

Foundations and Trends® in Machine Learning

Tutorial on Amortized Optimization

Suggested Citation: Brandon Amos (2023), "Tutorial on Amortized Optimization", Foundations and Trends® in Machine Learning: Vol. 16, No. 5, pp 592–732. DOI: 10.1561/2200000102.

Brandon Amos
Meta AI
brandon.amos.cs@gmail.com

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Contents

1	Introduction	593
2	Amortized Optimization Foundations	598
2.1	Defining the Model $\hat{y}_\theta(x)$	600
2.2	Learning the Model's Parameters θ	608
2.3	Extensions	620
3	Applications of Amortized Optimization	632
3.1	Variational Inference and Variational Autoencoders	632
3.2	Sparse Coding	635
3.3	Multi-task Learning and Meta-learning	637
3.4	Fixed-point Computations and Convex Optimization	643
3.5	Optimal Transport	649
3.6	Policy Learning for Control and Reinforcement Learning	653
4	Implementation and Software Examples	667
4.1	Amortization In the Wild: A Deeper Look	668
4.2	Training an Amortization Model on a Sphere	674
4.3	Other Useful Software Packages	676

5 Discussion	678
5.1 Surpassing the Convergence Rates of Classical Methods	678
5.2 Generalization and Convergence Guarantees	679
5.3 Measuring Performance	679
5.4 Successes and Limitations of Amortized Optimization	680
5.5 Some Open Problems and Under-explored Directions	682
5.6 Related Work	685
Acknowledgements	689
References	690

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Brandon Amos

Meta AI, USA; brandon.amos.cs@gmail.com

ABSTRACT

Optimization is a ubiquitous modeling tool and is often deployed in settings which repeatedly solve similar instances of the same problem. Amortized optimization methods use learning to predict the solutions to problems in these settings, exploiting the shared structure between similar problem instances. These methods have been crucial in variational inference and reinforcement learning and are capable of solving optimization problems many orders of magnitudes times faster than traditional optimization methods that do not use amortization. This tutorial presents an introduction to the amortized optimization foundations behind these advancements and overviews their applications in variational inference, sparse coding, gradient-based meta-learning, control, reinforcement learning, convex optimization, optimal transport, and deep equilibrium networks. The source code for this tutorial is available at <https://github.com/facebookresearch/amortized-optimization-tutorial>.

1

Introduction

This tutorial studies the use of machine learning to improve repeated solves of parametric optimization problems of the form

$$y^*(x) \in \arg \min_y f(y; x), \quad (1.1)$$

where the *non-convex* objective $f : \mathcal{Y} \times \mathcal{X} \rightarrow \mathbb{R}$ takes a *context* or *parameterization* $x \in \mathcal{X}$ which can be continuous or discrete, and the *continuous, unconstrained domain* of the problem is $y \in \mathcal{Y} = \mathbb{R}^n$. Eq. (1.1) implicitly defines a *solution* $y^*(x) \in \mathcal{Y}$. In most of the applications considered later in Section 3, $y^*(x)$ is unique and smooth, *i.e.*, the solution continuously changes in a connected way as the context change is illustrated in Figure 1.1.

Parametric optimization problems such as Eq. (1.1) have been studied for decades (Bank *et al.*, 1982; Fiacco and Ishizuka, 1990; Shapiro, 2003; Klatte and Kummer, 2006; Bonnans and Shapiro, 2013; Still, 2018; Fiacco, 2020) with a focus on sensitivity analysis. The general formulation in Eq. (1.1) captures many tasks arising in physics, engineering, mathematics, control, inverse modeling, and machine learning. For example, when controlling a continuous robotic system, \mathcal{X} is the space of *observations* or *states*, *e.g.*, angular positions and velocities describing

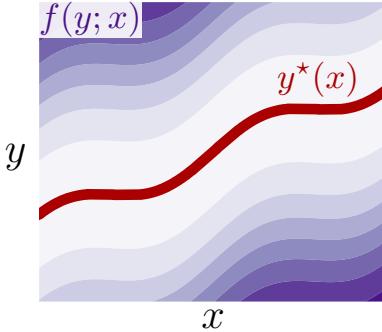


Figure 1.1: Illustration of the parametric optimization problem in Eq. (1.1). Each context x parameterizes an optimization problem that the objective $f(y; x)$ depends on. The contours show the values of the objectives where darker colors indicate higher values. The objective is then minimized over y and the resulting solution $y^*(x)$ is shown in red. In other words, each vertical slice is an optimization problem and this visualization shows a continuum of optimization problems.

the configuration of the system, the domain $\mathcal{Y} := \mathcal{U}$ is the *control space*, e.g., torques to apply to each actuated joint, and $f(u; x) := -Q(u, x)$ is the *control cost* or the negated *Q-value* of the state-action tuple (x, u) , e.g., to reach a goal location or to maximize the velocity. For every encountered state x , the system is controlled by solving an optimization problem in the form of Eq. (1.1). While $\mathcal{Y} = \mathbb{R}^n$ is over a deterministic real-valued space in Eq. (1.1), the formulation can also capture stochastic optimization problems as discussed in Section 2.3.1. For example, Section 3.1 optimizes over the (real-valued) parameters of a variational distribution and Section 3.6 optimizes over the (real-valued) parameters of a stochastic policy for control and reinforcement learning.

Optimization problems such as Eq. (1.1) quickly become a computational bottleneck in systems they are a part of. These problems often does not have a closed-form analytic solution and is instead solved with approximate numerical methods which iteratively search for the solution. This computational problem has led to many specialized solvers that leverage domain-specific insights to deliver fast solves. Specialized algorithms are especially prevalent in convex optimization methods for linear programming, quadratic programming, cone programming, and control and use theoretical insights of the problem structure to

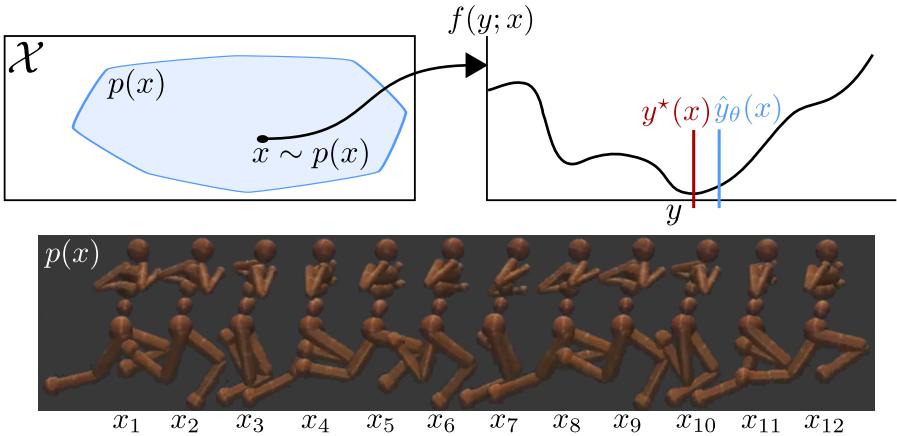


Figure 1.2: An amortized optimization method learns a model \hat{y}_θ to predict the minimum of an *objective* $f(y; x)$ to a parameterized optimization problem, as in Eq. (1.1), which depends on a *context* x . For example, in control, the context space \mathcal{X} is the state space of the system, e.g. angular positions and velocities describing the configuration of the system, the domain $\mathcal{Y} := \mathcal{U}$ is the control space, e.g. torques to apply to each actuated joint, the cost (or negated value) of a state-action pair is $f(u; x) := -Q(x, u)$, and the state distribution is $p(x)$. For an encountered state x , many reinforcement learning policies $\pi_\theta(x) := \hat{y}_\theta(x)$ amortize the solution to the underlying control problem with true solution $y^*(x)$. This humanoid policy was obtained with the model-based stochastic value gradient in Amos *et al.* (2021).

bring empirical gains of computational improvements and improved convergence (Boyd and Vandenberghe, 2004; Nocedal and Wright, 2006; Bertsekas, 2015; Bubeck, 2015; Nesterov *et al.*, 2018).

Mostly separate from optimization research and algorithmic advancements, the machine learning community has focused on developing generic function approximation methods for estimating non-trivial high-dimensional mappings from data (Murphy, 2012; Salakhutdinov, 2014; Deisenroth *et al.*, 2020). While machine learning models are often used to reconstruct mappings from data, e.g. for supervised classification or regression where the targets are given by human annotations. Many computational advancements on the software and hardware have been developed in recent years to make the prediction time fast: the forward pass of a neural network generating a prediction can execute in milliseconds on a graphics processing unit.

Overview. This tutorial studies the use of machine learning models to rapidly predict the solutions to the optimization problem in Eq. (1.1), which is referred to as *amortized optimization* or *learning to optimize*. Figure 1.2 illustrates a basic setup for control. Amortized optimization methods are capable of significantly improving the computational time of classical algorithms *on a focused subset of problems*. This is because the model is able to learn about the solution mapping from x to $y^*(x)$ that classical optimization methods usually do not assume access to. My goal in writing this is to explore a unified perspective of modeling approaches of amortized optimization in Section 2 to help draw connections between the applications in Section 3, *e.g.* between amortized variational inference, meta-learning, and policy learning for control and reinforcement learning, sparse coding, convex optimization, optimal transport, and deep equilibrium networks. These topics have historically been studied in isolation without connections between their amortization components. Section 4 presents a computational tour through source code for variational inference, policy learning, and a spherical optimization problem and Section 5 concludes with a discussion of challenges, limitations, open problems, and related work.

How much does amortization help? Amortized optimization has been revolutionary to many fields, especially including variational inference and reinforcement learning. Figure 4.1 shows that the amortization component of a variational autoencoder trained on MNIST is **25000** times faster (0.4ms vs. 8 seconds!) than solving a batch of 1024 optimization problems from scratch to obtain a solution of the same quality. These optimization problems are solved in every training iteration and can become a significant bottleneck if they are inefficiently solved. If the model is being trained for millions of iterations, then the difference between solving the optimization problem in 0.4ms vs. 8 seconds makes the difference between the entire training process finishing in a few hours or a month.

A historic note: amortization in control and statistical inference. Amortized optimization has arisen in many fields as a result to practical optimization problems being non-convex and not having easily computed, or closed-form solutions. Continuous control problems with linear dynamics and quadratic cost are convex and

often easily solved with the linear quadratic regulator (LQR) and many non-convex extensions and iterative applications of LQR have been successful over the decades, but becomes increasingly infeasible on non-trivial systems and in reinforcement learning settings where the policy often needs to be rapidly executed. For this reason, the reinforcement learning community almost exclusively amortizes control optimization problems with a learned policy (Sutton and Barto, 2018). Related to this throughline in control and reinforcement learning, many statistical optimization problems have closed form solutions for known distributions such as Gaussians. For example, the original Kalman filter is defined with Gaussians and the updates take closed-form. The extended Kalman filter generalizes the distributions to non-Gaussians, but the updates are in general no longer available analytically and need to be computationally estimated. Marino *et al.* (2018a) shows how amortization helps improve this computationally challenging step. Both of these control and statistical settings start with a simple setting with analytic solutions to optimization problems, generalize to more challenging optimization problems that need to be computationally estimated, and then add back some computational tractability with amortized optimization.

2

Amortized Optimization Foundations

The machine learning, statistics, and optimization communities are exploring methods of *learning to optimize* to obtain fast solvers for Eq. (1.1). I will refer to these methods as *amortized optimization* as they *amortize* the cost of solving the optimization problems across many contexts to approximate the solution mapping y^* . Amortized optimization is promising because in many applications, there are significant correlations and structure between the solutions which show up in y^* that a model can learn. This tutorial follows Shu (2017) for defining the core foundation of amortized optimization.

Definition 2.1. An *amortized optimization method* to solve Eq. (1.1) can be represented by $\mathcal{A} := (f, \mathcal{Y}, \mathcal{X}, p(x), \hat{y}_\theta, \mathcal{L})$, where $f : \mathcal{Y} \times \mathcal{X} \rightarrow \mathbb{R}$ is the unconstrained *objective* to optimize, \mathcal{Y} is the *domain*, \mathcal{X} is the *context space*, $p(x)$ is the *probability distribution over contexts* to optimize, $\hat{y}_\theta : \mathcal{X} \rightarrow \mathcal{Y}$ is the *amortization model* parameterized by θ which is learned by optimizing a *loss* defined on all the components $\mathcal{L}(f, \mathcal{Y}, \mathcal{X}, p(x), \hat{y}_\theta)$.

The objective f and domain \mathcal{Y} arise from the problem setting along with the context space \mathcal{X} and distribution over it $p(x)$, and the remaining definitions of the model \hat{y}_θ and loss \mathcal{L} are application-specific design

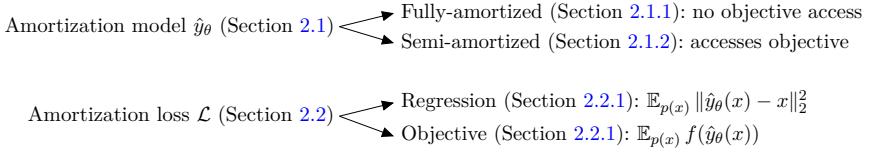


Figure 2.1: Overview of amortized optimization modeling and loss choices.

decisions that Sections 2.1 and 2.2 opens up. These sections present the modeling and loss foundations for the core problem in Definition 2.1 agnostic of specific downstream applications that will use them. The key choices highlighted in Figure 2.1 are how much information 1) the model \hat{y}_θ has about the objective f (fully- vs. semi-amortized), and 2) the loss has about the true solution y^* (regression- vs. objective-based). Figure 1.2 instantiates these components for amortizing the control of a robotic system. The model \hat{y}_θ solves the solution mapping y^* simultaneously for all contexts. The methods here usually assume the solution mapping y^* to be almost-everywhere smooth and well-behaved. The best modeling approach is an open research topic as there are many tradeoffs, and many specialized insights from the application domain can significantly improve the performance. The generalization capacity along with the model’s convergence guarantees are challenging topics which Section 5.2 covers in more detail.

Origins of the term “amortization” for optimization. The word “amortization” generally means to spread out costs and thus “amortized optimization” usually means to spread out computational costs of the optimization process. The term originated in the variational inference community for inference optimization (Kingma and Welling, 2014; Rezende *et al.*, 2014; Stuhlmüller *et al.*, 2013; Gershman and Goodman, 2014; Webb *et al.*, 2018; Ravi and Beatson, 2019; Cremer *et al.*, 2018; Wu *et al.*, 2020), and is used more generally in Xue *et al.* (2020), Sercu *et al.* (2021), and Xiao *et al.* (2021). Marino (2021, p. 28) give further background on the origins and uses of amortization. Concurrent to these developments, other communities have independently amortization methods without referring to them by the same terminology and analysis, such as in reinforcement learning, policy optimization, and sparse coding — Section 3 connects all of these under Definition 2.1.

Conventions and notation. The context space \mathcal{X} represents the sample space of a probability space that the distribution $p(x)$ is defined on, assuming it is Borel if not otherwise specified. For a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ in standard Euclidean space, $\nabla_x f(\bar{x}) \in \mathbb{R}^n$ denotes the *gradient* at a point \bar{x} and $\nabla_x^2 f(\bar{x}) \in \mathbb{R}^{n \times n}$ denotes the *Hessian*. For $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$, $D_x f(\bar{x}) \in \mathbb{R}^{m \times n}$ represents the *Jacobian* at \bar{x} with entries $[D_x f(\bar{x})]_{ij} := \frac{\partial f_i}{\partial x_j}(\bar{x})$. I abbreviate the loss to $\mathcal{L}(\hat{y}_\theta)$ when the other components can be inferred from the surrounding text and prefer the term “context” for x instead of “parameterization” to make the distinction between the x -parameterized optimization problem and the θ -parameterized model clear. I use “;” as separation in $f(y; x)$ to emphasize the separation between the domain variables y that Eq. (1.1) optimizes over from the context ones x that remain fixed. A model’s parameters θ are usually subscripts as $h_\theta(x)$ but I will equivalently write $h(x; \theta)$ sometimes.

2.1 Defining the Model $\hat{y}_\theta(x)$

The model $\hat{y}_\theta(x) : \mathcal{X} \times \Theta \rightarrow \mathcal{Y}$ predicts a solution to Eq. (1.1). In many applications, the best model design is an active area of research that is searching for models that are expressive and more computationally efficient than the algorithms classically used to solve the optimization problem. Section 2.1.1 starts simple with *fully-amortized* models that approximate the entire solution to the optimization problem with a single black-box model. Then Section 2.1.2 shows how to open up the model to include more information about the optimization problem that can leverage domain knowledge with *semi-amortized* models.

2.1.1 Fully-amortized models

Definition 2.2. A *fully-amortized* model $\hat{y}_\theta : \mathcal{X} \rightarrow \mathcal{Y}$ maps the context to the solution of Eq. (1.1) and does *not* access the objective f .

I use the prefix “fully” to emphasize that the entire computation of the solution to the optimization problem is absorbed into a black-box model that does *not* access the objective f . The prefix “fully” can be omitted when the context is clear because most amortization is fully

amortized. These are standard in amortized variational inference (Section 3.1) and policy leaning (Section 3.6), that typically use feedforward neural networks to map from the context space \mathcal{X} to the solution of the optimization problem living in \mathcal{Y} . Fully-amortized models are remarkable because they are often successfully able to predict the solution to the optimization problem in Eq. (1.1) *without* ever accessing the objective of the optimization problem after being trained.

Fully-amortized models are the most useful for attaining approximate solutions that are computationally efficient. They tend to work the best when the solution mappings $y^*(x)$ are predictable, the domain \mathcal{Y} is relatively small, usually hundreds or thousands of dimensions, and the context distribution isn't too large. When fully-amortized models don't work well, semi-amortized models help open up the black box and use information about the objective.

2.1.2 Semi-amortized models

Definition 2.3. A *semi-amortized* model $\hat{y}_\theta : \mathcal{X} \rightarrow \mathcal{Y}$ maps the context to the solution of the optimization problem and accesses the objective f of Eq. (1.1), typically iteratively.

Kim *et al.* (2018) and Marino *et al.* (2018b) proposed *semi-amortized* models for variational inference that add back domain knowledge of the optimization problem to the model \hat{y}_θ that the fully-amortized models do not use. These are brilliant ways of integrating the optimization-based domain knowledge into the learning process. The model can now internally integrate solvers to improve the prediction. Semi-amortized methods are typically iterative and update iterates in the domain \mathcal{Y} or in an *auxiliary* or *latent space* \mathcal{Z} . I refer to the space the semi-amortization iterates over as the *amortization space* and denote iterate t in these spaces, respectively, as \hat{y}_θ^t and z_θ^t . While the iterates and final prediction \hat{y}_θ can now query the objective f and gradient $\nabla_y f$, I notationally leave this dependence implicit for brevity and only reference these queries in the relevant definitions.

Semi-amortized models over the domain \mathcal{Y}

$$\hat{y}_\theta^0 \rightarrow \hat{y}_\theta^1 \rightarrow \cdots \rightarrow \hat{y}_\theta^K =: \hat{y}_\theta(x)$$

One of the most common semi-amortized model is to parameterize and integrate an optimization procedure used to solve Eq. (1.1) into the model \hat{y}_θ , such as gradient descent (Andrychowicz *et al.*, 2016; Finn *et al.*, 2017; Kim *et al.*, 2018). This optimization procedure is an internal part of the amortization model \hat{y}_θ , often referred to as the *inner-level* optimization problem in the bi-level setting that arises for learning.

Examples. This section instantiates a canonical semi-amortized model based gradient descent that learns the initialization as in model-agnostic meta-learning (MAML) by Finn *et al.* (2017), structured prediction energy networks (SPENs) by Belanger *et al.* (2017), and semi-amortized variational auto-encoders (SAVAEs) by Kim *et al.* (2018). The initial iterate $\hat{y}_\theta^0(x) := \theta$ is parameterized by $\theta \in \mathcal{X}$ for all contexts. Iteratively updating \hat{y}_θ^t for K gradient steps with a *learning rate* or *step size* $\alpha \in \mathbb{R}_+$ on the objective $f(y; x)$ gives

$$\hat{y}_\theta^t := \hat{y}_\theta^{t-1} - \alpha \nabla_y f(\hat{y}_\theta^{t-1}; x) \quad t \in \{1 \dots, K\}, \quad (2.1)$$

where model's output is defined as $\hat{y}_\theta := \hat{y}^K$.

Semi-amortized models over the domain can go significantly beyond gradient-based models and in theory, any algorithm to solve the original optimization problem in Eq. (1.1) can be integrated into the model. Section 2.2.2 further discusses the learning of semi-amortized models by unrolling that are instantiated later:

- Section 3.2 discusses how Gregor and LeCun (2010) integrate ISTA iterates (Daubechies *et al.*, 2004; Beck and Teboulle, 2009) into a semi-amortized model.
- Section 3.4.1 discusses models that integrate fixed-point computations into semi-amortized models. Venkataraman and Amos (2021) amortize convex cone programs by differentiating through the splitting cone solver (O'Donoghue *et al.*, 2016) and Bai *et al.* (2022) amortize deep equilibrium models (Bai *et al.*, 2019; Bai *et al.*, 2020).

- Section 3.4.5 discusses RLQP by Ichnowski *et al.* (2021) that uses the OSQP solver (Stellato *et al.*, 2018) inside of a semi-amortized model.

Semi-amortized models over a latent space \mathcal{Z}

$$\hat{z}_\theta^0 \rightarrow \hat{z}_\theta^1 \rightarrow \cdots \rightarrow \hat{z}_\theta^K \rightarrow \hat{y}_\theta(x)$$

In addition to only updating iterates over the domain \mathcal{Y} , a natural generalization is to introduce a latent space \mathcal{Z} that is iteratively optimized over *inside* of the amortization model. This is usually done to give the semi-amortized model more capacity to learn about the structure of the optimization problems that are being solved. The latent space can also be interpreted as a representation of the optimal solution space. This is useful for learning an optimizer that only searches over the *optimal* region of the solution space rather than the entire solution space.

Examples. The iterative gradient updates in Eq. (2.1) can be replaced with a learned update function as in Ravi and Larochelle (2017), Li and Malik (2017a), Andrychowicz *et al.* (2016), and Li and Malik (2017b). These model the past sequence of iterates and learn how to best-predict the next iterate, pushing them towards optimality. This can be done with a recurrent cell g such as an LSTM (Hochreiter and Schmidhuber, 1997) or GRU (Cho *et al.*, 2014) and leads to updates of the form

$$z_\theta^t, \hat{y}_\theta^t := g_\theta(z_\theta^{t-1}, x_\theta^{t-1}, \nabla_y f(\hat{y}_\theta^{t-1}; x)) \quad t \in \{1 \dots, K\} \quad (2.2)$$

where each call to the recurrent cell g takes a hidden state z along with an iterate and the derivative of the objective. This endows g with the capacity to learn significant updates leveraging the problem structure that a traditional optimization method would not be able to make. In theory, traditional update rules can also be fallen back on as the gradient step in Eq. (2.1) is captured by removing the hidden state z and setting

$$g(x, \nabla_y f(y; x)) := x - \alpha \nabla_y f(y; x). \quad (2.3)$$

Latent semi-amortized models are a budding topic and can excitingly learn many other latent representations that go beyond iterative gradient

updates in the original space. Luo *et al.* (2018) and Amos and Yarats (2020) learn a *latent domain* connected to the original domain where the latent domain captures hidden structures and redundancies present in the original high-dimensional domain \mathcal{Y} . Luo *et al.* (2018) consider gradient updates in the latent domain and Amos and Yarats (2020) show that the cross-entropy method (De Boer *et al.*, 2005) can be made differentiable and learned as an alternative to gradient updates. Amos *et al.* (2017) unrolls and differentiates through the bundle method (Smola *et al.*, 2007) in a convex setting as an alternative to gradient steps. The latent optimization could also be done over a learned parameter space as in POPLIN (Wang and Ba, 2020), which *lifts* the domain of the optimization problem Eq. (1.1) from \mathcal{Y} to the parameter space of a fully-amortized neural network. This leverages the insight that the parameter space of over-parameterized neural networks can induce easier non-convex optimization problems than in the original space, which is also studied in Hoyer *et al.* (2019).

Comparing semi-amortized models with warm-starting

Semi-amortized models are conceptually similar to learning a fully-amortized model to warm-start an existing optimization procedure that fine-tunes the solution. The crucial difference is that semi-amortized learning often end-to-end learns through the final prediction while warm-starting and fine-tuning only learns the initial prediction and does not integrate the knowledge of the fine-tuning procedure into the learning procedure. Choosing between these is an active research topic and while this tutorial will mostly focus on semi-amortized models, learning a fully-amortized warm-starting model brings promising results to some fields too, such as Zhang *et al.* (2019b), Baker (2019), and Chen *et al.* (2022b). In variational inference, Kim *et al.* (2018, Table 2) compare semi-amortized models (SA-VAE) to warm-starting and fine-tuning (VAE+SVI) and demonstrate that the end-to-end learning signal is helpful. In other words, amortization finds an initialization that is helpful for gradient-based optimization. Arbel and Mairal (2022) further study fully-amortized warm-started solvers that arise in bi-level optimization problems for hyper-parameter optimization and use the

theoretical framework from singularly perturbed systems (Habets, 2010) to analyze properties of the approximate solutions.

On second-order derivatives of the objective

Training a semi-amortized model is usually more computationally challenging than training a fully-amortized model. This section looks at how second-order derivatives of the objective may come up when unrolling and create a computational bottleneck when learning a semi-amortized model. The next derivation follows Nichol *et al.* (2018, §5) and Weng (2018) and shows the model derivatives that arise when composing a semi-amortized model with a loss.

Starting with a single-step model. This section instantiates a single-step model similar to Eq. (2.1) that parameterizes the initial iterate $\hat{y}_\theta^0(x) := \theta$ and takes one gradient step:

$$\hat{y}_\theta(x) := \hat{y}_\theta^0(x) - \alpha \nabla_y f(\hat{y}_\theta^0(x); x) \quad (2.4)$$

Interpreting $\hat{y}_\theta(x)$ as a model is non-standard in contrast to other parametric models because it makes the optimization step *internally part of the model*. Gradient-based optimization of losses with respect to the model’s parameters, such as Eqs. (2.9) and (2.10) requires the Jacobian of $\hat{y}_\theta(x)$ w.r.t. the parameters, *i.e.* $D_\theta[\hat{y}_\theta(x)]$ (or Jacobian-vector products with it). Because $\hat{y}_\theta(x)$ is an optimization step, the derivative of the model requires differentiating through the optimization step, which for Eq. (2.4) is

$$D_\theta[\hat{y}_\theta(x)] = I - \alpha \nabla_y^2 f(y_\theta^0(x); x) \quad (2.5)$$

and requires the Hessian of the objective. In Finn *et al.* (2017), $\nabla_y^2 f$ is the Hessian of the model’s parameters on the training loss (!) and is compute- and memory-expensive to instantiate for large models. In practice, the Hessian in Eq. (2.5) is often never explicitly instantiated as optimizing the loss only requires Hessian-vector products. The Hessian-vector product can be computed exactly or estimated without fully instantiating the Hessian, similar to how computing the derivative of a neural network with backprop does not instantiate the intermediate Jacobians and only computes the Jacobian-vector product. More information about efficiently computing Hessian-vector products is available

in Pearlmutter (1994) and Domke (2012). Jax’s [autodiff cookbook](#) (Bradbury *et al.*, 2020) further describes efficient Hessian-vector products. Before discussing alternatives, the next portion derives similar results for a K -step model.

Multi-step models. Eq. (2.4) can be extended to the K -step setting with

$$\hat{y}_\theta^K(x) := \hat{y}_\theta^{K-1}(x) - \alpha \nabla_y f(\hat{y}_\theta^{K-1}(x); x), \quad (2.6)$$

where the base $\hat{y}_\theta^0(x) := \theta$ as before. Similar to Eq. (2.5), the derivative of a single step is

$$D_\theta[\hat{y}_\theta^K(x)] = D_\theta[\hat{y}_\theta^{K-1}(x)] \left(I - \alpha \nabla_y^2 f(y_\theta^{K-1}(x); x) \right), \quad (2.7)$$

and composing the derivatives down to \hat{y}_θ^0 yields the product structure

$$D_\theta[\hat{y}_\theta^K(x)] = \prod_{k=0}^{K-1} \left(I - \alpha \nabla_y^2 f(y_\theta^k(x); x) \right), \quad (2.8)$$

where $D_\theta[\hat{y}_\theta^0(x)] = I$ at the base case. Computing Eq. (2.8) is now K times more challenging as it requires the Hessian $\nabla_y^2 f$ at *every* iteration of the model. While using Hessian-vector products can alleviate some computational burden of this term, it often still requires significantly more operations than most other derivatives.

Computationally cheaper alternatives. The first-order MAML baseline in Finn *et al.* (2017) suggests to simply not use the second-order terms $\nabla_y^2 f$ here, approximating the model derivative as the identity, *i.e.* $D_\theta[\hat{y}_\theta^K(x)] \approx I$, and relying on only information from the outer loss to update the parameters. They use the intuition from Goodfellow *et al.* (2015) that neural networks are locally linear and therefore these second-order terms of f are not too important. They show that this approximation works well in some cases, such as MiniImagenet (Ravi and Larochelle, 2017). The MAML++ extension by Antoniou *et al.* (2019) proposes to use first-order MAML during the early phases of training, but to later add back this second-order information. Nichol *et al.* (2018) further analyze first-order approximations to MAML and propose another approximation called Reptile that also doesn’t use this second-order information. These higher-order terms also come up

when unrolling in the different bi-level optimization setting for hyper-parameter optimization, and Lorraine *et al.* (2020, Table 1) gives a particularly good overview of approximations to these. Furthermore, memory-efficient methods for training neural networks and recurrent models with backpropagation and unrolling such as Gruslys *et al.* (2016) and Chen *et al.* (2016) can also help improve the memory utilization in amortization models.

Parameterizing and learning the objective. While this section has mostly not considered the setting when the objective f is also learned, the second-order derivatives appearing in Eq. (2.8) also cause issues in when the objective is parameterized and learned. In addition to learning an initial iterate, Belanger *et al.* (2017) learn the objective f representing an energy function. They parameterize f as a neural network and use softplus activation functions rather than ReLUs to ensure the objective’s second-order derivatives are non-zero.

2.1.3 Models based on differentiable optimization

As discussed in Section 2.2, the model typically needs to be (sub-)differentiable with respect to the parameters to attain the Jacobian $D_\theta[\hat{y}_\theta]$ (or compute Jacobian-vector products with it) necessary to optimize the loss. These derivatives are standard backprop when the model is, for example, a full-amortized neural network, but in the semi-amortized case, the model itself is often an optimization process that needs to be differentiated through. When the model updates are objective-based as in Eq. (2.1) and Eq. (2.2), the derivatives with respect to θ through the sequence of gradient updates in the domain can be attained by seeing the updates as a sequence of computations that are differentiated through, resulting in second-order derivatives. When more general optimization methods are used for the amortization model that may not have a closed-form solution, the tools of differentiable optimization (Domke, 2012; Gould *et al.*, 2016; Amos and Kolter, 2017; Amos, 2019; Agrawal *et al.*, 2019a) enable end-to-end learning.

2.1.4 Practically choosing a model

This section has taxonomized how to instantiate an amortization model in an application-agnostic way. As in most machine learning settings in practice, the modeling choice is often application-specific and needs to take into consideration many factors. This may include 1) the speed and expressibility of the model. 2) Adapting the model to specific context space \mathcal{X} . An MLP may be good for fixed-dimensional real-valued spaces but a convolutional neural network is likely to perform better for image-based spaces. 3) Taking the solution space \mathcal{Y} into consideration. For example, if the solution space is an image space, then a standard vision model capable of predicting high-dimensional images is reasonable, such as a U-net (Ronneberger *et al.*, 2015), dilated convolutional network (Yu and Koltun, 2016) or fully convolutional network (Long *et al.*, 2015). 4) The model also may need to adapt to a *variable-length* context or solution space. This arises in VeLO (Metz *et al.*, 2022) for learning to optimize machine learning models where the model needs to predict the parameters of different models that may have different numbers of parameters. Their solution is to decompose the structure of the parameter space and to formulate the semi-amortized model as a sequence model that predicts smaller MLPs that operate on smaller groups of parameters.

2.2 Learning the Model's Parameters θ

After specifying the amortization model \hat{y}_θ , the other major design choice is how to learn the parameters θ so that the model best-solves Eq. (1.1). Learning is often a *bi-level* optimization problem where the *outer level* is the parameter learning problem for a model $\hat{y}_\theta(x)$ that solves the *inner-level* optimization problem in Eq. (1.1) over the domain \mathcal{Y} . While defining the best loss is application-specific, most approaches can be roughly categorized as 1) regressing a ground-truth solution (Section 2.2.1), or 2) minimizing the objective (Sections 2.2.1 and 2.2.3), which Figure 2.2 illustrates. Optimizing the model parameters here can in theory be done with most parameter learning methods that incorporate zeroth-, first-, and higher-order information about the loss

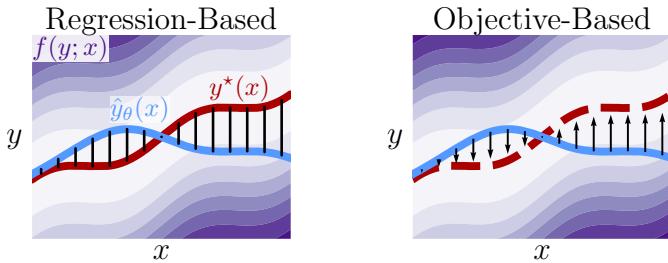


Figure 2.2: Overview of key losses for optimizing the parameters θ of the amortization model \hat{y}_θ . Regression-based losses optimize a distance between the model's prediction $\hat{y}_\theta(x)$ and the ground-truth $y^*(x)$. Objective-based methods update \hat{y}_θ using local information of the objective f and *without* access to the ground-truth solutions y^* .

being optimized, and this section mostly focuses on methods where θ is learned with a first-order gradient-based method such as Nesterov (1983), Duchi *et al.* (2010), Zeiler (2012), and Kingma and Ba (2015). The rest of this section discusses approaches for designing the loss and optimizing the parameters with first-order methods (Section 2.2.1) when differentiation is easy or zeroth-order methods (Section 2.2.3) otherwise, *e.g.*, in non-differentiable settings.

2.2.1 Choosing the objective for learning

Regression-based learning

Learning can be done by regressing the model's prediction $\hat{y}_\theta(x)$ onto a ground-truth solution $y^*(x)$. These minimize some distance between the predictions and ground-truth so that the expectation over the context distribution $p(x)$ is minimal. With a Euclidean distance, for example, regression-based learning solves

$$\arg \min_{\theta} \mathcal{L}_{\text{reg}}(\hat{y}_\theta) \quad \mathcal{L}_{\text{reg}}(\hat{y}_\theta) := \mathbb{E}_{x \sim p(x)} \|y^*(x) - \hat{y}_\theta(x)\|_2^2. \quad (2.9)$$

\mathcal{L}_{reg} is typically optimized with an adaptive first-order gradient-based method that is able to directly differentiate the loss with respect to the model's parameters.

Regression-based learning works the best for distilling known solutions into a faster model that can be deployed at a much lower cost, but

can otherwise start failing to work. In RL and control, regression-based amortization methods are referred to as *behavioral cloning* and is a widely-used way of recovering a policy using trajectories observed from an expert policy. Using regression is also advantageous when evaluating the objective $f(y; x)$ incurs a computationally intensive or otherwise complex procedure, such as an evaluation of the environment and dynamics in RL, or for computing the base model gradients when learning parameter optimizers. These methods work well when the ground-truth solutions are unique and semi-tractable, but can fail otherwise, *i.e.* if there are many possible ground-truth solutions for a context x or if computing them is too intractable. After all, solving Eq. (1.1) from scratch may be computationally expensive and amortization methods should improve the computation time.

Remark 2.1. Eq. (2.9) can be extended to other distances defined on the domain, such as non-Euclidean distances or the likelihood of a probabilistic model that predicts a distribution of possible candidate solutions. Adler *et al.* (2017) propose to use the Wasserstein distance for learning to predict the solutions to inverse imaging problems.

Objective-based learning

Instead of regressing onto the ground-truth solution, *objective-based* learning methods seek for the model’s prediction to be minimal under the objective f with:

$$\arg \min_{\theta} \mathcal{L}_{\text{obj}}(\hat{y}_{\theta}) \quad \mathcal{L}_{\text{obj}}(\hat{y}_{\theta}) := \mathbb{E}_{x \sim p(x)} f(\hat{y}_{\theta}(x); x). \quad (2.10)$$

These methods use local information of the objective to provide a descent direction for the model’s parameters θ . A first-order method optimizing Eq. (2.10) uses updates based on the gradient

$$\begin{aligned} \nabla_{\theta} \mathcal{L}_{\text{obj}}(\hat{y}_{\theta}) &= \nabla_{\theta} \left[\mathbb{E}_{x \sim p(x)} f(\hat{y}_{\theta}(x); x) \right] \\ &= \mathbb{E}_{x \sim p(x)} D_{\theta} [\hat{y}_{\theta}(x)]^{\top} \nabla_y [f(\hat{y}_{\theta}(x); x)], \end{aligned} \quad (2.11)$$

where the last step is obtained by the chain rule. This has the interpretation that the model’s parameters θ are updated by combining

the gradient information around the prediction $\nabla_y [f(\hat{y}_\theta(x); x)]$ shown in Figure 2.2 along with how θ impacts the model's predictions with the derivative $D_\theta [\hat{y}_\theta(x)]$. While this tutorial mostly focuses on optimizing Eq. (2.11) with first-order methods that explicitly differentiate the objective, Section 2.2.3 discusses alternatives to optimizing it with reinforcement learning and zeroth-order methods.

Objective-based methods thrive when the gradient information is informative and the objective and models are easily differentiable. Amortized variational inference methods and actor-critic methods both make extensive use of objective-based learning.

Remark 2.2. A standard gradient-based optimizer for Eq. (1.1) (without amortization) can be recovered from \mathcal{L}_{obj} by setting the model to the identity of the parameters, *i.e.* $\hat{y}_\theta(x) := \theta$, and $p(x)$ to be a Dirac delta distribution.

This can be seen by taking $D_\theta [\hat{y}_\theta(x)] = I$ in Eq. (2.11), resulting in $\nabla_\theta \mathcal{L}_{\text{obj}} (\hat{y}_\theta) = \nabla_y f(\hat{y}_\theta(x); x)$. Thus optimizing θ of this parameter-identity model with gradient descent is identical to solving Eq. (1.1) with gradient descent. Remark 2.2 shows a connection between a model trained with gradients of an objective-based loss and a non-amortized gradient-based solver for Eq. (1.1). The gradient update that would originally have been applied to an iterate $y \in \mathcal{Y}$ of the domain is now transferred into the model's parameters that are shared across all problem instances. This also leads to a hypothesis that objective-based amortization works best when a gradient-based optimizer is able to successfully solve Eq. (1.1) from scratch. However there may be settings where a gradient-based optimizer performs poorly but an amortized optimizer excels because it is able to use information from the other problem instances.

Remark 2.3. The objective-based loss in Section 2.2.1 provides a starting point for amortizing with other optimality conditions or reformulations of the optimization problem. This is done when amortizing for fixed-point computations and convex optimization in Section 3.4, as well as in optimal transport Section 3.5.

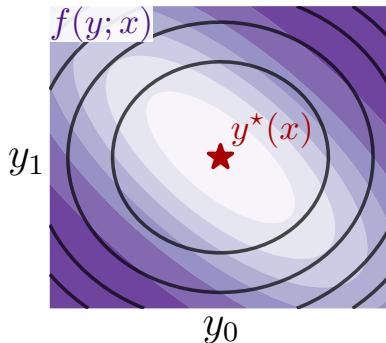


Figure 2.3: Contours of the regression-based amortization loss \mathcal{L}_{reg} (in black) alongside the contours of the objective (in purple where darker colors indicate higher values). This shows the inaccuracies of the regression-based loss, *e.g.* along a level set, may impact the overall objective differently.

Comparing the regression- and objective-based losses

Choosing between the regression- and objective-based losses is challenging as they measure the solution quality in different ways and have different convergence and locality properties. Liu *et al.* (2022) experimentally compare these losses for learning to optimize with fully-amortized set-based models. Figure 2.3 illustrates that the ℓ_2 -regression loss (the black contours) ignores the objective values (the purple contours) and thus gives the same loss to solutions that result in significantly different objective values. This could be potentially addressed by normalizing or re-weighting the dimensions for regression to be more aware of the curvature of the objective, but this is often not done. Another idea is to combine both the objective and regression losses. Combining the losses could work especially well when only a few contexts are labeled, such as the regression and residual terms in the physics-informed neural operator paper (Li *et al.*, 2021b). The following summarizes some other advantages (+) and disadvantages (-):

Regression-based losses \mathcal{L}_{reg}

- Often does not have access to $f(y; x)$
- + If $f(y; x)$ is computationally expensive, does not need to compute it
- + Uses global information with $y^*(x)$

- It may be expensive to compute $y^*(x)$
- + Does not need to compute $\nabla_y f(y; x)$
- May be hard when $y^*(x)$ is not unique

Objective-based losses \mathcal{L}_{obj}

- + Uses objective information of $f(y; x)$
- Can get stuck in local optima of $f(y; x)$
- + Faster, does not require $y^*(x)$
- Often requires computing $\nabla_y f(y; x)$
- + Easily learns non-unique $y^*(x)$

2.2.2 Learning iterative semi-amortized models

Fully-amortized or semi-amortized models can be learned with the regression- and objective-based losses. This section discusses how the loss can be further opened up and crafted to learn iterative semi-amortized methods. For example, if the model produces intermediate predictions \hat{y}_θ^i in every iteration i , then instead of optimizing the loss of just the final prediction, *i.e.* $\mathcal{L}(\hat{y}_\theta^K)$, a more general loss \mathcal{L}^Σ may consider the impact of every iteration of the model's prediction

$$\arg \min_{\theta} \mathcal{L}^\Sigma(\hat{y}_\theta) \quad \mathcal{L}^\Sigma(\hat{y}_\theta) := \sum_{i=0}^K w_i \mathcal{L}(\hat{y}_\theta^i), \quad (2.12)$$

where $w_i \in \mathbb{R}_+$ are weights in every iteration i that give a design choice of how important it is for the earlier iterations to produce reasonable solutions. For example, setting $w_i = 1$ encourages every iterate to be low.

Learning iterative semi-amortized methods also has (loose) connections to sequence learning models that arise in, *e.g.* text, audio, and language processing. Given the context x , an iterative semi-amortized model seeks to produce a sequence of predictions that ultimately result in the intermediate and final predictions, which can be analogous to a language model predicting future text given the previous text as context. One difference is that semi-amortized models do not necessarily attempt to model the probabilistic dependencies of a structured output space

(such as language) and instead only needs to predict intermediate computation steps for solving an optimization problem. The next section discusses concepts that arise when computing the derivatives of a loss with respect to the model’s parameters.

Unrolled optimization and backpropagation through time

$$\hat{z}_\theta^0 \rightarrow \hat{z}_\theta^1 \rightarrow \cdots \rightarrow \hat{z}_\theta^K \rightarrow \hat{y}_\theta(x) \rightarrow \mathcal{L}$$

The parameterization of *every* iterate z_θ^i can influence the final prediction \hat{y}_θ and thus losses on top of \hat{y}_θ need to consider the entire chain of computations. Differentiating through this kind of iterative procedure is referred to as *backpropagation through time* in sequence models and *unrolled optimization* (Pearlmutter and Siskind, 2008; Zhang and Lesser, 2010; Maclaurin *et al.*, 2015b; Belanger and McCallum, 2016; Metz *et al.*, 2017; Finn *et al.*, 2017; Han *et al.*, 2017; Belanger *et al.*, 2017; Belanger, 2017; Foerster *et al.*, 2017; Bhardwaj *et al.*, 2020; Monga *et al.*, 2021) when the iterates are solving an optimization problem. The term “unrolling” arises because the model computation is iterative and computing $D_\theta[\hat{y}_\theta(x)]$ requires saving and differentiating the “unrolled” intermediate iterations, as in Section 2.1.2. The terminology “unrolling” here emphasizes that the iterative computation produces a compute graph of operations and is likely inspired from *loop unrolling* in compiler optimization (Aho *et al.*, 1986; Davidson and Jinturkar, 1995) where loop operations are inlined for efficiency and written as a single chain of repeated operations rather than an iterative computation of a single operation.

Even though $D_\theta \hat{y}_\theta$ through unrolled optimization is well-defined, in practice it can be unstable because of exploding gradients (Pearlmutter, 1996; Pascanu *et al.*, 2013; Maclaurin, 2016; Parmas *et al.*, 2018) and inefficient for compute and memory resources because every iterate needs to be stored, as in Section 2.1.2. This is why most methods using unrolled optimization for learning often only unroll through *tens* of iterations (Metz *et al.*, 2017; Belanger *et al.*, 2017; Foerster *et al.*, 2017; Finn *et al.*, 2017) while solving the problems from scratch may

require 100k-1M+ iterations. This causes the predictions to be extremely inaccurate solutions to the optimization process and has sparked the research directions that the next section turns to that seek to make unrolled optimization more tractable.

Truncated backpropagation through time and biased gradients

$$\hat{z}_\theta^0 \rightarrow \hat{z}_\theta^1 \rightarrow \dots \rightarrow \hat{z}_\theta^{K-H} \rightarrow \dots \rightarrow \hat{z}_\theta^K \rightarrow \hat{y}_\theta(x) \rightarrow \mathcal{L}$$

Truncated backpropagation through time (TBPTT) (Werbos, 1990; Jaeger, 2002) is a crucial idea that has enabled the training of sequence models over long sequences. TBPTT's idea is that not every iteration needs to be differentiated through and that the derivative can be computed using smaller subsequences from the full sequence of model predictions by truncating the history of iterates. For example, the derivative of a model running for K iterations with a truncation length of H can be approximated by considering the influence of the last H iterates $\{\hat{z}_\theta^i\}_{i=K-H}^H$ on the loss \mathcal{L} .

Truncation significantly helps improve the computational and memory efficiency of unrolled optimization procedure but results in harmful *biased gradients* as these approximate derivatives do not contain the full amount of information that the model used to compute the prediction. This is especially damaging in approaches such as MAML (Finn *et al.*, 2017) that *only* parameterize the first iterate and is why MAML-based approaches often don't use TBPTT. Tallec and Ollivier (2017), Wu *et al.* (2018), Liao *et al.* (2018), Shaban *et al.* (2019), and Vicol *et al.* (2021) seek to further theoretically understand the properties of TBPTT, including the bias of the estimator and how to unbias it.

Other gradient estimators for sequential models

In addition to truncating the iterations, other approaches attempt to improve the efficiency of learning through unrolled iterations with other approximations that retain the influence of the entire sequence of predictions on the loss (Finn *et al.*, 2017; Nichol *et al.*, 2018; Lorraine

et al., 2020) which will be further discussed in Section 2.1.2. Some optimization procedures, such as gradient descent with momentum, can also be “reversed” without needing to retain the intermediate states (Maclaurin *et al.*, 2015b; Franceschi *et al.*, 2017). *Real-Time Recurrent Learning* (RTRL) by Williams and Zipser (1989) uses forward-mode automatic differentiation to compute unbiased gradient estimates in an online fashion. *Unbiased Online Recurrent* (UORO) by Tallec and Ollivier (2018) improves upon RTRL with a rank-1 approximation of the gradient of the hidden state with respect to the parameters. Silver *et al.* (2022) considers the directional derivative of a recurrent model along a candidate direction, which can be efficiently computed to construct a descent direction.

Semi-amortized learning with shrinkage and implicit differentiation

A huge issue arising in semi-amortized models is that adapting to long time horizons is computationally and memory inefficient and even if it wasn’t, causes exploding, vanishing, or otherwise unstable gradients. An active direction of research seeks to solve these issues by solving a smaller, local problem with the semi-amortized model, such as in Chen *et al.* (2020) and Rajeswaran *et al.* (2019). Implicit differentiation is an alternative to unrolling through the iterations of a semi-amortized model in settings where the model is able to successfully solve an optimization problem.

This section briefly summarizes *Implicit MAML* (iMAML) by Rajeswaran *et al.* (2019), which notably brings this insight to MAML. MAML methods usually only take a few gradient steps and are usually not enough to globally solve Eq. (1.1), especially at the beginning of training. Rajeswaran *et al.* (2019) observe that adding a penalty to the objective around the initial iterate \hat{y}_θ^0 makes it easy for the model to *globally* (!) solve the problem

$$\hat{y}_\theta(x) \in \arg \min_y f(y; x) + \frac{\lambda}{2} \|y - \hat{y}_\theta^0\|_2^2, \quad (2.13)$$

where the parameter λ encourages the solution to stay close to some initial iterate. Figure 2.4 visualizes a function $f(y; x)$ in black and add penalties in grey with $\lambda \in [0, 12]$ and see that a global minimum is

difficult to find without adding a penalty around the initial iterate. This global solution can then be implicitly differentiated to obtain a derivative of the loss with respect to the model's parameters *without* needing to unroll, as it requires significantly less computational and memory resources. Huszár (2019) further analyzes and discusses iMAML. They compare it to a Bayesian approach and observe that the insights from iMAML can transfer from gradient-based meta-learning to other amortized optimization settings.

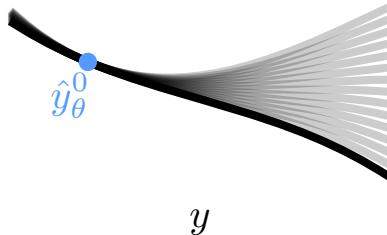


Figure 2.4: Illustration of the penalty used in the Implicit MAML by Rajeswaran *et al.* (2019) in Eq. (2.13). The original loss $f(y; x)$ is shown in black for a fixed context x and the lighter grey colors show the impact of varying λ . This shows that the quadratic term of the penalization eventually overtakes the original loss and makes an optimum appear close to \hat{y}_θ^0

Warning. Implicit differentiation is only useful when optimization problems are exactly solved and satisfy the conditions of the implicit function theorem in Theorem 2.1. This is why Rajeswaran *et al.* (2019) needed to add a penalty to MAML's inner optimization problem in Eq. (2.13) to make the problem exactly solvable. While they showed that this works and results in significant improvements for differentiation, it comes at the expense of changing the objective to penalize the distance from the previous iterate. In other words, iMAML modifies MAML's semi-amortized model and in general is not helpful for estimating the derivative through the original formulation of MAML. Furthermore, computing the implicit derivative by solving the linear system with the Jacobian in Eq. (2.30) may be memory and compute expensive to form and estimate exactly. In practice, some methods such as Bai *et al.* (2019) successfully use indirect and approximation methods to solve for the system in Eq. (2.30).

2.2.3 Learning with zeroth-order methods and reinforcement learning

Computing the derivatives to learn \hat{y}_θ with a first-order method may be impossible or unstable. These problems typically arise when learning components of the model that are truly non-differentiable, or when attempting to unroll a semi-amortized model for a lot of steps. In these settings, research has successfully explored other optimizers that do *not* need the gradient information. These methods often consider settings that improve an objective-based loss with small local perturbations rather than differentiation. Figure 2.5 illustrates that most of these methods can be interpreted as locally perturbing the model’s prediction and updating the parameters to move towards the best perturbations.

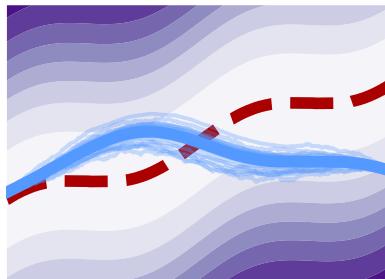


Figure 2.5: Illustration of perturbing \hat{y}_θ . A zeroth-order optimizers may make perturbations like this to search for an improved parameterization

Reinforcement learning

Li and Malik (2017a), Li and Malik (2017b), and Ichnowski *et al.* (2021) view their semi-amortized models as a Markov decision process (MDP) that they solve with reinforcement learning. The MDP interpretation uses the insight that the iterations x^i are the actions, the context and previous iterations or losses are typically the states, the associated losses $\mathcal{L}(x^i)$ are the rewards, and $\hat{y}_\theta^i(x)$ is a (deterministic) policy, and transitions given by updating the current iterate, either with a quantity defined by the policy or by running one or more iterations from an existing optimizer. Once this viewpoint is taken, then the optimal amortized model can be found by using standard reinforcement learning

methods, *e.g.* Li and Malik (2017a) and Li and Malik (2017b) uses Guided Policy Search (Levine and Koltun, 2013) and Ichnowski *et al.* (2021) uses TD3 (Fujimoto *et al.*, 2018). The notation \mathcal{L}^{RL} indicates that a loss is optimized with reinforcement learning, typically on the objective-based loss.

Loss smoothing and optimization with zeroth-order methods

Objective-based losses can have a high-frequency structure with many poor local minimum. Metz *et al.* (2019a) overcome this by smoothing the loss with a Gaussian over the *parameter space*, *i.e.*,

$$\mathcal{L}^{\text{smooth}}(\hat{y}_\theta) := \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \sigma^2 I)} [\mathcal{L}(\hat{y}_{\theta+\epsilon})], \quad (2.14)$$

where σ^2 is a fixed variance. Figure 2.6 illustrates a loss function \mathcal{L} in black and shows smoothed versions in color. They consider learning the loss with reparameterization gradients and zeroth-order evolutionary methods. Merchant *et al.* (2021) further build upon this for learned optimization in atomic structural optimization and study 1) clipping the values of the gradient estimator, and 2) parameter optimization with genetic algorithms.

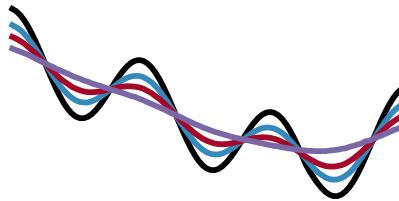


Figure 2.6: Gaussian smoothing of a loss using Eq. (2.14). The colors show different values of the variance σ^2 of the Gaussian. Selecting a high enough variance results in smoothing out most of the suboptimal minima.

Remark 2.4. While smoothing can help reduce suboptimal local minima, it may also undesirably change the location of the global minimum. One potential solution to this is to decay the smoothing throughout training, as done in Amos *et al.* (2021, Appendix A.1).

Connection to smoothing in reinforcement learning. The Gaussian smoothing of the objective \mathcal{L} in Eq. (2.14) is conceptually

similar to Gaussian smoothing of the objective in reinforcement learning, *i.e.* the $-Q$ -value, by a Gaussian policy. This happens in Eq. (3.39) and is further discussed in Section 3.6. The policy’s variance is typically controlled to match a target entropy (Haarnoja *et al.*, 2018) and the learning typically starts with a high variance so the policy has a broad view of the objective landscape and is then able to focus in on an optimal region of the value distribution. Amos *et al.* (2021) uses a fixed entropy decay schedule to explicitly control this behavior. In contrast, Metz *et al.* (2019a) and Merchant *et al.* (2021) do not turn the loss into a distribution and more directly smooth the loss with a Gaussian with a fixed variance σ^2 that is not optimized over.

2.3 Extensions

I have intentionally scoped Definition 2.1 to optimization problems over *deterministic, unconstrained, finite-dimensional, Euclidean* domains \mathcal{Y} where the context distribution $p(x)$ remains *fixed* the entire training time to provide a simple mental model that allows us to focus on the core amortization principles that consistently show up between applications. This section covers extensions from this setting that may come up in practice.

2.3.1 Extensions of the domain \mathcal{Y}

Deterministic \rightarrow stochastic optimization

A crucial extension is from optimization over deterministic vector spaces \mathcal{Y} to *stochastic optimization* where \mathcal{Y} represents a space of distributions, turning $y \in \mathcal{Y}$ from a vector in Euclidean space into a distribution. This comes up in Section 3.6 for control, for example.

Transforming parameterized stochastic problems back into deterministic ones. This portion will mostly focus on settings that optimize over the parametric distributions. This may arise in stochastic domains for variational inference in Section 3.1 and stochastic control in Section 3.6. These settings optimize over a constrained parametric family of distributions parameterized by some λ , for example over a multivariate normal $\mathcal{N}(\mu, \Sigma)$ parameterized by $\lambda := (\mu, \Sigma)$. Here,

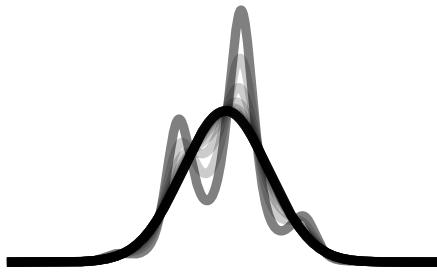


Figure 2.7: The Gaussian distribution can be characterized as the result of the optimization problem in Eq. (2.16): constrained to the space of continuous distributions with a given mean and variance, the Gaussian distribution has the maximum entropy in comparison to every other distribution. This example parameterizes a non-Gaussian density (shown in grey) and optimizes over it using gradient steps of Eq. (2.16), eventually converging to a Gaussian. An animated version is available [in the repository associated with this tutorial](#). While the Gaussian is the known closed-form solution to this optimization problem and analytically known, more general optimization problems over densities without known solutions can also be amortized.

problems can be transformed back to Eq. (1.1) by optimizing over the parameters with

$$\lambda^*(x) \in \arg \min_{\lambda} f(\lambda; x), \quad (2.15)$$

where λ induces a distribution that the objective f may use. When λ is not an unconstrained real space, the differentiable projections discussed in Section 2.3.1 could be used to transform λ back into this form for amortization.

Optimizing over distributions and densities. More general stochastic optimization settings involve optimizing over spaces representing distributions, such as the functional space of all continuous densities. Many standard probability distributions can be obtained and characterized as the solution to a maximum entropy optimization problem and is explored, *e.g.*, in Cover and Thomas (2006, Ch. 12), Guiasu and Shenitzer (1985, p. 47), and Pennec (2006, p. 6.2). For example, a Gaussian distribution $\mathcal{N}(\mu, \Sigma)$ solves the following constrained maximum entropy optimization problem over the space of continuous densities \mathcal{P} :

$$p^*(\mu, \Sigma) \in \arg \max_{p \in \mathcal{P}} \mathbb{H}_p[X] \text{ subject to } \mathbb{E}_p[X] = \mu \text{ and } \text{Var}_p[X] = \Sigma, \quad (2.16)$$

where $\mathbb{H}_p[X] := - \int p(x) \log p(x) dx$ is the *differential entropy* and the constraints are on the mean $\mathbb{E}_p[X]$ and covariance $\text{Var}_p[X]$. Figure 2.7 visualizes an example of Eq. (2.16). Cover and Thomas (2006, Theorem 8.6.5 and Example 12.2.8) prove that the closed-form solution of p^* is the Gaussian density. This Gaussian setting therefore does not need amortization as the closed-form solution is known and easily computed, but more general optimization problems over densities do not necessarily have closed-form solutions and could benefit from amortization. While this tutorial does not study amortizing these problems, in some cases it may be possible to again transform them back into deterministic optimization problems over Euclidean space for amortization by approximating the density g_θ with an expressive family of densities parameterized by θ .

Unconstrained → constrained optimization

Amortized constrained optimization problems may naturally arise, for example in the convex optimization settings in Section 3.4 and for optimization over the sphere in Section 4.2. Constrained optimization problems for amortization can often be represented as an extension of Eq. (1.1) with

$$y^*(x) \in \arg \min_{y \in \mathcal{C}} f(y; x), \quad (2.17)$$

where the constraints \mathcal{C} may also depend on the context x . Remark 2.3 suggests one way of amortizing Eq. (2.17) by amortizing the objective-based loss associated with the optimality conditions of the constrained problem. A budding research area studies how to more generally include constraints into the formulation. Baker (2019), Dong *et al.* (2020), Zamzam and Baker (2020), and Pan *et al.* (2020) learn to warm-start for optimal power flow. Misra *et al.* (2021) learn active sets for constrained optimization. Kriváčhy *et al.* (2020) solves constrained feasibility semi-definite programs with a fully-amortized neural network model using an objective-based loss. Donti *et al.* (2021) learns a fully-amortized model and optimizes an objective-based loss with additional completion and correction terms to ensure the prediction satisfies the constraints of the original problem.

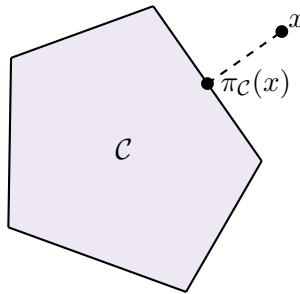


Figure 2.8: Illustration of Definition 2.4 showing a Euclidean projection $\pi_{\mathcal{C}}(x)$ of a point x onto a set \mathcal{C} .

Differentiable projections. When the constraints are relatively simple, a differentiable projection can transform a constrained optimization problem into an unconstrained one, *e.g.*, in reinforcement learning constrained action spaces can be transformed from the box $[-1, 1]^n$ to the reals \mathbb{R}^n by using the tanh to project from \mathbb{R}^n to $[-1, 1]^n$. Section 4.2 also uses a differentiable projection from \mathbb{R}^n onto the sphere \mathcal{S}^{n-1} . These are illustrated in Figure 2.8 and defined as:

Definition 2.4. A *projection* from \mathbb{R}^n onto a set $\mathcal{C} \subseteq \mathbb{R}^n$ is

$$\pi_{\mathcal{C}} : \mathbb{R}^n \rightarrow \mathcal{C} \quad \pi_{\mathcal{C}}(x) \in \arg \min_{y \in \mathcal{C}} D(x, y) + \Omega(y), \quad (2.18)$$

where $D : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ is a distance and $\Omega : \mathbb{R}^n \rightarrow \mathbb{R}$ is a regularizer that can ensure invertibility or help spread \mathbb{R}^n more uniformly throughout \mathcal{C} . A *(sub)differentiable projection* has (sub)derivatives $\nabla_x \pi_{\mathcal{C}}(x)$. I sometimes omit the dependence of π on the choice of D , Ω , and \mathcal{C} when they are given by the surrounding context.

Lack of idempotency. In linear algebra, a projection is defined to be *idempotent*, *i.e.* applying the projection twice gives the same result so that $\pi \circ \pi = \pi$. Unfortunately, projections as defined in Definition 2.4, such as Bregman projections, are *not* idempotent in general and often $\pi_{\mathcal{C}} \circ \pi_{\mathcal{C}} \neq \pi_{\mathcal{C}}$ as the regularizer Ω may cause points that are already on \mathcal{C} to move to a different position on \mathcal{C} .

Differentiable projections for constrained amortization. These can be used to cast Eq. (2.17) as the unconstrained problem Eq. (1.1) by composing the objective with a projection $f \circ \pi_{\mathcal{C}}$.

(Sub)differentiable projections enable gradient-based learning through the projection and is the most easily attainable when the projection has an explicit closed-form solution. For intuition, the ReLU, sigmoid, and softargmax can be interpreted as differentiable projections that solve convex optimization problems in the form of Eq. (2.18). Amos (2019, p. 2.4.4) further discusses these and proves them using the KKT conditions:

- The standard Euclidean projection onto the *non-negative orthant* \mathbb{R}_+^n is defined by

$$\pi(x) \in \arg \min_y \frac{1}{2} \|x - y\|_2^2 \text{ s.t. } y \geq 0, \quad (2.19)$$

and has a closed-form solution given by the ReLU, *i.e.* $\pi(x) := \max\{0, x\}$.

- The interior of the *unit hypercube* $[0, 1]^n$ can be projected onto with the entropy-regularized optimization problem

$$\pi(x) \in \arg \min_{0 < y < 1} -x^\top y - H_b(y), \quad (2.20)$$

where

$$H_b(y) := \left(\sum_i y_i \log y_i + (1 - y_i) \log(1 - y_i) \right) \quad (2.21)$$

is the binary entropy function. Eq. (2.20) has a closed-form solution given by the *sigmoid* or *logistic* function, *i.e.* $\pi(x) := (1 + e^{-x})^{-1}$.

- The interior of the $(n - 1)$ -*simplex* defined by

$$\Delta_{n-1} := \{p \in \mathbb{R}^n \mid 1^\top p = 1 \text{ and } p \geq 0\} \quad (2.22)$$

can be projected onto with the entropy-regularized optimization problem

$$\pi(x) \in \arg \min_{0 < y < 1} -x^\top y - H(y) \text{ s.t. } 1^\top y = 1 \quad (2.23)$$

where $H(y) := -\sum_i y_i \log y_i$ is the entropy function. Eq. (2.23) has a closed-form solution given by the *softargmax*, *i.e.* $\pi(x)_j = e^{x_j} / \sum_i e^{x_i}$, which is historically referred to as the *softmax*.

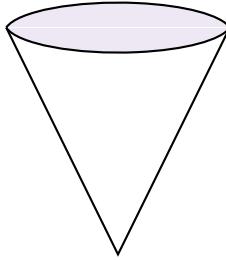


Figure 2.9: Illustration of the second-order cone in Eq. (2.24).

This section goes beyond these to differentiable projections onto *convex cones*. These can also be softened or regularized to help with continuity when composed with learning and amortization methods. Ali *et al.* (2017) and Busseti *et al.* (2019) discuss differentiating the standard Euclidean projections onto these, including:

- The *second-order, Lorentz, or ice cream cone* defined by

$$\mathcal{K}_{\text{soc}} := \{(x, y) \in \mathbb{R}^{m-1} \times \mathbb{R} : \|x\|_2 \leq y\}, \quad (2.24)$$

which is illustrated in Figure 2.9. The standard Euclidean projection is given in closed form as

$$\pi(x, y) := \begin{cases} 0 & \|x\|_2 \leq -y \\ (x, y) & \|x\|_2 \leq y \\ \frac{1}{2}(1 + \frac{y}{\|x\|_2})(x, \|x\|_2) & \text{otherwise.} \end{cases} \quad (2.25)$$

and can be explicitly differentiated.

- The *positive semidefinite cone* \mathcal{S}_+^m of the space of $m \times m$ positive semidefinite matrices. The Euclidean projection is obtained in closed-form by projecting the eigenvalues to be non-negative with $\pi(X) := \sum_i \max\{\lambda_i, 0\} q_i q_i^\top$, where the eigenvalue decomposition of X is given by $X = \sum_i \lambda_i q_i q_i^\top$. The derivative can be computed by differentiating through the eigenvalue decomposition and projection of the eigenvalues.
- The *exponential cone* is given by

$$\begin{aligned} \mathcal{K}_{\text{exp}} = & \{(x, y, z) : x \in \mathbb{R}, y > 0, z \geq y \exp(x/y)\} \\ & \cup \{(x, 0, z) : x \leq 0, z \geq 0\}. \end{aligned} \quad (2.26)$$

The standard Euclidean projection onto this does *not* have a known closed-form solution but can be computed using a Newton method as discussed in Parikh and Boyd (2014, p. 6.3.4). Ali *et al.* (2017) differentiate through this projection using implicit differentiation of the KKT system.

Other uses of projections in machine learning include:

- Adams and Zemel (2011), Cruz *et al.* (2017), and Mena *et al.* (2018) project onto the *Birkhoff polytope* of *doubly stochastic* matrices with row and column sums of 1, *i.e.*

$$\mathcal{B}_m := \{X \in \mathbb{R}^{m \times m} : X\mathbf{1} = X^\top \mathbf{1} = \mathbf{1}\}. \quad (2.27)$$

- Amos *et al.* (2019) project onto the capped simplex for a differentiable top- k layer.
- Blondel (2019) perform structure prediction and learning methods building on Fenchel-Young losses (Blondel *et al.*, 2020) and use projections onto the simplex, unit cube, knapsack polytope, Birkhoff polytope, permutohedron, and order simplex.

In many of these, the projections have explicit closed-form solutions that make it easy to compute and differentiate through the projections for learning. When a closed-form solution to the projection is not available to the project, but the projection can be numerically computed, projections can often still be differentiated through using implicit differentiation.

Euclidean → non-Euclidean optimization

Manifold optimization (Absil *et al.*, 2009; Hu *et al.*, 2019) over non-Euclidean spaces is a thriving topic in optimization as these problems arise frequently over complex geometries in nature. One form of manifold optimization takes \mathcal{Y} to be a Riemannian manifold rather than a real-valued spaced. This area of research has studied acceleration methods, (Duruisseaux and Leok, 2022), but less exploration has been done on amortized optimization. Section 4.2 discusses amortizing a simple

constrained spherical optimization problem that can be transformed into an unconstrained Euclidean optimization problem by using projections from ambient Euclidean space. When this is not possible, a budding area of research investigates more directly including the manifold structure into the amortization process. Gao *et al.* (2020) amortize optimization problems over SPD spaces.

2.3.2 Extensions of the model \hat{y}_θ

Finding the best model for an amortized optimization setup is an active research topic in many areas. While the tutorial is mostly scoped to differentiable parametric models that are end-to-end learned, variations and extensions can be considered.

Symbolic models: uncovering human-interpretable update rules

A huge issue of neural-network based amortization models is that they are uninterpretable and it is often impossible for us as humans to learn any new insights about the optimization problems being modeled, *e.g.* how to better-solve them. Symbolic models are one potential answer to this that attempt to search over a symbolic space that is much closer to the operations that humans would use to implement update rules for an optimization solver. Early studies of these methods include Bengio *et al.* (1994) and Runarsson and Jonsson (2000). Bello *et al.* (2017) significantly advances this direction by posing the learned optimizer as a reinforcement learning problem where the actions produce the operations underlying the update rules. They show how existing methods can be symbolically implemented using this formulation, and learn better update rules for classification and machine translation tasks. Symbolic methods are further studied and scaled in Real *et al.* (2020) and Zheng *et al.* (2022). Maheswaranathan *et al.* (2021) reverse engineer learned optimizers and show that they have learned interpretable behavior, including momentum, gradient clipping, learning rate schedules, and learning rate adaptation.

This direction of work challenges the best accelerated and adaptive gradient-based optimizers that are used for machine learning. Nesterov acceleration (Nesterov, 1983) has a provably optimal convergence rate

among first-order methods for solving convex optimization problems, but unfortunately breaks down in the non-convex setting. This has led to a stream of variations of acceleration methods for non-convex problems that come up in machine learning, such as Duchi *et al.* (2010), Zeiler (2012), and Kingma and Ba (2015), that typically add components that adapt the update rules to how much the objective is moving in each dimension. None of these algorithms are theoretically or provably the best in non-convex settings, and is often empirically validated depending on the domain. Using amortized optimization with a symbolic model to search the design space of optimizers can result in significantly better optimizers and insights into the optimization problems being solved, especially when this is done on new classes of problems beyond the parameter learning problems typically considered in machine learning settings.

2.3.3 Uncertainty-aware and Bayesian optimization

An active research direction combines *uncertainty* estimation and amortized optimization.

Amortization for Bayesian optimization. Chen *et al.* (2017) propose to use an RNN-based amortization in Bayesian optimization settings that predict the optimal solution to commonly used acquisition functions such as the expected improvement and observed improvement. This is powerful as optimizing the acquisition function is often a computational bottleneck. Swersky *et al.* (2020) consider amortized Bayesian optimization in discrete spaces and show applications to protein sequence design. Ravi and Beatson (2019) propose amortized Bayesian meta-learning for meta-learning with uncertainty estimation over the posterior and show applications to contextual bandits and few-shot learning.

Bayesian methods for amortization. You *et al.* (2022) investigate *optimizer uncertainty* or *Bayesian learning to optimize*. This setting explores the uncertainty that an optimizer, *e.g.* the amortization model, is the best optimizer for the problem.

2.3.4 Settings with additional learnable contexts φ

The amortization model is often a component within a larger system with other learnable parameters that are being optimized over. This is done in, for example, 1) variational autoencoders where the ELBO also depends on the decoder's parameters that are also being optimized over, 2) deep equilibrium models where the fixed point is parameterized and optimized over, and 3) reinforcement learning where the value estimate is also parameterized and learned over.

These dependencies can be captured by writing an explicit dependence of the context distribution and objective on an additional parameter φ , *i.e.* as $p(x; \varphi)$ and $f(y; x, \varphi)$. φ can be learned with a higher-level optimization process with a loss ℓ defined on the *solutions*. This could take the form of the bi-level problem

$$\arg \min_{\varphi} \mathbb{E}_{x \sim p(x)} \ell(y^*(x, \varphi); x, \varphi) \text{ subject to } y^*(x, \varphi) \in \arg \min_y f(y; x, \varphi) \quad (2.28)$$

where $y^*(x, \varphi)$ can be replaced with an approximation by a learned amortization model $\hat{y}_\theta \approx y^*$. The parameters φ in Eq. (2.28) can often be end-to-end learned *through the solution* of Eq. (1.1) to update the influence that φ has on the solutions. The next section turns to methods that show how to differentiate through the value $f(y^*(x, \varphi); x, \varphi)$ and solution $y^*(x, \varphi)$ to enable gradient-based learning of φ in Eq. (2.28).

Learning φ by differentiating the objective value $f(y^*(x, \varphi); x, \varphi)$

Methods can end-to-end learn through the *optimal objective value* $f(y^*(x, \varphi); x, \varphi)$ to update parameters φ that show up in the context — *i.e.* by taking $\ell = f$ in Eq. (2.28). For example, variational autoencoders differentiate through the objective value, *i.e.* the best approximation to the ELBO, to optimize the data log-likelihood of a parameterized decoder $\log p(x | z; \varphi)$. The theory around this is rooted in the optimization community's studies of *envelope theorems*, which describe settings where the minimum value can be differentiated by just differentiating the objective. *Danskin's envelope theorem* (Danskin, 1966) in convex settings is one of the earliest and has been extended into more general settings, *e.g.*, in (Bertsekas, 1971, Prop. A.22) and Carter, 2001; Mil-

grom and Segal, 2002; Bonnans and Shapiro, 2013. In the unconstrained and non-convex Eq. (1.1), the envelope theorem gives

$$\nabla_\varphi \min_y f(y; x, \bar{\varphi}) = \nabla_\varphi f(y^*(x, \bar{\varphi}); x, \bar{\varphi}) \quad (2.29)$$

at a point $\bar{\varphi}$ under mild assumptions, showing that differentiating through the min operation is equivalent to differentiating through just the objective at the optimal solution $y^*(x, \varphi)$.

Learning φ by differentiating the solution $y^*(x, \varphi)$

In addition to differentiating through the objective value, the solution $y^*(x, \varphi)$ can be implicitly differentiated. The derivative $D_\varphi y^*(x, \varphi)$ is referred to as the *adjoint derivative*, and it is often used for end-to-end learning (Domke, 2012; Gould *et al.*, 2016; Amos and Kolter, 2017; Barratt, 2018; Amos, 2019; Agrawal *et al.*, 2019a; Bai *et al.*, 2019; Bai *et al.*, 2020) and perturbation and sensitivity analysis (Bank *et al.*, 1982; Fiacco and Ishizuka, 1990; Shapiro, 2003; Klatte and Kummer, 2006; Bonnans and Shapiro, 2013; Still, 2018; Fiacco, 2020).

Computing the adjoint derivative $D_\varphi y^*(x, \varphi)$ is more involved than the value derivative using the envelope theorem in Eq. (2.29) as more components of $y^*(x)$ can change as x moves infinitesimally. An explicit closed-form solution to $y^*(x)$ is not available in most cases, which means that standard methods for explicitly computing the derivative through this computation may not work well or may break down. For example, an optimizer to compute $y^*(x)$ may be explicitly unrolled through, but this may be unstable and extremely memory- and compute-intensive to track all of the iterations. The adjoint derivative is typically computed with implicit differentiation by seeing $y^*(x)$ as an *implicit* function of x . This uses the implicit function theorem, which is originally from Dini (1878), and is presented in Dontchev and Rockafellar (2009, Theorem 1B.1).

Theorem 2.1 (Dini's implicit function theorem). Let the roots of $g(y; \varphi)$ define an implicit mapping $Y^*(\varphi)$ given by $Y^*(\varphi) := \{y \mid g(y; \varphi) = 0\}$, where $\varphi \in \mathbb{R}^m$, $y \in \mathbb{R}^n$, and $g : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n$. Let g be continuously differentiable in a neighborhood of $(\bar{y}; \bar{\varphi})$ such that $g(\bar{y}; \bar{\varphi}) = 0$, and

let the Jacobian of g with respect to y at $(\bar{y}, \bar{\varphi})$, *i.e.* $D_y g(\bar{y}; \bar{\varphi})$, be non-singular. Then Y^* has a single-valued localization y^* around $\bar{\varphi}$ for \bar{y} which is continuously differentiable in a neighborhood Q of $\bar{\varphi}$ with Jacobian satisfying

$$D_\varphi y^*(\tilde{\varphi}) = -D_y^{-1} g(y^*(\tilde{\varphi}); \tilde{\varphi}) D_\varphi g(y^*(\tilde{\varphi}); \tilde{\varphi}) \quad \text{for every } \tilde{\varphi} \in Q. \quad (2.30)$$

The adjoint derivative $D_\varphi y^*(\varphi)$ can be computed by seeing y^* as the root of an implicit function $g(y; x, \varphi)$, which needs to be selected to make the solution equivalent to the solution of Eq. (1.1). Typically $g(y; x, \varphi)$ is an optimality system of the optimization problem, *e.g.* the KKT system for constrained convex optimization problems. For the unconstrained problem here, the first-order optimality of the objective $g(y; x, \varphi) := \nabla_y f(y; x, \varphi)$ can be used with Theorem 2.1 to compute $D_\varphi y^*(x, \varphi)$.

3

Applications of Amortized Optimization

This section takes a review and tour of many key applications of amortized optimization to show some unifying ideas that can be shared between all of these topics. Table 3.1 summarizes the methods. The subsections in here are meant to be standalone and can be randomly accessed and read in any order. I scope closely to providing the relevant context for just the amortized optimization components and under-emphasize the remaining context of each research area.

Warning. Even though I try to provide the relevant background and notation to present the amortized optimization components, each section is meant to be a review rather than an introduction to these research topics. I defer further background to the original literature.

3.1 Variational Inference and Variational Autoencoders

Key ideas in amortized optimization originated in the variational inference (VI) community’s interest in approximating intractable densities and integrals via optimization. This section focuses only on the relevant components of amortized variational inference (AVI) used in machine learning for the variational autoencoder (VAE) and related generative models (Kingma and Welling, 2014; Rezende *et al.*, 2014; Mnih and

Table 3.1: Applications of amortized optimization covered in Section 3

\S	Application	Objective f	Domain \mathcal{Y}	Context Space \mathcal{X}	Amortization model \hat{g}_θ	Loss \mathcal{L}
3.1	VAE SAVAE/IVAE	– ELBO 	variational posterior 	data 	full semi	\mathcal{L}_{obj}
3.2	PSD LISTA	reconstruction 	sparse code 	data 	full semi	\mathcal{L}_{reg}
3.3	HyperNets LM MAML Neural Potts	task loss pseudo-likelihood	model parameters 	tasks protein sequences	full semi full	\mathcal{L}_{obj} $\mathcal{L}_{\text{RL}}^{\text{obj}}$ \mathcal{L}_{obj} \mathcal{L}_{obj}
3.4	NeuralFP HyperAA NeuralSCS HyperDEQ NeuralNMF RLQP	FP residual CP residual DEQ residual NMF residual R_{RLQP}	FP iterates CP iterates DEQ iterates factorizations QP iterates	FP contexts CP parameters DEQ parameters input matrices QP parameters	semi 	$\mathcal{L}_{\text{obj}}^\Sigma$ $\mathcal{L}_{\text{reg}}^\Sigma$ $\mathcal{L}_{\text{obj}}^\Sigma$ $\mathcal{L}_{\text{reg}}^\Sigma$ $\mathcal{L}_{\text{obj}}^\Sigma$ $\mathcal{L}_{\text{RL}}^{\text{obj}}$
3.5	Meta OT CondOT AmorConj A -SW	dual OT cost dual OT cost c -transform obj max-sliced dist	optimal couplings optimal couplings $\text{supp}(\alpha)$ slices Θ	input measures contextual information $\text{supp}(\beta)$ mini-batches	full 	\mathcal{L}_{obj} \mathcal{L}_{obj} \mathcal{L}_{obj} \mathcal{L}_{obj}
3.6	BC/IL (D)DPG/TD3 PILCO POPLIN DCEM IAPO SVG SAC GPS	$-Q$ -value D_Q or $-\mathcal{E}_Q$ 	controls control dists	state space 	full full or semi semi full 	\mathcal{L}_{reg} \mathcal{L}_{obj} \mathcal{L}_{obj} \mathcal{L}_{reg} \mathcal{L}_{reg} \mathcal{L}_{obj} \mathcal{L}_{obj} \mathcal{L}_{obj} \mathcal{L}_{KL}

Gregor, 2014; Rezende and Mohamed, 2015; Higgins *et al.*, 2017; Doersch, 2016; Kingma and Welling, 2019) and refer to references such as Jordan *et al.* (1999), Wainwright and Jordan (2008), and Blei *et al.* (2017) for a complete background in variational inference. Kim (2020) and Marino (2021) provide additional background on the use of amortization and semi-amortization in these settings. Historically, the use of an encoder network for amortized inference is often traced back to the Helmholtz machine (Dayan *et al.*, 1995), which uses a fully-amortized model but without a proper gradient estimator. Sjölund (2023) provides further background information and a tutorial on parametric variational inference.

3.1.1 The variational autoencoder (VAE) by Kingma and Welling (2014)

A VAE models a density $p(x)$ over a high-dimensional space, for example images, text, or videos, given samples $x \sim p(x)$. They introduce a lower-dimensional latent space with a known distribution $p(z)$, such as an isotropic Gaussian, designed to capture hidden structure present in $p(x)$. VAEs parameterize a likelihood model $p(x; \varphi)$ with φ . Optimizing the log-likelihood $\log p(x; \varphi) = \log \int_z p(x | z; \varphi)p(z)dz$ with this latent structure is typically intractable because of the integral over the latent space. Variational methods overcome this by introducing a tractable lower-bound called the *evidence lower bound* (ELBO) defined by

$$\log p(x; \varphi) \geq \text{ELBO}_\varphi(\lambda; x) := \mathbb{E}_{q(z; \lambda)} [\log p(x | z; \varphi)] - D_{\text{KL}}(q(z; \lambda) || p(z)), \quad (3.1)$$

where $q(z; \lambda)$ is a variational distribution over the latent space parameterized by λ and $p(z)$ is the prior. Given a sample $x \sim p(x)$ and fixed encoder's parameters φ the *best* lower bound λ^* satisfying

$$\log p(x) \geq \text{ELBO}_\varphi(\lambda^*; x) \geq \text{ELBO}_\varphi(\lambda; x) \quad (3.2)$$

for all λ can be obtained by solving the optimization problem

$$\lambda_\varphi^*(x) \in \arg \max_{\lambda} \text{ELBO}(\lambda; x, \varphi). \quad (3.3)$$

Gaussians are a common choice of the variational distribution $q(z; \lambda)$ in Kingma and Welling (2014), but may cause a loose inequality in Eq. (3.2). Rezende and Mohamed (2015) and Cremer *et al.* (2018) explore more expressive distributions to help make $\text{ELBO}(\lambda^*; x, \varphi)$ equal to $\log p(x)$.

Amortized VI (AVI) methods predict the solution to Eq. (3.3) while stochastic variational methods (Hoffman *et al.*, 2013) explicitly solve it. AVI methods learn a model $\hat{\lambda}_\theta : \mathcal{X} \rightarrow \Lambda$ with parameters θ , which is usually a feedforward neural network, to predict the maximum value of the ELBO by optimizing the objective-based loss

$$\arg \max_{\theta} \mathbb{E}_{x \sim p(x)} \text{ELBO}_\varphi(\hat{\lambda}_\theta(x); x) \quad (3.4)$$

where the expectation is usually approximated with a Monte Carlo estimate from the samples.

Summary. This standard AVI formulation is therefore an amortized optimization method $\mathcal{A}_{\text{VAE}} := (-\text{ELBO}, \Lambda, \mathcal{X}, p(x), \hat{\lambda}_\theta, \mathcal{L}_{\text{obj}})$ over the (negated) ELBO where the domain of the optimization problem is the variational parameter space Λ , the context space \mathcal{X} is the sample space for the generative model, the samples are given from $p(x)$, $\hat{\lambda}_\theta : \mathcal{X} \rightarrow \Lambda$ is the *fully-amortized* model optimized with the gradient-based loss \mathcal{L}_{obj} over $-\text{ELBO}$.

Extensions. Analyzing and extending the amortization components has been a key development in AVI methods. Cremer *et al.* (2018) investigate suboptimality in these models and categorize it as coming from an *amortization gap* where the amortized model for Eq. (3.4) does not properly solve it, or the *approximation gap* where the variational posterior is incapable of approximating the true distribution. Semi-amortization plays a crucial role in addressing the amortization gap and is explored in the semi-amortized VAE (SAVAE) by Kim *et al.* (2018) and iterative VAE (IVAE) by Marino *et al.* (2018b). AVI methods are also used in hierarchical (Sønderby *et al.*, 2016) and sequential settings (Chung *et al.*, 2015).

The full VAE loss. This section has left the parameterization φ of the model $p(x; \varphi)$ fixed to allow us to scope into the amortized optimization component in isolation. For completeness, the final step necessary to train a VAE is to optimize the ELBO over the training data of *both* $p(x; \varphi)$ along with the $\hat{\lambda}_\theta(x)$ with

$$\arg \max_{\varphi, \theta} \mathbb{E}_{x \sim p(x)} \text{ELBO}_\varphi(\hat{\lambda}_\theta(x); x). \quad (3.5)$$

3.2 Sparse Coding

Another early appearance of amortized optimization has been in sparse coding (Kavukcuoglu *et al.*, 2010; Gregor and LeCun, 2010). The connection to the broader amortized optimization and learning to optimize work has also been made by, *e.g.*, Chen *et al.* (2021a). *Sparse coding methods* seek to reconstruct an input from a sparse linear combination of bases (Olshausen and Field, 1996; Chen *et al.*, 2001; Donoho and Elad,

2003). Given a *dictionary* W_d of the basis vectors and an input $x \in \mathcal{X}$, the *sparse code* y^* is typically recovered by solving the optimization problem

$$y^*(x) \in \arg \min_y E(y; x) \quad E(y; x) := \frac{1}{2} \|x - W_d y\|_2^2 + \alpha \|y\|_1, \quad (3.6)$$

where E is the regularized reconstruction energy and $\alpha \in \mathbb{R}_+$ is a coefficient of the ℓ_1 term. Eq. (3.6) is traditionally solved with the Iterative Shrinkage and Thresholding Algorithm (ISTA) such as in Daubechies *et al.* (2004). Fast ISTA (FISTA) by Beck and Teboulle (2009) improves ISTA even more by adding a momentum term. The core update of ISTA methods is

$$y^{t+1} := h_\beta \left(W_e x + S y^t \right) \quad (3.7)$$

$W_e := (1/L)W_d^\top$ is the *filter matrix*, L is an *upper bound on the largest eigenvalue* of $W_d^T W_d$, $S := I - W_e W_d$ is the *mutual inhibition matrix*, and $h_\beta(v) := \text{sign}(v) \max \{0, |v| - \beta\}$ is the *shrinkage function* with threshold β , usually set to α/L . ISTA methods are remarkably fast ways of solving Eq. (3.6) and the machine learning community has explored the use of learning to make ISTA methods even faster that can be seen as instances of amortized optimization.

3.2.1 Predictive Sparse Decomposition (PSD) by Kavukcuoglu *et al.* (2010)

PSD predicts the best sparse code using fully-amortized models of the form

$$\hat{y}_\theta(x) := D \tanh(Fx), \quad (3.8)$$

where the parameters are $\theta = \{D, F\}$. Then, given a distribution over vectors $p(x)$, PSD regresses the prediction onto the true sparse code $y^*(x)$ by solving

$$\arg \min_\theta \mathbb{E}_{x \sim p(x)} \|\hat{y}_\theta(x) - y^*(x)\|_2^2, \quad (3.9)$$

where instead of solving for $y^*(x)$ directly with (F)ISTA, they also iteratively approximate it while iteratively learning the model.

Summary. $\mathcal{A}_{\text{PSD}} := (E, \mathcal{Y}, \mathcal{X}, p(x), \hat{y}_\theta, \mathcal{L}_{\text{reg}})$

3.2.2 Learned ISTA (LISTA) by Gregor and LeCun (2010)

LISTA further explores the idea of predicting solutions to sparse coding problems by proposing a semi-amortized model that integrates the iterative updates of ISTA into the model. LISTA leverages the soft-thresholding operator h and considers a semi-amortized model over the domain \mathcal{Y} that starts with $x_\theta^0 := 0$ and iteratively updates $x_\theta^{t+1} := h_\beta(Fx + Gx_\theta^t)$. Running these updates for K steps results in a final prediction $\hat{y}(x) := x_\theta^K$ parameterized by $\theta = \{F, G, \beta\}$ that is also optimized with the regression-based loss to the ground-truth sparse codes as in Eq. (3.9).

Summary. $\mathcal{A}_{\text{LISTA}} := (E, \mathcal{Y}, \mathcal{X}, p(x), \hat{y}_\theta, \mathcal{L}_{\text{reg}})$

3.3 Multi-task Learning and Meta-learning

Many multi-task learning and meta-learning methods also use amortized optimization for parameter learning. This section takes a glimpse at this viewpoint, which has also been observed before in Shu (2017) and Gordon *et al.* (2019).

Background. *Multi-task learning* (Caruana, 1997; Ruder, 2017) methods use shared representations and models to learn multiple tasks simultaneously. *Meta-learning* methods (Ward, 1937; Harlow, 1949; Schmidhuber, 1987; Kehoe, 1988; Schmidhuber, 1995; Thrun and Pratt, 1998; Baxter, 1998; Hochreiter *et al.*, 2001; Vilalta and Drissi, 2002; Lv *et al.*, 2017; Li and Malik, 2017a; Li and Malik, 2017b; Lake *et al.*, 2017; Weng, 2018; Hospedales *et al.*, 2020) seek to learn how to learn and are often used in multi-task settings. Multi-task and meta-learning settings typically define *learning tasks* $\mathcal{T} \sim p(\mathcal{T})$ that each consist of a classification or regression task. The tasks could be different hyper-parameters of a model, different datasets that the model is trained on, or in some cases different samples from the same dataset. Each task has an associated *task loss* $\mathcal{L}_{\mathcal{T}}(\hat{y}_\theta)$ that measures how well a parameterized model \hat{y}_θ performs on it. There is typically a distribution over tasks $p(\mathcal{T})$ and the goal is to find a model that best-optimizes the expectation over task losses by solving

$$\arg \min_{\theta} \mathbb{E}_{\mathcal{T} \sim p(\mathcal{T})} \mathcal{L}_{\mathcal{T}}(\hat{y}_\theta). \quad (3.10)$$

The motivation here is that there is likely shared structure and information present between the tasks that learning methods can leverage. The next section goes through methods that solve Eq. (3.10) using objective-based amortized optimization methods.

3.3.1 Fully-amortized hyper networks (HyperNets)

HyperNEAT (Stanley *et al.*, 2009) and Hypernetworks (Ha *et al.*, 2017) predict the optimal parameters to a network given a data sample and can be seen as fully-amortized optimization. The tasks here $\mathcal{T} = (x, y^*(x))$ usually consist of a sample from some data distribution $x \sim p(x)$ along with a target $y^*(x)$ for classification or regression, inducing a task distribution $p(\mathcal{T})$. HyperNets propose to predict $y^*(x)$ with a *prediction model* $\hat{y}_\varphi(x)$ parameterized by φ . Instead of learning this model directly, they propose to use an *amortization model* $\hat{\varphi}_\theta(x) \in \Phi$ to predict the parameters to the model $\hat{y}_{\hat{\varphi}_\theta(x)}(x) =: \hat{y}_\theta(x)$ that best-optimize the *task loss* $\mathcal{L}_{\mathcal{T}}(\hat{y}_\theta(x), y^*(x))$ for each data point. The amortization model is usually a black-box neural network that is fully-amortized and predicts the parameters from only the task's data without accessing the task loss. The models are learned with an objective-based loss

$$\arg \min_{\theta} \mathbb{E}_{\mathcal{T} \sim p(\mathcal{T})} \mathcal{L}_{\mathcal{T}}(\hat{y}_\theta(x), y^*(x)). \quad (3.11)$$

Summary. $\mathcal{A}_{\text{HyperNet}} := (\mathcal{L}_{\mathcal{T}}, \Phi, \mathcal{T}, p(\mathcal{T}), \hat{\varphi}_\theta, \mathcal{L}_{\text{obj}})$

3.3.2 Learning to optimize (LM) by Li and Malik (2017a)

Li and Malik (2017a) consider three multi-task settings for logistic regression, robust linear regression, and neural network classification where the different tasks are different datasets the models are trained on. Given a dataset $\mathcal{T} = \{x_i, y_i\}_{i=1}^N$ to train on, they again search for the parameters $\hat{\varphi}_\theta(\mathcal{T}) \in \Phi$ of another prediction model $\hat{y}_{\hat{\varphi}_\theta(\mathcal{T})}(x) =: \hat{y}_\theta(x)$ that performs well on a loss $\mathcal{L}_{\mathcal{T}}(\hat{y}_\theta)$ that measures how well the model fits to the dataset. In contrast to HyperNets, LM consider each task to be an entire dataset rather than just a single data point, and LM considers semi-amortized models that are able to iteratively refine the

prediction. They use a semi-amortized model that starts with an initial iterate $\hat{\varphi}_\theta^0(\mathcal{T})$ and then predicts the next iterate with

$$\hat{\varphi}_\theta^{t+1} = g_\theta(\{\varphi^i, \mathcal{L}_{\mathcal{T}}(\hat{\varphi}^i), \nabla_{\varphi} \mathcal{L}_{\mathcal{T}}(\hat{\varphi}^i), \Delta^i\}), \quad (3.12)$$

where the update model g_θ takes the last $i \in \{t - H, \dots, t\} \cap \mathcal{Z}_{\geq 0}$ iterates as the input, along with the objective, gradient, and objective improvement as auxiliary information. This model generalizes methods such as gradient descent that would just use the previous iterate and gradient. The experiments use $H = 25$ and typically run the model updates for 100 iterations. They want to learn the model with an objective-based loss here and take the viewpoint that it can be seen as an MDP that can be solved with the guided policy search (Levine and Koltun, 2013) method for reinforcement learning. Li and Malik (2017b) further develops these ideas for learning to optimize neural network parameters.

Summary. $\mathcal{A}_{\text{LM}} := (\mathcal{L}_{\mathcal{T}}, \Phi, \mathcal{T}, p(\mathcal{T}), \hat{\varphi}_\theta, \mathcal{L}_{\text{obj}}^{\text{RL}})$

3.3.3 Model-agnostic meta-learning (MAML) by Finn et al. (2017)

As discussed in Section 2.1.2, MAML can be seen as a semi-amortized optimization method. They also seek to predict the parameters $\hat{\varphi}_\theta(\mathcal{T}) \in \Phi$ of prediction model $\hat{y}_{\hat{\varphi}_\theta(\mathcal{T})}(x) =: \hat{y}_\theta(x)$ in a multi-task setting with tasks $\mathcal{T} \sim p(\mathcal{T})$. They propose to only learn to predict an initial iterate $\hat{\varphi}_\theta^0(\mathcal{T}) = \theta$ and then update the next iterates with gradient-based updates such as

$$\hat{\varphi}_\theta^{t+1} = \varphi_\theta^t - \alpha \nabla_{\varphi} \mathcal{L}_{\mathcal{T}}(\hat{\varphi}_\theta^t), \quad (3.13)$$

where $\mathcal{L}_{\mathcal{T}}(\varphi)$ is the task loss obtained by the model \hat{y}_φ parameterized by φ . MAML optimizes this model with an objective-based loss through the final prediction.

Summary. $\mathcal{A}_{\text{MAML}} := (\mathcal{L}_{\mathcal{T}}, \Phi, \mathcal{T}, p(\mathcal{T}), \hat{\varphi}_\theta, \mathcal{L}_{\text{obj}})$

3.3.4 Protein MSA modeling with the Neural Potts Model

Sercu et al. (2021) proposes a fully-amortized solution to fit a Potts model to a protein's multiple sequence alignment (MSA). Each task consists of a finite MSA $\mathcal{M} := \{x_i\}$ and they use a fully-amortized model

$\varphi_\theta(\mathcal{M}) \in \Phi$ to predict the optimal parameters of a Potts model $p(\mathcal{M}; \varphi)$ fit to the data. The model φ_θ is a large attention-based sequence model that takes the MSA as the input. Learning is done with the objective-based loss

$$\arg \min_{\theta} \mathbb{E}_{\mathcal{M} \sim p(\mathcal{M})} \mathcal{L}_{\text{PL}}(\varphi_\theta(\mathcal{M})) \quad (3.14)$$

to optimize the *pseudolikelihood* \mathcal{L}_{PL} of the Potts model.

Sercu *et al.* (2021) surprisingly observes that amortization results in better solutions than the classical method for the Potts model parameter optimization with a finite MSA. They refer to this as the *inductive gain* and attribute it to the fact that they only have a finite MSA from each protein and thus amortizing effectively shares information between proteins

Summary. $\mathcal{A}_{\text{NeuralPotts}} = (\mathcal{L}_{\text{PL}}, \Phi, \mathcal{M}, p(\mathcal{M}), \hat{\varphi}_\theta, \mathcal{L}_{\text{obj}})$

3.3.5 Other relevant multi-task and meta-learning work

The literature of multi-task learning and meta-learning methods is immense and often build on the preceding concepts. The following selectively summarizes a few other relevant ideas:

1. Ravi and Larochelle (2017) also propose optimization-based semi-amortized models that use a recurrent neural network to predict parameter updates for meta-learning in multi-task learning settings.
2. Latent embedding optimization (LEO) by Rusu *et al.* (2019) and fast context adaptation (CAVIA) by Zintgraf *et al.* (2019) perform semi-amortization over a learned latent space. This uses the powerful insight that semi-amortizing over the low-level parameters φ had a lot of redundancies and may not be able to easily capture task-specific variations that can be learned in a latent space.
3. Andrychowicz *et al.* (2016) consider semi-amortized models based on recurrent neural networks and show applications to amortizing quadratic optimization, neural networks for MNIST and CIFAR-10 classification, and neural style transfer.

4. Chen *et al.* (2017) consider RNN-based semi-amortized models in settings where the gradient of the objective is not used as part of the model and show applications in Bayesian optimization, Gaussian process bandits, control, global optimization, and hyperparameter tuning.
5. Wichrowska *et al.* (2017) continue studying RNN-based semi-amortized models for classification. They scale to Inception V3 (Szegedy *et al.*, 2016) and ResNet V2 (He *et al.*, 2016) architectures and scale to classification tasks on ImageNet (Russakovsky *et al.*, 2015), presenting many insightful ablations along the way.
6. Franceschi *et al.* (2018) further analyze the bilevel optimization aspects of gradient-based meta-learning and present new theoretical convergence results and empirical demonstrations.
7. MetaOptNet (Lee *et al.*, 2019b) and R2D2 (Bertinetto *et al.*, 2019) consider semi-amortized models based on differentiable optimization and propose to use differentiable SVMs and ridge regression as part of the amortization model.
8. Almost No Inner Loop by Raghu *et al.* (2020) study what parameters should be adapted within the amortization model and demonstrate settings where adapting only the final layer performs well, indicating that the shared model between tasks works well because it is learning shared features for all the tasks to use.
9. Wang *et al.* (2021) further connect gradient-based meta learning methods to multi-task learning methods.
10. HyperTransformer (Zhmoginov *et al.*, 2022) study amortized models based on transformers (Vaswani *et al.*, 2017) and show applications to few-shot classification.
11. Metz *et al.* (2021) study and emphasize the difficulty of optimizing objective-based loss with just gradient information due to natural chaotic-based failure models of the amortization model. They focus on iterated dynamical systems and study where chaotic losses

arise in physics and meta-learning. They identify the spectrum of the Jacobian as one source of these issues and give suggestions for remedying these undesirable behaviors to have learning systems that are well-behaved and stable.

12. Metz *et al.* (2019b) learn optimizers for robust classification tasks. They find that optimizers can uncover ways of quickly finding robust parameterizations that generalize to settings beyond the corruptions used during training.
13. Metz *et al.* (2019a) study semi-amortized optimization of convolutional architectures and identify and focus on key issues of 1) biased gradients from truncated BPTT and 2) exploding gradient norms from unrolling for many timesteps. They overcome both of these issues by optimizing the smoothed loss in Eq. (2.14) with a variant of the gradient estimator proposed in Parmas *et al.* (2018) for reinforcement learning. This estimator re-weights reparameterization gradients and likelihood ratio gradients using inverse variance weighting (Fleiss, 1993). Parmas and Sugiyama (2021) further unify the likelihood ratio and reparameterization gradients by connecting them with the divergence theorem which enables them to create a generalized estimator combining them.
14. Merchant *et al.* (2021) further build on the advancements of Metz *et al.* (2019a) for semi-amortized atomic structural optimization, which is a setting rife with poor local minima. Their models learn to “hop” out of these minima and are able to generalize more efficiently to new elements or atomic compositions.
15. Zhang *et al.* (2019a) and Knyazev *et al.* (2021) explore the fully-amortized HyperNets for architecture search for predicting parameters on CIFAR-10 and ImageNet. These models take a model’s compute graph as the context and use a graph neural network to predict the optimal parameters of that architecture on a task.
16. Huang *et al.* (2022) show how to use information from existing classes of “teacher” optimizers to learn a new “student” one that can result in even better performance, which they refer to

as *optimizer amalgamation*. This is done by optimizing for the objective-based loss with additional regression-based terms that encourage the learned optimizer to match one or more trajectories of the existing optimizers.

17. Harrison *et al.* (2022) look at the stability of learned optimization methods from a dynamical systems perspective and propose a number of modifications to improve the stability and generalization.
18. Metz *et al.* (2022) continue scaling a semi-amortized learned optimizer that predicts parameter updates for training machine learning models with millions of parameters. They train the optimizer for four thousand ATP-months and show that it outperforms many standard parameter optimization methods on standard learning tasks. One standout feature is that their amortization model does not assume a fixed-size context or prediction space but instead is able to predict updates for models with varying numbers of parameters. The key insight to supporting a variable number of parameters is to decompose the amortization model across parameter groups using an LSTM and hyper-network.

3.4 Fixed-point Computations and Convex Optimization

Definition 3.1. A *fixed point* $y^* \in \mathbb{R}^n$ of a map $g : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is where $g(y^*) = y^*$.

Continuous fixed-point problems as in Definition 3.1 and illustrated in Figure 3.1 are ubiquitous in engineering and science and amortizing their solutions is an active research area. Let $\mathcal{R}(y; x) := g(y; x) - y$ be the *fixed-point residual* with squared norm $\mathcal{N}(y; x) := \|\mathcal{R}(y; x)\|_2^2$. Fixed-point computations are connected to continuous unconstrained optimization as any fixed-point problem can be transformed into Eq. (1.1) by optimizing the residual norms with:

$$y^*(x) \in \arg \min_y \mathcal{N}(y; x), \quad (3.15)$$

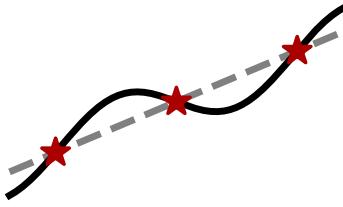


Figure 3.1: Illustration of the fixed points of a map $f(x)$. The map is shown in black and the fixed points (red stars) are where the map is equal to the identity (shown in grey), *i.e.* $f(x) = x$.

and conversely Eq. (1.1) can be transformed into a fixed-point problem via first-order optimality to find the fixed-point of $\nabla f(y; x) - y = 0$. Thus methods that amortize the solutions to Eq. (1.1) can help amortize the solutions to fixed-point computations Definition 3.1.

Solving and accelerating fixed-point computations. Fixed points can be found with *fixed-point iterations* $y^{t+1} := f(y^t)$ or by using *Newton's root-finding method* on the fixed-point residuals with

$$y^{t+1} := y^t - \left(D_y g(y^t) \right)^{-1} g(y^t). \quad (3.16)$$

These methods can also be *accelerated* by using a sequence of past iterates instead of just the most recent iterate. *Anderson acceleration* methods (Anderson, 1965; Walker and Ni, 2011; Zhang *et al.*, 2020) are standard and generate updates that combine the previous $M + 1$ iterates $\{y^i\}_{i=t-M}^t$ with an update of the form

$$\text{AA_Update}^t(\{y_i\}, \alpha, \beta) := \beta \sum_{i=0}^M \alpha_i g(y^{t-M+i}) + (1 - \beta) \sum_{i=0}^M \sum_{j=0}^M \alpha_i y^{t-M+j}, \quad (3.17)$$

where $\beta \in [0, 1]$ is a coefficient that controls whether the iterates or application of g on the iterates should be used, and $\alpha \in \mathbb{R}^{M+1}$ where $1^\top \alpha = 1$ are the coefficients used to combine the previous iterates. A basic AA method sets $\beta = 1$ and solves

$$\alpha^* := \arg \min_{\alpha} \|\mathcal{R}(y^i)\alpha\|_2 \text{ subject to } 1^\top \alpha = 1 \quad (3.18)$$

for $i \in \{t - M, t\}$ with least squares. Other methods such as *Broyden's method* (Broyden, 1965) can also accelerate fixed-point computations by turning them into root-finding problems.

3.4.1 Neural fixed-point acceleration (**NeuralFP**) and conic optimization with the splitting cone solver (**NeuralSCS**)

Neural fixed-point acceleration (Venkataraman and Amos, 2021) proposes a semi-amortized method for computing fixed-points and use it for convex cone programming. Representing a latent state at time t with \hat{h}^t , they parameterize the initial iterate $(\hat{y}^0, \hat{h}^0) = \text{init}_\theta(x)$ with an *initialization model* init_θ and perform the fixed-point computations

$$\begin{aligned}\tilde{x}^{t+1} &= f(\hat{y}^t; x) \\ (\hat{y}^{t+1}, \hat{h}^{t+1}) &= \text{acc}_\theta(\hat{y}^t, \tilde{x}^{t+1}, \hat{h}^t)\end{aligned}\tag{3.19}$$

using an *acceleration model* acc_θ that is typically a recurrent model that predicts the next iterate given the past sequence of iterates. Venkataraman and Amos (2021, Prop. 1) discuss how this model captures standard AA as an instance by setting the models equal to the standard update that doesn't use learning. They learn this model to amortize Eq. (3.15) over a distribution of contexts $p(x)$ with an objective-based loss that solves

$$\arg \min_{\theta} \mathbb{E}_{x \sim p(x)} \sum_{t=0}^K \mathcal{N}(\hat{y}_\theta^t(x)),\tag{3.20}$$

where the fixed-point residual norm \mathcal{N} is scaled by a context-specific *normalization factor*.

NeuralSCS (Venkataraman and Amos, 2021) applies this neural fixed-point acceleration to solve *constrained convex cone programs* solved by the splitting cone solver (SCS) (O'Donoghue *et al.*, 2016) of the form

$$\begin{array}{lll}\text{minimize } c^T x & \text{maximize } -b^T y \\ \text{s. t. } Ax + s = b & \text{s. t. } -A^T y + r = c \\ (x, s) \in \mathbb{R}^n \times \mathcal{K} & (r, y) \in \{0\}^n \times \mathcal{K}^*\end{array}\tag{3.21}$$

where $x \in \mathbb{R}^n$ is the primal variable, $s \in \mathbb{R}^m$ is the primal slack variable, $y \in \mathbb{R}^m$ is the dual variable, and $r \in \mathbb{R}^n$ is the dual residual. The set $\mathcal{K} \in \mathbb{R}^m$ is a non-empty convex cone with dual cone $\mathcal{K}^* \in \mathbb{R}^m$. where $x \in \mathbb{R}^n$ is the primal variable, $s \in \mathbb{R}^m$ is the primal slack variable, $y \in \mathbb{R}^m$ is the dual variable, and $r \in \mathbb{R}^n$ is the dual residual. The set $\mathcal{K} \in \mathbb{R}^m$ is a non-empty convex cone. SCS uses the *homogeneous*

self-dual embedding to view Eq. (3.21) as a fixed-point computation over $\mathcal{Z} = \mathbb{R}^{n \times m \times 1}$ with a scalar-valued scaling factor as the last component.

NeuralSCS proposes a semi-amortized model to predict the solution to the fixed point of the self-dual embedding that solves Eq. (3.21). Their semi-amortized model $\hat{z}_\theta(\phi)$ takes a context ϕ as the input and outputs a solution to the self-dual embedding by composing the SCS iterations f with the learned fixed-point acceleration modules $(\text{init}_\theta, \text{acc}_\theta)$.

Summary. $\mathcal{A}_{\text{NeuralSCS}} := (\mathcal{N}, \mathcal{Z}, \phi, p(\phi), \hat{z}_\theta, \mathcal{L}_{\text{obj}}^\Sigma)$

3.4.2 Neural acceleration for matrix factorization (NeuralNMF)

Sjölund and Bänkestad (2022) use semi-amortized neural acceleration to find low-rank factorizations of an input matrix V of the form:

$$V \approx WH^\top, \quad W \geq 0, H \geq 0, \quad (3.22)$$

where the basis matrix $W \in \mathbb{R}^{m \times r}$ and mixture matrix $H \in \mathbb{R}^{n \times r}$ are elementwise non-negative matrices of rank $r \leq \min(m, n)$. Let $Z = (W, H)$. Taking the norm of the residual of Eq. (3.22) leads to the optimization formulation

$$Z^*(V) \in \arg \min_{W, H \geq 0} \mathcal{N}_{\text{NMF}}(W, H; V) \quad \mathcal{N}_{\text{NMF}}(W, H; V) := \frac{1}{2} \|WH^\top - V\|_F^2, \quad (3.23)$$

which can be solved with ADMM (Boyd *et al.*, 2011) using alternating steps on H and V as done in Huang *et al.* (2016). Given a distribution over input matrices V , Sjölund and Bänkestad (2022), augment the ADMM approach from Huang *et al.* (2016) with transformer-based initialization and acceleration modules. This semi-amortized model is learned with an objective-based loss and unrolls through the ADMM iterations for learning.

Summary. $\mathcal{A}_{\text{NeuralNMF}} := (\mathcal{N}_{\text{NMF}}, \mathcal{Z}, V, p(V), \hat{Z}_\theta, \mathcal{L}_{\text{obj}}^\Sigma)$

3.4.3 HyperAnderson acceleration and deep equilibrium models (HyperDEQ)

Bai *et al.* (2022) similarly proposes a semi-amortized method for computing fixed-points and use it to improve *Deep equilibrium (DEQ)*

models (Bai *et al.*, 2019; Bai *et al.*, 2020; Gurumurthy *et al.*, 2021). Their learned variant of AA, called *HyperAnderson acceleration* uses models that predict the initial point $\hat{y}_\theta^0(x)$ and coefficients $\alpha_\theta(x; G)$ and $\beta_\theta(x; G)$ and result in iterations of the form

$$G_\theta^{t+1}, \hat{y}_\theta^{t+1} := \text{AA_Update}(\{\hat{y}_\theta^t\}, \alpha_\theta^t(x; G_\theta^t), \beta_\theta^t(x; G_\theta^t)), \quad (3.24)$$

where $G^t := \mathcal{R}(x^t)$ is the fixed-point residual at iteration t and the model's final prediction is $\hat{y}_\theta(x) := x^K$. Learning is performed by optimizing a summed regression-based loss that encourages the fixed-point iterations to converge as fast as possible by optimizing

$$\arg \min_{\theta} \mathcal{L}_{\text{HyperAA}}(\hat{y}_\theta) \quad \mathcal{L}_{\text{HyperAA}}(\hat{y}_\theta) := \mathbb{E}_{x \sim p(x)} \sum_{t=0}^K w_t \|y^* - \hat{y}_\theta^t\|_2^2 + \Omega(\alpha^t), \quad (3.25)$$

where Ω is a regularizer on α^t that is annealed to equal zero by the end of training and the weights (w_t) are set to be monotonically increasing to penalize the later iterations for not reaching the fixed point.

Deep equilibrium (DEQ) models (Bai *et al.*, 2019; Bai *et al.*, 2020) investigate implicit layers that parameterize and solve fixed-point computations and have been a flagship for “infinite depth” vision and language models. Given an input $x \in \mathcal{X}$, such as an image or language sequence to process, a DEQ model finds a fixed point $y^*(x)$ of $g_\varphi(y; x)$ to make a prediction for a task, such as regression or classification. This fixed-point problem can again be interpreted as finding the minimum norm of the residual $\mathcal{N}(y; x) := \|y - g_\varphi(y; x)\|_2^2$ as

$$y^*(x) \in \arg \min_x \mathcal{N}(y; x). \quad (3.26)$$

Bai *et al.* (2022) propose to use the HyperAnderson Acceleration model and loss to semi-amortize DEQs by learning the initial iterate and AA update coefficients, resulting in a setup of the form $\mathcal{A}_{\text{HyperDEQ}} := (\mathcal{N}, \mathcal{Y}, \mathcal{X}, p(x), \hat{y}_\theta, \mathcal{L}_{\text{HyperAA}})$.

3.4.4 Comparing NeuralFP and HyperAA

Neural fixed-point acceleration (NeuralFP) by Venkataraman and Amos (2021) and HyperAnderson Acceleration (HyperAA) by Bai *et al.* (2022)

can both generally be applied to semi-amortize fixed-point computations by parameterizing updates based on Anderson Acceleration, even though they are instantiated and evaluated on very different classes of fixed-point computations. Here is a brief comparison of the methods:

Neural fixed-point Acceleration

- Learn the initial iterate
- Learn the entire update
- Use an objective-based loss

HyperAnderson Acceleration

- Learn the initial iterate
- Learn α, β for the update
- Use an regression-based loss.

3.4.5 RLQP by Ichnowski et al. (2021)

RLQP (Ichnowski *et al.*, 2021) amortizes solutions to constrained convex quadratic optimization problems of the form

$$x^*(\phi) \in \arg \min_x \frac{1}{2} x^\top P x + q^\top x \text{ subject to } l \leq Ax \leq u, \quad (3.27)$$

where $x \in \mathbb{R}^n$ is the *domain* of the optimization problem and $\phi = \{P, q, l, A, u\}$ is the *context* or *parameterization* (from a larger space $\phi \in \Phi$) of the optimization problem with $P \succ 0$ (symmetric positive semi-definite). They build on the OSQP solver (Stellato *et al.*, 2018) for these optimization problems, which is based on operator splitting. Without over-relaxation, the core of OSQP uses updates that first solve the system

$$\begin{bmatrix} P + \sigma I & A^\top \\ A & -\text{diag}(\rho^t)^{-1} \end{bmatrix} \begin{bmatrix} x^{t+1} \\ v^{t+1} \end{bmatrix} = \begin{bmatrix} \sigma x^t - q \\ z^t - \text{diag}(\rho^t)^{-1} y^t \end{bmatrix} \quad (3.28)$$

and then updates

$$\begin{aligned} \tilde{z}^{t+1} &:= z^t + \text{diag}(\rho^t)^{-1}(v^{t+1} - y^t) \\ z^{t+1} &:= \Pi(\tilde{z}^{t+1} + \text{diag}(\rho^t)^{-1}y^t) \\ y^{t+1} &:= x^t + \text{diag}(\rho)(\tilde{z}^{t+1} - z^t + 1), \end{aligned} \quad (3.29)$$

where y, v are dual variables, z, \tilde{z} are auxiliary operator splitting variables, σ is a regularization parameter, and $\rho^t \in \mathbb{R}_+^m$ is a step-size parameter. Combining all of the variables into a state $s := (y, \lambda, \tilde{z}, z)$ living in $s \in \mathcal{S}$, the update can be written as $s^{t+1} := \text{OSQP_UPDATE}(s^t, \rho^t)$.

RLQP proposes to use these OSQP iterates as a semi-amortized model with the iterates $\{s^t, \rho^t\}$. They propose to only parameterize and learn to predict the step size $\rho^{t+1} := \pi_\theta(s^t)$, with a neural network amortization model π_θ . They model the process of predicting the optimal ρ as an MDP and define a reward $R_{\text{RLQP}}(s, \rho)$ that is -1 if the QP is not solved (based on thresholds of the primal and dual residuals) and 0 otherwise, *i.e.* each episode rolls out the OSQP iterations with a policy predicting the optimal step size. They solve this MDP with TD3 by Fujimoto *et al.* (2018) to find the parameters θ .

Summary. $\mathcal{A}_{\text{RLQP}} := (R_{\text{RLQP}}, \mathcal{S} \times \mathbb{R}_+^m, \Phi, p(\phi), \pi_\theta, \mathcal{L}_{\text{obj}}^{\text{RL}})$

3.5 Optimal Transport

Preliminaries. Optimal transport methods seek to optimally move mass between measures. Standard references and introductions include Villani (2009), Santambrogio (2015), and Peyré and Cuturi (2019), and this section concisely reviews key concepts. Given two measures (α, β) supported on spaces $(\mathcal{X}, \mathcal{Y})$, the *Kantorovich problem* (*e.g.* in Peyré and Cuturi (2019, Remark 2.13)) solves

$$\pi^\star(\alpha, \beta, c) \in \arg \inf_{\pi \in \mathcal{U}(\alpha, \beta)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y), \quad (3.30)$$

where the *coupling* π is joint distributions over the product of the measures, \mathcal{U} is the set of admissible couplings, c is a cost. The *dual* of Eq. (3.30), *e.g.* in Peyré and Cuturi (2019, Eq. 2.31), can be represented by

$$f^\star(\alpha, \beta, c) \in \arg \sup_f J(f) \quad (3.31)$$

where the *dual objective* is defined by

$$J(f) := \int_{\mathcal{X}} f(x) d\alpha(x) + \int_{\mathcal{Y}} f^c(y) d\beta(y) \quad (3.32)$$

over continuous dual potential functions $f : \mathcal{X} \rightarrow \mathbb{R}$ where

$$f^c(y) := \inf_x c(x, y) - f(x) \quad (3.33)$$

is the *c-transform* operation. In Euclidean spaces with the negative inner product cost (Villani, 2009, eq. 5.12), f is a convex function and the *c*-transform operation f^c in Eq. (3.33) is the standard Legendre-Fenchel transform, also known as the convex conjugate. When the measures α, β are discrete, a coupling π in the primal (Eq. (3.30)) can be represented as a matrix, and the potential f in the dual (Eq. (3.31)) can be represented as a finite-dimensional vector and solved with a linear programming formulation or Sinkhorn iterations (Cuturi, 2013) in the entropic setting.

The following sections overview methods that amortize these optimization problems arising for optimal transport. Section 3.5.1 discusses methods that amortize multiple OT problems and map from the measures and cost to the optimal coupling in Eq. (3.30) or duals in Eq. (3.31). Section 3.5.2 discusses methods that amortize the *c*-transform operation in Eq. (3.33) that arises as a repeatedly-solved subproblem when solving a single OT problem. Section 3.5.3 overviews amortizing a slicing optimization problem that arises when projecting measures down to a single dimension for more computationally efficient solves.

Remark 3.1. The Wasserstein GAN (WGAN) by Arjovsky *et al.* (2017) is not amortized optimization. While the continuous Wasserstein-1 potentials are estimated using samples from the generated and real data distributions, this is not performing amortized optimization because these potentials only optimize a single optimization transport problem between the generated and real data distributions. Changing the generated distribution indeed changes the optimal transport problem, but it's not important to solve the optimal transport problem between older generated distributions. The WGAN potentials during training can better be interpreted as warm-starting new optimal transport problems given by the generator's distribution.

3.5.1 Amortizing solutions to optimal transport problems

Many computational OT methods focus on computing the solution mapping from the measures and cost to the optimal coupling (Eq. (3.30)) or duals (Eq. (3.31)). When repeatedly solving optimal transport problems, this solution mapping is an optimization problem that can be amortized. These methods for predicting the optimal duals of OT problems are also related to Dinitz *et al.* (2021) and Khodak *et al.* (2022), which predicts the dual solutions to matching problems. They are also related to other heuristic-based initializations for OT problems that do not use amortization such as Thornton and Cuturi (2022).

Meta Optimal Transport by Amos *et al.* (2023)

Meta OT proposes to use a hypernetwork for this amortization. Here, they consider settings where there is a *meta-distribution* over the measures to couple and costs to use, *i.e.* $p(\alpha, \beta, c)$ and map directly from representations of the input measures and cost to the optimal dual variables, *i.e.* $f_\theta(\alpha, \beta, c)$. They instantiate this idea for optimal transport between discrete and continuous measures where the prediction f_θ warm-starts standard dual-based solvers and can then be mapped to the optimal primal coupling π^* .

Summary. $\mathcal{A}_{\text{MetaOT}} := (g, \mathcal{F}, \mathcal{P}(\mathcal{X} \times \mathcal{Y}) \times \mathcal{C}, \mathcal{D}, \mathcal{L}_{\text{obj}})$, where g is the dual objective, \mathcal{F} represents the space of dual potentials, *i.e.* $f \in \mathcal{F}$, $\mathcal{P}(\mathcal{X} \times \mathcal{Y})$ is a space of distributions over $\mathcal{X} \times \mathcal{Y}$ that α, β are sampled from, \mathcal{C} is a representation of the space of costs, and \mathcal{D} is a meta-distribution over α, β, c .

Conditional Optimal Transport by Bunne *et al.* (2022)

CondOT parameterizes a partially input-convex neural network (PICNN) (Amos *et al.*, 2017) to condition the amortized OT solution on contextual information. They focus primarily on the application of optimal transport in predicting the effect of drugs on cellular populations for patients. One of their key insights is to observe that OT problems need to be repeatedly solved in this setting for different combinations of drugs and patients. Instead of conditioning the amortization

model directly on the input measures, they condition it using auxiliary information about the patient and drug. This enables them to obtain an OT coupling and prediction of the drug effect even without knowing the target measure! Parameterizing their amortization model as a PICNN has connections to conditional neural processes (Garnelo *et al.*, 2018) and is especially useful for conditioning the high-dimensional potentials on the contextual information.

Summary. $\mathcal{A}_{\text{CondOT}} := (g, \mathcal{F}, \mathcal{Z}, \mathcal{D}, \mathcal{L}_{\text{obj}})$, where g is the dual objective, \mathcal{F} represents the space of dual potentials, *i.e.* $f \in \mathcal{F}$, \mathcal{Z} is contextual information for the OT problems, and \mathcal{D} is a meta-distribution over the contexts.

3.5.2 Amortized convex conjugates (**AmorConj**) and c -transforms

Most methods for computing the dual in Eq. (3.31) between a *single* pair of measures needs to repeatedly compute the c -transform in Eq. (3.33) to evaluate the objective value J in Eq. (3.32). This transform is typically not a computational bottleneck in discrete settings when the measures have a few thousand points, *e.g.* in Sinkhorn solvers such as (Cuturi, 2013). Otherwise in some continuous settings, the conjugate operation may be computationally challenging because it is an optimization problem that needs to be repeatedly solved from scratch to obtain a single Monte-Carlo estimate of $\int_{\mathcal{Y}} f^c(y) d\beta(y)$ to evaluate J in Eq. (3.32) *once*.

Scoping to computing the optimal transport maps between Euclidean measures with the negative inner product cost (Villani, 2009, eq. 5.12), f is a convex function and the c -transform operation f^c in Eq. (3.33) is the standard Legendre-Fenchel transform. Taghvaei and Jalali (2019) discusses a lot of the theoretical foundations underpinning Wasserstein-2 optimal transport and experimentally use a numerical method that solves each conjugate operation from scratch. To alleviate the computational bottleneck of this, many methods using similar theoretical foundations amortize this conjugate operation (Dam *et al.*, 2019; Makkuvu *et al.*, 2020; Korotin *et al.*, 2021; Amos, 2023). The simplest instantiation of this amortization uses a fully-amortized model $\hat{x}_\theta(y)$ trained with objective-based learning of the conjugate objective. Amos

(2023) further discusses the modeling and loss choices in this setting and also discusses the idea of fine-tuning the amortized prediction with a numerical solver to ensure the dual objective is accurately estimated.

Summary. $\mathcal{A}_{\text{AmorConj}} := (c(\cdot, y) - f(\cdot), \mathcal{X}, \mathcal{Y}, \beta, \hat{x}_\theta, \mathcal{L}_{\text{obj}})$.

Remark 3.2. Separate from amortizing the convex conjugate for optimal transport, Garcia *et al.* (2023) proposes to amortize the solution to a convex conjugation problem arising when computing the natural gradient. Also related is Bae *et al.* (2022), which amortizes the solution to a proximal optimization problem for updating parameters and can also amortize the solution to the natural gradient update (but doesn't explicitly go through the convex conjugate perspective).

3.5.3 Amortized Sliced Wasserstein (\mathcal{A} -SW) by Nguyen and Ho (2022)

Computing the Wasserstein distance between measures is computationally challenging. The *max-sliced* Wasserstein distance (Deshpande *et al.*, 2019) approximates $W(\alpha, \beta)$ between measures with $\mathcal{X} = \mathcal{Y} = \mathbb{R}^d$ by linearly projecting (or slicing) the atoms of the measures down into 1-dimensional measures where the 1-Wasserstein distance has a closed-form solution. Max-sliced Wasserstein distances search over slices on the d -dimensional sphere \mathcal{S}^{d-1} with

$$\text{Max-SW}(\alpha, \beta) := \max_{\theta \in \mathcal{S}^{d-1}} W(\theta; \alpha, \beta) \quad W(\theta; \alpha, \beta) := W(\theta_\# \alpha, \theta_\# \beta), \quad (3.34)$$

where $\theta_\# \alpha$ is the push-forward measure of μ through $T_\theta(x) = \theta^\top x$. Nguyen and Ho (2022) proposal to amortize Eq. (3.34) over mini-batches \mathcal{D} of size m sampled from each measure.

Summary. $\mathcal{A}_{\text{SW}} := (W(\theta), \mathcal{S}^{d-1}, \mathcal{X}^m \times \mathcal{Y}^m, \mathcal{D}, \mathcal{L}_{\text{obj}})$.

3.6 Policy Learning for Control and Reinforcement Learning

Many control and reinforcement learning methods amortize the solutions to a control optimization problem as illustrated in Figures 1.2 and 3.2.

Distinction. This section is on *amortization for reinforcement learning and control* and *not* the opposite direction of using *reinforcement*

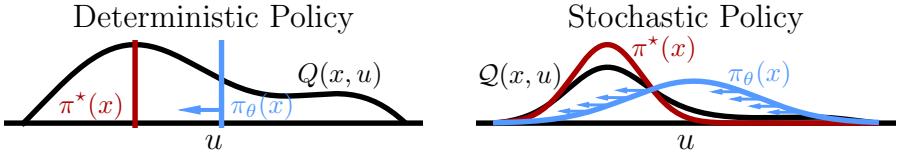


Figure 3.2: Many policy learning methods amortize optimization problem over the Q -values. Given a fixed input state x , the policy $\pi_\theta(x)$ predicts the maximum value $\pi^*(x)$. A stochastic policy predicts a distribution that minimizes some probabilistic distance to the Q -distribution, such as the expected value or KL.

learning for amortization that Section 2.2.3 discusses for parameter learning.

3.6.1 Background

Preliminaries in Markov decision processes.

Definition 3.2. A *Markov decision process* (MDP) can be represented with $\mathcal{M} := (\mathcal{X}, \mathcal{U}, p, r)$, where \mathcal{X} are the continuous *states*, \mathcal{U} are the continuous *actions* or *controls*, $p(x' | x, u)$ is the *transition dynamics* (also referred to as the *system*, *model*, or *world model*), which is a *Markov kernel* providing the probability the next state x' given the current state-action (x, u) , and $r : \mathcal{X} \times \mathcal{U}$ is the *reward function*.

This section scopes to methods that control a fully-observable and continuous MDP. A *policy* π that *controls* the MDP provides a distribution over actions to sample from for every state x and induces *state* and *state-control marginals* $\rho_t^\pi(\cdot)$ for each time step t , which can be constrained to start from an initial state x_0 as $\rho_t(\cdot|x)$. In the non-discounted, infinite-horizon case an *optimal policy* π^* maximizes the reward over rollouts of the MDP with

$$\pi^*(x) \in \arg \max_{\pi} \mathbb{E}_{x \sim p_{\text{init}}(x)} V^\pi(x) \quad V^\pi(x) := \sum_t \mathbb{E}_{(x_t, u_t) \sim \rho_t^\pi(\cdot|x)} r(x_t, u_t), \quad (3.35)$$

where p_{init} is the *initial state distribution* and $V^\pi(x)$ is the expected *value* of a policy π starting from a state x and that is taken over all possible future rewards induced by the stochastic policy and dynamics.

Given the *action-conditional value* Q of a policy defined by

$$Q^\pi(x, u) := r(x, u) + \mathbb{E}_{x' \sim p(\cdot|x, u)} [V^\pi(x')]. \quad (3.36)$$

In the deterministic setting with a fixed Q function, an optimal policy can be obtained by solving the *max-Q* optimization problem

$$\pi^*(x) \in \arg \max_u Q(x, u), \quad (3.37)$$

which is the form that can be used to interpret many control and reinforcement learning methods as amortized optimization. Instead of amortizing the solution to Eq. (3.37), methods such as Lowrey *et al.* (2019) and Ryu *et al.* (2020) explicitly solve the max-Q problem.

Control of deterministic MDPs with deterministic policies. If all of the components of the MDP are known, no learning needs to be done to obtain an optimal policy and standard *model predictive control* (MPC) methods often work well. In *deterministic MDPs*, the dynamics are deterministic and can be written as $x' := p(x, u)$. These can be solved with deterministic policies, which turns the expected value and marginal distributions into Dirac delta distributions that can be computed with single rollout. An optimal controller from an initial state x_1 can thus be obtained by solving the *finite-horizon* problem over the (negated) value approximated with a horizon length of H timesteps with

$$u_{1:H}^*(x_1) := \arg \min_{u_{1:H}} \sum_t C_t(x_t, u_t) \text{ subject to } x_{t+1} = p(x_t, u_t), \quad (3.38)$$

where the *cost* C at each time is usually the negated reward $C_t(x_t, u_t) := -r(x_t, u_t)$. The field of optimal control studies methods for solving control optimization problems of the form Eq. (3.38) and standard references include Bertsekas (2000), Kirk (2004), and Camacho and Alba (2013). Eq. (3.38) induces the policy $\pi(x) := u_1^*(x)$ that solves the MDP if the horizon H is long enough. Using a *terminal cost* at the end of the horizon can also give the controller information about how the system will perform beyond the finite-horizon rollouts being used, for example with $C_H(x_H, u_H) := -Q^\pi(x_H, u_H)$.

Reinforcement learning when the dynamics aren't known. Optimal control methods work well when the dynamics p of the MDP

are known, which is an unfortunately strong assumption in many settings where the system can only be sampled from. In these settings *reinforcement learning* (RL) methods thrive and solve the MDP given access to *only* samples from the dynamics. While summarizing all of the active RL methods is out-of-scope for this tutorial, the core of these methods is typically on 1) *policy evaluation* to estimate the *value* of a policy given only samples from the system, and 2) *policy improvement* to improve the policy using the value estimation.

Extensions in stochastic control. The max-Q problem in Eq. (3.37) can be extended to the stochastic optimization settings Section 2.3.1 briefly covered when the policy π represents a *distribution* over the action space \mathcal{U} . The most common objectives for stochastic policies are 1) the expected Q -value under the policy with

$$\pi^*(x) \in \arg \max_{\pi \in \Pi} \mathcal{E}_Q(\pi; x) \quad \mathcal{E}_Q(\pi; x) := \mathbb{E}_{u \sim \pi(\cdot)} Q(x, u), \quad (3.39)$$

or 2) the KL distance

$$\pi^*(x) \in \arg \min_{\pi \in \Pi} D_Q(\pi; x) \quad D_Q(\pi; x) := D_{\text{KL}}(\pi(\cdot) \parallel \mathcal{Q}(x, \cdot)), \quad (3.40)$$

where $\mathcal{Q}(x, \cdot) \propto \exp\{Q(x, \cdot)/\alpha\}$ is a Q -distribution induced by the Q values that is inversely scaled by $\alpha \in \mathbb{R}_+$. The policy π is usually represented as the parameters of a distribution and thus Π becomes the space of these parameters. In most cases, π is a Gaussian $\mathcal{N}(\mu, \Sigma)$ with a diagonal covariance Σ and thus Eqs. (3.39) and (3.40) can be turned into unconstrained continuous optimization problems of the form Eq. (1.1) by projecting onto the Gaussian parameters. Stochastic value gradient methods such as Heess *et al.* (2015) often amortize Eq. (3.39), while Levine and Koltun (2013) and Haarnoja *et al.* (2018) propose methods that build on Eq. (3.40), often adding additional softening and entropic terms to encourage the policy and value estimate to explore more and not converge too rapidly to a suboptimal minima. One last note is that the smoothing that the policy performs in Eq. (3.39) is nearly identical to the objective smoothing considered in Section 2.2.3, except in that setting the variance of the smoother remains fixed.

Connecting stochastic control back to deterministic control. This portion shows that taking stochastic policies to be Dirac delta

distributions in Eqs. (3.39) and (3.40) recovers the solutions to the deterministic control problem in Eq. (3.37). Taking a larger classes of policy distributions, such as Gaussians, can then be interpreted as smoothing the Q values to avoid 1) falling into poor local optima and 2) unstable regions where only a few actions have high value, but the rest have poor values. For the following, let $\delta_u(\cdot)$ be Dirac delta distribution with a parameter $u \in \mathbb{R}^n$ indicating the location of the mass.

Proposition 3.1. Let π be a Dirac delta distribution $\delta_u(\cdot)$. Then the solution $\pi^*(x)$ to the expected Q problem in Eq. (3.39) is the solution to the deterministic max- Q problem in Eq. (3.37).

Proof. Let $\Pi = \mathbb{R}^n$ be the parameter space of π and transform Eq. (3.39) to optimize over it:

$$\pi^*(x) \in \arg \max_{u \in \mathbb{R}^n} \mathbb{E}_{\tilde{u} \sim \delta_u(\cdot|x)} Q(x, \tilde{u}). \quad (3.41)$$

The expectation over the Dirac evaluates to

$$\mathbb{E}_{\tilde{u} \sim \delta_u(\cdot|x)} Q(x, \tilde{u}) = Q(x, u) \quad (3.42)$$

and thus Eq. (3.41) which is the max- Q operation in Eq. (3.37). \square

Similarly for the for the KL problem in Eq. (3.40):

Proposition 3.2. Let π be a Dirac delta distribution $\delta_u(\cdot)$. Then the solution $\pi^*(x)$ to the KL problem in Eq. (3.40) is the solution to the deterministic max- Q problem in Eq. (3.37).

Proof. Let $\Pi = \mathbb{R}^n$ be the parameter space of π and transform Eq. (3.40) to optimize over it:

$$\pi^*(x) \in \arg \min_{u \in \mathbb{R}^n} D_{KL}(\delta_u(\cdot) \parallel \mathcal{Q}(x, \cdot)). \quad (3.43)$$

Expanding the KL distance then gives the density of \mathcal{Q} at the mass:

$$\begin{aligned} D_{KL}(\delta_u(\cdot) \parallel \mathcal{Q}(x, \cdot)) &= \mathbb{E}_{\tilde{u} \sim \delta_u(\cdot)} [\log \delta_u(\tilde{u}) - \log \mathcal{Q}(x, \tilde{u})] \\ &= -\log \mathcal{Q}(x, u) + C \\ &= -\log \frac{1}{Z_x} \exp \{Q(x, u)\} + C \\ &= -Q(x, u) + \log Z_x + C \end{aligned} \quad (3.44)$$

where C is a constant that does not depend on u , $\mathcal{Q}(x, u)$ is the density at u , and \mathcal{Z}_x is the normalization constant for $\mathcal{Q}(x, \cdot)$ that does not depend on u . Putting Eq. (3.44) back into Eq. (3.43) and removing the constants that do not depend on u gives

$$\pi^*(x) \in \arg \min_{u \in \mathbb{R}^n} -\mathcal{Q}(x, u), \quad (3.45)$$

which is the max- Q operation in Eq. (3.37). \square

3.6.2 Behavioral cloning and imitation learning

This section starts in the setting where regression-based amortization is done to predict the solution of a controller that solves Eq. (3.35). These settings assume access to a controller, or samples from it, that uses traditional methods, and *not* learning, to solve Eq. (3.35) with the true or approximated dynamics. These solutions are typically available as samples from a policy $\pi^*(x)$ that provides the solution to the max-Q problem in Eq. (3.37) for regression-based amortization. In some settings these methods also use the optimal finite-horizon sequence $u_{1:H}^*(x)$ from a solution to Eq. (3.38).

Imitation learning methods such as behavioral cloning can be seen as a regression-based amortization that seek to distill, or clone, the expert's behavior into a learned model $\pi_\theta(x)$ that predicts the expert's action given the state x (Osa *et al.*, 2018, Chapter 3). Deterministic BC methods often regress onto the expert's state-action pairs $(x, \pi^*(x))$ sampled some distribution of states $p(x)$ with

$$\arg \min_{\theta} \mathbb{E}_{x \sim p(x)} \|\pi^*(x) - \pi_\theta(x)\|_2^2, \quad (3.46)$$

where, for example, the model π_θ could be a neural network. Thus BC in this setting performs regression-based amortization $\mathcal{A}_{\text{BC}} := (-Q, \mathcal{U}, \mathcal{X}, p(x), \pi_\theta, \mathcal{L}_{\text{reg}})$. Extensions from this setting could include when 1) the model π_θ is a sequence model that predicts the entire sequence $u_{1:H}^*$, and 2) the MDP or policy is stochastic and Eq. (3.46) turns into an amortized maximum likelihood problem rather than a regression problem.

Warning. One crucial difference between behavioral cloning and all of the other applications considered here is that behavioral cloning

does not assume knowledge of the original objective or cost used by the expert. This section assumes that an optimal objective exists for the purposes of seeing it as regression-based amortization. Settings such as inverse control and RL explicitly recover the expert’s objective, but are beyond the scope of our amortization focus.

3.6.3 The deterministic policy gradient

The policy learning of many model-free actor-critic reinforcement learning algorithms on continuous spaces can be seen as objective-based amortization of the max- Q operation in Eq. (3.37). This includes the policy improvement step for deterministic policies as pioneered by the deterministic policy gradient (DPG) by Silver *et al.* (2014), deep deterministic policy gradient (DDPG) by Lillicrap *et al.* (2016), and twin delayed DDPG (TD3) by Fujimoto *et al.* (2018). All of these methods interweave 1) *policy evaluation* to estimate the state-action value Q^{π_θ} of the current policy π_θ , and 2) *policy improvement* to find the policy that best-optimizes the max- Q operation with

$$\arg \max_{\theta} \mathbb{E}_{x \sim p(x)} Q(x, \pi_\theta(x)). \quad (3.47)$$

Summary. The DPG family of methods perform objective-based amortization of the max- Q optimization problem with

$$\mathcal{A}_{\text{DPG}} := (-Q, \mathcal{U}, \mathcal{X}, p(x), \pi_\theta, \mathcal{L}_{\text{obj}}). \quad (3.48)$$

3.6.4 The stochastic value gradient and soft actor-critic

This amortization viewpoint can be extended to *stochastic* systems and policies that use the *stochastic value gradient* (SVG) and covers a range of model-free to model-based method depending on how the value is estimated (Byravan *et al.*, 2019; Hafner *et al.*, 2020; Byravan *et al.*, 2022; Amos *et al.*, 2021). As observed in Haarnoja *et al.* (2018) and Amos *et al.* (2021), the policy update step in the soft actor-critic can also be seen as a model-free stochastic value gradient with the value estimate regularized or “softened” with an entropy term. These methods learn policies π_θ that amortize the solution to a stochastic optimization problem, such as Eqs. (3.39) and (3.40), over some distribution of states

$p(x)$, such as the stationary state distribution or an approximation of it with a replay buffer. Taking the expected value under the policy gives the policy loss

$$\arg \max_{\theta} \mathcal{L}_{\text{SVG}, \mathcal{E}}(\pi_{\theta}) \quad \mathcal{L}_{\text{SVG}, \mathcal{E}}(\pi_{\theta}) := \mathbb{E}_{x \sim p(x)} \mathbb{E}_{u \sim \pi_{\theta}(\cdot | x)} Q(x, u), \quad (3.49)$$

and taking the minimum KL distance gives the policy loss

$$\arg \min_{\theta} \mathcal{L}_{\text{SVG}, \text{KL}}(\pi_{\theta}) \quad \mathcal{L}_{\text{SVG}, \text{KL}}(\pi_{\theta}) := \mathbb{E}_{x \sim p(x)} D_{\text{KL}}(\pi_{\theta}(\cdot | x) \| \mathcal{Q}(x, \cdot)), \quad (3.50)$$

which softens the policy and value estimates with an entropy regularization as in Haarnoja *et al.* (2018) and Amos *et al.* (2021). Eq. (3.50) can be seen as an entropy-regularized value estimate by expanding the KL

$$\begin{aligned} \nabla_{\theta} \mathbb{E}_{x \sim p(x)} D_{\text{KL}}(\pi_{\theta}(\cdot | x) \| \mathcal{Q}(x, \cdot)) = \\ \nabla_{\theta} \mathbb{E}_{x \sim p(x)} \mathbb{E}_{u \sim \pi_{\theta}(u | x)} [\log(\pi_{\theta}(u | x)) - Q(x, u) / \alpha]. \end{aligned} \quad (3.51)$$

Mohamed *et al.* (2020) discusses standard ways of optimizing Eqs. (3.49) and (3.50), which could be with a likelihood ratio gradient estimator (Williams, 1992) or via reparameterization.

Summary. The policy update of methods based on the SVG and SAC perform objective-based amortization of a stochastic control optimization problem with

$$\mathcal{A}_{\text{SVG}} := (\mathcal{D}_{\mathcal{Q}} \text{ or } -\mathcal{E}_{\mathcal{Q}}, \mathcal{P}(\mathcal{U}), \mathcal{X}, p(x), \pi_{\theta}, \mathcal{L}_{\text{KL}}).$$

SVG-based amortization for model-free and model-based methods. SVG-based policy optimization provides a spectrum of model-free to model-based algorithms depending on if the value estimate is approximated in a model-free or model-based way, *e.g.* with rollouts of the true or approximate dynamics. Heess *et al.* (2015) explored this spectrum and proposed a few key instantiations. Byravan *et al.* (2019) and Amos *et al.* (2021) use learned models for the value approximation. The variation in Hafner *et al.* (2020) amortizes a model-based approximation using the *sum* of the value estimates of a model rollout. Henaff *et al.* (2019) explore uncertainty-based regularization to amortized policies learned with value gradients. Xie *et al.* (2021) consider

hierarchical amortized optimization that combine a higher-level planner based on CEM with a lower-level fully-amortized policy learned with stochastic value gradients. Byravan *et al.* (2022) perform a large-scale evaluation of amortization methods for control and study algorithmic variations and generalization capabilities, and consider methods based on the stochastic value gradient and behavioral cloning.

3.6.5 PILCO by Deisenroth and Rasmussen (2011)

PILCO is an early example that uses gradient-based amortization for control. They assume that only samples from the dynamics model are available, fit a Gaussian process to them, and then use that to estimate the finite-horizon Q -value of a deterministic RBF policy π_θ . The parameters θ are optimized by taking gradient steps to find the policy resulting in the maximum value over some distribution of states $p(x)$, *i.e.*

$$\arg \max_{\theta} \mathbb{E}_{x \sim p(x)} Q(x, \pi_\theta). \quad (3.52)$$

Summary. $\mathcal{A}_{\text{PILCO}} := (-Q, \mathcal{U}, \mathcal{X}, p(x), \pi_\theta, \mathcal{L}_{\text{obj}})$

3.6.6 Guided policy search (GPS)

The GPS family of methods (Levine and Koltun, 2013; Levine and Abbeel, 2014; Levine *et al.*, 2016; Montgomery and Levine, 2016) fits an approximate dynamics model to data and then amortizes the solutions of a controller that solves the MPC problem in Eq. (3.38) within a local region of the data to improve the amortization model. Given samples of π^* from a controller that solves Eq. (3.40), GPS methods typically optimize the KL divergence between the controller and these samples with

$$\arg \min_{\theta} \mathbb{E}_{x \sim p(x)} D_{\text{KL}}(\pi_\theta(\cdot | x) || \pi^*(\cdot | x)) \quad (3.53)$$

Summary. $\mathcal{A}_{\text{GPS}} := (\mathcal{D}_Q, \mathcal{P}(\mathcal{U}), \mathcal{X}, p(x), \pi_\theta, \mathcal{L}_{\text{KL}})$

Related methods such as Sacks and Boots (2022) study learning to optimize for imitating other controllers and are capable of working in cases when derivative information isn't available.

3.6.7 POPLIN by Wang and Ba (2020)

POPLIN explores behavioral cloning methods based on regression and generative modeling and observes that the parameter space of the amortized model is a reasonable space to solve new control optimization problems over. The methods discussed here

Distillation and amortization. POPLIN first trains a fully-amortized model on a dataset of trajectories with behavioral cloning or generative modeling. This section only considers the BC variant trained with \mathcal{A}_{BC} , which provides an *optimal* fully-amortized model π_{θ^*} .

Control. Next they explore ways of using the learned policy π_{θ^*} to solve the model predictive control optimization problem in Eq. (3.38). The *POPLIN-A* variant (“A” stands for “action”) uses π_{θ^*} to predict an initial control sequence $\hat{u}_{1:H}^0$ that is then passed as an input to a controller based on the cross-entropy method over the action space that uses a learned model on the trajectories. The *POPLIN-P* variant (“P” stands for “parameter”) suggests that the *parameter space* of the fully-amortized model has learned useful information about the structure of the optimal action sequences. As an alternative to solving the MPC problem in Eq. (3.38) over the action space, POPLIN-P proposes to use CEM to find a perturbation ω to the optimal parameters θ^* that maximizes the value from a state x with

$$\omega^*(x) \in \arg \max_{\omega} Q(x, u; \pi_{\theta^* + \omega}). \quad (3.54)$$

Thus the action produced by $\pi_{\theta^* + \omega^*}(x)$ is a solution to the control problem in Eq. (3.38) obtained by adapting the policy’s parameters to the state x .

Summary. POPLIN is an extension of behavioral cloning that amortizes control optimization problems with

$$\mathcal{A}_{\text{POPLIN}} := (-Q, \mathcal{U}, \mathcal{X}, p(x), \pi_{\theta}, \mathcal{L}_{\text{reg}}). \quad (3.55)$$

The initial phase is fully-amortized behavioral cloning. The second fine-tuning phase can be seen as semi-amortization that learns only the initialization θ and finds ω with CEM, with a regression-based loss \mathcal{L}_{reg} that *only* has knowledge of the initial model and does not include the adaptation.

3.6.8 The differentiable cross-entropy method by Amos and Yarats (2020)

Differentiable control (Amos *et al.*, 2018) is a budding area of work with the goal of integrating controllers into end-to-end modeling pipelines to overcome problems such as objective mismatch (Lambert *et al.*, 2020). The differentiable cross-entropy method (DCEM) was created towards the goal of doing this with controllers based on the cross-entropy method. Otherwise, as in Wang and Ba (2020), CEM needs to be done as a secondary step *after* learning and the learning process is not aware of the final policy that running CEM will induce. The key step to differentiate through CEM is to make the top- k operation smooth and differentiable by using the differentiable top- k operation proposed in Amos *et al.* (2019) called the limited multi-label projection layer.

Amos and Yarats (2020) considers a semi-amortized learning setting that learns a latent domain for control, which can be seen as a similarly-motivated alternative to the parameter-space control done in POPLIN. The key piece of *latent control* is to learn a *decoder* $\varphi_\theta : \mathcal{Z} \rightarrow \mathcal{U}^H$ that maps from a low-dimensional latent space \mathcal{Z} to the H -step control space that solves Eq. (3.38). Learning a latent space is useful if there are many redundancies and possibly bad local minima on the original control space \mathcal{U}^H that the latent space can get rid of. Given an initial state x_1 , the optimal latent representation can be obtained by solving the control optimization problem over \mathcal{Z} with

$$\hat{z}_\theta(x_1) \in \arg \min_{z \in \mathcal{Z}} C_\theta(z; x_1) \quad (3.56)$$

where $C_\theta(z; x_1)$ is the expected cost of rolling out the control sequence $u_{1:H} = \varphi(z)$ from the initial state x_1 , for example on deterministic systems C could be the sum of negated rewards

$$C(z; x) := - \sum_{t=1}^H r(x_t, u_t) \text{ subject to } x_{t+1} = p(x_t, u_t) \text{ and } x_{1:H} = \varphi_\theta(z) \quad (3.57)$$

Solving Eq. (3.56) with DCEM enables the optimal solution $\hat{z}_\theta(x)$ to be differentiated with respect to the parameters θ of the decoder φ_θ . The final predicted control sequence can be obtained with the decoder

$\hat{u}_{1:H}(x; \theta) := \varphi_\theta(\hat{z}_\theta(x))$ and the decoder can be learned by regressing onto ground-truth control sequences $u^*(x)$ with

$$\arg \min_{\theta} \mathcal{L}_{\text{DCEM}}(\hat{u}_{1:H}(\cdot; \theta)) \quad (3.58)$$

where the loss is given by

$$\mathcal{L}_{\text{DCEM}}(\hat{u}_{1:H}(\cdot; \theta)) := \mathbb{E}_{x \sim p(x)} \|u^*(x) - \hat{u}_{1:H}(x; \theta)\|_2^2. \quad (3.59)$$

Figure 3.3 visualizes an example on the cartpole task where this is able to learn a latent space that captures the cyclic and smoothness structure of the optimal control sequence space.

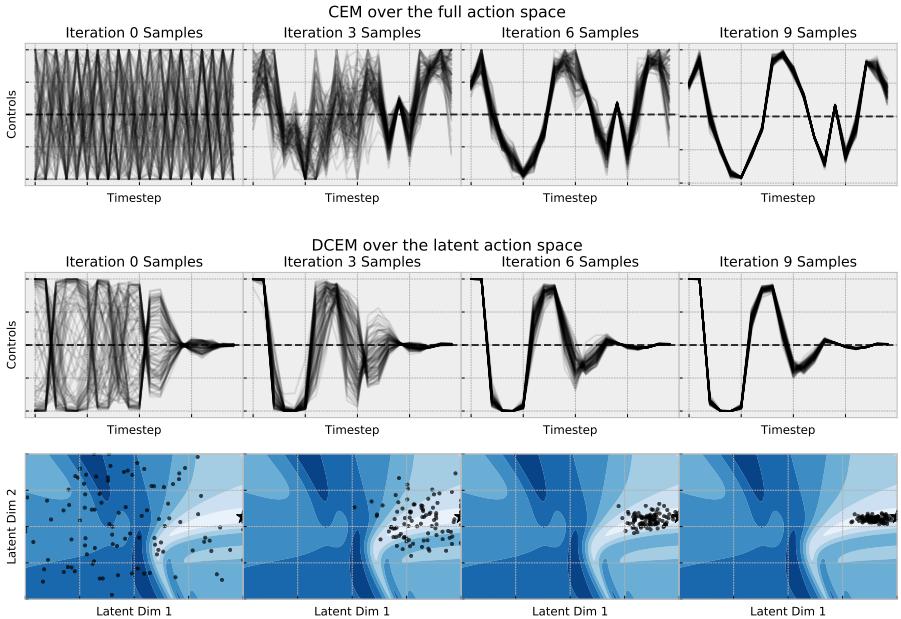


Figure 3.3: The differentiable cross-entropy method (DCEM) (Amos and Yarats, 2020) can be used to create semi-amortized controllers that learn a latent space \mathcal{Z} over control sequences. This visualization taken from the DCEM paper shows the samples that CEM and DCEM generate to solve the cartpole task starting from the same initial system state. The plots starting at the top-left show that CEM initially starts with no temporal knowledge over the control space whereas the latent space learned through DCEM generates a more feasible distribution over control sequences in each iteration that make them smooth and cyclic. The contours on the bottom show the controller's cost surface $C(z; x)$ for an initial state x where the lighter colors show regions with lower costs.

Overview. Learning a latent domain with the differentiable cross-entropy method is a semi-amortization method with

$$\mathcal{A}_{\text{DCEM}} := (-Q, \mathcal{U}, \mathcal{X}, p(x), \pi_\theta, \mathcal{L}_{\text{reg}}), \quad (3.60)$$

where the decoder φ_θ shows up from the policy π_θ solving the latent optimization problem with DCEM.

3.6.9 Iterative amortized policy optimization (IAPO) by Marino et al. (2021)

IAPO takes a probabilistic view and starts with the observation that DPG and SVG methods are amortized optimization problems with fully-amortized models with an objective-based loss. They then suggest to replace the model with an iterative semi-amortized model where the policy π_θ internally takes gradient steps on the actions of the underlying control optimization problem, and explore this semi-amortized policy in model-free and model-based reinforcement learning settings. Thus in the deterministic setting IAPO performs semi-amortized optimization

$$\mathcal{A}_{\text{IAPO}} := (-Q, \mathcal{U}, \mathcal{X}, p(x), \pi_\theta, \mathcal{L}_{\text{obj}}).$$

Warning. There's an interplay between the accuracy and quality of the policy optimizer and the value estimator. Because the value estimator is used to create its own target estimates, a better policy optimizer and controller can exploit optimistic inaccuracies in the value network. In other words, a seemingly better policy optimizing an inaccurate value estimate may result in a worse policy on the real system. This issue also arises when fully-amortized policies over-optimize the value estimate too early on in training, but is exacerbated with semi-amortized and iterative policies.

3.6.10 Learning the value function

The Q -value function Eq. (3.36) for finding an MDP policy is often unknown and needs to be estimated from data along with the policy π that is amortizing it, e.g. in Eq. (3.37). Actor-critic methods are a common reinforcement learning approach that jointly learn a policy π (the actor) and Q -value estimate (the critic) (Konda and Tsitsiklis, 1999; Sutton and Barto, 2018). The policy amortizes the current Q estimate,

e.g. by using an approach previously discussed in this section, and the Q function is fit to data sampled from the system. One way of learning the Q function is to replace the value estimate V^π in Eq. (3.36) with the Q -value estimate to yield the relationship

$$Q^\pi(x, u) := r(x, u) + \mathbb{E}_{x' \sim p(\cdot|x, u), u' \sim \pi(x')} [Q^\pi(x', u')] , \quad (3.61)$$

which is referred to as the *Bellman equation* (Bellman, 1966; Sutton and Barto, 2018). Eq. (3.61) is an equality that should hold over all states and actions in the system and a value estimate can be parameterized and learned to satisfy the relationship. While the best way of learning the Q estimate is an open research topic (Watkins and Dayan, 1992; Baird, 1995; Ernst *et al.*, 2005; Maillard *et al.*, 2010; Scherrer, 2010; Geist *et al.*, 2017; Le *et al.*, 2019; Fujimoto *et al.*, 2022), a common way is to optimize residual of Eq. (3.61) with

$$\arg \min_{\phi} \mathbb{E}_{(x, u) \sim \mathcal{D}} \left| Q_\phi^\pi(x, u) - \left(r(x, u) + \mathbb{E}_{x' \sim p(\cdot|x, u), u' \sim \pi(x')} Q_{\bar{\phi}}^\pi(x', u') \right) \right|^2 , \quad (3.62)$$

where $\bar{\phi}$ is a detached version of the rolling mean of the parameters.

4

Implementation and Software Examples

Turning now to the implementation details, this section looks at how to develop and analyze amortization software. The standard and easiest approach in most settings is to use automatic differentiation software such as Maclaurin *et al.* (2015a), Al-Rfou *et al.* (2016), Abadi *et al.* (2016), Bezanson *et al.* (2017), Agrawal *et al.* (2019b), Paszke *et al.* (2019), and Bradbury *et al.* (2020) to parameterize and learn the amortization model. There are many open source implementations and re-implementations of the methods in Section 3 that provide a concrete starting point to start building on them. This section looks closer at three specific implementations: Section 4.1 evaluates the amortization components behind existing implementations of variational autoencoders Section 3.1 and control Section 3.6 and Section 4.2 implements and trains an amortization model to optimize functions defined on a sphere. Table 4.1 summarizes the concrete dimensions of the amortization problems considered here and Section 4.3 concludes with other useful software references. The source code behind this section is available at <https://github.com/facebookresearch/amortized-optimization-tutorial>.

Table 4.1: Dimensions for the settings considered in this section

Setting	Context dimension $ \mathcal{X} $	Solution dimension $ \mathcal{Y} $
VAE on MNIST (4.1.1)	784 (=28 · 28, MNIST digits)	20 (parameterizing a 10D Gaussian)
Model-free control (4.1.2)	45 (humanoid states)	17 (action dimension)
Model-based control (4.1.3)	45 (humanoid states)	51 (=17 · 3, short action sequence)
Sphere (4.2)	16 (c -convex function parameterizations)	3 (sphere)

4.1 Amortization In the Wild: A Deeper Look

This section shows code examples of how existing implementations using amortized optimization define and optimize their models for variational autoencoders (Section 4.1.1) and control and policy learning (Sections 4.1.2 and 4.1.3). The amortization component in these systems is often a part of a larger system to achieve a larger task: VAEs also reconstruct the source data after amortizing the ELBO computation in Eq. (3.5) and policy learning methods also estimate the Q -value function in Section 3.6.10. This section scopes to the amortization components to show how they are implemented. I have also added evaluation code to the pre-trained amortization models from existing repositories and show that the amortized approximation often obtains a solution up to **25000 times** faster than solving the optimization problems from scratch on an NVIDIA Quadro GP100 GPU.

4.1.1 The variational autoencoder (VAE)

This section looks at the code behind standard VAE (Kingma and Welling, 2014) that follows the amortized optimization setup described in Section 3.1.1. While there are many implementations for training and reproducing a VAE, this section will use the implementation at <https://github.com/YannDubs/disentangling-vae>, which builds on the code behind Dupont (2018) at <https://github.com/Schlumberger/joint-vae>. While the repository is focused on disentangled representations and extensions of the original VAE formulation, this section only highlights the parts corresponding to the original VAE formulation. The code uses standard PyTorch in a minimal way that allow us to easily look at the amortization components.

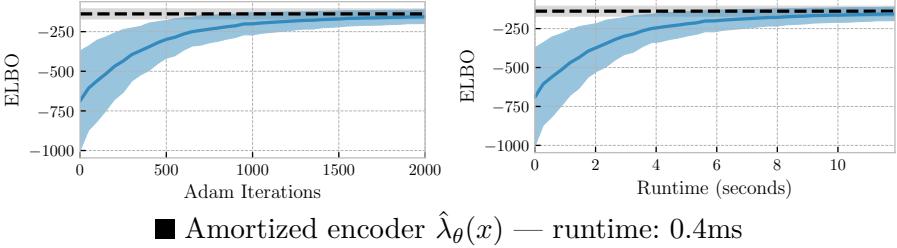


Figure 4.1: Runtime comparison between Adam and an amortized encoder $\hat{\lambda}_\theta$ to solve Eq. (3.3) for a VAE on MNIST. This uses a batch of 1024 samples and was run on an unloaded NVIDIA Quadro GP100 GPU. The values are normalized so that $\lambda(x) = 0$ takes a value of -1 and the optimal λ^* takes a value of 0. The amortized policy is approximately **25000** times faster than solving the problem from scratch.

Training the VAE. Figure 4.2 paraphrases the relevant snippets of code to implement the main amortization problem in Eq. (3.4) for image data where the likelihood is given by a Bernoulli. Figure 4.2a defines an encoder $\hat{\lambda}_\theta$, to predict a solution to the ELBO implemented in Figure 4.2b, which is optimized in a loop over the training data (images) in Figure 4.2c. The README in the repository contains instructions for running the training from scratch. The repository contains the binary of a model trained on the MNIST dataset (LeCun, 1998), which the next portion evaluates.

Evaluating the VAE. This section looks at how well the amortized encoder $\hat{\lambda}_\theta$ approximates the optimal encoder λ^* given by explicitly solving Eq. (3.3), which is referred to the *amortization gap* (Cremer et al., 2018). Eq. (3.3) can be solved with a gradient-based optimizer such as SGD or Adam (Kingma and Ba, 2015). Figure 4.4 shows the key parts of the PyTorch code for making this comparison, which can be run on the pre-trained MNIST VAE with `code/evaluate_amortization_speed_function_vae.py`.

Figure 4.1 shows that the amortized prediction from the VAE’s encoder predicts the solution to the ELBO **25000** times faster (!) than running 2k iterations of Adam on a batch of 1024 samples. This is significant as *every training iteration* of the VAE requires solving Eq. (3.3), and a large model may need millions of training iterations to converge. Amortizing the solution makes the difference between the training code running in a few hours instead of a few months if

```

1 class Encoder(nn.Module): # From disvae.models.encoders
2     def forward(self, x): # x is the amortization context: the
        original data
3         mu_logvar = self.convnet(x)
4         mu, logvar = mu_logvar.view(-1, self.latent_dim, 2).
            unbind(-1) # Split
5         return (mu, logvar) # = latent_dist or \lambda

```

(a) Forward definition for the encoder $\hat{\lambda}_\theta(x)$. `self.convnet` uses the architecture from Burgess *et al.* (2018).

```

1 # From disvae.models.losses.BetaHLoss with a Bernoulli likelihood
2 def estimate_elbo(data, latent_dist):
3     mean, logvar = latent_dist
4
5     reconstructed_batch = sample_and_decode(latent_dist)
6     log_likelihood = -F.binary_cross_entropy(
7         reconstructed_batch, x, reduce=False).sum(dim=[1,2,3])
8
9     # Closed-form distance to the prior
10    latent_kl = 0.5 * (-1 - logvar + mean.pow(2) + logvar.exp())
11    kl_to_prior = latent_kl.sum(dim=[-1])
12
13    loss = log_likelihood - kl_to_prior
14    return loss.mean()

```

(b) Definition of the ELBO in Eq. (3.1)

```

1 model = Encoder()
2 for batch in iter(data_loader):
3     latent_dist = model(batch)
4     loss = -estimate_elbo(batch, latent_dist)
5     self.optimizer.zero_grad()
6     loss.backward()
7     self.optimizer.step()

```

(c) Main VAE training loop for the encoder

Figure 4.2: Paraphrased PyTorch code examples of the key amortization components of a VAE from <https://github.com/YannDubs/disentangling-vae>.

0	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9
Adam ₂₅₀	9	8	8	6	9	7	7	9	3	9	3	9	0	0	9
Adam ₅₀₀	0	8	8	6	7	7	7	9	3	9	3	9	0	0	9
Adam ₁₀₀₀	0	9	8	6	7	7	7	9	3	9	3	9	0	0	9
Adam ₂₀₀₀	0	9	5	6	7	7	7	9	3	9	3	9	4	0	0
$\hat{\lambda}_\theta(x)$	0	9	5	6	7	7	7	9	3	9	3	9	3	4	0
Data	0	9	5	6	7	7	7	9	3	9	3	9	4	0	0

Figure 4.3: Decoded reconstructions of the variational distribution optimizing for the ELBO. Adam_{*n*} corresponds to the distribution from running Adam for *n* iterations, $\hat{\lambda}_\theta$ is the amortized approximation, and the ground-truth data, *i.e.* the context, is shown in the bottom row.

the problem was solved from scratch to the same level of optimality. Knowing only the ELBO values is not sufficient to gauge the quality of approximate variational distributions. To help understand the quality of the approximate solutions, Figure 4.3 plots out the decoded samples alongside the original data.

4.1.2 Control with a model-free value estimate

This section dives into the training and evaluation code for learning a deterministic model-free policy $\pi_\theta : \mathcal{X} \rightarrow \mathcal{Y}$ to amortize a model-free value estimate Q for controlling the humanoid MDP from Brockman *et al.* (2016) visualized in Figure 1.2. This MDP has $|\mathcal{X}| = 45$ states (angular positions and velocities describing the state of the system) and $|\mathcal{Y}| = 17$ actions (torques to apply to the joints). A model-free policy π maps the state to the optimal actions that maximize the value on the system. Given a known action-conditional value estimate $Q(x, u)$, the optimal policy π^* solves the optimization problem in Eq. (3.37) that the learned policy π tries to match, *e.g.* using policy gradient in Eq. (3.47).

The codebase behind Amos *et al.* (2021) at <https://github.com/facebookresearch/svg> contains trained model-free policy and value estimates on the humanoid in addition to model-based components the

```

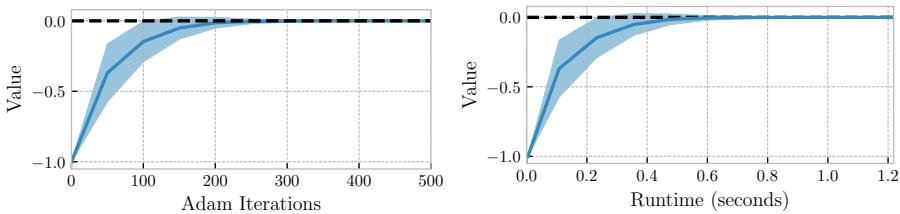
1 # amortization_model: maps contexts to a solution
2 # amortization_objective: maps an iterate and contexts to the
3 # objective
4
5 adam_lr, num_iterations = ...
6 contexts = sample_contexts()
7
8 # Predict the solutions with the amortization model
9 predicted_solutions = amortization_model(contexts)
10 amortized_objectives = amortization_objective(
11     predicted_solutions, contexts
12 )
13
14 # Use Adam (or another torch optimizer) to solve for the
15 # solutions
16 iterates = torch.nn.Parameter(torch.zeros_like(
17     predicted_solutions))
18 opt = torch.optim.Adam([iterates], lr=adam_lr)
19
20 for i in range(num_iterations):
21     objectives = amortization_objective(iterates, contexts)
22     opt.zero_grad()
23     objective.backward()
24     opt.step()

```

Figure 4.4: Evaluation code for comparing the amortized prediction \hat{y} to the true solution y^* solving Eq. (1.1) with a gradient-based optimizer. The full instrumented version of this code is available in the repository associated with this tutorial at `code/evaluate_amortization_speed_function.py`.

next section will use. The full training code there involves parameterizing a stochastic policy and estimating many additional model-based components, but the basic training loop for amortizing a deterministic policy from the solution there can be distilled into a form similar to Figure 4.2.

This section mostly focuses on evaluating the performance of the trained model-free policy in comparison to maximizing the model-free value estimate Eq. (3.37) from scratch for every state encountered. An exhaustive evaluation of a solver for Eq. (3.37) would need to ensure that the solution is not overly adapted to a bad part of the Q estimate space — because Q is also a neural network susceptible to adversarial examples,



■ Policy $\pi(x)$ — runtime: 0.65ms

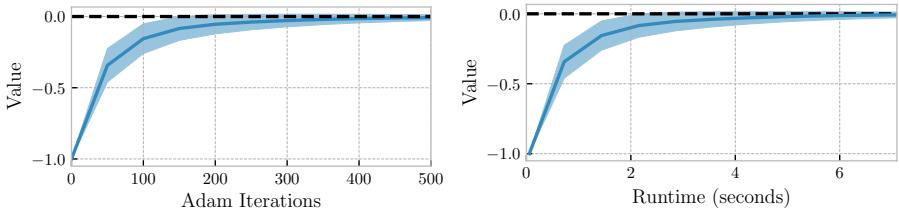
Figure 4.5: Runtime comparison between Adam and a learned policy π_θ to solve Eq. (3.37) on the humanoid MDP. This was evaluated as a batch on an expert trajectory with 1000 states and was run on an unloaded NVIDIA Quadro GP100 GPU. The values are normalized so that $\pi(x) = 0$ takes a value of -1 and the optimal π^* takes a value of 0. The amortized policy is approximately 1000 times faster than solving the problem from scratch.

it is very likely that directly optimizing Eq. (3.37) may result in a deceptively good policy when looking at the Q estimate that does not work well on the real system. For simplicity, this section ignores these issues and normalizes the values to $[-1, 0]$ where -1 will correspond to the value from taking a zero action and 0 will correspond to the value from taking the expert’s action. (This is valid in this example because the zero action and expert action never coincide.)

Figure 4.5 shows that the amortized policy is approximately 1000 times faster than solving the problem from scratch. The Q values presented there are normalized and clamped so that the expert policy has a value of zero and the zero action has a value of -1. This example can be run with `code/evaluate_amortization_speed_function_control.py`, which shares the evaluation code also used for the VAE in Figure 4.4.

4.1.3 Control with a model-based value estimate

Extending the results of Section 4.1.2, this section compares the trained humanoid policy from <https://github.com/facebookresearch/svg> to solving a short-horizon ($H = 3$) model-based control optimization problem defined in Eq. (3.38). The optimal action sequence solving Eq. (3.38) is $u_{1:H}^*$ can be approximated by interleaving a model-free policy π_θ with



■ Policy $\pi(x)$ — runtime: 5.8ms

Figure 4.6: Runtime comparison between Adam and a learned policy π_θ to solve a short-horizon ($H = 3$) model-based control problem (Eq. (3.38)) on the humanoid MDP. This was evaluated as a batch on an expert trajectory with 1000 states and was run on an unloaded NVIDIA Quadro GP100 GPU. The amortized policy is approximately 700 times faster than solving the problem from scratch.

the dynamics f . While standard model predictive control methods are often ideal for solving for $u_{1:H}^*$ from scratch, using Adam as a gradient-based shooting method is a reasonable baseline in this short-horizon setting.

Figure 4.6 shows that the amortized policy is approximately 700 times faster than solving the problem from scratch. This model-based setting has the same issues with the approximation errors in the models and the model-based value estimate is again normalized and clamped so that the expert policy has a value of zero and the zero action has a value of -1. The source code behind this example is also available in

`code/evaluate_amortization_speed_function_control.py`.

4.2 Training an Amortization Model on a Sphere

This section contains a new demonstration that applies the insights from amortized optimization to learn to solve optimization problems over spheres of the form

$$y^*(x) \in \arg \min_{y \in \mathcal{S}^2} f(y; x), \quad (4.1)$$

where \mathcal{S}^2 is the surface of the *unit 2-sphere* embedded in \mathbb{R}^3 as $\mathcal{S}^2 := \{y \in \mathbb{R}^3 \mid \|y\|_2 = 1\}$ and x is some parameterization of the function

$f : \mathcal{S}^2 \times \mathcal{X} \rightarrow \mathbb{R}$. Eq. (4.1) is relevant to physical and geographical settings seeking the extreme values of a function defined on the Earth or other spaces that can be approximated with a sphere. The full source code behind this experiment is available in `code/train-sphere.py`.

Amortization objective. Eq. (4.1) first needs to be transformed from a constrained optimization problem into an unconstrained one of the form Eq. (1.1). In this setting, one way of doing this is by using a projection:

$$y^*(x) \in \arg \min_{y \in \mathbb{R}^3} f(\pi_{\mathcal{S}^2}(y); x), \quad (4.2)$$

where $\pi_{\mathcal{S}^2} : \mathbb{R}^3 \rightarrow \mathcal{S}^2$ is the Euclidean projection onto \mathcal{S}^2 , *i.e.*,

$$\begin{aligned} \pi_{\mathcal{S}^2}(x) &:= \arg \min_{y \in \mathcal{S}^2} \|y - x\|_2 \\ &= x / \|x\|_2. \end{aligned} \quad (4.3)$$

c -convex functions on the sphere. A synthetic class of optimization problems defined on the sphere using the c -convex functions from Cohen *et al.* (2021) can be instantiated with:

$$f(y; x) = \min_{\gamma} \left\{ \frac{1}{2} d(x, z_i) + \alpha_i \right\}_{i=1}^m \quad (4.4)$$

where m components define the context $x = \{z_i\} \cup \{\alpha_i\}$ with $z_i \in \mathcal{S}^2$ and $\alpha_i \in \mathbb{R}$, $d(x, y) := \arccos(x^\top y)$ is the Riemannian distance on the sphere in the ambient Euclidean space, and $\min_{\gamma}(a_1, \dots, a_m) := -\gamma \log \sum_{i=1}^m \exp(-a_i/\gamma)$ is a soft minimization operator as proposed in Cuturi and Blondel (2017). The context distribution $p(x)$ is sampled with $z_i \sim \mathcal{U}(\mathcal{S}^2)$, *i.e.* uniformly from the sphere, and $\alpha_i \sim \mathcal{N}(0, \beta)$ with variance $\beta \in \mathbb{R}_+$.

Amortization model. The model $\hat{y}_\theta : \mathcal{X} \rightarrow \mathbb{R}$ is a fully-connected MLP. The predictions to Eq. (4.1) on the sphere can again be obtained by composing the output with the projection $\pi_{\mathcal{S}^2} \circ \hat{y}_\theta$.

Optimizing the gradient-based loss. Finally, it is reasonable to optimize the gradient-based loss \mathcal{L}_{obj} because the objective and model are tractable and easily differentiable. Figure 4.7 shows the model's predictions starting with the untrained model and finishing with the trained model, showing that this setup indeed enables us to predict the

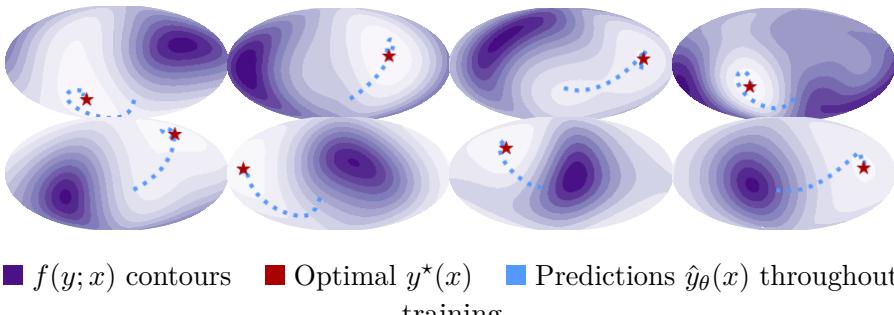


Figure 4.7: Visualization of the predictions of an amortized optimization model predicting the solutions to optimization problems on the sphere.

solutions to Eq. (4.1) with a single neural network $\hat{y}_\theta(x)$ trained with the gradient-based loss.

Summary. $\mathcal{A}_{\text{sphere}} := (f \circ \pi_{S^2}, \mathbb{R}^3, \mathcal{X}, p(x), \hat{y}_\theta, \mathcal{L}_{\text{obj}})$

4.3 Other Useful Software Packages

Implementing semi-amortized models are usually more challenging than fully-amortized models. Learning an optimization-based model that internally solves an optimization problem is not as widespread as learning a feedforward neural network. While most autodiff packages provide standalone features to implement unrolled gradient-based optimization, the following specialized packages provide crucial features that further enable the exploration of semi-amortized models:

- [cvxpylayers](#) (Agrawal *et al.*, 2019a) allows an optimization problem to be expressed in the high-level language CVXPY (Diamond and Boyd, 2016) and exported to PyTorch, JAX, and TensorFlow as a differentiable optimization layers.
- [jaxopt](#) (Blondel *et al.*, 2022) is a differentiable optimization library for JAX and implements many optimization settings and fixed-point computations along with their implicit derivatives.
- [higher](#) (Grefenstette *et al.*, 2019) is a PyTorch library that adds differentiable higher-order optimization support with 1) monkey-

patched functional `torch.nn` modules, and 2) differentiable versions of `torch.optim` optimizers such as Adam and SGD. This enables arbitrary torch modules and optimizers to be unrolled and used as a semi-amortized model.

- `TorchOpt` provides a functional and differentiable optimizer in PyTorch and has higher performance than `higher` in some cases.
- `functorch` (He and Zou, 2021) is a PyTorch library providing composable function transforms for batching and derivative operations, and for creating functional versions of PyTorch modules that can be used in optimization algorithms. All of these operations may arise in the implementation of an amortized optimization method and can become computational bottlenecks if not efficiently implemented.
- `DiffOpt.jl` provides differentiable optimization in Julia’s JuMP (Dunning *et al.*, 2017).
- `Torchmeta` (Deleu *et al.*, 2019) and `learn2learn` (Arnold *et al.*, 2020) are PyTorch libraries and collection of meta-learning algorithms that also focus on making data-loading and task definitions easy.
- `hypertorch` (Grazzi *et al.*, 2020) is a PyTorch package for computing hypergradients with a large focus on providing computationally efficient approximations to them.

5

Discussion

Many of the specialized methods discuss tradeoffs and limitations within the context of their application, and more generally papers such as Chen *et al.* (2021a) and Metz *et al.* (2021) provide even deeper probes into general paradigms for learning to optimize. This section emphasizes a few additional discussion points around amortized optimization.

5.1 Surpassing the Convergence Rates of Classical Methods

Theoretical and empirical optimization research often focuses on discovering algorithms with theoretically strong convergence rates in general or worst-case scenarios. Many of the algorithms with the best convergence rates are used as the state-of-the-art algorithms in practice, such as momentum and acceleration methods. Amortized optimization methods can surpass the results provided by classical optimization methods because they are capable of tuning the initialization and updates to the best-case scenario within the distribution of contexts the amortization model is trained on. For example, the fully amortized models for amortized variational inference and model-free actor-critic methods for RL presented in Section 4.1 solve the optimization problems *in constant time* with just a single prediction of the solution from the context with-

out even looking at the objective! Further theoretical characterizations of this are provided in Khodak *et al.* (2022) and related literature on algorithms with predictions.

5.2 Generalization and Convergence Guarantees

Despite having powerful successes of amortized optimization in some settings, the field struggles to bring strong success in other domains. Despite having the capacity of surpassing the convergence rates of other algorithms, oftentimes in practice amortized optimization methods can deeply struggle to generalize and converge to reasonable solutions. In some deployments this inaccuracy may be acceptable if there is a quick way of checking the quality of the amortized model, *e.g.* the residuals for fixed-point and convex problems. If that is the case, then poorly-solved instances can be flagged and re-solved with a standard solver for the problem that may incur more computational time for that instance. Banert *et al.* (2021) and Prémont-Schwarz *et al.* (2022) add provable convergence guarantees to semi-amortized models by guarding the update and ensuring the learned optimizer does not deviate too much from a known convergent algorithm. A practical takeaway is that some models are more likely to result in convergent and stable semi-amortized models than others. For example, the semi-amortized model parameterized with gradient descent (which has some mild converge guarantees) in Finn *et al.* (2017) is often more stable than the semi-amortized model parameterized by a sequential model (without many convergence guarantees) in (Ravi and Larochelle, 2017). Other modeling and architecture tricks such as layer normalization (Ba *et al.*, 2016) help improve the stability of amortized optimization models.

5.3 Measuring Performance

Quantifying the performance of amortization models can be even more challenging than the choice between using a regression- or objective-based loss and is often tied to problem-specific metrics that are important. For example, even if a method is able to attain low objective values in a few iterations, the computation may take *longer* than a

specialized algorithm or another amortization model that can reach the same level of accuracy, thus not making it useful for the original goal of speeding up solves to Eq. (1.1).

5.4 Successes and Limitations of Amortized Optimization

While amortized optimization has standout applications in variational inference, reinforcement learning, and meta-learning, it struggles to bring value in other settings. Often, learning the amortized model is computationally more expensive than solving the original optimization problems and brings instabilities into a higher-level learning or optimization process deployed on top of potentially inaccurate solutions from the amortized model. This section summarizes principles behind successful applications of amortized optimization and characterize limitations that may arise.

Characteristics of successful applications

- **Objective $f(y; x)$ is smooth over the domain \mathcal{Y} and has unique solutions y^* .** With objective-based learning, non-convex objectives with few poor local optima are ideal. This behavior can be encouraged with smoothing as is often done for meta-learning and policy learning (Section 2.2.3).
- **A higher-level process should tolerate sub-optimal solutions given by \hat{y} in the beginning of training.** In variational encoders, the suboptimal bound on the likelihood is still acceptable to optimize the density model’s parameters over in Eq. (3.5). And in reinforcement learning policies, a suboptimal solution to the maximum value problem is still acceptable to deploy on the system in early phases of training, and may even be desirable for the exploration induced by randomly initialized policies.
- **The context distribution $p(x)$ is not too big and well-scoped and deployed on a specialized class of sub-problems.** For example, instead of trying to amortize the solution

to *every* possible ELBO maximization, VAEs amortize the problem only over the dataset the density model is being trained on. And in reinforcement learning, the policy π_θ doesn't try to amortize the solution to *every* possible control problem, but instead focuses only on amortizing the solutions to the control problems on the replay buffer of the specific MDP.

- **In semi-amortized models, parameterizing the initialization and specialized components for the updates.** While semi-amortized models are a thriving research topic, the most successful applications of them:
 1. **Parameterize and learn the initial iterate.** MAML (Finn *et al.*, 2017) *only* parameterizes the initial iterate and follows it with gradient descent steps. Bai *et al.* (2022) parameterizes the initial iterate and follows it with accelerated fixed-point iterations.
 2. **Parameterize and learn specialized components of the updates.** In sparse coding, LISTA (Gregor and LeCun, 2010) only parameterized $\{F, G, \beta\}$ instead of the entire update rule. Bai *et al.* (2022) only parameterizes α, β after the initial iterate, and RLQP (Ichnowski *et al.*, 2021) only parameterizing ρ .

While using a pure sequence model to update a sequence of iterations is possible and theoretically satisfying as it gives the model the power to arbitrarily update the sequence of iterates, in practice this can be unstable and severely overfit to the training instances. Metz *et al.* (2021) observes, for example, that semi-amortized recurrent sequence models induce chaotic behaviors and exploding gradients.

Limitations and failures

- **Amortized optimization does *not* magically solve otherwise intractable optimization problems!** At least not without

significant insights. In most successful settings, the original optimization problem can be (semi-)tractably solved for a context x with classical methods, such as using standard black-box variational inference or model-predictive control methods. Intractabilities indeed start arising when repeatedly solving the optimization problem, even if a single one can be reasonably solved, and amortization often thrive in these settings to rapidly solve problems with similar structure.

- **The combination of $p(x)$ and $y^*(x)$ are too hard for a model to learn.** This could come from $p(x)$ being too large, *e.g.* contexts of every optimization problem in the universe, or the solution $y^*(x)$ not being smooth or predictable. $y^*(x)$ may also not be unique, but this is perhaps easier to handle if the loss is carefully set up, *e.g.* objective-based losses handle this more nicely.
- **The domain requires accurate solutions.** Even though metrics that measure the solution quality of \hat{y} can be defined on top of Eq. (1.1), amortized methods typically cannot rival the accuracy of standard algorithms used to solve the optimization problems. In these settings, amortized optimization still has the potential at uncovering new foundations and algorithms for solving problems, but is non-trivial to successfully demonstrate. From an amortization perspective, one difficulty of safety-critical model-free reinforcement learning comes from needing to ensure the amortized policy properly optimizes a value estimate that (hopefully) encodes safety-critical properties of the state-action space.

5.5 Some Open Problems and Under-explored Directions

In most domains, introducing or significantly improving amortized optimization is extremely valuable and will likely be well-received. Beyond this, there are many under-explored directions and combinations of ideas covered in this tutorial that can be shared between the existing fields using amortized optimization, for example:

1. **Overcoming local minima with objective-based losses and connections to stochastic policies.** Section 2.2.3 covered the objective smoothing by Metz *et al.* (2019a) and Merchant *et al.* (2021) to overcome suboptimal local minima in the objective. These have striking similarities to stochastic policies in reinforcement learning that also overcome local minima, *e.g.* in Eq. (3.39). The stochastic policies, such as in Haarnoja *et al.* (2018), have the desirable property of starting with a high variance and then focusing in on a low-variance solution with a penalty constraining the entropy to a fixed value. A similar method is employed in GECO (Rezende and Viola, 2018) that adjusts a Lagrange multiplier in the ELBO objective to achieve a target conditional log-likelihood. These tricks seem useful to generalize and apply to other amortization settings to overcome poor minima.
2. **Widespread and usable amortized convex solvers.** When using off-the-shelf optimization packages such as Diamond and Boyd (2016), O’Donoghue *et al.* (2016), and Stellato *et al.* (2018), users are likely solving many similar problem instances that amortization can help improve. Venkataraman and Amos (2021) and Ichnowski *et al.* (2021) are active research directions that study adding amortization to these solvers, but they do not scale to the general online setting that also doesn’t add too much learning overhead for the user.
3. **Improving the wall-clock training time of implicit models and differentiable optimization.** Optimization problems and fixed-point problems are being integrated into machine learning models, such as with differentiable optimization (Domke, 2012; Gould *et al.*, 2016; Amos and Kolter, 2017; Amos, 2019; Agrawal *et al.*, 2019a; Lee *et al.*, 2019b) and deep equilibrium models (Bai *et al.*, 2019; Bai *et al.*, 2020). In these settings, the data distribution the model is being trained on naturally induces a distribution over contexts that seem amenable to amortization. Venkataraman and Amos (2021) and Bai *et al.* (2022) explore amortization in these settings, but often do not improve the wall-clock time it takes to train these models from scratch.

4. **Understanding the amortization gap.** Cremer *et al.* (2018) study the *amortization gap* in amortized variational inference, which measures how well the amortization model approximates the true solution. This crucial concept should be analyzed in most amortized optimization settings to understand the accuracy of the amortization model.
5. **Implicit differentiation and shrinkage.** Chen *et al.* (2020) and Rajeswaran *et al.* (2019) show that penalizing the amortization objective can significantly improve the computational and memory requirements to train a semi-amortized model for meta-learning. Many of the ideas in these settings can be applied in other amortization settings, as also observed by Huszár (2019).
6. **Distribution shift of $p(x)$ and out-of-distribution generalization.** This tutorial has assumed that $p(x)$ is fixed and remains the same through the entire training process. However, in some settings $p(x)$ may shift over time, which could come from 1) the data generating process naturally changing, or 2) a *higher-level* learning process also influencing $p(x)$. Furthermore, after training on some context distribution $p(x)$, a deploy model is likely not going to be evaluated on the same distribution and should ideally be resilient to out-of-distribution samples. The out-of-distribution performance can often be measured and quantified and reported alongside the model. Even if the amortization model fails at optimizing Eq. (1.1), it's detectable because the optimality conditions of Eq. (1.1) or other solution quality metrics can be checked. If the solution quality isn't high enough, then a slower optimizer could potentially be used as a fallback.
7. **Amortized and semi-amortized control and reinforcement learning.** Applications of semi-amortization in control and reinforcement learning covered in Section 3.6 are budding and learning sample-efficient optimal controllers is an active research area, especially in model-based settings where the dynamics model is known or approximated. Amos and Yarats (2020) shows how amortization can learn latent control spaces that are aware of the

structure of the solutions to control problems. Marino *et al.* (2021) study semi-amortized methods based on gradient descent and show that they better-amortize the solutions than the standard fully-amortized models.

5.6 Related Work

5.6.1 Other tutorials, reviews, and discussions on amortized optimization

My goal in writing this tutorial was to provide a perspective of existing amortized optimization methods for learning to optimize with a categorization of the modeling (fully-amortized and semi-amortized) and learning (gradient-based, objective-based, or RL-based) aspects that I have found useful and have not seen emphasized as much in the literature. The other tutorials and reviews on amortized optimization, learning to optimize, and meta-learning over continuous domains that I am aware of are excellent resources:

- Chen *et al.* (2021a) captures many other emerging areas of learning to optimize and discuss many other modeling paradigms and optimization methods for learning to optimize, such as plug-and-play methods (Venkatakrishnan *et al.*, 2013; Meinhardt *et al.*, 2017; Chang *et al.*, 2017; Zhang *et al.*, 2017). They emphasize the key aspects and questions to tackle as a community, including model capacity, trainability, generalization, and interpretability. They propose *Open-L2O* as a new benchmark for learning to optimize and review many other applications, including sparse and low-rank regression, graphical models, differential equations, quadratic optimization, inverse problems, constrained optimization, image restoration and reconstruction, medical and biological imaging, wireless communications, seismic imaging.
- Shu (2017) is a blog post that discusses fully-amortized models with gradient-based learning and includes applications in variational inference, meta-learning, image style transfer, and survival-based classification.

- Weng (2018) is a blog post with an introduction and review of meta-learning methods. After defining the problem setup, the review discusses metric-based, model-based, and optimization-based approaches, and discusses approximations to the second-order derivatives that come up with MAML.
- Hospedales *et al.* (2020) is a review focused on meta-learning, where they categorize meta-learning components into a meta-representation, meta-optimizer, and meta-objective. The most relevant connections to amortization here are that the meta-representation can instantiate an amortized optimization problem that is solved with the meta-optimizer.
- Kim (2020) is a dissertation on deep latent variable models for natural language and contextualizes and studies the use of amortization and semi-amortization in this setting.
- Marino (2021) is a dissertation on learned feedback and feedforward information for perception and control and contextualizes and studies the use of amortization and semi-amortization in these settings.
- Monga *et al.* (2021) is a review on algorithm unrolling that starts with the unrolling in LISTA (Gregor and LeCun, 2010) for amortized sparse coding, and then connects to other methods of unrolling specialized algorithms. While some unrolling methods have applications in semi-amortized models, this review also considers applications and use-cases beyond just amortized optimization.
- Banert *et al.* (2020) consider theoretical foundations for data-driven nonsmooth optimization and show applications in deblurring and solving inverse problems for computed tomography.
- Liu *et al.* (2022) study fully-amortized models based on deep sets (Zaheer *et al.*, 2017) and set transformers (Lee *et al.*, 2019a). They consider regression- and objective-based losses for regression, PCA, core-set creation, and supply management for cyber-physical systems.

5.6.2 Amortized optimization over discrete domains

A significant generalization of Eq. (1.1) is to optimization problems that have discrete domains, which includes combinatorial optimization and mixed discrete-continuous optimization. I have chosen to not include these works in this tutorial as many methods for discrete optimization are significantly different from the methods considered here, as learning with derivative information often becomes impossible. Key works in discrete and combinatorial spaces include Khalil *et al.* (2016), Khalil *et al.* (2017), Jeong and Song (2019), Bertsimas and Stellato (2019), Shao *et al.* (2021), Bertsimas and Stellato (2021), and Cappart *et al.* (2021) and the surveys (Lodi and Zarpellon, 2017; Bengio *et al.*, 2021; Kotary *et al.*, 2021) capture a much broader view of this space. Banerjee and Roy (2015) consider repeated ILP solves and show applications in aircraft carrier deck scheduling and vehicle routing. For architecture search, Luo *et al.* (2018) learn a continuous latent space behind the discrete architecture space. Many reinforcement learning and control methods over discrete spaces can also be seen as amortizing or semi-amortizing the discrete control problems, for example: Cauligi *et al.* (2020) and Cauligi *et al.* (2021) use regression-based amortization to learn mixed-integer control policies. Fickinger *et al.* (2021) fine-tune the policy optimizer for every encountered state. Tennenholz and Mannor (2019), Chandak *et al.* (2019), and Van de Wiele *et al.* (2020) learn latent action spaces for high-dimensional discrete action spaces with shared structure.

5.6.3 Learning-augmented and amortized algorithms beyond optimization

While many algorithms can be interpreted as solving an optimization problems or fixed-point computations and can therefore be improved with amortized optimization, it is also fruitful to use learning to improve algorithms that have nothing to do with optimization. Some key starting references in this space include data-driven algorithm design (Balcan, 2020), algorithms with predictions (Dinitz *et al.*, 2021; Sakaue and Oki, 2022; Chen *et al.*, 2022a; Khodak *et al.*, 2022), learning to prune (Alabi *et al.*, 2019), learning solutions to differential equations (Li *et al.*, 2021a;

Poli *et al.*, 2020; Karniadakis *et al.*, 2021; Kovachki *et al.*, 2021; Chen *et al.*, 2021b; Blechschmidt and Ernst, 2021; Marwah *et al.*, 2021; Berto *et al.*, 2022) learning simulators for physics (Grzeszczuk *et al.*, 1998; Ladický *et al.*, 2015; He *et al.*, 2019; Sanchez-Gonzalez *et al.*, 2020; Wiewel *et al.*, 2019; Usman *et al.*, 2021; Vinuesa and Brunton, 2021), and learning for symbolic math (Lample and Charton, 2020; Charton, 2021; Charton *et al.*, 2021; Drori *et al.*, 2021; d’Ascoli *et al.*, 2022) Salimans and Ho (2022) progressively amortizes a sampling process for diffusion models. Schwarzschild *et al.* (2021) learn recurrent neural networks to solve algorithmic problems for prefix sum, mazes, and chess.

5.6.4 Continuation and homotopy methods

Amortized optimization settings share a similar motivation to continuation and homotopy methods that have been studied for over four decades (Richter and Decarlo, 1983; Watson and Haftka, 1989; Allgower and Georg, 2012). These methods usually set the context space to be the interval $\mathcal{X} = [0, 1]$ and simultaneously solve (without learning) problems along this line. This similarity indicates that problem classes typically studied by continuation and homotopy methods could also benefit from the shared amortization models here.

Acknowledgements

I would like to thank Nil-Jana Akpinar, Alfredo Canziani, Samuel Cohen, Georgina Hall, Misha Khodak, Boris Knyazev, Hane Lee, Joe Marino, Maximilian Nickel, Paavo Parmas, Rajiv Sambharya, Jens Sjölund, Bartolomeo Stellato, Alex Terenin, Eugene Vinitsky, and Atlas Wang for insightful discussions and feedback on this tutorial. I am also grateful to the anonymous FnT reviewers who gave a significant amount of helpful and detailed feedback.

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