Tangent-Space Regularization for Neural-Network Models of Dynamical Systems

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Abstract—This work introduces the concept of tangent space regularization for neural-network models of dynamical systems. The tangent space to the dynamics function of many physical systems of interest in control applications exhibits useful properties, e.g., smoothness, motivating regularization of the model Jacobian along system trajectories using assumptions on the tangent space of the dynamics. Without assumptions, large amounts of training data are required for a neural network to learn the full non-linear dynamics without overfitting. We compare different network architectures on one-step prediction and simulation performance and investigate the propensity of different architectures to learn models with correct input-output Jacobian. Furthermore, the influence of $L_2$ weight regularization on the learned Jacobian eigenvalue spectrum, and hence system stability, is investigated.

I. INTRODUCTION

Dynamical control systems are often described in continuous time by differential state equations on the form

$$\dot{x}(t) = f_c(x(t), u(t))$$

where $x$ is a Markovian state-vector, $u$ is the input and $f_c$ is a function that maps the current state and input to the state time-derivative. An example of such a model is a rigid-body dynamical model of a robot

$$\dot{x} = -M^{-1}(x)(C(x, \dot{x})\dot{x} + G(x) + F(\dot{x}) - u)$$  \hspace{1cm} (1)

where $M, C, G$ and $F$ model phenomena such as inertia, Coriolis, gravity and friction.

In the discrete time domain, we may consider models on the form

$$x_{t+1} = f(x_t, u_t)$$  \hspace{1cm} (2)

where $f$ is a function that maps the current state and input to the state at the next time-instance. Learning a globally valid dynamics model $\hat{f}$ of an arbitrary non-linear system $f$ with little or no prior information is a challenging problem. Although in principle, any sufficiently complex function approximator, such as a deep neural network (DNN), could be employed, high demands are put on the amount of data required to prevent overfitting and obtain a faithful representation of the dynamics over the entire state space.

In many applications, the linearization of $f$ is important, a typical example being linear control design.

Identification of $f$ must thus not only yield a good model for prediction/simulation, but also the Jacobian $J_f$ of $f$ must be close to the true system Jacobian $J$. In applications such as iterative learning control (ILC) and trajectory centric, episode-based reinforcement learning (TCRL), the linearization of the nonlinear dynamics along a trajectory is often all that is needed for optimization. Linear time-varying (LTV) models on the form

$$x_{t+1} = A_t x_t + B_t u_t$$  \hspace{1cm} (3)

where the matrices $A$ and $B$ constitute the output Jacobian, can be learned (data-)efficiently, in special cases extremely (time-)efficiently using dynamic programming [2]. A problem with learning an LTV model around a finite length trajectory is insufficient excitation provided by the control input. Prior knowledge regarding the evolution of the dynamics, encoded in form of carefully designed regularization, is required in order to obtain a well-posed optimization problem and a meaningful result. When model identification is a sub-task in an outer algorithm that optimizes a control-signal trajectory or a feedback policy, excessive noise added for identification purposes may be undesirable, making regularization solely over time as in [2] insufficient.

The discussion so far indicates two issues open for future work. 1) Complex non-linear models have the potential to be valid globally, but may suffer from overfitting and thus not learn a function with the correct linearization. 2) LTV models can be learned efficiently and can represent the linearized dynamics well, but are time-based and valid only locally.

In this work, we make use of the regularization methods detailed in [2] for incremental learning of a general, non-linear black-box model, $\hat{f}$. We further develop a method to perform sampled tangent-space regularization for use with deep-learning frameworks without support for higher-order derivatives. To this end, we consider an episode-based setting where the dynamical model is updated after each episode. Each episode, a new trajectory $\tau_i = \{x_t, u_t\}_{t=1}^T$ is obtained, to which we fit an LTV model, $l_i$, on the form (3) using the methods presented in [2]—this model will provide the regularization for the non-linear model. We then update the non-linear state-space model $\hat{f}$ by adding $\tau_i$ to the set of training data for $\hat{f}$, while using $l_i$, which we assume have learned a good approximation of $J_f$ along $\tau_i$, for tangent-space regularization of $J_f$.

We proceed to introduce the problem of learning a dynamics model $\hat{f}$ in Section II. We then introduce tan-

[github.com/baggepinnen/LTVModels.jl]
gent space regularization in Section~\[\text{III}\] and finally discuss the influence of weight decay on different formulations of the learning problem before conducting numerical evaluations.

II. Estimating the global model

To frame the learning problem we let the dynamics of a system be described by a neural-network $\hat{f}$ to be fitted to input-output data $\tau$ according to

Learning Objective 1:

$$x_{t+1} = \hat{f}(x_t, u_t) \in \mathbb{R}^n$$

which we will frequently write on the form $x^+ = \hat{f}(x, u)$ by omitting the time index $t$ and letting $\cdot^+$ indicate $\cdot_{t+1}$. We further consider the linearization of $\hat{f}$ around a trajectory

$$x_{t+1} = Ax_t + B_t u_t$$

where the matrices $A$ and $B$ constitute the input-output Jacobian $J_f$ of $f$

$$J_f = \begin{bmatrix}
    \nabla_x f_1^T & \nabla_u f_1^T \\
    \vdots & \vdots \\
    \nabla_x f_n^T & \nabla_u f_n^T
\end{bmatrix} \in \mathbb{R}^{n \times (n+m)} = [A \ B] \quad (5)$$

Our estimate $\hat{f}(x, u, w)$ of $f(x, u)$ will be parameterized by a vector $w$. The distinction between $f$ and $\hat{f}$ will, however, be omitted unless required for clarity.

We frame the learning problem as an optimization problem with the goal of adjusting the parameters $w$ of $\hat{f}$ to minimize a cost function $V(w)$ by means of gradient descent. The cost function $V(w)$ can take many forms, but we will limit the scope of this article to quadratic loss functions of the one-step prediction error, i.e.,

$$V(w) = \frac{1}{2} \sum_i \|x^+ - \hat{f}(x, u, w)\|^2 (x^+ - \hat{f}(x, u, w)) \quad (6)$$

It is well known that the Jacobian of the discrete-time model $f$ has eigenvalues different from that of the continuous-time counterpart $f_c$. In particular, if the sample rate is high, most eigenvalues of $f_c$ are close to 0. The eigenvalues for the discrete-time model $f$ however tend to cluster around 1 when sample rate is high. Another formulation of the discrete-time model, which we introduce as a new learning objective, is

Learning Objective 2:

$$x^+ - x = \Delta x = g(x, u)$$

$$f(x, u) = g(x, u) + x$$

with the second form being equivalent to the first, but highlighting a convenient implementation form that does not require transformation of the data. Classical theory for sampling of linear systems indicates that the eigenvalues of $g$ tend to those of $f_c$ as sample rate increases [3].

To gain insight into how this seemingly trivial change in representation may affect performance, we note that this transformation will alter the Jacobian according to

$$J_g = [A - I_n \ B] \quad (7)$$

with a corresponding unit reduction of the eigenvalues of $A$. For systems with integrators, or slow dynamics in general, this transformation leads to a better conditioned estimation problem [4]. In Section~\[\text{V}\] we investigate whether or not this transformation leads to a better prediction/simulation result and whether modern neural network training techniques such as the ADAM optimizer [5] and batch normalization [6] render this transformation superfluous. We further investigate how weight decay affects the eigenvalue spectrum of the Jacobian of $f$ and $g$ and hence, system stability.

A. Optimization landscape

To gain insight into the training of $f$ and $g$, we analyse the expressions for the gradients and Hessians of the cost functions. For a linear model $x^+ = Ax + Bu$ and a least-squares cost-function $V(\theta) = \frac{1}{2}(y - \Phi \theta)^T(y - \Phi \theta)$, where the linear model is written on regressor form $y = \Phi \theta$ with all parameters of $A$ and $B$ concatenated into the vector $\theta$, the gradient and the Hessian are given by

$$\nabla_\theta V = -\Phi^T(y - \Phi \theta) \quad (8)$$

$$\nabla^2_\theta V = \Phi \Phi^T \quad (9)$$

The Hessian is clearly independent of both the output $y$ and the parameters $\theta$ and differentiating the output does not have any major impact on gradient-based learning. For a nonlinear model, this is not necessarily the case:

$$V(w) = \frac{1}{2} \sum_i (x^+ - f(x, u, w))^T(x^+ - f(x, u, w)) \quad (10)$$

$$\nabla_w V = \sum_{i=1}^n \sum_{i=1}^n - (x^+ - f_i(x, u, w)) \nabla_w f_i \quad (11)$$

$$\nabla^2_w V = \sum_{i=1}^n \sum_{i=1}^n \nabla_w f_i \nabla_w f_i^T - (x^+ - f_i(x, u, w)) \nabla^2_w f_i \quad (12)$$

In this case, the Hessian depends on both the parameters and the target $x^+$. The transformation from $f$ to $g$ changes the gradients and Hessians according to

$$\nabla_w V = \sum_{i=1}^n \sum_{i=1}^n - (\Delta x_i - g_i(x, u, w)) \nabla_w (g_i) \quad (13)$$

$$\nabla^2_w V = \sum_{i=1}^n \sum_{i=1}^n \nabla_w g_i \nabla_w g_i^T - (\Delta x_i - g_i(x, u, w)) \nabla^2_w g_i \quad (14)$$

Since the output of $g$ is closer to zero compared to $f$ for systems of lowpass character, i.e., where $\|\Delta x\|$ is small, the transformation can be seen as preconditioning the problem by decreasing the influence of the term.
\[ \nabla^2_w g = \nabla^2_w f \] in the Hessian. With only the positive semi-
definite term \( \nabla_w(g) \nabla_w(f) = \nabla_w(f) \nabla_w(f)^T \) corresponding
to \( \Phi^T \Phi \) in the linear case remaining, the optimization
problem becomes easier. Similarly, \( g \) starts out closer to a
critical point \( \nabla_w V = 0 \), making convergence rapid.

III. TANGENT-SPACE REGULARIZATION

For systems where the function \( f \) is known to be
smooth, the Jacobian \( J_f(t) \) will vary slowly. In the rigid-
body dynamical model (1), for instance, the intertial and
gravitational forces are changing smoothly with the joint
configuration. A natural addition to the cost function of
the optimization problem would thus be a tangent-space
regularization term on the form
\[
\sum_i \| \hat{J}_{t+1} - \hat{J}_t \| \tag{15}
\]
which penalizes change in the input-output Jacobian of
the model over time, a strategy we refer to as Jacobian
propagation. A somewhat related strategy was proposed
in [7], where a tangent-dependent term in the cost
function was successfully used to enforce invariance of an
image classifier to rotations and translations of the input
image.

Taking the gradient of terms depending on the model
Jacobian requires calculation of higher order derivatives.
Depending on the framework used for optimization, this
can limit the applicability of the method. We thus
proceed to describe a sampled version of tangent space
regularization requiring only first order gradients.

Estimation of an LTV model with the regularization
term \([15]\) is straightforward and is the subject of [2].
Given a good estimate \( \hat{J}_f(t) \) provided by an LTV model,
one may regularize the learning of \( f \) by penalizing
\[ \sum_i \| J_f(t) - \hat{J}_f(t) \| . \]
An approximation to Jacobian propagation is obtained by augmenting the dataset with input
data perturbed in the direction of the Jacobian. For the
regression task at hand, we can implement such a strategy
by perturbing the input data \( \{ \hat{x}, \tilde{u} \} = \{ x + \epsilon_x, u + \epsilon_u \} \) by
some small noise terms \( \epsilon \), and generating a new target
\( x^+ \) using the LTV model \( \tilde{x}^+ = A\tilde{x} + B\tilde{u} \). If this was
done for each component of \( x \) and \( u \) separately, this
would correspond exactly to finite-difference Jacobian
propagation. However, due to the smoothness assumption
of \( f \) together with the smooth inductive bias of neural
networks, we get reasonable results by only perturbing
each input instance by a small Gaussian random vector.
We refer to this strategy as sampled Jacobian propagation.
Section [14] demonstrates how this approach enables learn-
ing of neural-network models with high-fidelity Jacobians.
The procedure is summarized in Algorithm 1.

Algorithm 1 An algorithm for efficient learning of a
nonlinear neural-network dynamics model. The sampling
of a rollout may entail using the estimated models for,
e.g., iterative learning control, trajectory optimization or
reinforcement learning.

1. Initialize a model \( f \).
2. \textbf{loop}
   1. Sample rollout trajectory \( \tau_i = \{ x_t, u_t \}_{t=1}^T \)
   2. Fit LTV model \( l_i \) using method in [2]
   3. Generate perturbed trajectories \( \hat{\tau}_i = \{ \hat{x}_t, \tilde{u}_t \} \) using \( l_i \).
   4. Fit \( f \) to \( \tau_i \) and \( \hat{\tau}_i \)
   5. (Optimize controller or control signal trajectory)
3. \textbf{end loop}

IV. WEIGHT DECAY

Weight decay is commonly an integral part of model
fitting used to combat overfitting, and can be thought of as
either penalizing complexity of the model or as encoding
prior knowledge about the size of the model coefficients.
\( L_2 \) weight decay is, however, a blunt weapon. While often
effective at mitigating overfitting, the procedure might
introduce a bias in the estimate. Since the bias always
is directed towards smaller weights, it can have different
consequences depending on what small weights imply
for a particular model architecture. For a discrete-time
model \( f \), small weights imply small eigenvalues and a
small output. For \( x^+ = g(x, u) + x \), on the other hand,
small weights imply eigenvalues closer to 1. Weight decay
thus has a vastly different effect on learning \( f \) and \( g \), and
since a high sample rate implies eigenvalues closer to 1,
weight decay is likely to bias the result of learning \( g \) in a
milder way as compared to when learning \( f \). We explore
the effect of weight decay in the next section by fitting
models to data generated by linear systems.

A natural question to ask is if weight decay can bias the
eigenvalues of the learned function to arbitrary chosen
locations. A generalized form of model formulation is
\( x^+ - Ax - Bu = h(x, u) \) where \( A \) and \( B \) can be seen
as a nominal linear model around which we learn the
nonlinear behavior. Weight decay will for this formulation
bias the Jacobian towards \( A \) and \( B \) which can be chosen
arbitrarily. Obviously, choosing a nominal linear model
is not always easy, and may in some cases not make
sense. One can however limit the scope to formulations
like \( x^+ - \tau x = h(x, u) \), where \( \tau \) is a scalar or a diagonal
matrix that shifts the nominal eigenvalues along the real
axis to, e.g., encourage stability.

V. EVALUATION

The previously described methods were evaluated on
two benchmarks problems. We compared performance on
one-step prediction as well as simulation from a known
initial condition. We further compared the fidelity of the
Jacobian of the estimated models, an important
property for optimization algorithms making use of the
models. The benchmarks consist of a simulated robot
arm with two revolute joints, friction and gravity and

3In the beginning of learning, the output of \( \hat{g} \) is small due to the
initialization of \( w \).
4New targets can be sampled each epoch.
Algorithm 2 Generation of random, stable linear systems.

\[ A_0 = 10 \times 10 \text{ matrix of random coefficients} \]
\[ A = A_0 - A_0^T \text{ skew-symmetric } \Rightarrow \text{pure imaginary eigenvalues} \]
\[ A = A - \Delta t I \text{ make 'slightly' stable} \]
\[ A = \exp(\Delta A) \text{ discrete time, sample time } \Delta t \]
\[ B = \text{random coefficients} \]

randomized, stable linear systems. Code to reproduce results are presented in the online repository.

We initially describe a baseline neural network approximator used in the experimental evaluation which we use to draw conclusions regarding the different learning objectives. We describe how deviations from this baseline model alter the conclusions drawn in Appendix II. The first examples demonstrate the effectiveness of tangent-space regularization, whereas later examples demonstrate the influence of weight decay.

A. Nominal model

Both functions \( f \) and \( g \) are modeled as ensembles, \( \mathcal{E} \), of 4 distinct single-layer neural networks with 20 neurons each. The 4 networks in the ensemble are trained on the same data with the same objective function, but with different random initializations of the weights and different non-linear activation functions.\(^5\) After a comparative study of 6 different activation functions, presented in Appendix II we selected networks with the activation functions elu, sigmoid, tanh and swish to form the components of the ensemble \( \mathcal{E} \). We train the models using the ADAM optimizer with a fixed step-size and fixed number of epochs, 2000 for \( f \) and 1000 for \( g \). The entire framework including all simulation experiments reported in this article is published at \(^6\) and is implemented in the Julia programming language \(^8\) and the Flux machine learning library.

When training with tangent-space regularization, a single perturbed trajectory was added with

\[ \{\epsilon_x, \epsilon_u\} \sim \mathcal{N}(0, \{0.1^2 \text{ diag } \Sigma_x, 0.1^2 \text{ diag } \Sigma_u\}) \]

and the network was trained for half the number of epochs compared to the nominal baseline model.

B. Randomized linear system

To assess the effectiveness of sampled Jacobian propagation we create random, stable linear systems according to Algorithm II and evaluate the Jacobian of the learned model for points sampled randomly in the state space. The results are illustrated in Fig. 1. During training, the model trained without tangent-space regularization reaches far lower training error, but validation data indicate that overfitting has occurred. The model trained with tangent-space regularization learns better Jacobians and produces smaller prediction- and simulation errors.

\(^5\)The variation in the ensemble predictions may serve as a bootstrap estimate of the variance of the estimator.

\(^6\)github.com/FluxML/Flux.jl

Fig. 1. Learned Jacobian eigenvalues of \( g \) for randomly sampled points in the state-space (blue) together with the eigenvalues of the true model (red). Tangent-space regularization (right) leads to better estimation of the Jacobian with eigenvalues in a tighter cluster around the true eigenvalues close to the unit circle.

The effect of weight decay on the learned Jacobian is illustrated in Fig. 2. Due to overparamterization, heavy overfitting is expected without adequate regularization. Not only is it clear that learning of \( g \) has been more successful than learning of \( f \) in the absence of weight decay, but we also see that weight decay has had a deteriorating effect on learning \( f \), whereas it has been beneficial in learning \( g \). This indicates that the choice of architecture interacts with the use of standard regularization techniques and must be considered while modeling.

C. Robot task

The robot has non-linear dynamics and thus a changing Jacobian along a trajectory. This task demonstrates the utility of tangent-space regularization for systems where the regularization term is not the theoretically perfect choice, as was the case with the linear system. We simulate

\(^7\)We are referring to the Jacobian of the dynamics, as opposed to the Jacobian of the forward kinematic encountered in robotics.
the system with a low-pass filtered random input and compare prediction and simulation error as well as the error in the estimated Jacobian.

The prediction and simulation errors for validation data, i.e., trajectories not seen during training, are shown in Fig. 3. The results indicate that tangent-space regularization leads to reduced prediction and simulation errors compared to baseline, with lower mean error and smaller spread, indicating more robust learning. In particular, divergence of the state was encountered during some simulations of the baseline model, a behavior which was not encountered for models trained with tangent-space regularization.

To assess the fidelity of the learned Jacobian, we average the input-output Jacobian over the ensemble $\mathcal{E}$ and compare it to the ground-truth Jacobian of the simulator. We display the distribution of errors in the estimated Jacobians over 35 Monte-Carlo runs in Fig. 4. The error was calculated as the mean over time steps of the Frobenius norm of the difference in coefficients between the true Jacobian and the ensemble average Jacobian:

$$\sqrt{\frac{1}{T} \sum_t \left\| J_t - \frac{1}{|E|} \sum_{\mathcal{E}} J_t^\mathcal{E} \right\|^2_F}$$

The results show a significant benefit of tangent-space regularization over baseline, with a reduction of the mean error as well as a smaller spread of errors, indicating a more stable and reliable training.

VI. DISCUSSION

We note that $g$ generally trains faster and reaches a lower value of the objective function compared to $f$. The structure of $g$ resembles that of a residual network [9], where a skip connection is added between the input and a layer beyond the first adjacent layer, in our case, directly to the output. While skip connections have helped to enable successful training of very deep architectures for tasks such as image recognition, we motivated the benefit of the skip connection with classical theory for sampling of continuous-time systems [3] and an analysis of the model Hessian. Exploring the similarities with residual networks remains an interesting avenue for future work.

The scope of this article was limited to settings where a state-sequence is known. In a more general setting, learning the transformation of past measurements and inputs to a state-representation is required and networks with recurrence (RNNs) are required. Initial results indicate that the conclusions drawn regarding the formulation ($f$ vs. $g$) of the model and the effect of weight decay remains valid in the RNN setting, but a more detailed analysis is the target of future work.

VII. CONCLUSIONS

We have demonstrated how tangent-space regularization by means of sampled Jacobian propagation can be used to regularize the learning of a neural network model of a dynamical system with an increase in prediction and simulation performance as well as increasing the fidelity of the learned Jacobians as result.

We investigated different architectures of the NN model and found that the relationship between sample time and system bandwidth affects the preferred choice of architecture, where one approximator architecture ($g$) train faster and generally generalize better in terms of all metrics if the sample rate is high. An analysis of gradient and Hessian expressions motivated the difference and conclusions were reinforced by experiment with different sample rates.

The effect of including $L_2$ weight decay was investigated and shown to vary greatly with the model architecture. Implications on the stability and eigenvalues of the learned model highlights the need to consider the architecture choice carefully.

APPENDIX I

COMPARISON OF ACTIVATION FUNCTIONS

Figure 5 displays the distribution of prediction errors over 200 Monte-Carlo runs with different random seeds.
and different activation functions. The results indicate that the relu and leaky relu functions are worse suited for the considered task and are thus left out from the set of selected bootstrap ensemble activation functions.

**Appendix II**

**Deviations from the nominal model**

*Sample rate:* The sample rate determines the location of the eigenvalues of the Jacobian for a discrete-time dynamical system. Faster sampling moves the eigenvalues closer to 1, with implications for numerical accuracy for very small sampling times [4]. Faster sampling also leads to a function $g$ closer to zero and $f$ closer to 1. With 5 times slower sampling, the difference between $f$ and $g$ in prediction performance was less pronounced for the validation data and both methods performed comparably with respect to the estimated Jacobians. With 5 times faster sampling, method $g$ performs much better on prediction and Jacobian estimation but much worse on simulation.

*Number of neurons:* Doubling or halving the number of neurons generally led to worse performance.

*Number of layers:* Adding a fully connected layer with the same number of neurons did not change any conclusions.

*Dropout:* Inclusion of dropout (20%) increases prediction and simulation performance for $g$ while performance is decreased for $f$. Performance on Jacobian estimation was in general worse.

*Layer normalization:* Prediction and simulation performance remained similar or slightly worse, whereas Jacobian estimation broke down completely.

*Measurement noise:* Although not a hyper parameter, we investigate the influence of measurement noise on the identification results. Increasing degree of measurement noise degrades all performance metrics in predictable ways and does not change any qualitative conclusions.

*Ensemble size:* A three times larger ensemble of network yields marginally better performance on all metrics, with a three times longer training time.

*Number of perturbed trajectories for sampled Jacobian propagation:* We found that sampling a single trajectory was sufficient and adding additional samples did not alter the performance significantly. A larger state dimension might require more samples, although we have not quantified this.

*Optimizer, Batch normalization, Batch size:* Neither of these modifications altered the performance significantly.

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