Differentiable Convex Modeling in Robotic Planning and Control

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To all of the people that light up my life. ♡

Abstract

Domain-specific modeling priors and specialized components are becoming increasingly important to the machine learning field. These components integrate specialized knowledge that we have as humans into model. We argue in this thesis that optimization methods provide an expressive set of operations that should be part of the machine learning practitioner's modeling toolbox.

We present two foundational approaches for optimization-based modeling: 1) the *OptNet* architecture that integrates optimization problems as individual layers in larger end-to-end trainable deep networks, and 2) the *input-convex neural network (ICNN)* architecture that helps make inference and learning in deep energy-based models and structured prediction more tractable.

We then show how to use the OptNet approach 1) as a way of combining model-free and model-based reinforcement learning and 2) for top-k learning problems. We conclude by showing how to differentiate cone programs and turn the `cvxpy` domain specific language into a differentiable optimization layer that enables rapid prototyping of the approaches in this thesis.

The source code for this thesis document is available in open source form at:
https://github.com/bamos/thesis

Acknowledgments

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Chapter 1

Introduction

Algorithm 1 CPEG Algorithm

input x_0, U ▷ nominal control plan
while $\|\delta U\| >$ tolerance **do**
    $\bar{X}, \bar{U} = \text{simulate}(x_0, U)$ ▷ predict trajectory
    $A, B = \text{linearize}(\bar{X}, \bar{U})$ ▷ linearize about prediction
    $\delta X, \delta U = \text{cvx}(\bar{X}, \bar{U}, A, B)$ ▷ solve for correction
    $U \mathrel{+}= \delta U$ ▷ correct control plan
end while
return U ▷ return updated control plan

The field of machine learning has grown rapidly over the past few years and has a growing set of well-defined and well-understood operations and paradigms that allow a practitioner to inject domain knowledge into the modeling procedure. These operations include linear maps, convolutions, activation functions, random sampling, and simple projections (e.g. onto the simplex or Birkhoff polytope). In addition to these layers, the practitioner can also inject domain knowledge at a higher-level of how modeling components interact. Paradigms are becoming well-established for modeling images, videos, audio, sequences, permutations, and graphs, among others. This thesis proposes a new set of primitive operations and paradigms based on optimization that allow the practitioner to inject specialized domain knowledge into the modeling procedure.

Optimization plays a large role in machine learning for parameter optimization or architecture search. In this thesis, we argue that optimization should have a third role in machine learning separate from these two, that it can be used as a modeling tool inside of the inference procedure. Optimization is a powerful modeling tool and as we show in Section 2.4.4, many of the standard operations such as the ReLU, sigmoid, and softmax can all be interpreted as explicit closed-form solutions to constrained convex optimization problems. We also highlight in Section 2.2.1 that the standard feedforward supervised learning setup can be captured by an energy-based optimization problem. Thus these techniques are captured as special cases of the general optimization-based modeling methods we study

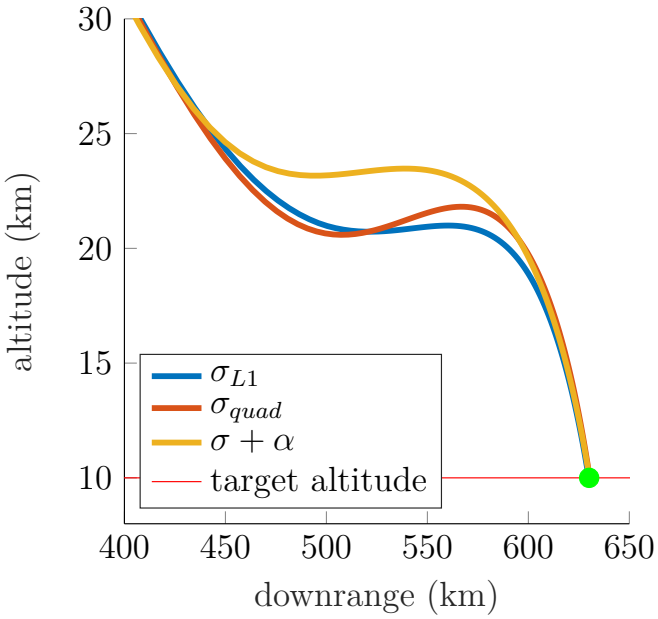

Figure 1.1: Caption my bruddah

in this thesis that don't necessarily have explicit closed-form solutions. This generalization adds new modeling capabilities that were not possible before and enables new ways that practitioners can inject domain knowledge into the models.

From an optimization viewpoint, the techniques we propose in this thesis can be used for partial modeling of optimization problems. Traditionally a modeler needs to have a complete analytic view of their system if they want to use optimization to solve their problem, such as in many control, planning, and scheduling tasks. The techniques in this thesis lets the practitioner leave latent parts in their optimization-based modeling procedure that can then be learned from data.

1.1 Summary of research contributions

The first portion of this thesis presents foundational modeling techniques that use optimization-based modeling:

- **??** presents the *OptNet* architecture that shows how to use constrained convex optimization as a layer in an end-to-end architecture.
  - **??** presents the formulation of these architectures and shows how backpropagation can be done in them by implicitly differentiating the KKT conditions.
  - **??** studies the representational power of these architectures and proves how they can represent any piecewise linear function including the ReLU.
  - **??** presents our efficient QP solver for these layers and **??** shows how we can compute the backwards pass with almost no computational overhead.

    - **??** shows empirical results that uses OptNet for a synthetic denoising task and to learn the rules of the Sudoku game.
- **??** presents the *input-convex neural network* architecture.
    - **??** discusses efficient inference techniques for these architectures. We propose a new inference technique called the Bundle-Entropy method in **??**.
    - **??** discusses efficient learning techniques for these architecture.
    - **??** shows empirical results applying ICNNs to structured prediction, data imputation, and continuous-action Q learning.

The remaining portions discuss applications and extensions of OptNet.

- **??** presents our *differentiable model predictive control* (MPC) work as a step towards leveraging MPC as a differentiable policy class for reinforcement learning in continuous state-action spaces.
    - **??** shows how to efficiently differentiate through the Linear Quadratic Regulator (LQR) by solving another LQR problem. This result comes from implicitly differentiating the KKT conditions of LQR and interpreting the resulting system as solving another LQR problem.
    - **??** shows how to differentiate through non-convex MPC problems by differentiating through the fixed point obtained when solving the MPC problem with sequential quadratic programming (SQP).
    - **??** shows our empirical results using imitation learning in the pendulum and cartpole environments. Notably, we show why doing end-to-end learning with a controller is important in tasks when the expert is non-realizable.

- ?? presents the Limited Multi-Layer Projection (LML) layer for top-k learning problems.
  - ?? introduces the LML projection problem that we study.
  - ?? shows how to efficiently solve the LML projection problem by solving the dual with a parallel bracketed root-finding method.
  - ?? presents how to maximize the top-k recall with the LML layer.
  - ?? shows our empirical results on top-k image classification and scene graph generation.
- ?? shows how to make differentiable `cvxpy` optimization layers by differentiating through the internal transformations and internal cone program solver. This enables rapid prototyping of all of the convex optimization-based modeling methods we consider in this thesis.
  - ?? shows how to differentiate cone programs (including non-polyhedral cone programs) by implicitly differentiating the residual map of Minty's parameterization of the homogeneous self-dual embedding.
  - ?? shows examples of using our package to implement optimization layers for the ReLU, sigmoid, softmax; projections onto polyhedral and ellipsoidal sets; and the OptNet QP.

1.2 Summary of open source contributions

The code and experiments developed for this thesis are free and open-source:

- https://github.com/locuslab/icnn: TensorFlow experiments for the input-convex neural networks work presented in **??**.
- https://locuslab.github.io/qpth/ and https://github.com/locuslab/qpth: A stand-alone PyTorch library for the OptNet QP layers presented in **??**.
- https://github.com/locuslab/optnet: PyTorch experiments for the OptNet work presented in **??**.
- https://locuslab.github.io/mpc.pytorch and https://github.com/locuslab/mpc.pytorch: A stand-alone PyTorch library for the differentiable model predictive control approach presented in **??**.
- https://github.com/locuslab/differentiable-mpc: PyTorch experiments for the differentiable MPC work presented in **??**.

I have also created the following open source projects during my Ph.D.:

- https://github.com/bamos/block: An intelligent block matrix library for numpy, PyTorch, and beyond.
- https://github.com/bamos/dcgan-completion.tensorflow: Image Completion with Deep Learning in TensorFlow.
- https://github.com/cmusatyalab/openface: Face recognition with deep neural networks.
- https://github.com/bamos/densenet.pytorch: A PyTorch implementation of DenseNet.

1.3 Summary of publications

The content of **??** appears in:

> [5] Brandon Amos and J. Zico Kolter. "OptNet: Differentiable Optimization as a Layer in Neural Networks". In: *Proceedings of the International Conference on Machine Learning*. 2017

The content of **??** appears in:

> [7] Brandon Amos, Lei Xu, and J. Zico Kolter. "Input Convex Neural Networks". In: *Proceedings of the International Conference on Machine Learning*. 2017

The content of **??** appears in:

> [4] Brandon Amos, Ivan Jimenez, Jacob Sacks, Byron Boots, and J. Zico Kolter. "Differentiable MPC for End-to-end Planning and Control". In: *Advances in Neural Information Processing Systems*. 2018, pp. 8299–8310

Non-thesis research: I have also pursued the following research directions during my Ph.D. studies. These are excluded from the remainder of this thesis.

> [3] Brandon Amos, Laurent Dinh, Serkan Cabi, Thomas Rothörl, Sergio Gómez Colmenarejo, Alistair Muldal, Tom Erez, Yuval Tassa, Nando de Freitas, and Misha Denil. "Learning Awareness Models". In: *International Conference on Learning Representations*. 2018
>
> [6] Brandon Amos, Bartosz Ludwiczuk, and Mahadev Satyanarayanan. *OpenFace: A general-purpose face recognition library with mobile applications*. Tech. rep. Technical Report CMU-CS-16-118, CMU School of Computer Science, 2016
> **Available online at:** https://cmusatyalab.github.io/openface

I have also contributed to the following publications as a non-primary author.

> Priya L Donti, Brandon Amos, and J. Zico Kolter. "Task-based End-to-end Model Learning". In: *NIPS*. 2017
>
> Han Zhao, Tameem Adel, Geoff Gordon, and Brandon Amos. "Collapsed Variational Inference for Sum-Product Networks". In: *ICML*. 2016
>
> Zhuo Chen et al. "An Empirical Study of Latency in an Emerging Class of

Edge Computing Applications for Wearable Cognitive Assistance". In: *Proceedings of the Second ACM/IEEE Symposium on Edge Computing*. ACM. 2017, p. 12

Zhuo Chen, Lu Jiang, Wenlu Hu, Kiryong Ha, Brandon Amos, Padmanabhan Pillai, Alex Hauptmann, and Mahadev Satyanarayanan. "Early Implementation Experience with Wearable Cognitive Assistance Applications". In: *WearSys*. 2015

Nigel Andrew Justin Davies, Nina Taft, Mahadev Satyanarayanan, Sarah Clinch, and Brandon Amos. "Privacy mediators: helping IoT cross the chasm". In: *HotMobile*. 2016

Junjue Wang, Brandon Amos, Anupam Das, Padmanabhan Pillai, Norman Sadeh, and Mahadev Satyanarayanan. "A Scalable and Privacy-Aware IoT Service for Live Video Analytics". In: *Proceedings of the 8th ACM on Multimedia Systems Conference*. ACM. 2017, pp. 38–49

Wenlu Hu, Brandon Amos, Zhuo Chen, Kiryong Ha, Wolfgang Richter, Padmanabhan Pillai, Benjamin Gilbert, Jan Harkes, and Mahadev Satyanarayanan. "The Case for Offload Shaping". In: *HotMobile*. 2015

Mahadev Satyanarayanan, Pieter Simoens, Yu Xiao, Padmanabhan Pillai, Zhuo Chen, Kiryong Ha, Wenlu Hu, and Brandon Amos. "Edge Analytics in the Internet of Things". In: *IEEE Pervasive Computing* 2 (2015), pp. 24–31

Ying Gao, Wenlu Hu, Kiryong Ha, Brandon Amos, Padmanabhan Pillai, and Mahadev Satyanarayanan. *Are Cloudlets Necessary?* Tech. rep. Technical Report CMU-CS-15-139, CMU School of Computer Science, 2015

Kiryong Ha, Yoshihisa Abe, Thomas Eiszler, Zhuo Chen, Wenlu Hu, Brandon Amos, Rohit Upadhyaya, Padmanabhan Pillai, and Mahadev Satyanarayanan. "You can teach elephants to dance: agile VM handoff for edge computing". In: *Proceedings of the Second ACM/IEEE Symposium on Edge Computing*. ACM. 2017, p. 12

Wenlu Hu, Ying Gao, Kiryong Ha, Junjue Wang, Brandon Amos, Zhuo Chen, Padmanabhan Pillai, and Mahadev Satyanarayanan. "Quantifying the impact of edge computing on mobile applications". In: *Proceedings of the 7th ACM SIGOPS Asia-Pacific Workshop on Systems*. ACM. 2016, p. 5

Chapter 2

Preliminaries and Background

This section provides a broad overview of foundational ideas and background material relevant to this thesis. In most chapters of this thesis, we include a deeper discussion of the related literature relevant to that material.

2.1 Preliminaries

The content in this thesis builds on the following topics. We assume preliminary knowledge of these topics and give a limited set of key references here. The reader should have an understanding of statistical and machine learning modeling paradigms as described in Wasserman [147], Bishop [22], and Friedman, Hastie, and Tibshirani [45]. Our contributions mostly focus on end-to-end modeling with deep architectures as described in Schmidhuber [117] and Goodfellow, Bengio, Courville, and Bengio [49] with applications in computer vision as described in Forsyth and Ponce [44], Bishop [22], and Szeliski [132]. Our contributions also involve optimization theory and applications as described in Bertsekas [19], Boyd and Vandenberghe [25], Bonnans and Shapiro [24], Griewank and Walther [57], Nocedal and Wright [100], Sra, Nowozin, and Wright [124], and Wright [152]. One application area of this thesis work focuses on control and reinforcement learning. Control is one kind of optimization-based modeling and is further described in Bertsekas, Bertsekas, Bertsekas, and Bertsekas [20], Sastry and Bodson [115], and Levine [82]. Reinforcement learning methods are summarized in Sutton, Barto, et al. [131] and Levine [81].

2.2 Energy-based Learning

Energy-based learning is a machine learning method typically used in supervised settings that explicitly adds relationships and dependencies to the model's output space. This is in contrast to purely feed-forward models that typically cannot explicitly capture dependencies in the output space. At the core of energy-based learning methods is a scalar-valued *energy* function $E_\theta(x, y) : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ parameterized by θ that measures the fit between some input x and output y. Inference in energy-based models is done by solving the

optimization problem

$$\hat{y} = \underset{y}{\operatorname{argmin}}\, E_\theta(x, y). \tag{2.1}$$

We note that this is a powerful formulation for modeling and learning and subsumes the representational capacity of standard deep feedforward models, which we show how to do in Section 2.2.1. The energy function can also be interpreted from a probabilistic lens as the negated unnormalized joint distribution over the input and output spaces.

Energy-based methods have been in use for over a decade and the tutorial LeCun, Chopra, Hadsell, Ranzato, and Huang [78] overviews many of the foundational methods and challenges in energy-based learning. The two main challenges for energy-based learning are 1) learning the parameters θ of the energy function E_θ and 2) efficiently solving the inference procedure in Equation (2.1). These challenges have historically been tamed by using simpler energy functions consisting of hand-engineered feature extractors for the inputs x and linear functions of y. This captures models such as Markov random fields [85] and conditional random fields [77, 129]. Standard gradient-based methods are difficult to use for parameter learning because $\hat{y}$ depends on θ through the argmin operator, which is not always differentiable. Historically, a common approach to doing parameter learning in energy-based models has been to directly shape the energy function with a max-margin approach Taskar, Guestrin, and Koller [138] and Taskar, Chatalbashev, Koller, and Guestrin [137].

More recently, there has been a strong push to further incorporate structured prediction methods like conditional random fields as the "last layer" of a deep network architecture [109, 159, 29] as well as in deeper energy-based architectures [16, 17, 15, 145]. We further discuss Structured Prediction Energy Networks (SPENs) in Section 2.2.2.

An ongoing discussion in the community argues whether adding the dependencies explicitly in an energy-based is useful or not. Feedforward models have a remarkable representational capacity that can implicitly learn the dependencies and relationships from data without needing to impose additional structure or modeling assumptions and without making the model more computationally expensive with an optimization-based inference procedure. One argument against this viewpoint that supports energy-based modeling is that explicitly including modeling information improves the data efficiency and requires less samples to learn because some structure and knowledge is already present in the model and does not have to be learned from scratch.

2.2.1 Energy-based Models Subsume Feedforward Models

We highlight the power of energy-based modeling for supervised learning by noting how they subsume deep feedforward models. Let $\hat{y} = f_\theta(x)$ be a deep feedforward model. The energy-based representation of this model is $E(x, y) = ||y - f_\theta(x)||_2^2$ and inference becomes the convex optimization problem $\hat{y} = \operatorname{argmin}_y E(x, y)$, which has the exact solution $\hat{y} = f_\theta(x)$. An energy function that has more structure over the output space adds representational capacity that a feedforward model wouldn't be able to capture explicitly.

2.2.2 Structured Prediction Energy Networks

Structured Prediction Energy Networks (SPENs) [16, 17, 15] are a way of bridging the gap between modern deep learning methods and classical energy-based learning methods. SPENs provide a deep structure over input and output spaces by representing the energy function $E_\theta(x, y)$ with a standard feed-forward neural network. This expressive formulation comes at the cost of making the inference procedure in Equation (2.1) difficult and non-convex. SPENs typically use an approximate inference procedure by taking a fixed-number of gradient descent steps for inference. For learning, SPENs typically replace the inference with an *unrolled gradient-based optimizer* that starts with some prediction y_0 and takes a fixed number of gradient steps to minimize the energy function

$$y_{i+1} = y_i - \alpha \nabla_y E_\theta(x, y_i).$$

The final iterate as then taken as the prediction $\hat{y} \triangleq y_N$. Gradient-based parameter learning can be done by differentiating the prediction $\hat{y}$ with respect to θ by unrolling the inference procedure. Unrolling the inference procedure can be done in most autodiff frameworks such as PyTorch [107] or TensorFlow [1]. activation functions with smooth first derivatives such as the sigmoid or softplus [48] should be used to avoid discontinuities because unrolling the inference procedure involves computing $\nabla_\theta \nabla_y E_\theta(x, y)$.

2.3 Modeling with Domain-Specific Knowledge

The role of domain-specific knowledge in the machine learning and computer vision fields has been an active discussion topic over the past decade and beyond. Historically, domain knowledge such as fixed hand-crafted feature and edge detectors were rigidly part of the computer vision pipeline and have been overtaken by learnable convolutional models LeCun, Cortes, and Burges [79] and Krizhevsky, Sutskever, and Hinton [75]. To highlight the power of convolutional architectures, they provide a reasonable prior for vision tasks even without learning [141]. Machine learning models extend far beyond the reach of vision tasks and the community has a growing interest on domain-specific priors rather than just using fully-connected architectures. These priors ideally can be integrated as end-to-end learnable modules into a larger system that are learned as a whole with gradient-based information. In contrast to pure fully-connected architectures, specialized submodules ideally improve the data efficiency of the model, add interpretability, and enable grey-box verification.

Recent work has gone far beyond the classic examples of adding modeling priors by using convolutional or sequential models. A full discussion of all of the recent improvements is beyond the scope of this thesis, and here we highlight a few key recent developments.

- Differentiable beam search [53] and differentiable dynamic programming [92]
- Differentiable protein simulator [68]
- Differentiable particle filters [70]
- Neural ordinary differential equations [30] and applications to reversible generative models [54]

- Relational reasoning on sets, graphs, and trees [14, 157, 74, 47, 114, 62, 13, 156, 41, 122]
- Geometry-based priors [27, 60, 97, 135, 87]
- Memory [127, 55, 56, 155, 64, 105]
- Attention [8, 142, 146]
- Capsule networks [113, 65, 154]
- Program synthesis [112, 99, 9, 35, 104]

2.4 Optimization-based Modeling

Optimization can be used for modeling in machine learning. Among many other applications, these architectures are well-studied for generic classification and structured prediction tasks [50, 126, 26, 78, 16, 17]; in vision for tasks such as denoising [136, 118] or edge-aware smoothing [12]. Diamond, Sitzmann, Heide, and Wetzstein [36] presents unrolled optimization with deep priors. Metz, Poole, Pfau, and Sohl-Dickstein [93] uses unrolled optimization within a network to stabilize the convergence of generative adversarial networks [51]. Indeed, the general idea of solving restricted classes of optimization problem using neural networks goes back many decades [73, 89], but has seen a number of advances in recent years. These models are often trained by one of the following four methods.

2.4.1 Explicit Differentiation

If an analytic solution to the argmin can be found, such as in an unconstrained quadratic minimization, the gradients can often also be computed analytically. This is done in Tappen, Liu, Adelson, and Freeman [136] and Schmidt and Roth [118]. We cannot use these methods for the constrained optimization problems we consider in this thesis because there are no known analytic solutions.

2.4.2 Unrolled Differentiation

The argmin operation over an unconstrained objective can be approximated by a first-order gradient-based method and unrolled. These architectures typically introduce an optimization procedure such as gradient descent into the inference procedure. This is done in Domke [38], Belanger, Yang, and McCallum [17], Metz, Poole, Pfau, and Sohl-Dickstein [93], Goodfellow, Mirza, Courville, and Bengio [50], Stoyanov, Ropson, and Eisner [126], Brakel, Stroobandt, and Schrauwen [26], and Finn, Abbeel, and Levine [43]. The optimization procedure is unrolled automatically or manually [38] to obtain derivatives during training that incorporate the effects of these in-the-loop optimization procedures.

Given an unconstrained optimization problem with a parameterized objective

$$\operatorname*{argmin}_x f_\theta(x),$$

gradient descent starts at an initial value x_0 and takes steps

$$x_{i+1} = x_i - \alpha \nabla_x f_\theta(x).$$

For learning, the final iterate of this procedure x_N can be taken as the output and $\partial x_N / \partial \theta$ can be computed with automatic differentiation.

In all of these cases, the optimization problem is unconstrained and unrolling gradient descent is often easy to do. When constraints are added to the optimization problem, iterative algorithms often use a projection operator that may be difficult to unroll through and storing all of the intermediate iterates may become infeasible.

2.4.3 Implicit argmin differentiation

Most closely related to this thesis work, there have been several applications of the implicit function theorem to differentiating through constrained convex argmin operations. These methods typically parameterize an optimization problem's objective or constraints and then applies the *implicit function theorem* (Theorem 1) to optimality conditions of the optimization problem that implicitly define the solution, such as the *KKT conditions* [25, Section 5.5.3]. We will first review the implicit function theorem and KKT conditions and then discuss related work in this space.

Implicit function analysis [39] typically focuses on solving an equation $f(p, x) = 0$ for x as a function s of p, *i.e.* $x = s(p)$. *Implicit differentiation* considers how to differentiate the solution mapping with respect to the parameters, *i.e.* $\nabla_p s(p)$. The *implicit function theorem* used in standard calculus textbooks can be traced back to the lecture notes from 1877-1878 of Dini [37] and is presented in Dontchev and Rockafellar [39, Theorem 1.B.1] as follows.

Theorem 1 (Implicit function theorem)**.** *Let $f : \mathbb{R}^d \times \mathbb{R}^n \to \mathbb{R}^n$ be continuously differentiable in a neighborhood of $(\bar{p}, \bar{x})$ and such that $f(\bar{p}, \bar{x}) = 0$, and let the partial Jacobian of f with respect to x at $(\bar{p}, \bar{x})$, namely $\nabla_x f(\bar{p}, \bar{x})$, be nonsingular. Then the solution mapping $S(p) = \{x \in \mathbb{R}^n \mid f(p, x) = 0\}$ has a single-valued localization s around $\bar{p}$ for $\bar{x}$ which is continuously differentiable in a neighborhood Q of $\bar{p}$ with Jacobian satisfying $\nabla s(p) = -\nabla_x f(p, s(p))^{-1} \nabla_p f(p, s(p))$ for every $p \in Q$.*

In addition to the content in this thesis, several other papers apply the implicit function theorem to differentiate through the argmin operators. This approach frequently comes up in bilevel optimization [52, 76] and sensitivity analysis [19, 42, 18, 24]. [11] is a note on applying the implicit function theorem to the KKT conditions of convex optimization problems and highlights assumptions behind the derivative being well-defined. Gould, Fernando, Cherian, Anderson, Santa Cruz, and Guo [52] describes general techniques for differentiation through optimization problems, but only describe the case of exact equality constraints rather than both equality and inequality constraints (they add inequality constraints via a barrier function). Johnson, Duvenaud, Wiltschko, Adams, and Datta [69] performs implicit differentiation on (multi-)convex objectives with coordinate subspace constraints. The older work of Mairal, Bach, and Ponce [90] considers argmin differentiation for a LASSO problem, derives specific rules for this case, and presents an efficient

algorithm based upon our ability to solve the LASSO problem efficiently. Jordan-Squire [71] studies convex optimization over probability measures and implicit differentiation in this context. Bell and Burke [18] adapts automatic differentiation to obtain derivatives of implicitly defined functions.

2.4.4 An optimization view of the ReLU, sigmoid, and softmax

In this section we note how the commonly used ReLU, sigmoid, and softmax functions can be interpreted as explicit closed-form solutions to constrained convex optimization (argmin) problems. Bibi, Ghanem, Koltun, and Ranftl [21] presents another view that interprets other layers as proximal operators and stochastic solvers. We use these as examples to further highlight the power of optimization-based inference, not to provide a new analysis of these layers. The main focus of this thesis is *not* on learning and re-discovering existing activation functions. In this thesis, we rather propose new optimization-based inference layers that do *not* have explicit closed-form solutions like these examples and show that they can still be efficiently turned into differentiable building blocks for end-to-end architectures.

Theorem 2. *The ReLU, defined by* $f(x) = \max\{0, x\}$*, can be interpreted as projecting a point* $x \in \mathbb{R}^n$ *onto the non-negative orthant as*

$$f(x) = \underset{y}{\operatorname{argmin}} \quad \frac{1}{2}||x - y||_2^2 \quad \text{s.t.} \quad y \geq 0. \tag{2.2}$$

Proof. The usual solution can be obtained by looking at the KKT conditions of Equation (2.2). Introducing a dual variable $\lambda \geq 0$ for the inequality constraint, the Lagrangian of Equation (2.2) is

$$L(y, \lambda) = \frac{1}{2}||x - y||_2^2 - \lambda^\top y. \tag{2.3}$$

The stationarity condition $\nabla_y L(y^\star, \lambda^\star) = 0$ gives a way of expressing the primal optimal variable $y^\star$ in terms of the dual optimal variable $\lambda^\star$ as $y^\star = x + \lambda^\star$. Complementary slackness $\lambda_i^\star(x_i + \lambda_i^\star) = 0$ shows that $\lambda_i^\star \in \{0, -x_i\}$. Consider two cases:

- **Case 1:** $x_i \geq 0$. Then $\lambda_i^\star$ must be 0 since we require $\lambda^\star \geq 0$. Thus $y_i^\star = x_i + \lambda_i^\star = x_i$.
- **Case 2:** $x_i < 0$. Then $\lambda_i^\star$ must be $-x_i$ since we require $y \geq 0$. Thus $y_i^\star = x_i + \lambda_i^\star = 0$.

Combining these cases gives the usual solution of $y^\star = \max\{0, x\}$. □

Theorem 3. *The sigmoid or logistic function, defined by* $f(x) = (1 + e^{-x})^{-1}$*, can be interpreted as projecting a point* $x \in \mathbb{R}^n$ *onto the interior of the unit hypercube as*

$$f(x) = \underset{0<y<1}{\operatorname{argmin}} \quad -x^\top y - H_b(y), \tag{2.4}$$

where $H_b(y) = -\left(\sum_i y_i \log y_i + (1 - y_i) \log(1 - y_i)\right)$ *is the binary entropy function.*

Proof. The usual solution can be obtained by looking at the first-order optimality condition of Equation (2.4). The domain of the binary entropy function H_b restricts us to $0 < y < 1$ without needing to explicitly represent this as a constraint in the optimization problem. Let $g(y; x) = -x^\top y - H_b(y)$ be the objective. The first-order optimality condition $\nabla_y g(y^\star; x) = 0$ gives us $-x_i + \log y_i^\star - \log(1 - y_i^\star) = 0$ and thus $y^\star = (1 + e^{-x})^{-1}$. □

Theorem 4. *The softmax, defined by* $f(x)_j = e^{x_j} / \sum_i e^{x_i}$*, can be interpreted as projecting a point* $x \in \mathbb{R}^n$ *onto the interior of the* $(n-1)$*-simplex*

$$\Delta_{n-1} = \{p \in \mathbb{R}^n \mid 1^\top p = 1 \;\text{ and }\; p \geq 0\}$$

as

$$f(x) = \underset{0<y<1}{\operatorname{argmin}} \quad -x^\top y - H(y) \quad \text{s.t.} \quad 1^\top y = 1 \tag{2.5}$$

where $H(y) = -\sum_i y_i \log y_i$ *is the entropy function.*

Proof. The usual solution can be obtained by looking at the KKT conditions of Equation (2.5). Introducing a scalar-valued dual variable ν for the equality constraint, the Lagrangian is

$$L(y, \nu) = -x^\top y - H(y) + \nu(1^\top y - 1) \tag{2.6}$$

The stationarity condition $\nabla_y L(y^\star, \nu^\star) = 0$ gives a way of expressing the primal optimal variable $y^\star$ in terms of the dual optimal variable $\nu^\star$ as

$$y_j^\star = \exp\{x_j - 1 - \nu^\star\}. \tag{2.7}$$

Putting this back into the equality constraint $1^\top y^\star = 1$ gives us $\sum_i \exp\{x_i - 1 - \nu^\star\} = 1$ and thus $\nu^\star = \log \sum_i \exp\{x_i - 1\}$. Substituting this back into Equation (2.7) gives us the usual definition of $y_j = e^{x_j} / \sum_i e^{x_i}$. □

Corollary 1. *A temperature-scaled softmax scales the entropy term in the objective and the sparsemax [91] replaces the objective's entropy penalty with a ridge section.*

2.5 Reinforcement Learning and Control

The fields of reinforcement learning (RL) and optimal control typically involve creating agents that act optimally in an environment. These environments can typically be represented as a Markov decision process (MDP) with a continuous or discrete state space and a continuous or discrete action space. The environment often has some oracle-given reward associated with each state and the goal of RL and control is to find a policy that maximizes the cumulative reward achieved.

Using the notation from [81], *policy search* methods learn a policy $\pi_\theta(u_t|x_t)$ parameterized by θ that predicts a distribution over next action to take given the current state x_t. The goal of policy search is to find a policy that maximizes the expected return

$$\underset{\theta}{\operatorname{argmax}} \ \mathbb{E}_{\tau\sim p_\theta(\tau)}\left[\sum_t \gamma^t r(x_t, u_t)\right], \tag{2.8}$$

where $p_\theta(\tau) = p(x_1)\prod \pi_\theta(u_t|x_t)p(x_{t+1}|x_t, u_t)$ is the distribution over trajectories, $\gamma \in (0, 1]$ is a discount factor, $r(x_t, u_t)$ is the state-action reward at time t, and $p(x_{t+1}|x_t, u_t)$ is the state-transition probability. In many scenarios, the reward r is assumed to be a black-box function that derivative information cannot be obtained from. *Model-free* techniques for policy search typically do not attempt to model the state-transition probability while *model-based* and *control* approaches do.

Control approaches typically provide a policy by planning based on known state transitions. For example, in continuous state-action spaces with deterministic state transitions, the finite-horizon model predictive control problem is

$$\underset{x_{1:T}\in\mathcal{X}, u_{1:T}\in\mathcal{U}}{\operatorname{argmin}} \ \sum_{t=1}^{T} C_t(x_t, u_t) \ \text{ subject to } \ x_{t+1} = f(x_t, u_t), \ \ x_1 = x_{\text{init}}, \tag{2.9}$$

where x_{init} is the current system state, the cost C_t is typically hand-engineered and differentiable, and $x_{t+1} = f(x_t, u_t)$ is the deterministic next-state transition, *i.e.* the point-mass given by $p(x_{t+1}|x_t, u_t)$. While this thesis focuses on the continuous and deterministic setting, control approaches can also be applied in discrete and stochastic settings.

Pure model-free techniques for policy search have demonstrated promising results in many domains by learning *reactive polices* which directly map observations to actions [95, 101, 59, 88, 120, 121, 58]. Despite their success, model-free methods have many drawbacks and limitations, including a lack of interpretability, poor generalization, and a high sample complexity. **Model-based methods** are known to be more sample-efficient than their model-free counterparts. These methods generally rely on learning a dynamics model directly from interactions with the real system and then integrate the learned model into the control policy [119, 2, 34, 63, 23]. More recent approaches use a deep network to learn low-dimensional latent state representations and associated dynamics models in this learned representation. They then apply standard trajectory optimization methods on these learned embeddings [80, 148, 84]. However, these methods still require a manually specified and hand-tuned cost function, which can become even more difficult in a

latent representation. Moreover, there is no guarantee that the learned dynamics model can accurately capture portions of the state space relevant for the task at hand.

To leverage the benefits of both approaches, there has been significant interest in **combining the model-based and model-free paradigms.** In particular, much attention has been dedicated to utilizing model-based priors to accelerate the model-free learning process. For instance, synthetic training data can be generated by model-based control algorithms to guide the policy search or prime a model-free policy [130, 140, 83, 59, 143, 84, 28, 98, 128]. [10] learns a controller and then distills it to a neural network policy which is then fine-tuned with model-free policy learning. However, this line of work usually keeps the model separate from the learned policy.

Alternatively, the policy can include an **explicit planning module** which *leverages learned models* of the system or environment, both of which are learned through model-free techniques. For example, the classic Dyna-Q algorithm [130] simultaneously learns a model of the environment and uses it to plan. More recent work has explored incorporating such structure into deep networks and learning the policies in an end-to-end fashion. Tamar, Wu, Thomas, Levine, and Abbeel [134] uses a recurrent network to predict the value function by approximating the value iteration algorithm with convolutional layers. Karkus, Hsu, and Lee [72] connects a dynamics model to a planning algorithm and formulates the policy as a structured recurrent network. Silver, Hasselt, Hessel, Schaul, Guez, Harley, Dulac-Arnold, Reichert, Rabinowitz, Barreto, et al. [123] and Oh, Singh, and Lee [102] perform multiple rollouts using an abstract dynamics model to predict the value function. A similar approach is taken by Weber, Racanière, Reichert, Buesing, Guez, Rezende, Badia, Vinyals, Heess, Li, et al. [149] but directly predicts the next action and reward from rollouts of an explicit environment model. Farquhar, Rocktäschel, Igl, and Whiteson [41] extends model-free approaches, such as DQN [96] and A3C [94], by planning with a tree-structured neural network to predict the cost-to-go. While these approaches have demonstrated impressive results in discrete state and action spaces, they are not applicable to continuous control problems.

To tackle continuous state and action spaces, Pascanu, Li, Vinyals, Heess, Buesing, Racanière, Reichert, Weber, Wierstra, and Battaglia [106] propose a neural architecture which uses an abstract environmental model to plan and is trained directly from an external task loss. Pong, Gu, Dalal, and Levine [111] learn goal-conditioned value functions and use them to plan single or multiple steps of actions in an MPC fashion. Similarly, Pathak, Mahmoudieh, Luo, Agrawal, Chen, Shentu, Shelhamer, Malik, Efros, and Darrell [108] train a goal-conditioned policy to perform rollouts in an abstract feature space but ground the policy with a loss term which corresponds to true dynamics data. The aforementioned approaches can be interpreted as a distilled optimal controller which does not separate components for the cost and dynamics. Taking this analogy further, another strategy is to differentiate through an optimal control algorithm itself. Okada, Rigazio, and Aoshima [103] and Pereira, Fan, An, and Theodorou [110] present a way to differentiate through path integral optimal control [151, 150] and learn a planning policy end-to-end. Srinivas, Jabri, Abbeel, Levine, and Finn [125] shows how to embed differentiable planning (unrolled gradient descent over actions) within a goal-directed policy. In a similar vein, Tamar, Thomas, Zhang, Levine, and Abbeel [133] differentiates through an iterative LQR (iLQR)

solver [86, 153, 139] to learn a cost-shaping term offline. This shaping term enables a shorter horizon controller to approximate the behavior of a solver with a longer horizon to save computation during runtime.

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