Tutorial on amortized optimization for learning to optimize over continuous domains

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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. This leverages the shared structure between similar problem instances. In this tutorial, we will discuss the key design choices behind amortized optimization, roughly categorizing 1) models into fully-amortized and semi-amortized approaches, and 2) learning methods into regression-based and objective-based. We then view existing applications through these foundations to draw connections between them, including for manifold optimization, variational inference, sparse coding, meta-learning, control, reinforcement learning, convex optimization, and deep equilibrium networks. This framing enables us easily see, for example, that the amortized inference in variational autoencoders is conceptually identical to value gradients in control and reinforcement learning as they both use fully-amortized models with an objective-based loss.

The source code for this tutorial is available at:

https://github.com/facebookresearch/amortized-optimization-tutorial
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1. Introduction

We study the use of machine learning to improve repeated solves of optimization problems

\[ y^* (x) \in \arg \min_y f(y; x), \]  

(1)

where the non-convex objective \( f : \mathcal{Y} \times \mathcal{X} \to \mathbb{R} \) takes a context or parameterization \( x \in \mathcal{X} \) which can be continuous or discrete, and the continuous, unconstrained domain of the problem is \( y \in \mathcal{Y} = \mathbb{R}^n \). A solution \( y^*(x) \in \mathcal{Y} \), which we will often assume to be unique, is implicitly defined via the optimization procedure and captures the similarities between problems with different contexts. Parametric optimization problems of this form 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 large focus on sensitivity analysis. This general formulation captures many tasks arising in physics, engineering, mathematics, control, and machine learning. For example, when controlling a continuous robotic system, \( \mathcal{X} \) is the space of observations or states, the domain \( \mathcal{Y} := \mathcal{U} \) is the control space, and \( f(u; x) := -Q(u, x) \) is the control cost or the negated \( Q \)-value of the state-action tuple \( (x, u) \). For every encountered state \( x \), the system is controlled by solving an optimization problem in the form of eq. (1).

Optimization problems such as eq. (1) quickly become a computational bottleneck in systems. Eq. (1) 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 bring empirical gains of computational improvements and improved convergence.

Overview. This is a tutorial on amortized optimization, which is the use of machine learning and statistical methods to augment and computationally speed up optimization methods which solve eq. (1). We focus on the modeling and learning tools necessary for building learning-augmented solvers and extensions of classical optimization methods. Amortized optimization methods are capable of significantly surpassing the convergence bounds derived for classical algorithms on a focused subset of problems because the convergence bounds are typically for worst- or average-case analysis. My goal in writing this is to explore a unified perspective of modeling approaches of amortized optimization to help draw connections between applications, for example between amortized variational inference, meta-learning, and policy learning for control and reinforcement learning. I also connect to selected applications in manifold optimization, sparse coding, convex optimization, and deep equilibrium networks and discuss extensions and other applications beyond the scope here.

2. Amortized optimization foundations for learning to optimize

The machine learning, statistics, and optimization communities are exploring methods of learning to optimize to obtain fast solvers for eq. (1). We will refer to these methods as
Figure 2: An amortized optimization method learns a model $\hat{y}_\theta$ to predict the minimum of an objective $f(y; x)$ to a parameterized optimization problem, as in eq. (1), which depends on a context $x$. For example, in control, the context space $\mathcal{X}$ is the state space of the system, the domain $\mathcal{Y} := \mathcal{U}$ is the control space, 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).

 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. We follow Shu (2017) for defining the core foundation of amortized optimization as:

**Definition 1** An AMORTIZED OPTIMIZATION METHOD to solve eq. (1) can be represented by $\mathcal{A} := (f, \mathcal{Y}, \mathcal{X}, p(x), \hat{y}_\theta, \mathcal{L})$, where $f : \mathcal{Y} \times \mathcal{X} \to \mathbb{R}$ 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, $\hat{y}_\theta : \mathcal{X} \to \mathcal{Y}$ is the AMORTIZATION MODEL parameterized by $\theta$ 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 $\hat{y}_\theta$ and loss $\mathcal{L}$ are application-specific design decisions that sections 3 and 4 opens up. Figure 2 illustrates these components. The model $\hat{y}_\theta$ solves the solution mapping $y^*$ simultaneously for all contexts. We also usually (informally) 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 8.2 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, 2013; Rezende et al., 2014; Stuhlmüller et al., 2013; Gershman and Goodman, 2014; Webb et al., 2017; Ravi and Beatson, 2018; Cremer et al., 2018; Wu et al., 2020), and is used more generally in (Xue et al., 2020; Sercu et al., 2021; Xiao et al., 2021). Marino (2021, p. 28) give further background on the origins and uses of amortization.

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 $f: \mathbb{R}^n \to \mathbb{R}$ in standard Euclidean space, we denote the gradient at a point $\bar{x}$ with $\nabla_{\bar{x}}f(\bar{x}) \in \mathbb{R}^n$ and the Hessian with $\nabla^2_{\bar{x}}f(\bar{x}) \in \mathbb{R}^{n \times n}$. For $f: \mathbb{R}^n \to \mathbb{R}^m$, $D_{\bar{x}}f(\bar{x}) \in \mathbb{R}^{m \times n}$ represents the Jacobian at $\bar{x}$ with entries $[D_{\bar{x}}f(\bar{x})]_{ij} = \frac{\partial f_i}{\partial x_j}(\bar{x})$. We 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 $\theta$-parameterized model clear. We use “;” as separation in $f(y; x)$ to emphasize the separation between the domain variables $y$ that eq. (1) optimizes over from the context ones $x$ that remain fixed. A model’s parameters $\theta$ are usually subscripts as $h_\theta(x)$ but we will equivalently write $h(x; \theta)$ sometimes.

3. Defining the model $\hat{y}_\theta(x)$

The model $\hat{y}_\theta(x): \mathcal{X} \times \Theta \to \mathcal{Y}$ predicts a solution to eq. (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. We will start simple with fully-amortized models in section 3.1 that approximate the entire solution to the optimization problem with a single black-box model. Then section 3.2 shows how to open up the model to include more information about the optimization problem that can leverage domain knowledge with semi-amortized models.

3.1 Fully-amortized models

Definition 2 A FULLY-AMORTIZED model $\hat{y}_\theta: \mathcal{X} \to \mathcal{Y}$ maps the context to the solution of eq. (1) and does NOT access the objective $f$.

We use the non-standard 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 $f$. These are standard in amortized variational inference (section 6.1) and model-free reinforcement leaning (section 6.5), 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 can also be interpreted as a zero-shot approximation to solving eq. (1) from the context without accessing the optimization problem.

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, we open up the black box and turn to semi-amortized models.

3.2 Semi-amortized models

**Definition 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), typically iteratively.

Kim et al. (2018); Marino et al. (2018) proposed semi-amortized models for variational inference that add back domain knowledge of the optimization problem to the model \( \hat{y}_\theta \) that the fully-amortized models do not use. The model itself can now internally integrates 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 \( \mathcal{Z} \). We refer to the space the semi-amortization iterates over as the **amortization space** and denote iterate \( t \) in these spaces, respectively, as \( \hat{y}_t^\theta \) and \( z_t^\theta \). While the iterates and final prediction \( \hat{y}_\theta \) can now query the objective \( f \) and gradient \( \nabla_y f \), we notationally leave this dependence implicit for brevity and only reference these queries in the relevant definitions.

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

One of the most common semi-amortized model is to parameterize and integrate an optimization procedure used to solve eq. (1) into the model \( \hat{y}_\theta \), such as gradient descent (Andrychowicz et al., 2016; Finn et al., 2017; Kim et al., 2018). We emphasize that this optimization procedure is an internal part of the amortization model \( \hat{y}_\theta \), often referred to as the **inner-level** optimization problem in the bi-level setting that arises for learning.

**Examples.** We now instantiate 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 \( \hat{y}_0^\theta(x) := \theta \) is parameterized by \( \theta \in \mathcal{X} \) for all contexts. We then use the knowledge of the objective \( f(y; x) \) for a given context \( x \) and iteratively update

\[
\hat{y}_t^\theta := \hat{y}_{t-1}^\theta - \alpha \nabla_y f(\hat{y}_{t-1}^\theta; x) \quad t \in \{1, \ldots, K\}
\]

for \( K \) steps with a learning rate \( \alpha \in \mathbb{R}_+ \) and set the model’s output to be \( \hat{y}_\theta := \hat{y}^K \).

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) can be integrated into the model. We will further discuss the learning of semi-amortized models by unrolling in section 4.2.1 and will then later see many other instantiations of it:

- **Section 6.2** discusses how Gregor and LeCun (2010) integrate ISTA iterates (Daubechies et al., 2004; Beck and Teboulle, 2009) into a semi-amortized model.
- **Section 6.4.1** 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, 2020).
• Section 6.4.5 discusses RLQP by Ichnowski et al. (2021) that uses the OSQP solver (Stellato et al., 2018) inside of a semi-amortized model.

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

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

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.

**Examples.** The iterative gradient updates in eq. (2) can be replaced with a learned update function as in Ravi and Larochelle (2016); Li and Malik (2016, 2017). These model the past sequence of iterates and learn how to best-predict the next iterate so that the overall sequence is optimal. 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

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

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) is captured by removing the hidden state $z$ and setting

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

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); Amos and Yarats (2019) 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 (2019) 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, 2019), which lifts the domain of the optimization problem eq. (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).

3.2.3 Semi-amortized models vs. warm-starting and fine-tuning

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 we 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. (2019); Baker (2019); Chen et al. (2022). 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. Arbel and Mairal (2021) 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.

### 3.2.4 On second-order derivatives of the objective

Second-order derivatives of the objective often arise when optimizing semi-amortized models and may be a computational bottleneck. Finn et al. (2017); Nichol et al. (2018); Lorraine et al. (2020) propose alternatives to forming the full unrolled derivative, and in this section we will take a closer look at where the second-order terms come from and discuss alternatives. Finn et al. (2017) observed these second-order terms and the following derivation is similar to the ones that Nichol et al. (2018, §5) and Weng (2018) perform by composing the model with the loss, as we will expand on in eq. (12). We focus only on the model derivatives.

**Starting with a single-step model.** We first instantiate a single-step model similar to eq. (2) that parameterizes the initial iterate $\hat{y}_0(x) := \theta$ and takes one gradient step:

$$\hat{y}_\theta(x) := \hat{y}_0(x) - \alpha \nabla_y f(\hat{y}_0(x); x)$$

(5)

The Jacobian of $\hat{y}_\theta(x)$ with respect to the parameters is

$$D_\theta[\hat{y}_\theta(x)] = I - \alpha \nabla_y^2 f(\hat{y}_0(x); x),$$

(6)

which 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 obtain for large models. Before discussing alternatives, we derive similar results for a $K$-step model.

**Multi-step models.** We extend eq. (5) to the $K$-step setting with

$$\hat{y}_K^K(x) := \hat{y}_0(x) - \alpha \nabla_y f(\hat{y}_0(x); x),$$

(7)

where the base $\hat{y}_0(x) := \theta$ as before. Similar to eq. (6), the derivative of a single step is

$$D_\theta[\hat{y}_K^K(x)] = D_\theta[\hat{y}_0(x)] \left( I - \alpha \nabla_y^2 f(\hat{y}_0(x); x) \right),$$

(8)

and composing the derivatives down to $\hat{y}_0$ yields the product structure

$$D_\theta[\hat{y}_K^K(x)] = \prod_{k=0}^{K-1} \left( I - \alpha \nabla_y^2 f(\hat{y}_0(x); x) \right),$$

(9)

where we use $D_\theta[\hat{y}_0(x)] = I$ at the base case. Computing and storing eq. (9) is now $K$ times more challenging as it requires storing the Hessian $\nabla_y^2 f$ at every iteration of the model!
Computationally cheaper alternatives. The first-order MAML baseline in Finn et al. (2017) suggests to simply not use the second-order terms $\nabla^2_\theta f$ 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. (2014) 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, 2016). The MAML++ extension by Antoniou et al. (2018) 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.

Parameterizing and learning the objective. While we mostly do not consider the setting when the objective $f$ is also learned, the second-order derivatives appearing in eq. (9) also cause issues in when the objective is parameterized and learned. In addition to learning an initial iterate, Belanger et al. (2017) the 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 exist.

3.3 Models based on differentiable optimization

As we will see in the next section, the model typically needs to be (sub-)differentiable with respect to the parameters to attain the derivative $D_\theta [\hat{y}_\theta]$ 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) and eq. (3), the derivatives with respect to $\theta$ 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.

4. Learning the model’s parameters $\theta$

Given an amortization model $\hat{y}_\theta$, the last remaining design choice is how to learn the parameters $\theta$ so that the model best-solves eq. (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) over the domain $\mathcal{Y}$. While defining the best loss is application-specific, most approaches can be roughly categorized as 1) matching a ground-truth solution (section 4.1.1), or 2) minimizing the objective (sections 4.1.2 and 4.3), which fig. 3 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 being optimized, and in here we mostly focus on methods where $\theta$ is learned.
4.1 Choosing the objective for learning

4.1.1 Regression-based learning

The first learning method we consider is to regress 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

\[
\arg \min_\theta \mathcal{L}_{\text{reg}}(\hat{y}_\theta) \quad \mathcal{L}_{\text{reg}}(\hat{y}_\theta) := \mathbb{E}_{x \sim p(x)} \| y^*(x) - \hat{y}_\theta(x) \|^2_2. \tag{10}
\]

\( \mathcal{L}_{\text{reg}} \) 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 control, regression-based amortization methods are referred to as behavioral cloning. 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) from scratch may be computationally expensive and amortization methods should improve the computation time.

4.1.2 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:

\[
\arg \min_\theta \mathcal{L}_{\text{obj}}(\hat{y}_\theta) \quad \mathcal{L}_{\text{obj}}(\hat{y}_\theta) := \mathbb{E}_{x \sim p(x)} f(\hat{y}_\theta(x); x). \tag{11}
\]
These methods use local information of the objective to provide a descent direction for the model. A first-order method optimizing eq. (11) uses updates based on the gradient
\[
\nabla_\theta \mathcal{L}_{\text{obj}}(\hat{y}_\theta) = \nabla_\theta \left[ \mathbb{E}_{x \sim p(x)} f(\hat{y}_\theta(x); x) \right] = \mathbb{E}_{x \sim p(x)} D_\theta [\hat{y}_\theta(x)]^T \nabla_y [f(\hat{y}_\theta(x); x)],
\]
(12)
where the last step is obtained by the chain rule. This has the interpretation that the model’s parameters are updated by combining the gradient information around the prediction \( \nabla_x [f(\hat{y}_\theta(x); x)] \), which we show in fig. 3, with how \( \theta \) impacts the model’s predictions with the derivative \( D_\theta [\hat{y}_\theta(x)] \). While we mostly focus on optimizing eq. (12) with first-order methods that explicitly differentiate the objective, section 4.3 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. We will see that amortized variational inference methods and actor-critic methods both make extensive use of objective-based learning.

Remark 1. A standard gradient-based optimizer for eq. (1) (without amortization) can be recovered from \( \mathcal{L}_{\text{obj}} \) 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. (12), resulting in \( \nabla_\theta \mathcal{L}_{\text{obj}}(\hat{y}_\theta) = \nabla_y f(\hat{y}_\theta(x); x) \). Thus optimizing \( \theta \) of this parameter-identity model with gradient descent is identical to solving eq. (1) with gradient descent. Remark 1 shows a connection between a model trained with gradients of an objective-based loss and a non-amortized gradient-based solver for eq. (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 us to the intuition that objective-based amortization works best when a gradient-based optimizer is able to successfully solve eq. (1) from scratch.

4.1.3 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 4 illustrates that the \( \ell_2 \)-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. The following summarizes some other advantages (+) and disadvantages (−):

![Figure 4: \( \mathcal{L}_{\text{reg}} \) contours.](image-url)
Regression-based losses $L_{\text{reg}}$

- Does not consider $f(y; x)$
- Uses global information with $y^*(x)$
- Expensive to compute $y^*(x)$
- Does not compute $\nabla_y f(y; x)$
- Hard to learn non-unique $y^*(x)$

Objective-based losses $L_{\text{obj}}$

- 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 $y^*(x)$

4.2 Learning iterative semi-amortized models

Fully-amortized or semi-amortized models can be learned with the regression- and objective-based losses. Here we discuss how the loss can be further opened up and crafted to learn iterative semi-amortized methods. For example, if the model produces intermediate predictions $\hat{y}_\theta^i$ in every iteration $i$, instead of optimizing the loss of just the final prediction, i.e. $L(\hat{y}_{\theta^K})$, we can consider more generally variants of the losses that we will denote as $L^\Sigma$ that consider the impact of every iteration of the model’s prediction

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

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 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. We next discuss concepts that arise when computing the derivatives of a loss with respect to the model’s parameters.

4.2.1 Unrolled optimization and backpropagation through time

The parameterization of every iterate $z_\theta^i$ can influence the final prediction $\hat{y}_\theta$ and thus losses on top of $\hat{y}_\theta$ need to consider the entire chain of computations. Differentiating through an iterative procedure such as this is referred to as backpropagation through time in sequence models and unrolled optimization (Pearlmutter and Siskind, 2008; Zhang and Lesser, 2010; Maclaurin et al., 2015a; Belanger and McCallum, 2016; Metz et al., 2016; 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 as the model computation is iterative and computing $D_\theta[\hat{y}_\theta(x)]$ requires saving and differentiating the “unrolled” intermediate iterations, as we saw in section 3.2.4. 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 $D_{\theta} \hat{y}_\theta$ is well-defined, in practice it can be instable because of exploding gradients, and inefficient for compute and memory resources because every iterate needs to be stored, as we saw in section 3.2.4. This is why most methods using unrolled optimization for learning often only unroll through tens of iterations (Metz et al., 2016; Belanger et al., 2017; Foerster et al., 2017; Finn et al., 2017) while solving the problems from scratch typically require millions (!) of iterations. This causes the predictions to be extremely inaccurate solutions to the optimization process and has sparked the research directions that we next turn to that seek to make unrolled optimization more tractable.

4.2.2 Truncated backpropagation through time and biased gradients

$z_0^{\theta} \rightarrow \hat{z}_0^{\theta} \rightarrow \cdots \rightarrow \hat{z}_{K-H}^{\theta} \rightarrow \cdots \rightarrow \hat{z}_K^{\theta} \rightarrow \hat{y}_\theta(x) \rightarrow \mathcal{L}$

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 $\{z_i^{\theta}\}_{i=K-H}$ 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); Vicol et al. (2021) seek to further theoretically understand the properties of TBPTT, including the bias of the estimator and how to unbias it.

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) we will further discuss in section 3.2.4.

4.2.3 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 instable 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. (2019); 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
Here we briefly summarize 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), especially at the beginning of training. Rajeswaran et al. (2019) observe that adding a penalty to the objective around the initial iterate $\hat{y}_\theta^0$ makes it easy for the model to globally (!) solve the problem

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

where the parameter $\lambda$ that encourages the solution to stay close to some initial iterate. In fig. 5, we visualize 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.

4.3 Parameter learning with zeroth-order methods and reinforcement learning

Computing the derivatives to learn $\hat{y}_\theta$ 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 6 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.

4.3.1 Reinforcement learning

Li and Malik (2016, 2017); 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 $x^t$ are the actions, the context and previous iterations or losses are typically the states, the associated losses $\mathcal{L}(x^t)$ are the rewards, and $\hat{y}_\theta^t(x)$ 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 (2016, 2017) uses Guided Policy Search (Levine and Koltun, 2013) and Ichnowski et al. (2021) uses TD3 (Fujimoto et al., 2018). We use $\mathcal{L}^{RL}$ to indicate that a loss is optimized with reinforcement learning, typically on the objective-based loss.
4.3.2 Loss smoothing and optimization with zeroth-order methods

Metz et al. (2019a) observe that objective-based losses can have a high-frequency structure with many poor local minimum. To overcome this, they use Gaussian smoothing:

$$L^{\text{smooth}}(\hat{y}_\theta) := \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \sigma^2 I)} [L(\hat{y}_\theta + \epsilon)], \quad (15)$$

where $\sigma^2$ is a fixed variance. Figure 7 illustrates a loss function $L$ 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.

Connection to smoothing in reinforcement learning. The Gaussian smoothing of the objective $L$ in eq. (15) is conceptually similar to Gaussian smoothing of the objective in reinforcement learning, i.e. the $-Q$-value, by a Gaussian policy that we will see in eq. (64) and further discuss in section 6.5. 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. In contrast, Metz et al. (2019a); 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 $\sigma^2$ that is not optimized over.

5. Extensions of the amortization setting we consider here

I have intentionally scoped definition 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. Here, we cover extensions from this setting that may come up in practice.

5.1 Extensions of the domain $\mathcal{Y}$

5.1.1 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 6.5 for control, for example.

Transforming parameterized stochastic problems back into deterministic ones. We will mostly focus on settings that optimize over the parametric distributions. We use this for the stochastic domains arising in amortized variational inference in section 6.1 and stochastic control in section 6.5. These settings optimize over a constrained parametric family of distributions parameterized by some $\lambda$, for example over a multivariate normal $\mathcal{N}(\mu, \Sigma)$ parameterized by $\lambda := (\mu, \Sigma)$. Here, problems can be transformed back to eq. (1) by optimizing over the parameters with

$$\lambda^*(x) \in \arg \min_{\lambda} f(\lambda; x), \quad (16)$$
where \( \lambda \) induces a distribution that the objective \( f \) may use. When \( \lambda \) is not an unconstrained real space, the differentiable projections we will discuss in section 5.1.2 could be used to transform \( \lambda \) 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, §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 \( \mathcal{P} \):

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

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 \( \text{Var}_p[X] \). 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 we do 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 \( g_\theta \) with an expressive family of densities parameterized by \( \theta \).

### 5.1.2 Unconstrained \( \rightarrow \) Constrained Optimization

Amortized constrained optimization problems may naturally arise, for example in the convex optimization settings we consider in section 6.4 and for optimization over the sphere we discuss in section 7. Constrained optimization problems for amortization can often be represented as an extension of eq. (1) with

\[
y^*(x) \in \arg \min_{y \in \mathcal{C}} f(y; x),
\]  

where the constraints \( \mathcal{C} \) may also depend on the context \( x \). A budding research area studies how to more generally include constraints into the formulation. Baker (2019); Dong et al. (2020); Zamzam and Baker (2020); Pan et al. (2020) learn to warm-start for optimal power flow. Misra et al. (2021) learn active sets for constrained optimization. Kriváčy et al. (2020) solves constrained feasibility SDPs 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.
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 7 also uses a differentiable projection from $\mathbb{R}^n$ onto the sphere $S^{n-1}$. We define these as:

**Definition 4** A projection from $\mathbb{R}^n$ onto a set $C \subseteq \mathbb{R}^n$ is

$$\pi_C : \mathbb{R}^n \to C \quad \pi_C(x) \in \arg \min_{y \in C} D(x, y) + \Omega(y), \quad (19)$$

where $D : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a distance and $\Omega : \mathbb{R}^n \to \mathbb{R}$ is a regularizer that can ensure invertibility or help spread $\mathbb{R}^n$ more uniformly throughout $C$. A (sub)differentiable projection has (sub)derivatives $\nabla_{x} \pi_C(x)$. We sometimes omit the dependence of $\pi$ on the choice of $D$, $\Omega$, and $C$ 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 4, such as Bregman projections, are not idempotent in general and often $\pi_C \circ \pi_C \neq \pi_C$ as the regularizer may cause points that are already on $C$ to move to a different position on $C$.

Differentiable projections for constrained amortization. These can be used to cast Eq. (18) as the unconstrained problem eq. (1) by composing the objective with a projection $f \circ \pi_C$. (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, we first interpret the ReLU, sigmoid, and softargmax as differentiable projections that solve convex optimization problems in the form of eq. (19). Amos (2019, §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

$$\pi(x) \in \arg \min_y \frac{1}{2} \|x - y\|_2^2 \quad \text{s.t.} \quad y \geq 0, \quad (20)$$

and has a closed-form solution given 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

$$\pi(x) \in \arg \min_{0 < y < 1} -x^\top y - H_b(y), \quad (21)$$

where

$$H_b(y) := \left( \sum_i y_i \log y_i + (1 - y_i) \log (1 - y_i) \right) \quad (22)$$

is the binary entropy function. Eq. (21) 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
\[
\Delta_{n-1} := \{ p \in \mathbb{R}^n \mid 1^\top p = 1 \text{ and } p \geq 0 \}
\] (23)
can be projected onto with the entropy-regularized optimization problem
\[
\pi(x) \in \arg \min_{0 < y < 1} -x^\top y - H(y) \quad \text{s.t.} \quad 1^\top y = 1
\] (24)
where \(H(y) := -\sum_i y_i \log y_i\) is the entropy function. Eq. (24) 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.

Going beyond these, we next cover differentiable projections onto convex cones, noting that they can also be softened or regularized to help with continuity when composed with learning and amortization methods. Ali et al. (2017); Busseti et al. (2019) discuss differentiating the standard Euclidean projections onto these, including:

• The second-order, Lorentz, or ice cream cone defined by
\[
\mathcal{K}_{soc} := \{(x, y) \in \mathbb{R}^{m-1} \times \mathbb{R} : \|x\|_2 \leq y\}
\] (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
\[
\mathcal{K}_{exp} = \{(x, y, z) : x \in \mathbb{R}, y > 0, z \geq y \exp(x/y)\} \cup \{(x, 0, z) : x \leq 0, z \geq 0\}
\] (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, §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); Santa Cruz et al. (2017); Mena et al. (2018) project onto the Birkhoff polytope of doubly stochastic matrices with row and column sums of 1, i.e.
\[
\mathcal{B}_m := \{X \in \mathbb{R}^{m \times m} : X1 = X^\top 1 = 1\}
\] (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, permutahedron, 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.

5.1.3 Euclidean \(\rightarrow\) 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. This area of research has studied acceleration methods, (Duruisseaux and Leok, 2022), less exploration has been done on amortized optimization. Section 7 discusses amortizing a simple constrained spherical optimization problem that we are able to transform 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.

5.2 Extensions of the model \(\hat{y}_\theta\)

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

5.2.1 Symbolic models: Uncovering human-interpretable update rules

One of the largest issues in the models we consider is that they are uninterpretable and it is often impossible for us as humans to learn any new insights about the optimization problems we are modeling, 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); 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); Zheng et al. (2022).

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. (2011); Zeiler (2012); Kingma and Ba (2014), 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.

5.3 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 (2018) 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.

5.4 Settings where \( p(x) \) changes and can be end-to-end learned

We will mostly assume that \( p(x) \) is fixed and remains the same through the entire training process to allow us to scope to the amortization aspects in all of the settings. 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 \( p(x) \).

Higher-level learning processes can use end-to-end learning to update a context distribution parameterized by \( \varphi \), which we write as \( p(x; \varphi) \). This is done in, for example, variational inference and deep equilibrium models, and involves optimizing a higher-level loss \( \ell \) defined on the solutions, which could take the form of the bi-level problem

\[
\arg\min_{\varphi} \mathbb{E}_{x \sim p(x; \varphi)} \ell(y^* (x); x) \quad \text{subject to} \quad y^* (x) \in \arg\min_y f(y; x) \tag{28}
\]

where \( y^* (x) \) can be replaced with an approximation by a learned amortization model \( \hat{y}_\theta \approx y^* \). The parameters \( \varphi \) in eq. (28) can often be end-to-end learned through the solution of eq. (1) to update the influence that \( p(x; \varphi) \) has on the solutions. We next turn to methods that show how to differentiate through the value \( f(y^* (x); x) \) and solution \( y^* (x) \) to enable gradient-based learning of \( \varphi \) in eq. (28).

5.4.1 End-to-end learning \( p(x; \varphi) \) by differentiating the value \( f(y^* (x); x) \)

Methods can end-to-end learn through the optimal value \( f(y^* (x); x) \) to update other parameters that show up in the context. For example, variational autoencoders differentiate through the value, i.e. the best approximation to the ELBO, to optimize their density
model. The theory of why this works is rooted in the optimization community’s studies of envelope theorems that 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); Milgrom and Segal (2002); Bonnans and Shapiro (2013). In the unconstrained and non-convex eq. (1), the envelope theorem gives

\[
\nabla_x \min_{y} f(y; \bar{x}) = \nabla_x f(y^*(\bar{x}); \bar{x})
\]

(29)

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

5.4.2 End-to-end learning \( p(x) \) by differentiating the solution \( y^*(x) \)

In addition to differentiating through the value, the solution \( y^*(x) \) can be implicitly differentiated. We will refer to the derivative \( D_2 y^*(x) \) 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, 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 \( D_2 y^*(x) \) is more involved than the value derivative using the envelope theorem in eq. (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 as we have seen in the other settings, this may be unstable and tracking all of the iterations is extremely memory- and compute-intensive. 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) as:

**Theorem 1 (Dini’s implicit function theorem)** Let the roots of \( g(y; x) \) define an implicit mapping \( Y^*(x) \) given by \( Y^*(x) := \{y \mid g(y; x) = 0\} \), where \( x \in \mathbb{R}^m \), \( y \in \mathbb{R}^n \), and \( g : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n \). Let \( g \) be continuously differentiable in a neighborhood of \((\bar{y}, \bar{x})\) such that \( g(\bar{y}; \bar{x}) = 0 \), and let the Jacobian of \( g \) with respect to \( y \) at \((\bar{y}, \bar{x})\), i.e. \( D_y g(\bar{y}; \bar{x}) \), be non-singular. Then \( Y^* \) has a single-valued localization \( y^* \) around \( \bar{x} \) for \( \bar{y} \) which is continuously differentiable in a neighborhood \( Q \) of \( \bar{x} \) with Jacobian satisfying

\[
D_2 y^*(\bar{x}) = -D_y^{-1} g(y^*(\bar{x}); \bar{x}) D_2 g(y^*(\bar{x}); \bar{x}) \quad \text{for every} \ \bar{x} \in Q.
\]

(30)

The adjoint derivative \( D_2 y^*(x) \) can be computed by seeing \( y^* \) as the roots of an implicit function \( g(y; x) \), which we need to select to make the solution equivalent to the solution of eq. (1). Typically \( g(y; x) \) is an optimality system of the optimization problem, e.g. the KKT system for constrained convex optimization problems. For the unconstrained problem we consider here, we can take the first-order optimality of the objective \( g(y; x) := \nabla_y f(y; x) \) and apply theorem 1 to compute \( D_2 y^*(x) \).
### Table 1: We tour the following applications of amortized optimization.

| §   | Application | Objective | Domain | Context Space | Amortization model | Loss L |
|-----|-------------|-----------|--------|---------------|--------------------|-------|
| 6.1 | VAE         | - ELBO    | Variational posterior | Data | Full | $\mathcal{L}_{\text{obj}}$ |
|     | SAVAE/IVAE | | | | Semi | $\mathcal{L}_{\text{reg}}$ |
| 6.2 | PSD         | Reconstruction | Sparse code | Data | Full | $\mathcal{L}_{\text{obj}}$ |
|     | LISTA       | | | | Semi | $\mathcal{L}_{\text{reg}}$ |
| 6.3 | HyperNets   | Task loss | Model parameters | Tasks | Full | $\mathcal{L}_{\text{obj}}$ |
|     | LM          | | | | Semi | $\mathcal{L}_{\text{reg}}$ |
|     | MAML        | | | | | $\mathcal{L}_{\text{obj}}$ |
|     | Neural Potts| Pseudo-likelihood | | Protein sequences | Full | $\mathcal{L}_{\text{obj}}$ |
| 6.4 | NeuralFP    | FP residual | FP iterates | FP contexts | Semi | $\mathcal{L}_{\Sigma\text{obj}}$ |
|     | HyperAA     | | | | | $\mathcal{L}_{\Sigma\text{reg}}$ |
|     | NeuralSCS   | CP residual | CP iterates | CP parameters | | $\mathcal{L}_{\Sigma\text{obj}}$ |
|     | HyperDEQ    | DEQ residual | DEQ iterates | DEQ parameters | | $\mathcal{L}_{\Sigma\text{reg}}$ |
|     | NeuralNMF   | NMF residual | Factorizations | Input matrices | | $\mathcal{L}_{\Sigma\text{obj}}$ |
|     | RLQP        | $R_{\text{RLQP}}$ | | | | $\mathcal{L}_{\Sigma\text{obj}}$ |
| 6.5 | BC/IL       | $-Q$-value | Controls | State space | Full | $\mathcal{L}_{\text{reg}}$ |
|     | (D)DPG/TD3  | | | | Full or semi | $\mathcal{L}_{\text{obj}}$ |
|     | PILCO       | | | | | $\mathcal{L}_{\text{obj}}$ |
|     | POPLIN      | | | | | $\mathcal{L}_{\text{reg}}$ |
|     | DCEM        | | | | Semi | $\mathcal{L}_{\text{reg}}$ |
|     | IAPO        | | | | | $\mathcal{L}_{\text{obj}}$ |
|     | SVG         | $D_Q$ or $-\mathcal{E}_Q$ | Control dists | | Full | $\mathcal{L}_{\text{obj}}$ |
|     | SAC         | | | | | $\mathcal{L}_{\text{obj}}$ |
|     | GPS         | | | | | $\mathcal{L}_{\text{KL}}$ |
| 7   | Synthetic Sphere | $c$-convex functions | $S^2 \rightarrow \mathbb{R}^3$ | RCPM parameters | Full | $\mathcal{L}_{\text{obj}}$ |

### 6. Review and tour of existing research that uses amortized optimization

We now take a review and tour of the key applications of amortized optimization to show some unifying ideas that can be shared between all of these topics. Table 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.

#### 6.1 Amortized 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. We focus 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, 2013; Rezende et al., 2014; Mnih and Gregor, 2014; Rezende and Mohamed, 2015; Higgins et al., 2016; Doersch, 2016; Kingma et al., 2019) and refer to references such as Jordan.
et al. (1999); Wainwright and Jordan (2008); Blei et al. (2017) for a complete background in variational inference. Kim (2020); 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.

6.1.1 The variational autoencoder (VAE) by Kingma and Welling (2013)

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 \( p(x) \). Before defining the amortization model, VAEs parameterize a likelihood model \( p(x; \varphi) \) with \( \varphi \). 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

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

where \( q(z; \lambda) \) is a variational distribution over the latent space parameterized by \( \lambda \) and \( p(z) \) is the prior. Given a sample \( x \sim p(x) \), we can find the best lower bound \( \lambda^* \) that satisfies

\[
\log p(x) \geq \text{ELBO}(\lambda^*; x, \varphi) \geq \text{ELBO}(\lambda; x, \varphi)
\]

for all \( \lambda \) by solving the optimization problem

\[
\lambda^* \in \arg \max_{\lambda} \text{ELBO}(\lambda; x, \varphi).
\]

Amortized VI (AVI) methods predict the solution to eq. (33) while stochastic variational methods (Hoffman et al., 2013) explicitly solve it. AVI methods learn a model \( \hat{\lambda}_\theta : \mathcal{X} \to \Lambda \) with parameters \( \theta \), which is usually a feedforward neural network, to predict the maximum value of the ELBO by optimizing the objective-based loss

\[
\arg \max_{\theta} \mathbb{E}_{x \sim p(x)} \text{ELBO}(\hat{\lambda}_\theta(x); x, \varphi)
\]

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 \( \Lambda \), the context space \( \mathcal{X} \) is the sample space for the generative model, the samples are given from \( p(x) \), \( \hat{\lambda}_\theta : \mathcal{X} \to \Lambda \) is the fully-amortized model optimized with the gradient-based loss \( \mathcal{L}_{\text{obj}} \) 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. (34) 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. (2018).

The full VAE loss. This section has left the parameterization $\varphi$ 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 $\hat{\lambda}_\theta(x)$ with

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

6.2 Amortized 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

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

where $E$ is the regularized reconstruction energy and $\alpha \in \mathbb{R}_+$ is a coefficient of the $\ell_1$ term. Eq. (36) 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 momentum term. The core update of ISTA methods is

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

$W_e := (1/L)W_d^T$ 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 $\beta$, usually set to $\alpha/L$. ISTA methods are remarkably fast ways of solving eq. (36) 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.

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

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

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

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

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

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

Summary. $A_{PSD} := (E, \mathcal{Y}, \mathcal{X}, p(x), \hat{y}_\theta, \mathcal{L}_{reg})$
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 \( Y \) that starts with \( x^0_\theta := 0 \) and iteratively updates \( x^{t+1}_\theta := h_\beta(Fx + Gx^t_\theta) \). Running these updates for \( K \) steps results in a final prediction \( \hat{y}(x) := x^K_\theta \) parameterized by \( \theta = \{F, G, \beta\} \) that is also optimized with the regression-based loss to the ground-truth sparse codes as in eq. (39).

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

### 6.3 Amortized multi-task learning and meta-learning

Many multi-task learning and meta-learning methods also use amortized optimization for parameter learning. Here we will take a glimpse at this viewpoint, which has also been observed before in Shu (2017); Gordon et al. (2018).

**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; Ly et al., 2017; Li and Malik, 2016, 2017; 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 \( T \sim p(T) \) 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 \( \mathcal{L}_T(\hat{y}_\theta) \) that measures how well a parameterized model \( \hat{y}_\theta \) performs on it. There is typically a distribution over tasks \( p(T) \) and the goal is to find a model that best-optimizes the expectation over task losses by solving

\[
\arg\min_\theta \mathbb{E}_{T \sim p(T)} \mathcal{L}_T(\hat{y}_\theta).
\]  

(40)

The motivation here is that there is likely shared structure and information present between the tasks that learning methods can leverage. We will next go through methods that solve eq. (40) using objective-based amortized optimization methods.

### 6.3.1 Fully-amortized hyper networks (HyperNets)

HyperNEAT (Stanley et al., 2009) and Hypernetworks (Ha et al., 2016) predict the optimal parameters to a network given a data sample and can be seen as fully-amortized optimization. The tasks here \( T = (x, y^*(x)) \) 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 \( p(T) \). HyperNets propose to predict \( y^*(x) \) with a prediction model \( \hat{y}_\varphi(x) \) parameterized by \( \varphi \). 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 \( \mathcal{L}_T(\hat{y}_\theta(x), y^*(x)) \) 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
\[
\arg\min_{\theta} \mathbb{E}_{T \sim p(T)} L_T(\hat{y}_\theta(x), y^*(x)). \tag{41}
\]

**Summary.** \(A_{\text{HyperNet}} := (L_T, \Phi, T, p(T), \hat{\varphi}_\theta, L_{\text{obj}})\)

### 6.3.2 Learning to Optimize (LM) by Li and Malik (2016)

Li and Malik (2016) 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 \(T = \{x_i, y_i\}_{i=1}^N\) to train on, they again search for the parameters \(\hat{\varphi}_\theta(T) \in \Phi\) of another prediction model \(\hat{y}_{\hat{\varphi}_\theta(T)}(x) =: \hat{y}_\theta(x)\) that performs well on a loss \(L_T(\hat{y}_\theta)\) 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 \(\hat{\varphi}_0^0\) and then predicts the next iterate with
\[
\hat{\varphi}_\theta^{t+1} = g_\theta(\{\varphi^t, L_T(\hat{\varphi}^t), \nabla \varphi L_T(\hat{\varphi}^t), \Delta^t\}), \tag{42}
\]
where the update model \(g_\theta\) takes the last \(i \in \{t-H, t\} \cap \mathbb{R}_+\) 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 (2017) further develops these ideas for learning to optimize neural network parameters.

**Summary.** \(A_{\text{LM}} := (L_T, \Phi, T, p(T), \hat{\varphi}_\theta, L_{\text{obj}})\)

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

As we discussed in section 3.2.1, MAML can be seen as a semi-amortized optimization method. They also seek to predict the parameters \(\hat{\varphi}_\theta(T) \in \Phi\) of prediction model \(\hat{y}_{\hat{\varphi}_\theta(T)}(x) =: \hat{y}_\theta(x)\) in a multi-task setting with tasks \(T \sim p(T)\). They propose to only learn to predict an initial iterate \(\hat{\varphi}_0^0(T) = \theta\) and then update the next iterates with gradient-based updates such as
\[
\hat{\varphi}_\theta^{t+1} = \varphi_t^t - \alpha \nabla \varphi L_T(\hat{\varphi}_\theta^t), \tag{43}
\]
where \(L_T(\varphi)\) is the task loss obtained by the model \(\hat{y}_\varphi\) parameterized by \(\varphi\). MAML optimizes this model with an objective-based loss through the final prediction.

**Summary.** \(A_{\text{MAML}} := (L_T, \Phi, T, p(T), \hat{\varphi}_\theta, L_{\text{obj}})\)

### 6.3.4 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 \(M := \{x_i\}\) and they use a fully-amortized model \(\varphi_\theta(M) \in \Phi\) to predict the optimal parameters of a Potts model.
The model $\varphi_\theta$ is a large attention-based sequence model that takes the MSA as the input. Learning is done with the objective-based loss

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

(44)

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

### 6.3.5 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. Here we selectively summarize a few other relevant ideas:

1. Ravi and Larochelle (2016) 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. (2018) performs semi-amortization over a learned latent space. This uses the powerful insight that semi-amortizing over the low-level parameters $\varphi$ 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 hyper-parameter 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., 2018) 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. (2019) 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 propose to overcome both of these issues by dynamically weighting reparameterization gradients and zeroth-order evolutionary methods to optimize the smoothed loss in eq. (15).

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 minimum. 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. (2018); 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.
6.4 Amortized fixed-point computations and convex optimization

**Definition 5** 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 5 are ubiquitous in engineering and science and amortizing their solutions is an active research area. Let \( R(y) := g(y) - y \) be the fixed-point residual with squared norm \( N(y) := \|R(y)\|_2^2 \). Fixed-point computations are connected to continuous unconstrained optimization as any fixed-point problem can be transformed into eq. (1) by optimizing the residual norms with:

\[
y^*(x) \in \arg\min_y N(y),
\]

and conversely eq. (1) can be transformed into a fixed-point problem via first-order optimality to find the fixed-point of \( \nabla f(y) - y = 0 \). Thus methods that to amortize the solutions to eq. (1) can help amortize the solutions to fixed-point computations definition 5.

**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

\[
y^{t+1} := y^t - (D_y g(y^t))^{-1} g(y^t).
\]

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

\[
\text{AA}_\text{Update}^t(\{y_i\}, \alpha, \beta) := \beta \sum_{i=0}^M \alpha_i y^{t-M+i} + (1 - \beta) \sum_{i=0}^M \sum_{j=0}^M \alpha_i y^{t-M+i},
\]

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

\[
\alpha^* := \arg\min_{\alpha} \|R(y)\alpha\|_2 \text{ subject to } 1^\top \alpha = 1
\]

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.

6.4.1 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 \( \text{init}_\theta \) and perform the fixed-point computations

\[
\hat{x}^{t+1} = f(\hat{y}^t; x)
\]

\[
(\hat{y}^{t+1}, \hat{h}^{t+1}) = \text{acc}_\theta(\hat{y}^t, \hat{x}^{t+1}, \hat{h}^t)
\]

Figure 9: Fixed points of a map.
using an \textit{acceleration model} $\text{acc}_\theta$ 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. (45) over a distribution of contexts $p(x)$ with an objective-based loss that solves

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

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 \textit{constrained convex cone programs} solved by the splitting cone solver (SCS) (O’donoghue et al., 2016) of the form

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

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 $\mathcal{K}^* \in \mathbb{R}^m$. SCS uses the \textit{homogeneous self-dual embedding} to view eq. (51) as a fixed-point computation over $Z = \mathbb{R}^{n \times m \times 1}$ 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. (51). Their semi-amortized model $\hat{z}_\theta(\phi)$ takes a context $\phi$ 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 ($\text{init}_\theta, \text{acc}_\theta$).

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

6.4.2 Neural acceleration for matrix factorization (\textit{NeuralNMF})

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

$$
V \approx WH^T, \quad W \geq 0, H \geq 0, 
$$

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. (52) leads to the optimization formulation

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

which can be solved with ADMM (Boyd et al., 2011). Given a distribution over input matrices $V$, Sjölund and Bänkestad (2022), augment a base ADMM method 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.

\textbf{Summary.} \ $A_{\text{NeuralNMF}} := \left( \mathcal{N}_{\text{NMF}}, Z, V, p(V), \hat{Z}_\theta, \mathcal{L}_{\text{obj}}^\Sigma \right)$
6.4.3 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, 2020; Gurumurthy et al., 2021). Their learned variant of AA, called HyperAnderson acceleration uses models that predict the initial point \( \hat{y}_0^\theta(x) \) and coefficients \( \alpha_\theta(x; G) \) and \( \beta_\theta(x; G) \) and result in iterations of the form

\[
G_{\theta}^{t+1}, \hat{y}_{\theta}^{t+1} := \text{AA}_\text{Update}(\{\hat{y}_0^t\}, \alpha_t^\theta(x; G_t^\theta), \beta_t^\theta(x, G_t^\theta)),
\]

where \( G_t^\theta \) 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

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

where \( \Omega \) is a regularizer on \( \alpha^t \) 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, 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 \( g_\phi(y; x) \) 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 \( \mathcal{N}(y; x) := \| y - g_\phi(y; x) \|_2^2 \) as

\[
y^*(x) \in \arg \min_x \mathcal{N}(y; x).
\]

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 \( \mathcal{A}_{\text{HyperDEQ}} := (\mathcal{N}, \mathcal{Y}, \mathcal{X}, p(x), \hat{y}_\theta, \mathcal{L}_{\text{HyperAA}}) \).

6.4.4 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 we briefly compare 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 \( \alpha, \beta \) for the update
- Use an regression-based loss
Figure 10: 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.

6.4.5 RLQP by Ichnowski et al. (2021)

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

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

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

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

and then updates

$$z^{t+1} := z^t + \text{diag}(\rho^t)^{-1} (v^{t+1} - y^t)$$

$$z^{t+1} := \Pi (z^{t+1} + \text{diag}(\rho^t)^{-1} y^t)$$

$$y^{t+1} := x^t + \text{diag}(\rho^t) (z^{t+1} - zt + 1),$$

where $y, v$ are dual variables, $z, \tilde{z}$ are auxiliary operator splitting variables, $\sigma$ is a regularization parameter, and $\rho^t \in \mathbb{R}^m_+$ is a step-size parameter. We combine all of the variables into a state $s := (y, \lambda, \tilde{z}, z)$ living in $s \in S$ and write the update as $s^{t+1} := \text{OSQP}_\text{UPDATE}(s^t, \rho^t)$.

RLQP proposes to use these OSQP iterates as a semi-amortized model with the iterates $\{s^t, \rho^t\}$. The propose to only parameterize and learn to predict the step size $\rho^{t+1} := \pi_\theta(s^t)$, with a neural network amortization model $\pi_\theta$. They model the process of predicting the optimal $\rho$ as an MDP and define a reward $R_{RLQP}(s, \rho)$ 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 $\theta$.

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

6.5 Amortized policy learning for control and reinforcement learning

Many control and reinforcement learning methods amortize the solutions to a control optimization problem as illustrated in figs. 2 and 10.
Distinction. This section is on amortization for reinforcement learning and control and not the different direction of using reinforcement learning for amortization that we discuss in section 4.3 for parameter learning.

6.5.1 BACKGROUND

Preliminaries in Markov decision processes.

Definition 6 We represent a Markov decision process (MDP) with \( \mathcal{M} := (\mathcal{X}, \mathcal{U}, p, r) \), where \( \mathcal{X} \) are the continuous states, \( \mathcal{U} \) are the continuous actions or controls, \( p(x' \mid x, u) \) 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.

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

\[
\pi^*(x) \in \arg \max_{\pi} \mathbb{E}_{x \sim p_{\text{init}}(x)} V^\pi(x) \quad V^\pi(x) := \sum_t \mathbb{E}_{(x_t, u_t) \sim \rho_{\pi}^t(\cdot \mid x)} r(x_t, u_t), \tag{60}
\]

where \( p_{\text{init}} \) is the initial state distribution and \( V^\pi(x) \) is the expected value of a policy \( \pi \) 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

\[
Q^\pi(x, u) := r(x, u) + \mathbb{E}_{x' \sim p(\cdot \mid x, u)} \left[ V^\pi(x') \right], \tag{61}
\]

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

\[
\pi^*(x) \in \arg \max_u Q(x, u), \tag{62}
\]

which is the form we will often use to interpret many control and reinforcement learning methods as amortized optimization. Instead of amortizing the solution to eq. (62), methods such as Lowrey et al. (2018); Ryu et al. (2019) 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, which we write 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

\[
u^*_{1:H}(x_1) := \arg \min_{u_{1:H}} \sum_t C_t(x_t, u_t) \text{ subject to } x_{t+1} = p(x_t, u_t), \tag{63}\]
where the cost $C$ at each time is usually the negated reward $C_t(x_t, u_t) := -r(x_t, u_t)$. Eq. (63) induces the policy $\pi(x) := u_\pi^*(x)$ 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 we are only able to sample from the system. 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. (62) can be extended to the stochastic optimization settings we briefly covered in section 5.1.1 when the policy $\pi$ 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

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

(64)

or 2) the KL distance

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

(65)

where $Q(x, \cdot) \propto \exp\{Q(x, \cdot)/\alpha\}$ is a $Q$-distribution induced by the $Q$ values that is inversely scaled by $\alpha \in \mathbb{R}_+$. The policy $\pi$ is usually represented as the parameters of a distribution and thus $\Pi$ becomes the space of these parameters. In most cases we take $\pi$ to be a Gaussian $\mathcal{N}(\mu, \Sigma)$ with a diagonal covariance $\Sigma$ and thus we thus we can turn eqs. (64) and (65) into unconstrained continuous optimization problems of the form eq. (1) by projecting onto the Gaussian parameters. We will see that stochastic value gradient methods such as Heess et al. (2015) often amortize eq. (64), while Levine and Koltun (2013); Haarnoja et al. (2018) propose methods that build on eq. (65), 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. Lastly, we note again that the smoothing that the policy performs in eq. (64) is nearly identical to the objective smoothing considered in section 4.3.2, except in that setting the variance of the smoother remains fixed.

**Connecting stochastic control back to deterministic control.** We show that taking stochastic policies to be Dirac delta distributions in eqs. (64) and (65) recovers the solutions to the deterministic control problem in eq. (62). 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) instable 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 1** Let $\pi$ be a Dirac delta distribution $\delta_u(\cdot)$. Then the solution $\pi^*(x)$ to the expected $Q$ problem in eq. (64) is the solution to the deterministic max-Q problem in eq. (62).
Proof Let \( \Pi = \mathbb{R}^n \) be the parameter space of \( \pi \) and transform eq. (64) to optimize over it:

\[
\pi^*(x) \in \arg \max_{u \in \mathbb{R}^n} E_{\tilde{u} \sim \delta_u(x)} Q(x, \tilde{u}).
\]  

(66)

The expectation over the Dirac evaluates to

\[
E_{\tilde{u} \sim \delta_u(x)} Q(x, \tilde{u}) = Q(x, u)
\]

(67)

and thus eq. (66) which is the max-Q operation in eq. (62).

Similarly for the KL problem in eq. (65):

Proposition 2 Let \( \pi \) be a Dirac delta distribution \( \delta_u(\cdot) \). Then the solution \( \pi^*(x) \) to the KL problem in eq. (65) is the solution to the deterministic max-Q problem in eq. (62).

Proof Let \( \Pi = \mathbb{R}^n \) be the parameter space of \( \pi \) and transform eq. (65) to optimize over it:

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

(68)

Expanding the KL distance then gives the density of \( Q \) at the mass:

\[
D_{KL}(\delta_u(\cdot) \parallel Q(x, \cdot)) = E_{\tilde{u} \sim \delta_u(x)} [\log \delta_u(\tilde{u}) - \log Q(x, \tilde{u})] = -\log Q(x, u) + C
\]

(69)

where \( C \) is a constant that does not depend on \( u \), \( Q(x, u) \) is the density at \( u \), and \( Z_x \) is the normalization constant for \( Q(x, \cdot) \) that does not depend on \( u \). Putting eq. (69) back into eq. (68) and removing the constants that do not depend on \( u \) gives

\[
\pi^*(x) \in \arg \min_{u \in \mathbb{R}^n} -Q(x, u),
\]  

(70)

which is the max-Q operation in eq. (62).

6.5.2 Behavioral cloning and imitation learning

We will start in the setting where regression-based amortization is done to predict the solution of a controller that solves eq. (60). In these settings, we have access to a controller, or samples from it, that uses traditional methods, and not learning, to solve eq. (60), and we either know the true dynamics or form an approximation to them that the control is done on top of. We typically have access to these solutions as samples from a policy \( \pi^*(x) \) that provides the solution to the max-Q problem in eq. (62) that we want to do regression-based amortization onto. In some settings these methods also use the optimal finite-horizon sequence \( u_{1:H}^*(x) \) from a solution to eq. (63).
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 $x$. Deterministic BC methods often regress onto the expert’s state-action pairs $(x, \pi^*(x))$ sampled some distribution of states $p(x)$ with

$$\arg\min_\theta \mathbb{E}_{x \sim p(x)} \|\pi^*(x) - \pi_\theta(x)\|^2_2,$$  \hspace{1cm} (71)

where, for example, the model $\pi_\theta$ could be a neural network. Thus BC in this setting performs regression-based amortization $A_{BC} := (-Q, U, X, p(x), \pi_\theta, L_{reg})$. Extensions from this setting could include when 1) the model $\pi_\theta$ is a sequence model that predicts the entire sequence $u^*_1:H$, and 2) the MDP or policy is stochastic and eq. (71) 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 that we consider is that in behavioral cloning, we also may not know the original objective that the expert solves. We assume 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.

### 6.5.3 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. (62). 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. (2015), and and twin delayed DDPG (TD3) by Fujimoto et al. (2018). All of these methods interweave 1) policy evaluation to estimate the state-action value $Q^\pi_\theta$ of the current policy $\pi_\theta$, and 2) policy improvement to find the policy that best-optimizes the max-$Q$ operation with

$$\arg\max_\theta \mathbb{E}_{x \sim p(x)} Q(x, \pi_\theta(x)).$$  \hspace{1cm} (72)

**Summary.** The DPG family of methods perform objective-based amortization of the max-$Q$ optimization problem with $A_{DPG} := (-Q, U, X, p(x), \pi_\theta, L_{obj})$.

### 6.5.4 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., 2019; Byravan et al., 2021; Amos et al., 2021). As observed in Haarnoja et al. (2018); 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 $\pi_\theta$ that amortize the solution to a stochastic optimization problem, such as eqs. (64) and (65), 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

$$\arg\max_\theta \mathcal{L}_{SVG, \mathcal{E}}(\pi_\theta) \quad \mathcal{L}_{SVG, \mathcal{E}}(\pi_\theta) := \mathbb{E}_{x \sim p(x)} \mathbb{E}_{u \sim \pi(\cdot|x)} Q(x, u),$$  \hspace{1cm} (73)
and taking the minimum KL distance gives the policy loss

\[ \arg\min_{\theta} L_{\text{SVG}}(\pi_{\theta}) := \mathbb{E}_{x \sim p(x)} D_{\text{KL}}(\pi_{\theta}(\cdot \mid x) \parallel \mathcal{Q}(x, \cdot)), \tag{74} \]

which softens the policy and value estimates with an entropy regularization as in Haarnoja et al. (2018); Amos et al. (2021). Eq. (74) can be seen as an entropy-regularized value estimate by expanding the KL

\[ \mathbb{E}_{x \sim p(x)} D_{\text{KL}}(\pi_{\theta}(\cdot \mid x) \parallel \mathcal{Q}(x, \cdot)) = \mathbb{E}_{x \sim p(x)} \mathbb{E}_{u \sim \pi_{\theta}(u \mid x)} [\alpha \log(\pi(u \mid x)) - \mathcal{Q}(x, u)]. \tag{75} \]

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

\[ A_{\text{SVG}} := (D_{\mathcal{Q}} \text{ or } -\mathcal{E}_{\mathcal{Q}}, \mathcal{P}(\mathcal{U}), \mathcal{X}, p(x), \pi_{\theta}, L_{\text{KL}}). \]

**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); Amos et al. (2021) use learned models for the value approximation. The variation in Hafner et al. (2019) 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. (2020) 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. (2021) 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.

6.5.5 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 \( \pi_{\theta} \). The parameters \( \theta \) are optimized by taking gradient steps to find the policy resulting in the maximum value over some distribution of states \( p(x) \), i.e.

\[ \arg\max_{\theta} \mathbb{E}_{x \sim p(x)} Q(x, \pi_{\theta}). \tag{76} \]

**Summary.** \( A_{\text{PILCO}} := (-Q, \mathcal{U}, \mathcal{X}, p(x), \pi_{\theta}, L_{\text{obj}}) \)

6.5.6 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. (63) within a local region of the data to improve the amortization model. Given samples of \( \pi^* \) from a
controller that solves eq. (65), GPS methods typically optimize the KL divergence between
the controller and these samples with
\[
\arg\min_{\theta} \mathbb{E}_{x \sim p(x)} D_{KL}(\pi_{\theta}(\cdot | x) \parallel \pi^{*}(\cdot | x))
\] (77)

**Summary.** \( \mathcal{A}_{GPS} := (D_{Q}, \mathcal{P}(U), \mathcal{X}, p(x), \pi_{\theta}, L_{KL}) \)

### 6.5.7 POPLIN by Wang and Ba (2019)

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. Here we only consider
the BC variant trained with \( \mathcal{A}_{BC} \), which provides an optimal fully-amortized model \( \pi_{\theta^{*}} \).

**Control.** Next they explore ways of using the learned policy \( \pi_{\theta^{*}} \) to solve the model
predictive control optimization problem in eq. (63). The POPLIN-A variant (“A” stands for
“action”) uses \( \pi_{\theta^{*}} \) to predict an initial control sequence \( \hat{u}_{1:H} \) 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. (63) over the action space, POPLIN-P proposes to use CEM to find a perturbation \( \omega \) to
the optimal parameters \( \theta^{*} \) that maximizes the value from a state \( x \) with
\[
\omega^{*}(x) \in \arg\max_{\omega} Q(x; u; \pi_{\theta^{*}+\omega}).
\] (78)

Thus the action produced by \( \pi_{\theta^{*}+\omega^{*}}(x) \) is a solution the control problem in eq. (63) obtained
by adapting the policy’s parameters to the state \( x \).

**Summary.** POPLIN is an extension of of behavioral cloning that amortizes control
optimization problems with \( \mathcal{A}_{POPLIN} := (-Q, U, \mathcal{X}, p(x), \pi_{\theta}, L_{reg}) \). The initial phase is fully-
amortized behavioral cloning. The second fine-tuning phase can seen as semi-amortization
that learns only the initialization \( \theta \) and finds \( \omega \) with CEM, with a regression-based loss \( L_{reg} \)
that only has knowledge of the initial model and does not include the adaptation.

### 6.5.8 The differentiable cross-entropy method by Amos and Yarats (2019)

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 (2019), 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.
Figure 11: The differentiable cross-entropy method (DCEM) can be used to create semi-amortized controllers that learn a latent space $\mathcal{Z}$ over control sequences. This visualization 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.

Amos and Yarats (2019) 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. (63). Learning a latent space is useful if there are many redundancies and possibly bad local minimum 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

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

(79)
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

$$C(z; x) := -\sum_{t=1}^{H} r(x_t, x_t) \text{ subject to } x_{t+1} = p(x_t, u_t) \text{ and } x_{1:H} = \varphi_\theta(z)$$  \hspace{1cm} (80)

Solving eq. (79) with DCEM enables the optimal solution $\hat{z}_\theta(x)$ to be differentiated with respect to the parameters $\theta$ of the decoder $\varphi_\theta$. 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

$$\arg\min_{\theta} \mathcal{L}_{\text{DCEM}}(\hat{u}_{1:H}(:, \theta)) \hspace{1cm} \mathcal{L}_{\text{DCEM}}(\hat{u}_{1:H}(:, \theta)) := \mathbb{E}_{x \sim p(x)} \| u_{1:H}^*(x) - \hat{u}_{1:H}(x; \theta) \|^2_2.$$  \hspace{1cm} (81)

Figure 11 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.

**Overview.** Learning a latent domain with the differentiable cross-entropy method is a semi-amortization method with $\mathcal{A}_{\text{DCEM}} := (-Q, \mathcal{U}, \mathcal{X}, p(x), \pi_\theta, \mathcal{L}_{\text{obj}})$, where the decoder $\varphi_\theta$ shows up from the policy $\pi_\theta$ solving the latent optimization problem with DCEM.

### 6.5.9 Iterative amortized policy optimization (IAPO) by Marino et al. (2020)

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 $\pi_\theta$ 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 $\mathcal{A}_{\text{IAPO}} := (-Q, \mathcal{U}, \mathcal{X}, p(x), \pi_\theta, \mathcal{L}_{\text{obj}})$. 
7. Manifold extension: Amortized optimization on the sphere

We conclude with a simple new demonstration that applies the insights from amortized optimization to learn to solve optimization problems over spheres of the form

\[ y^* (x) \in \arg \min_{y \in S^2} f(y; x), \]

(82)

where \( S^2 \) is the surface of the unit 2-sphere embedded in \( \mathbb{R}^3 \) as \( S^2 := \{ y \in \mathbb{R}^3 \mid \| y \|_2 = 1 \} \) and \( x \) is some parameterization of the function \( f : S^2 \times \mathcal{X} \to \mathbb{R} \). Eq. (82) 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.

**Amortization objective.** We first need to turn the constrained problem in eq. (82) into an unconstrained optimization problem of the form eq. (1). In this setting, one way of doing this is by using a projection:

\[ y^* (x) \in \arg \min_{y \in \mathbb{R}^3} f(\pi_{S^2}(y); x), \]

(83)

where \( \pi_{S^2} : \mathbb{R}^3 \to S^2 \) is the Euclidean projection onto \( S^2 \), i.e.,

\[
\pi_{S^2}(x) := \arg \min_{y \in S^2} \| y - x \|_2 \\
= x / \| x \|_2.
\]

(84)

c-convex functions on the sphere. We instantiate a synthetic class of optimization problems defined on the sphere using the c-convex functions from Cohen et al. (2021):

\[
f(y; x) = \min_{\gamma} \left\{ \frac{1}{2} d(x, z_i) + \alpha_i \right\}^m_{i=1}
\]

(85)

where \( m \) components define the context \( x = \{ z_i \} \cup \{ \alpha_i \} \) with \( z_i \in S^2 \) 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 \( \min_{\gamma} (a_1, \ldots, a_m) := -\gamma \log \sum_{i=1}^m \exp(-a_i/\gamma) \) is a soft minimization operator as proposed in Cuturi and Blondel (2017). We sample \( p(x) \) with \( z_i \sim \mathcal{U}(S^2) \), uniformly from the sphere, and \( \alpha_i \sim \mathcal{N}(0, \beta) \) with variance \( \beta \in \mathbb{R}_+ \).

**Amortization model.** We next instantiate the model \( \hat{y}_\theta : \mathcal{X} \to \mathbb{R} \) as a fully-connected MLP. The predictions to eq. (82) on the sphere can again be obtained by composing the output with the projection \( \pi_{S^2} \circ \hat{y}_\theta \).

**Optimizing the gradient-based loss.** Finally we choose to optimize the gradient-based loss \( L_{\text{obj}} \) as the objective and model are tractable and easily differentiable. Figure 12 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 solutions to eq. (82) with a single neural network \( \hat{y}_\theta(x) \) trained with the gradient-based loss.

**Summary.** \( \mathcal{A}_{\text{sphere}} := (f \circ \pi_{S^2}, \mathbb{R}^3, \mathcal{X}, p(x), \hat{y}_\theta, L_{\text{obj}}) \)
8. 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); Metz et al. (2021) provide even deeper probes into general paradigms for learning to optimize. Here we emphasize a few additional discussion points around amortized optimization.

8.1 Going beyond the known convergence rates of classical methods

Theoretical and empirical optimization research often focuses on discovering algorithms with theoretically strong convergence rates, and indeed many of the algorithms with the best convergence rates are used as the state-of-the-art algorithms in practice. Amortized optimization and the paradigm of learning to optimize can offer even better convergence rates in this space that surpass even the best theoretical rates when scoping to optimization problems sampled from a context space $p(x)$. For example, the fully amortized models for amortized variational inference and model-free actor-critic methods for RL solve the optimization problems in constant time with just a single prediction of the solution from the context without even looking at the objective! In semi-amortized settings, this intuition also enables parameterized versions of optimization algorithms to far surpass the known convergence bounds by similarly giving the amortization model the power of predicting a near-optimal solution in constant time.

8.2 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.

8.3 Measuring performance

Quantifying the performance of amortization models can 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).

8.4 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. Here we summarize principles behind successful applications of amortized optimization and characterize limitations that may arise.

8.4.1 Characteristics of successful applications

- **Objective** $f(y; x)$ is smooth over the domain $\mathcal{Y}$ and has unique solutions $y^\star$. With objective-based learning, non-convex objectives with few poor local optimum are ideal. This behavior can be encouraged with smoothing as is often done for meta-learning and policy learning (section 4.3.2).

- 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. (35). 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 $\pi_\theta$ 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 $\alpha, \beta$ after the initial iterate, and RLQP (Ichnowski et al., 2021) only parameterizing $\rho$.

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.
8.4.2 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), 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.

8.5 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.** In section 4.3.2, we covered the objective smoothing by Metz et al. (2019a); Merchant et al. (2021) to overcome local minima in the objective. These have striking similarities to stochastic policies in reinforcement learning that also overcome local minima, e.g. in eq. (64). 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. I have not seen this property in many amortization settings and it seems desirable for the same reasons.

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); Stellato et al. (2018), users are likely solving many similar problem instances that
amortization can help improve. Venkataraman and Amos (2021); 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, 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); 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. (2019); 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. Amortized and semi-amortized control and reinforcement learning. Applications of semi-amortization in control and reinforcement learning that we covered in section 6.5 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 (2019) shows how amortization can learn latent control spaces that are aware of the structure of the solutions to control problems. Marino et al. (2020) study semi-amortized methods based on gradient descent and show that they better-amortize the solutions than the standard fully-amortized models.

8.6 Coding and implementing amortized optimization

The approaches we consider here are most-easily implemented with automatic differentiation software such as Maclaurin et al. (2015b); Al-Rfou et al. (2016); Abadi et al. (2016); Bezanson et al. (2017); Agrawal et al. (2019b); Paszke et al. (2019); Bradbury et al. (2020). Many of the approaches cited in here have open-source implementations using many of these packages which provide a good starting point to start building on top of.

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., 2021) 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.

- **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.

9. Related work

9.1 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; Rick 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.

• Arridge et al. (2019) survey data-driven optimization methods for solving inverse problems. This survey covers the foundations and discuss tradeoffs between statistical accuracy and robustness, and functional complexity, stability, and interpretability. Their applications include image denoising, image deblurring, image inpainting, computed tomography, photoacoustic tomography, magnetic resonance imaging, and magnetic particle imaging.

• 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.

• Banert et al. (2020) consider theoretical foundations for data-driven nonsmooth optimization and show applications in deblurring and solving inverse problems for computed tomography and is further developed in Banert et al. (2021).

• 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.

• 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.

9.2 Amortized optimization over discrete domains

A significant generalization of eq. (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 what we cover here, as learning with derivative information often becomes impossible. Key works in discrete and combinatorial spaces include Khalil et al. (2016); Dai et al. (2017); Jeong and Song (2019); Bertsimas and Stellato (2019); Shao
et al. (2021); Bertsimas and Stellato (2021); 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, 2021) use regression-based amortization to learn mixed-integer control policies. Fickinger et al. (2021) fine-tune the policy optimizer for every encountered state. Tennenholtz and Mannor (2019); Chandak et al. (2019); Van de Wiele et al. (2020) learn latent action spaces for high-dimensional discrete action spaces with shared structure.

9.3 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), learning to prune (Alabi et al., 2019), learning solutions to differential equations (Li et al., 2020; 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., 2021) 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, 2019; 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.

9.4 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.

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