Learning with differentiable and amortized optimization

Brandon Amos • Meta AI (FAIR) NYC

<u>http://github.com/bamos/presentations</u>

Optimization is crucial technology

Optimization is a **modeling** and **decision-making** paradigm and **encodes reasoning operations**

Finds the **best way to interact** with a **representation of the world**

Focus: parametric optimization problems that are repeatedly solved



• \mathcal{X} vertical slices are optimization problems

Breakthroughs enabled by optimization include

1. controlling systems (robotic, autonomous, mechanical, and multi-agent)







objective optimal solution **CONTEXT** (or parameterization) $y^*(x) \in \operatorname{argmin} f(y; x)$ $y \in \mathcal{C}(x)$ optimization variable constraints



Breakthroughs enabled by optimization include

- 1. **controlling systems** (robotic, autonomous, mechanical, and multi-agent)
- 2. making operational decisions based on future predictions
- 3. efficiently **transporting** or **matching** resources, information, and measures
- 4. **allocating** budgets and portfolios
- 5. **designing** materials, molecules, and other structures
- 6. solving inverse problems (to infer underlying hidden costs, incentives, geometries, terrains)
- 7. parameter learning of predictive and statistical models





When optimization fails, machine learning helps

$$y^*(x) \in \underset{y \in \mathcal{C}(x)}{\operatorname{argmin}} f(y; x)$$

Bad representation of the world (unknown, mis-specified, or inaccurate) **Solving is computationally difficult**



When machine learning fails, optimization helps

Optimization provides an internal reasoning operation



This talk: integrating optimization and learning

Key: view **optimization as a function** from the context x to the solution $y^*(x) \in \operatorname{argmin} f(y; x)$ $y \in \mathcal{C}(x)$

Differentiable optimization $-\frac{\partial}{\partial x}y^{\star}(x)$

Task-based optimization Foundations: convex quadratic and cone programs **Applications**

Amortized optimization $-\hat{y}_{\theta}(x) \approx y^{\star}(x)$

RL as amortized optimization Foundations: modeling and loss choices Applications Amortization via learning latent subspaces





Demand prediction and scheduling



Using predictions for scheduling

Stage 1: maximum likelihood training



Using predictions for scheduling

Stage 1: maximum likelihood training



max-likelihood model \neq best model for the task Why? Modeling errors impact tasks in different ways

Task-based end-to-end model learning in stochastic optimization. Donti, Amos, and Kolter, NeurIPS 2017. *Objective mismatch in model-based reinforcement learning.* Lambert, Amos, Yadan, and Calandra, L4DC 2020.

Stage 2: deploy within a larger system



Idea: improve the model with the task loss



Stage 2: deploy within a larger system. Improve the model with the task information



Incorporating the task loss is crucial

Task-based end-to-end model learning in stochastic optimization. Donti, Amos, and Kolter, NeurIPS 2017.



How to differentiate an optimization problem?



Stage 2: deploy within a larger system. Improve the model with the task information



Differentiable optimization layers

Definition. A **differentiable optimization layer** for a machine learning model internally solves an optimization problem and is learned with backpropagation



Differentiable convex quadratic programs

OptNet: Differentiable Optimization as a Layer in Neural Networks. Amos and Kolter, ICML 2017.

Differentiable convex conic programs

Section 7 of Differentiable optimization-based modeling for machine learning. Amos, PhD Thesis 2019 Differentiating through a cone program. Agrawal et al., 2019

Differentiable convex optimization layers. Agrawal*, Amos*, Barratt*, Boyd*, Diamond*, Kolter*, NeurIPS 2019.

$$x^{\star} = \underset{x}{\operatorname{argmin}} c^{\top} x$$

subject to $b - Ax \in \mathcal{K}$
$$\overbrace{\text{Second-order (Lorentz): } \{(t, x) \in \mathbb{R}_{+} \times \mathbb{R}^{n} | \|x\|_{2} \le t\}}$$

$$\overbrace{\text{Second-order (Lorentz): } \{(t, x) \in \mathbb{R}_{+} \times \mathbb{R}^{n} | \|x\|_{2} \le t\}}$$

$$\overbrace{\text{Semidefinite: } \mathbb{S}_{+}^{n}}$$

$$\overbrace{\text{Exponential: } \{(x, y, z) \in \mathbb{R}^{3} | ye^{x/y} \le z, y > 0\} \cup \mathbb{R}_{-} \times \{0\} \times \mathbb{R}_{+}}$$

Conic Optimality

Find z^* s.t. $\mathcal{R}(z^*, \theta) = 0$ where $z^* = [x^*, ...]$ and $\theta = \{A, b, c\}$

Implicitly differentiating \mathcal{R} gives $D_{\theta}(z^{\star}) = -(D_{z}\mathcal{R}(z^{\star}))^{-1}D_{\theta}\mathcal{R}(z^{\star})$

Task-based end-to-end model learning in stochastic optimization. Donti, Amos, and Kolter, NeurIPS 2017.

Task-based learning (task-aware predictions, decision-focused learning)





OptNet: Differentiable Optimization as a Layer in Neural Networks. Amos and Kolter, ICML 2017.

Task-based learning (task-aware predictions, decision-focused learning)

Learning hard constraints (Sudoku from data)

 $y^{\star}(x) = \underset{y}{\operatorname{argmin}} \operatorname{dist}(x, y)$ subject to $Gy \leq h$

parameters $\theta = \{G, h\}$





Limited multi-label projection layer. Amos et al., 2019.

Task-based learning (task-aware predictions, decision-focused learning)

Learning hard constraints (Sudoku from data)

Modeling projections (ReLU, sigmoid, softmax; differentiable top-k, and sorting)

$$\operatorname{argtopk}_{\tau}(x) = \operatorname{argmin}_{y} -y^{\mathsf{T}}x - \tau H_{b}(y)$$

subject to $0 \le y \le 1$
 $1^{\mathsf{T}}y = k$
$$H_{b}(y) \coloneqq -\sum_{i} (y_{i} \log y_{i} + (1 - y_{i}) \log(1 - y_{i}))$$

is the binary cross-entropy function
$$001$$

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Learning latent permutations with Gumbel-Sinkhorn networks. Mena et al., ICLR 2018.

Task-based learning (task-aware predictions, decision-focused learning)

Learning **hard constraints** (Sudoku from data)

Modeling projections (ReLU, sigmoid, softmax; differentiable top-k, and sorting)

Gumbel-Sinkhorn: projection onto the **Birkhoff polytope** \mathcal{B}_N :

$$\pi_{\mathcal{B}_N,\tau}(X) = \underset{P \in \mathcal{B}_N}{\operatorname{argmax}} \langle P, X \rangle_F + \tau H(P)$$

$$\mathcal{B}_N = \left\{ X \colon X \ge 0, \Sigma_i X_{ij} = \Sigma_j X_{ij} = 1 \right\}$$



What Game Are We Playing? End-to-end Learning in Normal and Extensive Form Games. Ling et al., IJCAI 2018.

Task-based learning (task-aware predictions, decision-focused learning)

Learning hard constraints (Sudoku from data)

Modeling projections (ReLU, sigmoid, softmax; differentiable top-k, and sorting)

Game theory (differentiable equilibrium finding)



 $\min_{u} \max_{v} u^{\mathsf{T}} P v \text{ subject to } \mathbf{1}^{\mathsf{T}} u = \mathbf{1} \quad \mathbf{1}^{\mathsf{T}} v = \mathbf{1} \quad u, v \ge 0$ Parameterize and learn payoff *P*

Differentiable MPC for end-to-end planning and control. Amos et al., NeurIPS 2018. The differentiable cross-entropy method. Amos and Yarats, ICML 2020.

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Game theory (differentiable equilibrium finding)

RL and control (differentiable control-based policies, enforcing safety constraints)

$$x_{1:T}^{\star}, u_{1:T}^{\star} \in \underset{x_{1:T}, u_{1:T}}{\operatorname{argmin}} \sum_{t} \underbrace{\underset{t}{\overset{\text{cost}}{\bigcap(x_t, u_t)}}}_{t} \text{ s.t. } \underbrace{\underset{x_1 = x_{\text{init}}}{\overset{\text{initial state}}{\inf(x_{t+1})}} \underbrace{\underset{t}{\overset{\text{dynamics}}{y_{t+1}}}_{t} \underbrace{\underset{u_t \in \mathcal{U}}{\overset{\text{constraints}}}}_{u_t \in \mathcal{U}}$$

Parameterize and learn cost and dynamics

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Meta-learning with differentiable convex optimization. Lee et al., CVPR 2019.

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Game theory (differentiable equilibrium finding)

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Meta-learning (differentiable SVMs and optimizers, implicit MAML)

MetaOptNet:

Differentiate the decision boundary w.r.t. the dataset

$$w^{\star}(\mathcal{D}) = \underset{w}{\operatorname{argmin}} \|w\|^{2} + C \sum_{i} \max\{0, 1 - y_{i}f(x_{i})\}$$



Input-convex neural networks. Amos, Xu, Kolter, ICML 2017.

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Energy-based learning and structured prediction (differentiable inference with, e.g., ICNNs)

$$y^{\star}(x) = \underset{y}{\operatorname{argmin}} E_{\theta}(x, y)$$

Applications of differentiable optimization Differentiable convex optimization layers. Agrawal*, Amos*, Barratt*, Boyd*, Diamond*, Kolter*, NeurIPS 2019.

Task-based learning (task-aware predictions, decision-focused learning)

Learning hard constraints (Sudoku from data)

Modeling **projections** (ReLU, sigmoid, softmax; differentiable top-k, and sorting)

Game theory (differentiable equilibrium finding)RL and control (differentiable control-based policies, er

Meta-learning (differentiable SVMs and optimizers, imp o

Energy-based learning and structured prediction (diff⁻²

Sensitivity analysis (differentiable logistic regression)

$$\theta^{\star}(\mathcal{D}) \in \operatorname*{argmax}_{\theta} \sum_{i} \log p_{\theta}(y_i \mid x_i)$$



Task-based learning (task-aware predictions, decision-focused learning)

Learning hard constraints (Sudoku from data)

Modeling projections (ReLU, sigmoid, softmax; differentiable top-k, and sorting)

Game theory (differentiable equilibrium finding)

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Sensitivity analysis (differentiable logistic regression)

Differentiable CVXPY layers

Differentiable convex optimization layers. Agrawal*, Amos*, Barratt*, Boyd*, Diamond*, Kolter*, NeurIPS 2019.



$$z_{i+1} = \underset{z}{\operatorname{argmin}} \frac{1}{2} z^{\top} Q(z_i) z + q(z_i)^{\top} z$$

subject to $A(z_i) z = b(z_i)$
 $G(z_i) z \le h(z_i)$

Parameters/Submodules : Q, q, A, b, G, h

Before: 1k lines of code, now:

```
import cvxpy as cp
from cvxpyth import CvxpyLayer
obj = cp.Minimize(0.5*cp.quad_form(x, Q) + p.T * x)
cons = [A*x == b, G*x <= h]
prob = cp.Problem(obj, cons)
layer = CvxpyLayer(prob, params=[Q, p, A, b, G, h], out=[x])
```

This talk

Differentiable optimization $-\frac{\partial}{\partial x}y^{\star}(x)$

Task-based optimization Foundations: convex quadratic and cone programs Applications

Amortized optimization $-\hat{y}_{\theta}(x) \approx y^{\star}(x)$

RL as amortized optimization Foundations: modeling and loss choices Applications Amortization via learning latent subspaces





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Deploying optimization and repeated solves

Tutorial on amortized optimization for learning to optimize over continuous domains. Amos, Foundations and Trends in Machine Learning 2023. *On the model-based stochastic value gradient for continuous reinforcement learning*. Amos et al., L4DC 2021.



Repeatedly solved problems share structure

Tutorial on amortized optimization for learning to optimize over continuous domains. Amos, Foundations and Trends in Machine Learning 2023.



Amortization: approximate the solution map

Tutorial on amortized optimization for learning to optimize over continuous domains. Amos, Foundations and Trends in Machine Learning 2023.

A fast amortization model \hat{y}_{θ} can be 25,000 times faster than solving y^* from scratch for VAEs

Amortization model $\hat{y}_{\theta}(x)$ tries to approximate $y^{*}(x)$ **Example:** A neural network mapping from x to the solution

Loss \mathcal{L} measures how well \hat{y} fits y^* and optimized with $\min_{\theta} \mathcal{L}(\hat{y}_{\theta})$ **Regression:** $\mathcal{L}(\hat{y}_{\theta}) \coloneqq \mathbb{E}_{p(x)} \|\hat{y}_{\theta}(x) - y^*(x)\|_2^2$ **Objective:** $\mathcal{L}(\hat{y}_{\theta}) \coloneqq \mathbb{E}_{p(x)} f(\hat{y}_{\theta}(x))$



Tutorial on amortized optimization for learning to optimize over continuous domains. Amos, Foundations and Trends in Machine Learning 2023.

Reinforcement learning and control (actor-critic methods, SAC, DDPG, GPS, BC)



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Reinforcement learning and **control** (actor-critic methods, SAC, DDPG, GPS, BC)

Variational inference (VAEs, semi-amortized VAEs)

Given a VAE model $p(x) = \log \int_z p(x|z)p(x)$, encoding amortizes the optimization problem

 $\lambda^{\star}(x) = \underset{\lambda}{\operatorname{argmax}} \operatorname{ELBO}(\lambda; x) \quad \text{where} \quad \operatorname{ELBO}(\lambda; x) \coloneqq \mathbb{E}_{q(z;\lambda)}[\log p(x|z)] - \mathcal{D}_{\operatorname{KL}}(q(x;\lambda)|p(z)).$



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Variational inference (VAEs, semi-amortized VAEs)

Meta-learning (HyperNets, MAML)

Given a task \mathcal{T} , amortize the computation of the optimal parameters of a model

 $\theta^{\star}(\mathcal{T}) = \operatorname*{argmax}_{\theta} \ell(\mathcal{T}, \theta)$

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Sparse coding (PSD, LISTA)

Given a **dictionary** W_d of **basis vectors** and **input** x, a **sparse code** is recovered with

$$y^{*}(x) \in \underset{y}{\operatorname{argmin}} ||x - W_{d}y||_{2}^{2} + \alpha ||y||_{1}$$

Predictive sparse decomposition (PSD) and Learned ISTA (LISTA) **amortize this problem** Kavukcuoglu, Ranzato, and LeCun, 2010. Gregor and LeCun, 2010.

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Roots, fixed points, and convex optimization (NeuralDEQs, RLQP, NeuralSCS)



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Roots, fixed points, and convex optimization (NeuralDEQs, RLQP,

Optimal transport (slicing, conjugation, Meta Optimal Transport)

 $T^{\star}(\alpha,\beta) \in \underset{T \in \mathcal{C}(\alpha,\beta)}{\operatorname{argmin}} \mathbb{E}_{x \sim \alpha} \|x - T(x)\|_{2}^{2}$ Meta Optimal Transport. Amos et al., 2022





Tutorial on amortized optimization for learning to optimize over continuous domains. Amos, Foundations and Trends in Machine Learning 2023.

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Roots, fixed points, and convex optimization (NeuralDEQs, RLQP, N

Optimal transport (slicing, conjugation, Meta Optimal Transport)

$$f^{c}(y) = -\inf_{x} f(x) - x^{\mathsf{T}} y$$

On amortizing convex conjugates for optimal transport. Amos, ICLR 2023



Reinforcement learning and **control** (actor-critic methods, SAC, DDPG, GPS, BC)

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Foundations and Trends[®] in Machine Learning

Tutorial on amortized optimization for learning to optimize over continuous domains

Brandon Amos Facebook AI Research, Meta

BDA@FB.COM

Amortization via learning latent subspaces

The differentiable cross-entropy method. Amos and Yarats, ICML 2020.

Full control sequence space

Amortize the problem by learning a latent subspace of optimal solutions Only search over optimal solutions rather than the entire space

$$x_{1:T}^{\star}, u_{1:T}^{\star} \in \underset{x_{1:T}, u_{1:T}}{\operatorname{argmin}} \sum_{t} \underbrace{\underset{t}{\overset{\text{cost}}{\mathcal{C}_{\theta}(x_t, u_t)}}_{t} \text{ s.t.} \underbrace{\underset{x_1 = x_{\text{init}}}{\overset{\text{initial state}}{x_{t+1} = f_{\theta}(x_t, u_t)}}_{t} \underbrace{\underset{u_t \in \mathcal{U}}{\overset{\text{constraints}}}_{u_t \in \mathcal{U}}} \underbrace{\underset{u_t \in \mathcal{U}}{\overset{\text{subspace of optimal solutions}}}_{t}$$



Amortization via learning latent subspaces

The differentiable cross-entropy method. Amos and Yarats, ICML 2020.



Future directions and open questions

Goal: build intelligent systems that **understand and interact** with the world **Why?** To advance scientific and engineering discoveries

Advancing optimization and machine learning foundations is crucial



How to handle discrete spaces?

CombOptNet. Paulus, Rolínek, Musil, Amos, and Martius, ICML 2021.



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How to transfer knowledge between structures?

Cross-domain imitation learning via optimal transport. Fickinger, Cohen, Russell, Amos, ICLR 2022.

Optimization (optimal transport) connects disparate spaces to enable knowledge transfer





How can latent representations gain an awareness of unobserved concepts?

Learning awareness models. Amos et al., ICLR 2018.

Situation awareness is the perception of the elements in the environment within a volume of time and space, and the comprehension of their meaning, and the projection of their status in the near future.

— Mica Endsley (1987) Former Chief Scientist of the U.S. Air Force



How to model and control non-trivial systems?



On the model-based stochastic value gradient for continuous reinforcement. B. Amos et al., L4DC 2021.



Nocturne: a driving benchmark for multi-agent learning. Vinitsky et al., NeurIPS Datasets and Benchmarks 2022



Learning Neural Event Functions for Ordinary Differential Equations. Chen, Amos, Nickel, ICLR 2021.

How to perform machine learning and optimization over non-Euclidean spaces?

Riemannian convex potential maps. Cohen*, Amos*, and Lipman, ICML 2021.



How to perform machine learning and optimization over non-Euclidean spaces?

Matching Normalizing Flows and Probability Paths on Manifolds. Ben-Hamu et al., ICML 2022.



Learning with differentiable and amortized optimization

Summary

Optimization expresses **non-trivial reasoning operations**

Integrates nicely with machine learning by seeing it as a function





Learning with differentiable and amortized optimization

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[ICML 2017] <i>Differentiable QPs: OptNet</i>	[ICML 2021] <u>Riemannian Convex Potential Maps</u>
[ICML 2017] Input-convex neural networks	[L4DC 2021] On the model-based stochastic value gradient
[NeurIPS 2017] <i>Differentiable Task-based Model Learning</i>	[ICLR 2021] Learning Neural Event Functions for ODEs
[NeurIPS 2018] Differentiable MPC for End-to-end Planning and Control	[ICLR 2021] <u>Neural Spatio-Temporal Point Processes</u>
[ICLR 2018] <u>Learning Awareness Models</u>	[NeurIPS 2021] <u>Online planning via RL amortization</u>
[NeurIPS 2019] <i>Differentiable Convex Optimization Layers</i>	[ICML 2022] <u>Matching Flows and Probability Paths on Manifolds</u>
[Ph.D. Thesis 2019] <i>Differentiable Optimization-Based Modeling for ML</i>	[NeurIPS 2022] <u>Theseus: Differentiable Nonlinear Optimization</u>
[arXiv 2019] <u>Differentiable Top-k and Multi-Label Projection</u>	[NeurIPS 2022] <i>Differentiable Voronoi tessellation</i>
[arXiv 2019] <u>Generalized Inner Loop Meta-Learning: ⊽higher</u>	[NeurIPS 2022] <u>Nocturne self-driving benchmark</u>
[ICML 2020] <u>Differentiable Cross-Entropy Method</u>	[ICLR 2022] <u>Cross-Domain Imitation Learning via Optimal Transport</u>
[L4DC 2020] <u>Objective Mismatch in MBRL</u>	[arXiv 2022] <u>Meta Optimal Transport</u>
[MLCB 2020] <u>Neural Potts Model</u>	[ICLR 2023] <u>On amortizing convex conjugates for optimal transport</u>
[ICML 2021] Differentiable Combinatorial Optimization: CombOptNet	[L4DC 2023] <u>End-to-End Learning to Warm-Start for QPs</u>
[AISTATS 2021] <u>Gromov-DTW time series alignment</u>	[Foundations and Trends in ML 2023] <i>Tutorial on amortized optimization</i>

Collaborators: Akshay Agrawal, Andrew Gordon Wilson, Anselm Paulus, Arnaud Fickinger, Byron Boots, Denis Yarats, Edward Grefenstette, Eugene Vinitsky, Franziska Meier, Georg Martius, Giulia Luise, Heli Ben-Hamu, Hengyuan Hu, Ievgen Redko, Ivan Jimenez, Jacob Sacks, Jakob Foerster, Joseph Ortiz, Laurent Dinh, Luis Pineda, Marc Deisenroth, Maximilian Nickel, Michal Rolínek, Mikael Henaff, Misha Denil, Mustafa Mukadam, Nando de Freitas, Nathan Lambert, Noam Brown, Omry Yadan, Priya Donti, Ricky Chen, Roberto Calandra, Samuel Cohen, Samuel Stanton, Shane Barratt, Shobha Venkataraman, Soumith Chintala, Stephen Boyd, Steven Diamond, Stuart Russell, Tom Erez, Tom Sercu, Vít Musil, Xiaomeng Yang, Yann LeCun, Yaron Lipman, Yuval Tassa, Zeming Lin, Zico Kolter