

ADAPTIVE NONLINEAR MPC BASED ON EKF

• By combining online EKF-based learning of the model parameters with nonlinear MPC we get an adaptive nonlinear MPC controller

• Do we really need to train the full model online?

• Output integrators: only update the bias term d_k on the output. Conceived to track constant set-points

• Can we train more general nonlinear disturbance models to better track time-varying references?

NONLINEAR DISTURBANCE MODELS FOR MPC

(Krupa, Zanon, Bemporad, arXiv, 2023)

• Consider the following general prediction model with unmeasured disturbance:

$$\begin{aligned} x(k+1) &= f(x(k), u(k), d(k)) \\ d(k) &= h(x(k), u(k), \theta(k)) \\ y(k) &= g(x(k), d(k)) \end{aligned}$$

- Key idea: only train the disturbance model online to refine the prediction model only where the system is operating
- The nominal model f, g is trained offline and frozen
- **Motivation**: train the full model online may be difficult (lack of excitation, catastrophic forgetting, computational demand, etc.)
- Under certain assumptions, we can show that the tracking error y(k) r(k) asymptotically converges to zero, even if r(k) is not constant
EXAMPLE: CSTR PROCESS

- MPC control of a diabatic continuous stirred tank reactor (CSTR)
- Process model is nonlinear (Seborg, Edgar, Mellichamp, 2004)

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{Af} - C_A) - C_A k_0 e^{-\frac{\Delta E}{RT}}$$
$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \frac{UA}{\rho C_p V}(T_j - T) - \frac{\Delta H}{\rho C_p} C_A k_0 e^{-\frac{\Delta E}{RT}}$$



- T: temperature inside the reactor [K] (state)
- C_A : concentration of the reactant in the reactor $[kgmol/m^3]$ (state)
- T_j : jacket temperature [K] (input)
- T_f : feedstream temperature [K] (measured disturbance)
- C_{Af} : feedstream concentration $[kgmol/m^3]$ (measured disturbance)
- Objective: manipulate T_j to regulate C_A on desired setpoint

- **Model**: nominal (white-box) NL model with slightly different model coefficients and three different disturbance models:
 - Constant Disturbance Model: y = v + d, $\theta = d$
 - Polynomial Disturbance Model: a polynomial function $d_x = h_x(x, u, \theta)$ entering the white-box model in a way that, for a suitable (unknown) θ , it matches the exact CSTR dynamics
 - Feedforward Neural Network: perturb both y(k) and x(k + 1) by setting d_x = FNN with input (x, u), 2 layers with 6 neurons each, sigmoid activation, d_y = FNN with input x, single layer with 4 neurons. Total # parameters = 97
- NLMPC: N = 5, $\cot = (x x_r)'(x x_r) + (u u_r)'(u u_r)$, terminal constraint $x(k + N) = x_r(k + N)$, no other constraints.

EXAMPLE: CSTR PROCESS

• Generic trackable reference signal r(k) (w/ preview)



- Constant disturbance model is worse than FNN disturbance model, especially when r(k) changes rapidly

TRAINING RNNS VIA SEQUENTIAL LEAST SQUARES

TRAINING RNNS BY SEQUENTIAL LEAST-SQUARES

(Bemporad, 2023)

• RNN training problem = optimal control problem:

$$\begin{array}{ll} \min_{\theta_x,\theta_y,x_0,x_1,\dots,x_{N-1}} & r(x_0,\theta_x,\theta_y) + \sum_{k=0}^{N-1} \ell(y_k,\hat{y}_k) \\ \text{s.t.} & x_{k+1} = f_x(x_k,u_k,\theta_x) \\ & \hat{y}_k = f_y(x_k,u_k,\theta_y) \end{array} \qquad \qquad \begin{array}{l} \text{inputs} = \theta_x,\theta_y,x_0 \\ \text{output} = \hat{y} \\ \text{reference} = y_k \\ \text{weas. dist.} = u_k \end{array}$$

- $r(x_0, \theta_x, \theta_y)$ = input penalty
- $\ell(y_k, \hat{y}_k)$ = output penalty
- prediction horizon = N steps, control horizon = 1 step
- Linearized model: given a current guess $\theta_x^{h}, \theta_y^{h}, x_0^{h}, \ldots, x_{N-1}^{h}$, approximate

$$\begin{aligned} \Delta x_{k+1} &= (\nabla_x f_x)' \Delta x_k + (\nabla_{\theta_x} f_x)' \Delta \theta_x \\ \Delta y_k &= (\nabla_x f_y)' \Delta x_k + (\nabla_{\theta_y} f_y)' \Delta \theta_y \end{aligned}$$

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TRAINING RNNS BY SEQUENTIAL LEAST-SQUARES

• Linearized dynamic response: $\Delta x_k = M_{kx} \Delta x_0 + M_{k\theta_x} \Delta \theta_x$

(Bemporad, 2023)

$$\begin{split} M_{0x} &= I, \quad M_{0\theta_x} = 0\\ M_{(k+1)x} &= \nabla_x f_x(x_k^h, u_k, \theta_x^{-h}) M_{kx}\\ M_{(k+1)\theta_x} &= \nabla_x f_x(x_k^h, u_k, \theta_x^{-h}) M_{k\theta_x} + \nabla_{\theta_x} f_x(x_k^h, u_k, \theta_x^{-h}) \end{split}$$

- Take 2^{nd} -order expansion of the loss ℓ and regularization term r
- Solve least-squares problem to get increments Δx_0 , $\Delta \theta_x$, $\Delta \theta_y$
- Update x_0^{h+1} , θ_x^{h+1} , θ_y^{h+1} by applying either a
 - line-search (LS) method based on Armijo rule
 - or a trust-region method (Levenberg-Marquardt) (LM)
- The resulting training method is a Generalized Gauss-Newton method
 very good convergence properties (Messerer, Baumgärtner, Diehl, 2021)
- No guarantee to converge to a global minimum (multiple runs may be required)

Example: magneto-rheological fluid damper

N=2000 data used for training, 1499 for testing the model

(Wang, Sano, Chen, Huang, 2009)



RNN model: 4 states, shallow NNs w/ 4 neurons, I/O feedthrough



NAILS = GNN method with **line search** NAILM = GNN method with **LM steps**

 $\mathsf{BFR} = 100 (1 - \frac{\|Y - \hat{Y}\|_2}{\|Y - \bar{u}\|_2})$ BFR (Best Fit Rate) training

NAILS	94.41 (0.27)	89.35 (2.63)
NAILM	94.07 (0.38)	89.64 (2.30)
AMSGrad	84.69 (0.15)	80.56 (0.18)
EKF	91.41 (0.70)	87.17 (3.06)

MSE loss on training data,

initial weights

mean value and range over 20 runs from different random

test

• We also want to handle non-smooth/non-convex regularization terms

$$\min_{\theta_x, \theta_y, x_0} \quad r(x_0, \theta_x, \theta_y) + \sum_{k=0}^{N-1} \ell(y_k, f_y(x_k, \theta_y)) + g(\theta_x, \theta_y)$$

s.t. $x_{k+1} = f_x(x_k, u_k, \theta_x)$

E.g.: $g(\theta_x, \theta_y) = \tau(\|\theta_x\|_1 + \|\theta_y\|_1)$ (Lasso regularization)

Idea: use alternating direction method of multipliers (ADMM) by splitting

$$\min_{\theta_x, \theta_y, x_0, \nu_x, \nu_y} \quad r(x_0, \theta_x, \theta_y) + \sum_{k=0}^{N-1} \ell(y_k, f_y(x_k, \theta_y)) + g(\nu_x, \nu_y)$$
s.t.
$$x_{k+1} = f_x(x_k, u_k, \theta_x)$$

$$\begin{bmatrix} \nu_x \\ \nu_y \end{bmatrix} = \begin{bmatrix} \theta_x \\ \theta_y \end{bmatrix}$$

ADMM + Seq. LS = NAILS algorithm (Nonconvex ADMM Iterations and Sequential LS)

$$\begin{bmatrix} x_0^{t+1} \\ \theta_x^{t+1} \\ \theta_y^{t+1} \end{bmatrix} = \arg\min_{x_0, \theta_x, \theta_y} V(x_0, \theta_x, \theta_y) + \frac{\rho}{2} \left\| \begin{bmatrix} \theta_x - \nu_x^t + w_x^t \\ \theta_y - \nu_y^t + w_y^t \end{bmatrix} \right\|_2^2 \quad \text{(sequential) LS}$$

$$\begin{bmatrix} \nu_x^{t+1} \\ \nu_y^{t+1} \end{bmatrix} = \operatorname{prox}_{\frac{1}{\rho}g}(\theta_x^{t+1} + w_x^t, \theta_y^{t+1} + w_y^t) \quad \text{proximal step}$$

$$\begin{bmatrix} w_x^{t+1} \\ w_y^{t+1} \end{bmatrix} = \begin{bmatrix} w_x^h + \theta_x^{t+1} - \nu_x^{t+1} \\ w_y^h + \theta_y^{t+1} - \nu_y^{t+1} \end{bmatrix} \quad \text{update dual variable}$$

- ADMM + Levenberg-Marquardt steps = NAILM algorithm
- Fluid-damper example: Lasso regularization $g(\nu_x, \nu_y) = \tau(\|\nu_x\|_1 + \|\nu_y\|_1)$



(mean results over 20 runs from different initial weights)

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• Fluid-damper example: Lasso regularization $g(\nu_x, \nu_y) = 0.2(\|\nu_x\|_1 + \|\nu_y\|_1)$

training	BFR	BFR	sparsity	CPU	#
algorithm	training	test	%	time	epochs
NAILS	91.00 (1.66)	87.71 (2.67)	65.1 (6.5)	11.4 s	250
NAILM	91.32 (1.19)	87.80 (1.86)	64.1 (7.4)	11.7 s	250
AMSGrad	91.04 (0.47)	88.32 (0.80)	16.8 (7.1)	64.0 s	2000
Adam	90.47 (0.34)	87.79 (0.44)	8.3 (3.5)	63.9 s	2000
DiffGrad	90.05 (0.64)	87.34 (1.14)	7.4 (4.5)	63.9 s	2000
EKF	89.27 (1.48)	86.67 (2.71)	47.9 (9.1)	13.2 s	50

 \approx same fit than SGD/EKF but sparser models and faster (Apple M1 Pro)

• Fluid-damper example: group-Lasso regularization $g(\nu_i^g) = \tau_g \sum_{i=1}^{n_x} \|\nu_i^g\|_2$ to zero entire rows/columns and reduce the state-dimension automatically



good choice: $n_x = 3$ (best fit on test data)

(Bemporad, 2023)

• Fluid-damper example: quantization of θ_x , θ_y for simplifying model arithmetic +leaky-ReLU activation function

$$g(\theta_i) = \begin{cases} 0 & \text{if } \theta_i \in \mathcal{Q} \\ +\infty & \text{otherwise} \end{cases} \qquad \qquad \mathcal{Q} = \text{multiples of } 0.1 \text{ between } -0.5 \text{ and } 0.5 \end{cases}$$

- BFR = 84.36 (training), 78.43 (test) ← NAILS w/ quantization
- BFR = 17.64 (training), 12.79 (test) ← no ADMM, just quantize after training
- Training time: \approx 12 s (w/ quantization), 7 s (no ADMM)

- Note: no convergence to a global minimum is guaranteed
- NAILS/LM = flexible & efficient algorithm for training control-oriented RNNs

TRAINING RNNS - SILVERBOX BENCHMARK

(Wigren, Schoukens, 2013)

• Silverbox benchmark (Duffin oscillator): 10 traces (\approx 8600 samples each) used for training, 40000 for testing





(Schoukens, Ljung, 2019)

Data download: http://www.nonlinearbenchmark.org

TRAINING RNNS - SILVERBOX BENCHMARK

(Bemporad, 2023)

- RNN model: 8 states, 3 layers of 8 neurons, atan activation, no I/O feedthrough
- Initial-state: encode x_0 as the output of a NN with atan activation, 2 layers of 4 neurons, receiving 8 past inputs and 8 past outputs

$$\min_{\theta_{x_0}, \theta_x, \theta_y} \quad r(\theta_{x_0}, \theta_x, \theta_y) + \sum_{j=1}^{M} \sum_{k=0}^{N-1} \ell(y_k^j, \hat{y}_k^j) \\ \text{s.t.} \quad x_{k+1}^j = f_x(x_k^j, u_k^j, \theta_x), \ \hat{y}_k^j = f_y(x_k^j, u_k^j, \theta_y) \\ \quad x_0^j = f_{x_0}(v^j, \theta_{x_0})$$
 $v = \begin{bmatrix} y_{-1} \\ \vdots \\ y_{-8} \\ u_{-1} \\ \vdots \\ u_{-8} \end{bmatrix}$

[cf. (Beintema, Toth, Schoukens, 2021)]

- ℓ_2 -regularization: $r(\theta_{x_0}, \theta_x, \theta_y) = \frac{0.01}{2}(\|\theta_x\|_2^2 + \|\theta_y\|_2^2) + \frac{0.1}{2}\|\theta_{x_0}\|_2^2$
- Total number of parameters $n_{\theta_x} + n_{\theta_y} + n_{\theta_{x_0}} = 296 + 225 + 128 = 649$
- Training: use NAILM over 150 epochs

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TRAINING RNNS - SILVERBOX BENCHMARK

• Identification results on test data ¹:

identification method	RMSE [mV]	BFR [%]
ARX (ml) [1]	16.29 [4.40]	69.22 [73.79]
NLARX (ms) [1]	8.42 [4.20]	83.67 [92.06]
NLARX (mlc) [1]	1.75 [1.70]	96.67 [96.79]
NLARX (ms8c50) [1]	1.05 [0.30]	98.01 [99.43]
Recurrent LSTM model [2]	2.20	95.83
SS encoder [3] ($n_x = 4$)	[1.40]	[97.35]
NAILM	0.35	99.33

Ljung, Zhang, Lindskog, Juditski, 2004
 Ljung, Andersson, Tiels, Schön, 2020
 Beintema, Toth, Schoukens, 2021

RMSE =
$$\sqrt{\frac{1}{N} \sum_{k=1}^{N} (y_k - \hat{y}_k)^2}$$

- NAILM training time \approx 400 s (MATLAB+CasADi on Apple M1 Max CPU)
- Repeat training with ℓ_1 -regularization:



¹ Trained RNN: http://cse.lab.imtlucca.it/~bemporad/shared/silverbox/rnn888.zip

LINEAR AND NONLINEAR IDENTIFICATION VIA L-BFGS

SYSTEM IDENTIFICATION PROBLEM

• Class of dynamical models with n_x states, n_u inputs, n_y outputs:

 $x_{k+1} = Ax_k + Bu_k + f_x(x_k, u_k; \theta_x)$ $\hat{y}_k = Cx_k + Du_k + f_y(x_k, u_k; \theta_y)$

Special cases:

linear model, RNN, ...

• Loss function (open-loop prediction error + regularization)

• Condense the problem by eliminating the hidden states x_k and get

(nonconvex) nonlinear programming (NLP) problem

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 $\min f(z) + r(z)$

NLP PROBLEM

- If *f* and *r* differentiable: use any state-of-the-art unconstrained NLP solver, e.g., L-BFGS (Limited-memory Broyden–Fletcher–Goldfarb–Shanno) (Liu, Nocedal, 1989)
- The gradient $\nabla f(z)$ can be computed efficiently by automatic differentiation

• However, sparsifying the model requires non-smooth regularizers:

$$r_1(z) = au \|z\|_1$$
 $r_g(z) = au_g \sum_{i=1}^m \|I_i z\|_2$
 ℓ_1 -regularization group-Lasso penalty

• Examples of group-Lasso penalties:

 $m = n_x$ and I_i selected to reduce the number of states $m = n_u$ and I_i selected to reduce the number of inputs

HANDLING NON-SMOOTH REGULARIZATION TERMS

(Bemporad, 2024)

1. If $r(x) = \sum_{i=1}^{n} r_i(x_i)$ and $r_i : \mathbb{R} \to \mathbb{R}$ is convex and positive semidefinite, the ℓ_1 -regularized problem can be recast as a **bound-constrained NLP**:

$$\begin{split} \min_{x} f(x) + \tau \|x\|_{1} + r(x) \\ x^{*} &= y^{*} - z^{*} \\ \\ \textbf{Example:} r(x) &= \|x\|_{2}^{2} \operatorname{then} r(y) + r(-z) = \|[\frac{y}{z}]\|_{2}^{2} \quad \overset{\text{well-regularized}}{\underset{\text{augmented problem}}{\overset{\text{well-regularized}}{\overset{well-regularized$$

2. If r(x) is convex and symmetric wrt each component x_i and increasing for $x \ge 0$, and $\tau > 0$, then we can solve instead

 $\min_{y,z\geq 0} f(y-z) + \tau [1 \dots 1] \begin{bmatrix} y \\ z \end{bmatrix} + r(y+z)$

if r(x) differentiable for $x \neq 0$ then r(y+z) differentiable if any $y_i, z_j > 0$

Example: r(x) = group-Lasso penalty + constraint $y, z \ge \epsilon$ = machine precision

EXAMPLE: LINEAR SYSTEM IDENTIFICATION

• Cascaded-Tanks benchmark: (Schoukens, Mattson, Wigren, Noël, 2016)

						-	
	R^2 (training)			R^2 (test)			
n_x	lbfgs	sippy ²	matlab ³	lbfgs	sippy	MATLAB	
1	87.43	56.24	87.06	83.22	52.38	83.18	(ssest)
2	94.07	28.97	93.81	92.16	23.70	92.17	(ssest)
3	94.07	74.09	93.63	92.16	68.74	91.56	(ssest)
4	94.07	48.34	92.34	92.16	45.50	90.33	(ssest)
5	94.07	90.70	93.40	92.16	89.51	80.22	(ssest)
6	94.07	94.00	93.99	92.17	92.32	88.49	(n4sid)
7	94.07	92.47	93.82	92.17	90.81	< 0	(ssest)
8	94.49	< 0	94.00	89.49	< 0	< 0	(n4sid)
9	94.07	< 0	< 0	92.17	< 0	< 0	(ssest)
10	94.08	93.39	< 0	92.17	92.35	< 0	(ssest)

$z = (A, B, C, D, x_0)$, mean-squared error loss + ℓ_2 -regularization

(n4sid) 1024 test data (ssest) (ssest) (standard scaling)

 $n_y = n_u = 1$ 1024 training data

CPU time: 2.4 s (lbfgs), 30 ms (sippy), 50 ms (n4sid/pred.), 0.3 s (n4sid/sim.), 0.5 s (ssest) [Apple M1 Max]

NLP with bounds solved in JAX/JAXOPT using the L-BFGS-B solver (Byrd, Lu, Nocedal, Zhu, 1995)



pip install jax-sysid

github.com/bemporad/jax-sysid

- ² (Armenise, Vaccari, Bacci Di Capaci, Pannocchia, 2018)
- ³ (Ljung, SYS-ID Toolbox)

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JAX-SYSID LIBRARY

Python code to identify a linear time-invariant model:

```
from jax_sysid.models import LinearModel
from jax_sysid.utils import compute_scores
model = LinearModel(nx, ny, nu)
model.loss(rho_x0=1.e-3, rho_th=1.e-2)
model.optimization(lbfgs_epochs=1000)
model.fit(Y,U)
Yhat, Xhat = model.predict(model.x0, U)
A,B,C,D = model.ssdata()
```



(Bemporad, 2024)

• Python code for testing the model:

```
x0_test = model.learn_x0(U_test, Y_test)
Yhat_test, Xhat_test = model.predict(x0_test, U_test)
R2_train, R2_test, msg = compute_scores(Y, Yhat, Y_test, Yhat_test, fit='R2')
print(msg)
```

JAX-SYSID LIBRARY

• Sample Python code to identify a **nonlinear RNN** model:

```
jax-sysid
import numpy as np
from jax sysid.models import Model
def state fcn(x,u,params):
                               state-update function, x(k+1)
    . . .
def output fcn(x,u,params):
                               output function, y(k)
    . . .
model = Model(nx, ny, nu, state fcn=state fcn, output fcn=output fcn)
  = 0.5 * np.eye(nx)
А
     . . .
b4 = np.zeros(ny) # Parameter initialization:
model.init(params=[A,B,C,W1,W2,W3,b1,b2,W4,W5,b3,b4])
model.loss(rho x0=1.e-4, rho th=1.e-4)
model.optimization(adam epochs=1000, lbfgs epochs=1000)
model.fit(Y, U)
Yhat, Xhat = model.predict(model.x0, U)
```

(Bemporad, 2024)

EXAMPLE: LINEAR SYSTEM IDENTIFICATION

• Synthetic data generated by the cascaded 2x2 linear system

$$\begin{aligned} x_{k+1} &= \begin{bmatrix} \begin{array}{ccccc} 0.96 & 0.26 & 0.04 & 0 & 0 & 0 \\ -0.26 & 0.70 & 0.26 & 0.0 & 0 & 0 \\ 0 & 0 & 0.93 & 0.32 & 0.07 & 0 \\ 0 & 0 & -0.32 & 0.61 & 0.32 & 0 \\ 0 & 0 & 0 & 0 & 0.90 & 0.38 \\ 0 & 0 & 0 & 0 & -0.38 & 0.52 \end{bmatrix} x_k + \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0.22 & 0 \\ 0 & 0.10 \\ 0 & 0.38 \end{bmatrix} u_k + \xi_k \\ y_k &= \begin{bmatrix} x_1 \\ x_3 \end{bmatrix} + \eta_k \end{aligned}$$

$$\xi_{ki}, \eta_{kj} \in \mathcal{N}(0, 0.01)$$

N=2000 training data
 $\{(u_k, y_k)\}$

• Group-lasso penalty for model-order reduction:

model.group_lasso_x()

$$\min_{\theta_x, \theta_y, x_0} \frac{1}{1000} \|z\|_2^2 + 10^{-16} \|z\|_1 + \tau_g \sum_{i=1}^{n_x} \left\| \begin{bmatrix} A'_{i,:} \\ A_{:,i} \\ B'_{i,:} \\ C_{:,i} \end{bmatrix} \right\|_2 + \frac{1}{N} \sum_{k=0}^{N-1} \|y_k - Cx_k\|_2^2$$



best results out of 10 runs CPU time \approx 3.85 s per run [Apple M1 Max]

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EXAMPLE: LINEAR SYSTEM IDENTIFICATION

- Synthetic data generated by a random linear system with $n_x = 3$ states, $n_u = 10$ inputs, $n_u = 1$ outputs, noise in $\mathcal{N}(0, 0.01)$, N = 10000 training data
- The last 5 columns of the *B* matrix are **1000x smaller** than the first 5
- Group-lasso penalty for **input selection**:

model.group lasso u()

$$\min_{\substack{\theta_x, \theta_y, x_0}} 10^{-8} \|z\|_2^2 + 10^{-16} \|z\|_1 + \tau_g \sum_{i=1}^{n_u} \|B_{:,i}\|_2 + \frac{1}{N} \sum_{k=0}^{N-1} \|y_k - Cx_k\|_2^2$$

$$\sup_{\substack{\theta_x, \theta_y, x_0}} \frac{10^{-9} |\theta_x|^2 + 10^{-16} ||z||_1 + \tau_g \sum_{i=1}^{n_u} \|B_{:,i}\|_2 + \frac{1}{N} \sum_{k=0}^{N-1} \|y_k - Cx_k\|_2^2$$

$$\sup_{\substack{\theta_x, \theta_y, x_0}} \frac{10^{-9} |\theta_x|^2 + 10^{-16} ||z||_1 + \tau_g \sum_{i=1}^{n_u} \|B_{:,i}\|_2 + \frac{1}{N} \sum_{k=0}^{N-1} \|y_k - Cx_k\|_2^2$$

$$\sup_{\substack{\theta_x, \theta_y, x_0}} \frac{10^{-9} ||z||^2 + 10^{-16} ||z||_1 + \tau_g \sum_{i=1}^{n_u} \|B_{:,i}\|_2 + \frac{1}{N} \sum_{k=0}^{N-1} \|y_k - Cx_k\|_2^2$$

$$\sup_{\substack{\theta_x, \theta_y, x_0}} \frac{10^{-9} ||z||^2 + 10^{-16} ||z||_1 + \tau_g \sum_{i=1}^{n_u} \|B_{:,i}\|_2 + \frac{1}{N} \sum_{k=0}^{N-1} \|y_k - Cx_k\|_2^2$$

$$\sup_{\substack{\theta_x, \theta_y, x_0}} \frac{10^{-9} ||z||^2 + 10^{-16} ||z||_1 + \tau_g \sum_{i=1}^{n_u} \|B_{:,i}\|_2 + \frac{1}{N} \sum_{k=0}^{N-1} \|y_k - Cx_k\|_2^2$$

$$\sup_{\substack{\theta_x, \theta_y, x_0}} \frac{10^{-9} ||z||^2 + 10^{-16} ||z||_1 + \tau_g \sum_{i=1}^{n_u} \|B_{:,i}\|_2 + \frac{1}{N} \sum_{k=0}^{N-1} \|y_k - Cx_k\|_2^2$$

$$\sup_{\substack{\theta_x, \theta_y, x_0}} \frac{10^{-9} ||z||^2 + 10^{-16} ||z||_1 + \tau_g \sum_{i=1}^{n_u} \|B_{:,i}\|_2 + \frac{1}{N} \sum_{k=0}^{N-1} \|y_k - Cx_k\|_2^2$$

$$\sup_{\substack{\theta_x, \theta_y, x_0}} \frac{10^{-9} ||z||^2 + 10^{-16} ||z||_1 + \tau_g \sum_{i=1}^{n_u} \|B_{:i}\|_2 + \frac{1}{N} \sum_{i=1}^{N-1} \|y_i\|_1 + \frac{1}{N} \sum_{i=1}^{n_u} \|y_i\|_2 + \frac{1}{N} \sum_{i=1}^{N-1} \|y_i\|_1 + \frac{1}{N} \sum_{i=1}^{N-1} \|y_i\|_1$$

100

• Can be useful to identify Hammerstein models using basis functions on u

 10^{-1}

10-3

10-2

10-4

100.

LINEAR SYSTEM IDENTIFICATION W/ STABILITY CONSTRAINTS

- We try enforcing $||A||_2 \le 1$ by adding the loss $\rho_A \max\{||A||_2^2 1 + \epsilon_A, 0\}^2$
- Example: 1000 training + 1000 test data generated by the unstable LTI system

$$x_{k+1} = \begin{bmatrix} 1.0001 & 0.5 & 0.5 \\ 0 & 0.9 & -0.2 \\ 0 & 0 & 0.7 \end{bmatrix} x_k + Bu_k + \xi_k$$
$$y_k = Cx_k + z_k$$

where the entries of $B, C \in \mathcal{N}(0, 1), \xi_{ki} \in \mathcal{N}(0, 0.01^2), \zeta_k \in \mathcal{N}(0, 0.05^2)$, and u_k uniformly generated in $[-\frac{1}{2}, \frac{1}{2}]$

• Training setup:

model.force_stability(rho_A=1.e3, epsilon_A=1.e-3)

- $\rho_A = 10^3$, $\epsilon_A = 10^{-3}$
- 3000 Adam + 5000 L-BFGS iters
- CPU time \approx **5.38 s** [Apple M1 Max]

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BFR (Best Fit Rate)trainingtest98.293091.7369

Eigenvalues of identified matrix *A*: 0.99997, 0.92747, 0.59781

QUASI-LPV MODEL IDENTIFICATION

• Quasi-LPV (qLPV) models are defined by:

$$x_{k+1} = A(p_k)x_k + B(p_k)u_k$$
$$y_k = C(p_k)x_k + D(p_k)u_k$$
$$\begin{bmatrix} A(p_k) & B(p_k) \\ C(p_k) & D(p_k) \end{bmatrix} = \begin{bmatrix} A_0 & B_0 \\ C_0 & D_0 \end{bmatrix} + \sum_{i=1}^{n_p} \begin{bmatrix} A_i & B_i \\ C_i & D_i \end{bmatrix} p_{ki}$$

where $p_k \in \mathbb{R}^{n_p}$ is the scheduling parameter vector, such as

$$p_{ki} = \frac{1}{1 + e^{-f(x_k, u_k; \theta_i)}}, i = 1, \dots, n_p - 1$$

where $f(x_k, u_k; \theta_i)$ is a FNN with linear output layer and parameters θ_i

• qLPV models are a powerful class of control-oriented nonlinear models

EXAMPLE: QLPV MODEL IDENTIFICATION

• Generate 5000 training data and 1000 test data from the NL dynamics

$$x_{k+1} = \begin{bmatrix} 0.5\sin(x_{1k}) + 1.7\cos(0.5x_{2k})u_k\\ 0.6\sin(x_{1k} + x_{3k}) + 0.4\tan(x_{1k} + x_{2k})\\ 0.4e^{-x_{2k}} + 0.9\sin(-0.5x_{1k})u_k \end{bmatrix} + \xi_k$$
$$y_k = \operatorname{atan}(2.2x_{1k}^3) + \operatorname{atan}(1.8x_{2k}^3) + \operatorname{atan}(-x_{3k}^3) + z_k$$

where $\xi_k, z_k \in \mathcal{N}(0, 0.01^2)$ and u_k uniformly generated in $[-\frac{1}{2}, \frac{1}{2}]$

- p_k = 2-layer FNN (6 neurons each) + swish activation + sigmoid output function
- Training setup:
- warm start: identify LTI model (2000 L-BFGS iters)
- 1000 Adam + 5000 L-BFGS iters for qLPV-SYSID
- CPU time \approx **20 s** [Apple M1 Max]

BFR (Best Fit Rate)	n_p	training	test
LTI	0	74.7374	74.9277
qLPV	1	94.5179	94.5059
qLPV	2	96.3040	94.3056
qLPV	3	96.5766	96.4442

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EXAMPLE: QUASI-LPV MODEL OF SILVERBOX BENCHMARK

• **Quasi-LPV** model structure ($n_x = 8$ states):

$$x_{k+1} = (A_0 + A_1 p_k) x_k + (B_0 + B_1 p_k) u_k$$

$$y_k = C x_k$$

$$p_k = \text{swish}(W_2 \text{swish}(W_1 x_k + b_1) + b_2)$$

$$\operatorname{swish}(x) = \frac{x}{1+e^{-x}}$$

(Bemporad, NL-SYSID Workshop, 2024)



- Training setup:
 - ℓ_2 -regularization ($ho = 10^{-4}$)
 - warm start on first experiment (8,600 samples)
 500 Adam + 500 L-BFGS iterations
 - 5000 L-BFGS iterations on full dataset (86,114 samples)
 - CPU time \approx **265 s** [Apple M1 Max]
- RMSE on test data: 0.397 mV

 $(||A_0||_2 = 1.96, ||A_1||_2 = 0.35, ||B_0||_2 = 0.79, ||B_1||_2 = 0.09)$

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(LTI model: 14.090 mV)

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INDUSTRIAL ROBOT BENCHMARK

(Weigand, Götz, Ulmen, Ruskowski, 2022)

- KUKA KR300 R2500 ultra SE industrial robot, full robot movement
- 6 inputs (torques), 6 outputs (joint angles), w/ backlash, highly nonlinear and coupled, slightly over-sampled ($||y_k - y_{k-1}||$ is often very small)
- Identification benchmark dataset (forward model):
 - Sample time: $T_s = 100 \text{ ms}$
 - N = 39988 training samples
 - $N_{\rm test}$ = 3636 test samples
- Very challenging NL-SYSID benchmark on nonlinearbenchmark.org



nonlinearbenchmark.org

RECURRENT NEURAL NETWORKS IN RESIDUAL FORM

(Bemporad, 2024)

• Recurrent Neural Network (RNN) model in residual form:

$$\begin{array}{rcl} x_{k+1} &=& Ax_k + Bu_k + f_x(x_k, u_k, \theta_x^i) \\ y_k &=& Cx_k + f_y(x_k, \theta_y^i) \\ f_x, f_y &=& \textit{feedforward neural network} \end{array}$$



$$v_j = A_j f_{j-1}(v_{j-1}) + b_j$$

 $\theta = (A_1, b_1, \ldots, A_L, b_L)$

Goal: minimize open-loop simulation error under elastic net regularization

$$\min_{x_0, A, B, C, \theta_x, \theta_y} \frac{1}{N} \sum_{k=1}^N \|y_k - \hat{y}_k\|_2^2 + \frac{1}{2} \rho(\|\theta_x\|_2^2 + \|\theta_y\|_2^2) + \tau(\|\theta_x\|_1 + \|\theta_y\|_1)$$

s.t. model equations

*l*₁-regularization introduced to reduce # model coefficients (=simpler model)

TRAINING RNN W/ ℓ_1 -PENALTIES - INDUSTRIAL ROBOT

- Main issues with industrial robot benchmark:
 - many parameters to train, large dataset ⇒ complex NLP
 - high sensitivity wrt weights (dynamics gets easily unstable)
 - local minima (solution depends on initial guess)
 - cannot easily use mini-batches: open-loop simulation cost is not separable, long-term memory effects present due to small sample time
- More general residual networks + ℓ_1 /group-Lasso regularization possible



SOLUTION APPROACH

(Bemporad, 2024)

- 1. Standard-scale I/O data for numerical reasons $u_i \leftarrow \frac{u_i \mu_u^i}{\sigma_u^i}$, $y_i \leftarrow \frac{y_i \mu_y^i}{\sigma_y^i}$ $i = 1, \dots, 6$
- 2. Train (A, B, C, x_0) by **jax-sysid** (1000 L-BFGS iters) w/o ℓ_1 -regularization ($x \in \mathbb{R}^{12}$) (CPU time: 9.12 s) [Apple M1 Max]

For comparison: **n4sid** takes 36.21 s and gives lower \mathbb{R}^2 -scores on training & test data in MATLAB sippy fails

3. Fix $({\cal A},{\cal B},{\cal C})$ and train simple RESNET model with shallow NNs:

 $x_{k+1} = Ax_k + Bu_k + f_x(x_k, u_k, \theta_x), \qquad y_k = Cx_k + f_y(x_k, \theta_y)$

• Optimization: to handle $\tau \|\theta\|_1$, use jax-sysid running 2000 Adam iters first (for warm-start) and then 2000 L-BGFS-B iters

INDUSTRIAL ROBOT BENCHMARK: RESULTS

- State $x \in \mathbb{R}^{12}$, f_x , f_y with 36 and 24 neurons, swish activation for $\frac{x}{1+e^{-x}}$
- Total number of training parameters: $\dim(\theta_x) + \dim(\theta_y) = 1590$



• Model quality measured by average R^2 -score on all outputs:

$$R^{2} = \frac{1}{n_{y}} \sum_{i=1}^{n_{y}} 100 \left(1 - \frac{\sum_{k=1}^{N} (y_{k,i} - \hat{y}_{k,i|0})^{2}}{\sum_{k=1}^{N} (y_{k,i} - \frac{1}{N} \sum_{i=1}^{N} y_{k,i})^{2}} \right)$$

 Training time ≈ 12 min on a single core per run [Apple M1 Max] (3192 variables, 2000 Adam iterations + 2000 L-BFGS-B iterations)

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INDUSTRIAL ROBOT BENCHMARK: RESULTS

• **Open-loop simulation** errors ($\rho = 0.01, \tau = 0.008$):

	R^2 (training)	R^2 (test)	R^2 (training)	R^2 (test)	
	RNN model	RNN model	linear model	linear model	
average	77.1493	57.1784	48.2789	43.8573	jax-sysid
			39.2822	32.0410	n4sid

- More parameters/smaller regularization leads to overfitting training data
- Pure Adam vs LBFG-B+Adam vs OWL-QN (Andrew, Gao, 2007): (au=0.008)

	adam	fcn	$\overline{R^2}$	$\overline{R^2}$	# zeros	CPU
solver	iters	evals	training	test	$(heta_x, heta_y)$	time (s)
L-BFGS-B	2000	2000	77.1493	57.1784	556/1590	309.87
OWL-QN	2000	2000	74.7816	54.0531	736/1590	449.17
Adam	6000	0	71.0687	54.3636	1/1590	389.39

• Adam is unable to sparsify the model

INDUSTRIAL ROBOT BENCHMARK: RESULTS

• Compute *p*-step ahead prediction $\hat{y}_{k+p|k}$, with hidden state $x_{k|k}$ estimated by an Extended Kalman Filter based on identified RNN model



- This is a more relevant indicator of model quality for MPC purposes than open-loop simulation error $\hat{y}_{k|0}-y_k$

DEEP NONLINEAR MPC: AN EXAMPLE

DEEP NONLINEAR MPC FOR AUTONOMOUS DRIVING

- Goal: track desired longitudinal speed (v_y), lateral displacement (e_y) and orientation ($\Delta \Psi$)
- Inputs: wheel torque T_w and steering angle δ
- Constraints: on e_y and lateral displacement s (for obstacle avoidance) and manipulated inputs T_w, δ
- Sampling time: 100 ms
- Model: gray-box bicycle model
- kinematics is simple to model (white box)
- tire forces harder to model + stiff wheel slip ratio dynamics $(k_f, k_r) \Rightarrow$ small integration step required
- learn a black-box neural-network model !

(Boni, Capelli, Frascati @ODYS, 2021) "Model Predictive Control" - © 2025 A. Bemporad. All rights reserved.






DEEP NONLINEAR MPC FOR AUTONOMOUS DRIVING

- **ODYS Deep Learning Toolset** used to learn a neural-network with input $(v_x, v_y, \omega, k_f, k_r, T_w, \delta)$ @k and output $(v_x, v_y, \omega, k_f, k_r)$ @k + 1
- Data generated from high-fidelity simulation model with noisy measurements, sampled @10Hz
- Neural network model: 2 hidden layers, 55 neurons each
- Advantages of black-box (neural network) model:
 - No physical model required describing tire-road interaction
 - directly learn the model in discrete-time $(T_s = 100 \text{ ms})$



DEEP NONLINEAR MPC FOR AUTONOMOUS DRIVING

Model validation on test data:



• C-code (network+Jacobians) automatically generated for ODYS MPC



DEEP NONLINEAR MPC FOR AUTONOMOUS DRIVING

• Closed-loop MPC: overtake vehicle #1, keep safety distance from vehicle #2



• Good reference tracking, constraints on e_y, v_x satisfied, smooth command action

DIRECT DATA-DRIVEN MPC

DIRECT DATA-DRIVEN MPC



• Can we design an MPC controller without first identifying a model of the open-loop process ?

DATA-DRIVEN DIRECT CONTROLLER SYNTHESIS

(Campi, Lecchini, Savaresi, 2002) (Formentin et al., 2015)



- Collect a set of data $\{u(t), y(t), p(t)\}, t = 1, \dots, N$
- Specify a desired closed-loop linear model \mathcal{M} from r to y
- Compute $r_v(t) = \mathcal{M}^{\#} y(t)$ from pseudo-inverse model $\mathcal{M}^{\#}$ of \mathcal{M}
- Identify linear (LPV) model K_p from $e_v = r_v y$ (virtual tracking error) to u

DIRECT DATA-DRIVEN MPC

• Design a linear MPC (reference governor) to generate the reference r

(Bemporad, Mosca, 1994) (Gilbert, Kolmanovsky, Tan, 1994)



• MPC designed to handle input/output constraints and improve performance

(Piga, Formentin, Bemporad, 2017)

DIRECT DATA-DRIVEN MPC - AN EXAMPLE

• Experimental results: MPC handles soft constraints on $u,\Delta u$ and y

with MPC

without MPC



15

desired tracking performance achieved

Time [s]

20

4.5

3

2.5

5

10

 θ [rad]

θ



constraints on input increments satisfied

No open-loop process model was identified to design the MPC controller!

30



OPTIMAL DIRECT DATA-DRIVEN MPC

• Question: How to choose the reference model \mathcal{M} ?



• Can we choose \mathcal{M} from data so that K_p is an **optimal controller**?

OPTIMAL DIRECT DATA-DRIVEN MPC

(Selvi, Piga, Bemporad, 2018)

• Idea: parameterize desired closed-loop model $\mathcal{M}(\theta)$ and optimize

$$\min_{\theta} J(\theta) = \frac{1}{N} \sum_{t=0}^{N-1} \underbrace{W_y(r(t) - y_p(\theta, t))^2 + W_{\Delta u} \Delta u_p^2(\theta, t)}_{\text{performance index}} + \underbrace{W_{\text{fit}}(u(t) - u_v(\theta, t))^2}_{\text{identification error}}$$

- Evaluating $J(\theta)$ requires synthesizing $K_p(\theta)$ from data and simulating the nominal model and control law

$$y_p(\theta, t) = \mathcal{M}(\theta)r(t) \qquad u_p(\theta, t) = K_p(\theta)(r(t) - y_p(\theta, t))$$
$$\Delta u_p(\theta, t) = u_p(\theta, t) - u_p(\theta, t - 1)$$

• Optimal θ obtained by solving a (non-convex) nonlinear programming problem

OPTIMAL DIRECT DATA-DRIVEN MPC

• Results: linear process

$$G(z) = \frac{z - 0.4}{z^2 + 0.15z - 0.325}$$

Data-driven controller **only 1.3% worse** than model-based LQR (=SYS-ID on same data + LQR design)

• Results: nonlinear (Wiener) process

 $y_L(t) = G(z)u(t)$ $y(t) = |y_L(t)| \arctan(y_L(t))$

The data-driven controller is **24% better** than LQR based on identified open-loop model !

 $\begin{bmatrix} 0 & -\overline{T(t)} & -\overline{CL}(t) \\ 0 & -\overline{T(t)} & -\overline{T(t)} & -\overline{T(t)} \\ 0 & -\overline{T(t)} & -\overline{T(t)} \\ 0 & -\overline{T(t)} & -\overline{T(t)}$



(Selvi, Piga, Bemporad, 2018)

DATA-DRIVEN OPTIMAL POLICY SEARCH

DATA-DRIVEN OPTIMAL POLICY SEARCH

(Ferrarotti, Bemporad, 2019)

Plant + environment dynamics (unknown):

 $s_{t+1} = h(s_t, p_t, u_t, d_t)$

- s_t states of plant & environment
- p_t exogenous signal (e.g., reference)
- u_t control input
- d_t unmeasured disturbances
- Control policy: $\pi : \mathbb{R}^{n_s + n_p} \longrightarrow \mathbb{R}^{n_u}$ deterministic control policy

$$u_t = \pi(s_t, p_t)$$

Closed-loop performance of an execution is defined as

$$\mathcal{J}_{\infty}(\pi, s_0, \{p_{\ell}, d_{\ell}\}_{\ell=0}^{\infty}) = \sum_{\ell=0}^{\infty} \rho(s_{\ell}, p_{\ell}, \pi(s_{\ell}, p_{\ell}))$$

$$\rho(s_\ell, p_\ell, \pi(s_\ell, p_\ell)) \; = \; {\rm stage} \, {\rm cost}$$

OPTIMAL POLICY SEARCH PROBLEM

• Optimal policy:

$$\begin{aligned} \pi^* &= \arg \min_{\pi} \mathcal{J}(\pi) \\ \mathcal{J}(\pi) &= \mathbb{E}_{s_0, \{p_\ell, d_\ell\}} \left[\mathcal{J}_{\infty}(\pi, s_0, \{p_\ell, d_\ell\}) \right] & \text{expected performance} \end{aligned}$$

- Simplifications:
 - Finite parameterization: $\pi=\pi_K(s_t,p_t)$ with K = parameters to optimize

- Finite horizon:
$$\mathcal{J}_L(\pi, s_0, \{p_\ell, d_\ell\}_{\ell=0}^{L-1}) = \sum_{\ell=0}^{L-1} \rho(s_\ell, p_\ell, \pi(s_\ell, p_\ell))$$

Optimal policy search: use stochastic gradient descent (SGD)

$$K_t \leftarrow K_{t-1} - \alpha_t \mathcal{D}(K_{t-1})$$

with $\mathcal{D}(K_{t-1})$ = descent direction

DESCENT DIRECTION

- The descent direction $\mathcal{D}(K_{t-1})$ is computed by generating:
 - N_s perturbations $s_0^{(i)}$ around the current state s_t
 - N_r random reference signals $r_\ell^{(j)}$ of length L,
 - N_d random disturbance signals $d_\ell^{(h)}$ of length L,

$$\mathcal{D}(K_{t-1}) = \sum_{i=1}^{N_s} \sum_{j=1}^{N_p} \sum_{k=1}^{N_q} \nabla_K \mathcal{J}_L(\pi_{K_{t-1}}, s_0^{(i)}, \{r_\ell^{(j)}, d_\ell^{(k)}\})$$



SGD step = mini-batch of size $M = N_s \cdot N_r \cdot N_d$

- Computing $\nabla_K \mathcal{J}_L$ requires predicting the effect of π over L future steps
- We use a local linear model just for computing $\nabla_K \mathcal{J}_L$, obtained by running recursive linear system identification

OPTIMAL POLICY SEARCH ALGORITHM

- At each step *t*:
 - 1. Acquire current s_t
 - 2. Recursively update the local linear model
 - 3. Estimate the direction of descent $\mathcal{D}(K_{t-1})$
 - 4. Update policy: $K_t \leftarrow K_{t-1} \alpha_t \mathcal{D}(K_{t-1})$
- If policy is learned online and needs to be applied to the process:
 - Compute the nearest policy K_t^{\star} to K_t that stabilizes the local model

$$\begin{split} K_t^\star = & \arg\!\min_K & \|K - K_t^s\|_2^2 \\ & \text{s.t. } K \text{ stabilizes local linear model} \quad \textit{ linear matrix inequality} \end{split}$$

• When policy is learned online, exploration is guaranteed by the reference r_t

SPECIAL CASE: OUTPUT TRACKING

•
$$x_t = [y_t, y_{t-1}, \dots, y_{t-n_o}, u_{t-1}, u_{t-2}, \dots, u_{t-n_i}]$$

 $\Delta u_t = u_t - u_{t-1}$ control input increment

- Stage cost: $\| y_{t+1} r_t \|_{Qy}^2 + \| \Delta u_t \|_R^2 + \| q_{t+1} \|_{Q_q}^2$
- Integral action dynamics $q_{t+1} = q_t + (y_{t+1} r_t)$

$$s_t = \begin{bmatrix} x_t \\ q_t \end{bmatrix}, \quad p_t = r_t.$$

• Linear policy parametrization:

$$\pi_K(s_t, r_t) = -K^s \cdot s_t - K^r \cdot r_t, \qquad K = \begin{bmatrix} K^s \\ K^r \end{bmatrix}$$

EXAMPLE: RETRIEVE LQR FROM DATA

Online tracking performance (no disturbance, $d_t = 0$):



EXAMPLE: RETRIEVE LQR FROM DATA

Evolution of the error $||K_t - K_{opt}||_2$:



 $K_{\text{SGD}} = [-1.255, 0.218, 0.652, 0.895, 0.050, 1.115, -2.186]$

 $K_{\text{opt}} = [-1.257, 0.219, 0.653, 0.898, 0.050, 1.141, -2.196]$

NONLINEAR EXAMPLE



Continuously Stirred Tank Reactor (CSTR)

apmonitor.com

model is unknown

Feed:

- concentration: 10kg mol/m³
- temperature: 298.15K

$$T = \hat{T} + \eta_T, \ C_A = \hat{C}_A + \eta_C, \quad \eta_T, \ \eta_C \sim \mathcal{N}(0, \sigma^2), \quad \sigma = 0.01$$

$$Q_y = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad R = 0.1 \qquad Q_q = \begin{bmatrix} 0.01 & 0 \\ 0 & 0 \end{bmatrix}$$

NONLINEAR EXAMPLE





n_i	n_o	L
2	3	10
N ₀	N_r	Nq
50	20	20





Continuously Stirred Tank Reactor (CSTR) (courtesy: apmonitor.com)

SGD beats SYS-ID + LQR

• Extended to switching-linear and nonlinear policy, and to collaborative learning

(Ferrarotti, Bemporad, 2020a) (Ferrarotti, Bemporad, 2020b) (Ferrarotti, Breschi, Bemporad, 2021)

LEARNING OPTIMAL MPC CALIBRATION

MPC CALIBRATION PROBLEM

- The design depends on a vector x of MPC parameters
- Parameters can be many things:
 - MPC weights, prediction model coefficients, horizons
 - Covariance matrices used in Kalman filters
 - Tolerances used in numerical solvers



• Define a **performance index** *f* over a closed-loop simulation or real experiment. For example:



• Automatic calibration = find the best combination of parameters by solving the global optimization problem

 $\min_{x} f(x)$

GLOBAL OPTIMIZATION ALGORITHMS FOR AUTO-TUNING

What is a good optimization algorithm to solve $\min f(x)$?

• The algorithm should not require the gradient $\nabla f(x)$ of f(x), in particular if experiments are involved (derivative-free or black-box optimization)

• The algorithm should not get stuck on local minima (global optimization)

• The algorithm should make the **fewest evaluations** of the cost function *f* (which is expensive to evaluate)

AUTO-TUNING - GLOBAL OPTIMIZATION ALGORITHMS

- Several derivative-free global optimization algorithms exist: (Rios, Sahidinis, 2013)
 - Lipschitzian-based partitioning techniques:
 - DIRECT (DIvide in RECTangles) (Jones, 2001)
 - SHGO (Simplicial Homology Global Optimisation) (Endres, Sandrock, Focke, 2018)
 - Multilevel Coordinate Search (MCS) (Huyer, Neumaier, 1999)
 - Response surface methods
 - Kriging (Matheron, 1967), DACE (Sacks et al., 1989)
 - Efficient Global Optimization (EGO) (Jones, Schonlau, Welch, 1998)
 - Bayesian Optimization (BO) (Brochu, Cora, De Freitas, 2010)
 - Genetic Algorithms (GA) (Holland, 1975)
 - Particle Swarm Optimization (PSO) (Kennedy, 2010)
 - ...

GLIS method - radial basis function surrogates + inverse distance weighting

(Bemporad, 2020)

cse.lab.imtlucca.it/~bemporad/glis



AUTO-TUNING - GLIS

• Goal: solve the global optimization problem

$$\begin{aligned} \min_x & f(x) \\ \text{s.t.} & \ell \leq x \leq u \\ & g(x) \leq 0 \end{aligned}$$



- Step #0: Get random initial samples $x_1, \ldots, x_{N_{\text{init}}}$ (Latin Hypercube Sampling)
- Step #1: given N samples of f at x_1, \ldots, x_N , build the surrogate function

$$\hat{f}(x) = \sum_{i=1}^{N} \beta_i \phi(\epsilon ||x - x_i||_2)$$

 $\phi = radial \ basis \ function$

Example: $\phi(\epsilon d) = \frac{1}{1 + (\epsilon d)^2}$ (inverse quadratic)

Vector β solves $\hat{f}(x_i) = f(x_i)$ for all $i = 1, \dots, N$ (=linear system)

• Note: build and minimize $\hat{f}(x_i)$ iteratively may easily miss global optimum!

AUTO-TUNING - GLIS

• Step #2: construct the IDW exploration function

$$z(x) = \frac{2}{\pi} \Delta F \tan^{-1} \left(\frac{1}{\sum_{i=1}^{N} w_i(x)} \right)$$

or 0 if $x \in \{x_1, \dots, x_N\}$

where
$$w_i(x) = rac{e^{-\|x-x_i\|^2}}{\|x-x_i\|^2}$$

 ΔF = observed range of $f(x_i)$

• Step #3: optimize the acquisition function

$$\begin{aligned} x_{N+1} &= & \arg \min \quad \hat{f}(x) - \delta z(x) \\ &\text{s.t.} \quad \ell \leq x \leq u, \ g(x) \leq 0 \end{aligned}$$

 δ = exploitation vs exploration tradeoff

to get new sample x_{N+1}

• Iterate the procedure to get new samples $x_{N+2}, \ldots, x_{N_{\max}}$



GLIS VS BAYESIAN OPTIMIZATION



BO					
O GLIS					
-1					
5 10 15					
camelsixhumps					
БООО					
4000 GLIS					
2000					
2000					
5 10 15					
howtman6					
BO GLIS					
-2					
-4					
-4 20 40 60 80					
-4 20 40 60 80 3 ×10 ⁸ rosenbrock8					
4 20 40 60 $803 \times 10^8 rosenbrock8$					
-4 -20 40 60 80 3 ×10 ⁸ rosenbrock8					
-4 20 40 60 80 3 ×10 ⁸ rosenbrock8 2 GLIS					
3×10^9 rosenbrock8 20×10^9 rosenbrock8					
$\begin{array}{c} 4 \\ \hline 20 \\ \hline 40 \\ \hline 60 $					
4 20 40 60 $803 \times 10^8 rosenbrock82 0 6 10^6 10$					
$\begin{array}{c} 4 \\ \hline 20 \\ \hline 20 \\ \hline 40 \\ \hline 60 \\ \hline 80 \\ \hline 3 \\ 2 \\ \hline 0 \\ \hline 20 \\ \hline 0 \\ \hline 20 \\ \hline 0 \\ \hline $					
$\begin{array}{c} 4 \\ - \\ 20 \\ -$					
4 20 40 60 80 3 × 10 ⁸ rosenbrock8 1 0 20 40 60 80 styblinski-tang5 20 0 0 0 0 0 0 0					
$\begin{array}{c} 4 \\ \hline 20 \\ \hline 20 \\ \hline 40 \\ \hline 60 \\ \hline 80 \\ \hline \\ 3 \\ 2 \\ \hline 0 \\ \hline 20 \\ \hline 0 \\ \hline$					
$\begin{array}{c} 4 \\ \hline \\ 20 \\ 20$					

problem	n	BO [s]	GLIS [s]
ackley	2	29.39	3.13
adjiman	2	3.29	0.68
branin	2	9.66	1.17
camelsixhumps	2	4.82	0.62
hartman3	3	26.27	3.35
hartman6	6	54.37	8.80
himmelblau	2	7.40	0.90
rosenbrock8	8	63.09	13.73
stepfunction2	4	11.72	1.81
styblinski-tang5	5	37.02	6.10

Results computed on 20 runs per test BO = MATLAB's bayesopt fcn

- Comparable performance
- GLIS is computationally lighter
- GLIS is more flexible

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AUTO-TUNING: MPC EXAMPLE

• We want to auto-tune the linear MPC controller

$$\min \sum_{k=0}^{50-1} (y_{k+1} - r(t))^2 + (W^{\Delta u}(u_k - u_{k-1}))^2$$

s.t. $x_{k+1} = Ax_k + Bu_k$
 $y_c = Cx_k$
 $-1.5 \le u_k \le 1.5$
 $u_k \equiv u_{N_u}, \forall k = N_u, \dots, N-1$



- Calibration parameters: $x = [\log_{10} W^{\Delta u}, N_u]$
- Range: $-5 \le x_1 \le 3$ and $1 \le x_2 \le 50$
- Closed-loop performance objective:

$$f(x) = \sum_{t=0}^{T} \underbrace{(y(t) - r(t))^2}_{\text{track well}} + \underbrace{\frac{1}{2}(u(t) - u(t-1))^2}_{\text{smooth control action}} + \underbrace{2N_u}_{\text{small QR}}$$

AUTO-TUNING: EXAMPLE



• Result: $x^{\star} = [-0.2341, 2.3007]$

 $W^{\Delta u} = 0.5833, N_u = 2$

MPC AUTOTUNING EXAMPLE

• Linear MPC applied to cart-pole system: 14 parameters to tune



- sample time
- weights on outputs and input increments
- prediction and control horizons
- covariance matrices of Kalman filter
- absolute and relative tolerances of QP solver

• Closed-loop performance score:
$$J = \int_0^T |p(t) - p_{ref}(t)| + 30|\phi(t)|dt$$

- MPC parameters tuned using 500 iterations of GLIS
- Performance tested with simulated cart on two hardware platforms (PC, Raspberry PI)

MPC AUTOTUNING EXAMPLE



- MPC parameters tuned by GLIS global optimizer (500 fcn evals)
- Auto-calibration can squeeze max performance out of the available hardware
- Bayesian optimization gives similar results, but with larger computation effort

AUTO-TUNING: PROS AND CONS

- Pros:
 - $\mathbf{s} = \mathbf{s} = \mathbf{s} + \mathbf{s} +$
 - 🖕 Applicable to any calibration parameter (weights, horizons, solver tolerances, ...)
 - **d** Rather arbitrary performance index f(x) (tracking performance, response time, worst-case number of flops, ...)
- Cons:
 - **I** Need to **quantify** an objective function f(x)
 - No room for qualitative assessments of closed-loop performance
 - Often have multiple objectives, not clear how to blend them in a single one

ACTIVE PREFERENCE LEARNING

- Objective function f(x) is not available (latent function)
- We can only express a preference between two choices:

$$\pi(x_1, x_2) = \begin{cases} -1 & \text{if } x_1 \text{ "better" than } x_2 & [f(x_1) < f(x_2)] \\ 0 & \text{if } x_1 \text{ "as good as" } x_2 & [f(x_1) = f(x_2)] \\ 1 & \text{if } x_2 \text{ "better" than } x_1 & [f(x_1) > f(x_2)] \end{cases}$$

• We want to find a global optimum x^* (="better" than any other x)

find x^* such that $\pi(x^*, x) \leq 0, \ \forall x \in \mathcal{X}, \ \ell \leq x \leq u$

- Active preference learning: iteratively propose a new sample to compare
- Key idea: learn a surrogate of the (latent) objective function from preferences

PREFERENCE-LEARNING EXAMPLE

(Brochu, de Freitas, Ghosh, 2007)



- Realistic image synthesis of material appearance are based on models with many parameters x_1, \ldots, x_n
- Defining an objective function f(x) is hard, while a human can easily assess whether an image resembles the target one or not
- **Preference gallery** tool: at each iteration, the user compares two images generated with two different parameter instances

ACTIVE PREFERENCE LEARNING ALGORITHM



- Fit a surrogate $\hat{f}(x)$ that respects the preferences expressed by the decision maker at sampled points (by solving a QP)
- Minimize an acquisition function $\hat{f}(x) \delta z(x)$ to get a new sample x_{N+1}
- Compare x_{N+1} to the current "best" point ($\mathbf{A}, \mathbf{P}, \approx$) and iterate
SEMI-AUTOMATIC CALIBRATION BY PREF.-BASED LEARNING

- Use preference-based optimization (GLISp) algorithm for semi-automatic tuning of MPC (Zhu, Bemporad, Piga, 2021)
- Latent function = calibrator's (unconscious) score of closed-loop MPC performance
- GLISp proposes a new combination x_{N+1} of MPC parameters to test
- By observing test results, the calibrator expresses a **preference**, telling if x_{N+1} is "**better**", "**similar**", or "**worse**" than current best combination
- Preference learning algorithm: update the surrogate $\hat{f}(x)$ of the latent function, optimize the acquisition function, ask preference, and iterate





 Same performance index to assess closed-loop quality, but unknown: only preferences are available

• Result:
$$W^{\Delta u} = 0.6888$$
, $N_u = 2$



tested combinations of MPC params



Best function value

(latent) performance index

• Example: calibration of a simple MPC for lane-keeping (2 inputs, 3 outputs)

$$\begin{cases} \dot{x} = v \cos(\theta + \delta) \\ \dot{y} = v \sin(\theta + \delta) \\ \dot{\theta} = \frac{1}{L} v \sin(\delta) \end{cases}$$



• Multiple control objectives:

"optimal obstacle avoidance", "pleasant drive", "CPU time small enough", ... **not easy to quantify in a single function**

- 5 MPC parameters to tune:
 - sampling time
 - prediction and control horizons
 - weights on input increments $\Delta v, \Delta \delta$

• Preference query window:



• Convergence after 50 GLISp iterations (=49 queries):



Optimal MPC parameters:

- sample time = 85 ms (CPU time = 80.8 ms)
- prediction horizon = 16
- control horizon = 5
- weight on Δv = 1.82
- weight on $\Delta\delta$ = 8.28



- Note: no need to define a closed-loop performance index explicitly!
- Extended to handle also unknown constraints (Zhu, Piga, Bemporad, 2021)

WORST-CASE SCENARIO DETECTION

CORNER-CASE SCENARIO DETECTION PROBLEM

(Zhu, Bemporad, Kneissl, Esen, 2022)

- Goal: detect undesired simulation scenarios (=corner-cases)
- Let x = parameters defining the scenario, \mathcal{X}_{ODD} = operational design domain $x \in \mathcal{X}_{ODD} \subseteq \mathbb{R}^n$
- critical scenario = vector x^* for which the closed-loop behavior is critical
- Example:
 - x = (initial distance between ego car and obstacle, obstacle acceleration, ...)
 - Critical scenario: time-to-collision is too short, excessive jerk of ego car, ...
- Key idea: use global optimizer GLIS to generate critical corner-cases

 $x^* \in \operatorname*{arg\,min}_{x \in \mathcal{X}_{\mathrm{ODD}}} \quad f(x)$ s.t. $\ell \le x \le u$ f(x) = criticality of closed-loop simulation (or experiment) determined by scenario x(the smaller f(x), the more critical x is)

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CORNER-CASE DETECTION: CASE STUDY

- Problem: find critical scenarios in automated driving w/ obstacles
- MPC controller for lane-keeping and obstacle-avoidance based on simple kinematic bicycle model (Zhu, Piga, Bemporad, 2021)

$$\begin{aligned} \dot{x}_f = v \cos(\theta + \delta) \\ \dot{w}_f = v \sin(\theta + \delta) \\ \dot{\theta} = \frac{v \sin(\delta)}{L} \\ (x_f, w_f) \neq \text{front-wheel position} \end{aligned}$$



• Black-box optimization problem: given k obstacles, solve

$$\begin{split} \min_{\ell \leq x \leq u} \quad & \sum_{i=1}^k d_{x_f, \mathsf{critical}}^{\mathsf{SV}, i}(x) + d_{w_f, \mathsf{critical}}^{\mathsf{SV}, i}(x) \\ \text{s.t.} \quad & \mathsf{other constraints} \end{split}$$



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CORNER-CASE DETECTION: CASE STUDY

• Cost function terms to minimize: for each obstacle #i define

$$d_{x_{f},\text{critical}}^{\text{SV},i}(x) = \begin{cases} \min_{t \in T_{\text{collision}}} d_{x_{f}}^{\text{SV},i}(x,t) & \mathcal{I}_{\text{collision}}^{i} & \min \text{ dist. @collision with } \# \\ L & \sim \mathcal{I}_{\text{collision}}^{i} \& \mathcal{I}_{\text{collision}} & \text{collision with other } \#_{j} \neq \# \\ \sum_{t \in T_{\text{sim}}} d_{x_{f}}^{\text{SV},i}(x,t) & \sim \mathcal{I}_{\text{collision}} & \max \text{ dist. @collision with other } \#_{j} \neq \# \\ \end{cases}$$

$$d_{w_{f},\text{critical}}^{\text{SV},i}(x) = \begin{cases} \min_{t \in T_{\text{collision}}} d_{w_{f}}^{\text{SV},i}(x,t) & \mathcal{I}_{\text{collision}}^{i} \\ w_{f,\text{safe}} & \sim \mathcal{I}_{\text{collision}}^{i} \& \mathcal{I}_{\text{collision}} \\ \sum_{t \in T_{\text{sim}}} d_{w_{f}}^{\text{SV},i}(x,t) & \sim \mathcal{I}_{\text{collision}} \end{cases}$$

$$\begin{split} \mathcal{I}^{i}_{\text{collision}} &= \texttt{true} \quad \text{if} \quad \exists t \in T_{\text{sim}} \, \texttt{s.t.} \\ (d^{\text{SV},i}_{x_f}(x,t) \leq L) \, \& \, (d^{\text{SV},i}_{w_f}(x,t) \leq W) \\ \mathcal{I}_{\text{collision}} &= \texttt{true} \quad \text{if} \quad \exists h \quad \texttt{s.t.} \quad \mathcal{I}^{h}_{\text{collision}} = \texttt{true} \end{split}$$



CORNER-CASE DETECTION: CASE STUDY

Logical scenario 1: GLIS identifies 64 collision cases within 100 simulations

itor	<i>x</i>						
itei	x_{f1}^{0}	v_{1}^{0}	x_{f2}^{0}	v_2^0	x_{f3}^{0}	v_3^0	
51	15.00	30.00	44.14	10.00	49.10	47.39	
79	28.09	30.00	70.29	10.00	74.79	31.74	
40	34.30	30.00	60.59	10.00	77.80	35.97	



red = optimal solution found by GLIS solver

Ego car changes lane to avoid #1, but cannot brake fast enough to avoid #2

• Logical scenario 2: GLIS identifies 9 collision cases within 100 simulations

itor	x					
itei	x_{f1}^{0}	v_{1}^{0}	t_c			
28	12.57	46.94	16.75			
16	17.53	47.48	23.65			
88	44.54	41.26	16.02			

red = optimal solution found by GLIS solver



Ego car changes lane to avoid #1, but cannot decelerate in time for the sudden lane-change of #1

LEARNING-BASED MPC: FINAL REMARKS

LEARNING-BASED MPC: FINAL REMARKS

- ML very useful to get control-oriented models (and control laws) from data
- ML cannot replace control engineering:
 - Blindly applying deep NNs can lead to useless models for embedded control
 - Approximating MPC laws by NN's can fail, often still need online optimization
 - Model-free reinforcement learning can fail wrt model-based control design, which is more sample-efficient and better performs tasks it wasn't trained for



(Yann LeCun, Twitter/X, August 25, 2024)